Analyst® 1.7 Software with HotFix 1

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Introduction 1

The *Analyst® 1.7 Software with HotFix 1 Release Notes* describe the features in the Analyst® 1.7 Software with HotFix 1 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 *Analyst® 1.7 Software with HotFix 1 Installation Guide*.

Contact Us

SCIEX Support

- sciex.com/contact-us
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Customer Training

- In North America: NA.CustomerTraining@sciex.com
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Online Learning Center

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CyberSecurity

For the latest guidance on cybersecurity for SCIEX products, visit sciex.com/Documents/brochures/win7-SecurityGuidance.pdf.

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 Analyst® 1.7 Software with HotFix 1 release notes have been structured so that you only have to read the sections that are relevant to you.

Note: For reference, the name of the software patch or HotFixes release where the issue was previously fixed is included.

Read New Enhancements in Analyst® 1.7 Software with HotFix 1 on page 7 and Fixed Issues in Analyst® 1.7 Software with HotFix 1 on page 9 of the release notes.

Everyone should read Notes on Use, Known Issues, and Limitations on page 13, as this section applies specifically to issues that are known in the Analyst®1.7 Software with HotFix 1.

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

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

Technical Support

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

Enhancements and Fixes 2

This section describes the enhancements and fixes in the Analyst® 1.7 Software with HotFix 1. To view the enhancements and fixes for the previous releases of the Analyst® software, refer to the *Release Notes* that came with that version of the software.

New Enhancements in Analyst® 1.7 Software with HotFix 1

Support for the Windows 10 (64-bit) operating system

The Analyst® 1.7 Software with HotFix 1 supports the Windows 10 (64-bit) operating system. It continues to support Windows 7 (32-bit) SP1 and Windows 7 (64-bit) operating systems.

Support for electronic licensing

The Analyst® 1.7 Software with HotFix 1 supports both node-locked licensing (assigned to one computer) and server-based electronic licensing (concurrent licensing).

Added a new feature: Scheduled Ionization

The Analyst® 1.7 Software with HotFix 1 supports a new feature called Scheduled Ionization, which helps to reduce the risk of instrument contamination. It supports both electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) modes.

Support for Microsoft Office 2016

The Analyst® 1.7 Software with HotFix 1 supports Microsoft Office 2016.

Support for two new scripts

Two new scripts are now available in the Analyst® 1.7 Software with HotFix 1: sMRM Calculator and MSServiceLog (3500, 4500, 5500, 6500, and 6500+ series of instruments only). The logging for service support is on by default. Users can change the settings or disable the logging using the MSServicelog script.

Added enhancements for the *Scheduled* MRM™ Algorithm

- The sMRM Calculator script can be used to facilitate *Scheduled* MRM™ Algorithm method development. The user can see what the projected cycle time is for each cycle and the dwell time to be applied to each transition before running the method.

- Different Q1/Q3 resolution settings per transition are allowed.

- Users can use Target Scan Time per experiment or Target Cycle Time for all *Scheduled* MRM™ experiments.

- The Target Cycle Time option is selected by default in a new *Scheduled* MRM™ Algorithm method.

Enhancements and Fixes

- Users should review the value set for the Target Cycle Time after all *Scheduled* MRM™ experiments have been added to the method.

- The pause time between mass ranges is now included in the Target Scan Time or Target Cycle Time for dwell time calculation for all models of mass spectrometers.

- The file info now includes the dwell time applied to each transition.

- The user can now set the minimum dwell time and maximum dwell time per method.

Added enhancements for the *Scheduled* MRM™ Pro Algorithm

- In a *Scheduled* MRM™ Pro Algorithm method with IDA or without IDA, the user can now turn on or turn off the dynamic window extension.

- The user can set different trigger thresholds and extension thresholds to allow more triggering on the secondary transitions without having unnecessary extended windows.

- The user can now apply dynamic background subtraction for MRM-triggered-MRM without IDA (on primary *Scheduled* MRM™ transitions for triggering secondary *Scheduled* MRM™ transitions without IDA).

Editing the retention time (RT) for a full quantitation method is allowed

The Analyst® 1.7 Software with HotFix 1 now allows the user to modify the retention time (RT) for a full quantitation method to any reasonable RT in the Build Quantitation Method module, even if the new value is still in the RT window of the real peak.

Checksum is enabled by default

Checksum is enabled by default in a fresh installation of the Analyst® 1.7 Software with HotFix 1.

Six new report templates included

Six new report templates are included in the fresh installation of the Analyst® 1.7 Software with HotFix 1. The new report templates are listed below:

- Library Search - Best Candidate - 2perPage.docx

- Library Search - Confirmation - 2perPage.docx

- Library Search - Best Candidate - 1perPage.docx

- Library Search - Confirmation - 1perPage.docx

- Library Search - Best Candidate - 6perPage.docx

- Library Search - Confirmation - 6perPage.docx

If the software is being upgraded from a previous version of the Analyst® software to Analyst® 1.7 Software with HotFix 1, then the six new report templates are installed and the following existing templates are preserved:

- Library Search 3CE Best Candidate.docx

- Library Search 3CE Confirmation.docx

- Library Search CES Best Candidate.docx

- Library Search CES Confirmation.docx

Added support for Analyst® Device Driver 1.2

The Analyst® 1.7 Software with HotFix 1 adds support for the Analyst Device Driver 1.2, which is an HPLC device control application for the Analyst software.

Features not supported or tested in the Analyst® 1.7 Software with HotFix 1

- Microsoft Office 2007 is no longer supported in the Analyst® 1.7 Software with HotFix 1.

- Analyst Administrator console is not tested with the Analyst® 1.7 Software with HotFix 1.

Fixed Issues in Analyst® 1.7 Software with HotFix 1

Note: The software also includes all of the issues that were fixed in Analyst® 1.6.3 HotFix 1, Analyst® 1.6.3 HotFix 2, Analyst® 1.6.3 HotFix 3, Analyst® 1.6.3 HotFix 4, and Analyst® 1.7 software. Refer to the respective release notes for details.

The following issues have been fixed in this release:

Second level IDA not passing correct ions to dependent scan

If you have a method with two dependent EPI scans and an MS3 scan type, then only the most abundant ions from the second EPI scan are passed to the MS3 scan instead of the most abundant ions from both EPI scans. This issue has been fixed. (AN-157)

IDA is not adjusting the mass properly for ER scans when survey scans have a different polarity

When a method contains two survey scans of different polarities, the mass for the dependent ER scan might be adjusted for the polarity of the second survey scan even if a mass adjustment is not required. This issue has been fixed. (AN-259)

IDA acquisition might use compound grouping if the method once contained advanced *Scheduled* MRM™ parameters

If the user creates an IDA method that includes a *Scheduled* MRM™ survey scan that once contained advanced parameters but was changed to basic, then the IDA scan will continue to use the advanced parameters, including compound grouping, even though they are not visible. When creating IDA methods, if the user enters advanced parameters for *Scheduled* MRM™ survey scans and then change the scan to basic mode, make sure that all of the entries are removed from the advanced options before converting to a basic method. This issue has been fixed. (AN-300)

Secondary transitions for *Scheduled* MRM™ Pro algorithm stop acquiring while the peak is still eluting

When acquiring *Scheduled* MRM™ Pro algorithm data with secondary transitions in IDA with DBS (dynamic background subtraction), the secondary transitions stop acquiring on the back half of the peak. If DBS is turned off, then the entire peak is captured for the secondary transitions. This issue has been fixed. (AN-312)

No signal detected for the MRM experiment in the second period if the first period contains MS3 scan but the second period does not

In a two-period method with the first period containing MRM and MS3 scans and the second period containing just MRM but without MS3 scan, signal is not detected for the MRM experiment in the second period. There is no such a problem if the second period also contains an MS3 scan. This issue has been fixed. (AN-418)

Access to Hardware Configuration mode is restricted for a customized role without tune-related permissions

In Analyst® software, access to Hardware Configuration mode is not granted to a customized role unless one of the Tune operations is also allowed in Security Configuration while assigning permissions to that role. This issue has been fixed. (AN-472)

Values for DP, CE, CXP, and EP change automatically when a row is added in the mass table in an MRM acquisition method

When a new row is inserted in the mass ranges table in an MRM method, the DP, CE, CXP, and EP values revert to the default value for the last (bottom) transition in the table without notifying the user. This issue has been fixed. (AN-489)

Integration results are different between Analyst® software and the Reporter software

The Reporter software did not handle chromatograms that had exponential skim points on the left or the right. In addition, the baseline slopes of some chromatograms, with or without skim, were drawn incorrectly. This issue has been fixed. (AN-501)

Concentration for incorrect Internal Standard (IS) printed when multiple IS are used

Concentration for the incorrect Internal Standard is printed when multiple IS are used in the quantitation method. The printed IS concentration is not consistent with the value captured in the Results Table. This issue has been fixed. (AN-735)

Peak Review's Update Method operation on a Results Table created with semi-automatic quantitation method shows unexpected results

A Results Table created from a semi-automatic quantitation method was opened and Peak Review's Update Method operation was executed "on all peaks", the Record Modified checkbox became checked unexpectedly for some samples. In addition, the Analyte and IS Expected Retention Times for some samples were different. This issue has been fixed. (AN-747)

Some quantitation operations might take longer time on the Dell XE2 computer than on the Dell 9010 computer

For certain data files, some quantitation operations might take longer time (>10 seconds) on a Dell XE2 computer than on a Dell 9010 computer. The operations tend to be slower only when they are executed for the first time since the Analyst® software is launched. This issue has been fixed. (AN-766)

Incorrect mass adjustment in dual-survey IDA with polarity switch between the EMS survey scans

When an IDA method contains EMS survey scans with polarity switching, the algorithm is to select the most intense 1-n peaks among all peaks of both polarity survey scans combined, then perform mass adjustment for dependents scans if the polarity is different from the polarity of last survey scan. This was causing triggering on incorrect mass because of the incorrect mass adjustment. This issue has been fixed. Now the mass adjustment will only be done on an ER scan if it is used, and the candidate polarity is different from the ER experiment polarity. The selected candidates will be triggered in the first available dependent scans in their survey scan polarity without mass adjustment. The dependent scan experiments that are not assigned with a candidate are skipped. Maximum half of the dependent scan experiments will be triggered for each cycle. Make sure the number of dependent scan experiments is double the number of the most intense ions when creating the method. (AN-778)

Analyst® software might go into repair mode if a user with no Read permission to the Analyst Data folder attempts to open the software

When a user who does not have the Read permission to the Analyst Data folder attempts to open the Analyst® software, the Analyst® software might go into the repair mode. This issue has been fixed. (AN-789)

Formula columns were not being updated when a sample was removed from the Results Table

When a sample was removed from the Results Table, the data in the formula columns were not getting updated. This issue has been fixed. (AN-822)

IDA Explorer does not show EPI positive and EPI negative spectra

The IDA Explorer does not show the EPI positive and EPI negative spectra. There is no issue with data quality. Use the Analyst Explorer to view EPI positive and EPI negative spectra. This issue has been fixed in this version of the software but it might still occur when viewing dual-survey IDA data that was acquired using an older version of the software. (AN-833)

Update Method operation on a Results Table created with fully automatic quantitation method shows unexpected results

Results Table created with fully automatic quantitation method has wrong Record Modified settings after Update Method operation. This issue has been fixed. (AN-871)

The Make Exclusion List From Spectrum script does not work

The Make Exclusion List From Spectrum script does not work. This issue has been fixed. (AN-902)

Shimadzu systems with rack changers were injecting samples from the wrong vial position

Shimadzu systems with rack changers were injecting samples from the vial position and plate specified in the acquisition method even if those were different from the batch or actual physical plates on the rack changer. This issue has been fixed. If they do not match between the method and the batch, the user would not be able to submit the batch. (AN-977)

Audit Trail review - wrong chromatogram could be shown

Enhancements and Fixes

For multiple-analyte Results Tables, "Review" in the audit trail manager for an analyte of a sample might open the originally integrated chromatogram for a different analyte even though it is still for the correct sample. This issue has been fixed. (AN-1003)

Printing an acquisition method including an ExionLC™ might print all information only for the first time

Printing an acquisition method including an ExionLC™ might be only successful for the first time. With the method open, printing the method for the second time or more might only show the MS method portion. This issue has been fixed. To print everything, use the Print Pane option. (AN-1074)

Newly created Results Tables were associated with unknown versions of audit map

Newly created Results Tables were associated with an unknown version of an audit map that could not be located on the local disk or network drive. This issue has been fixed now for Results Tables that are created using version 1.7 of the Analyst® software. However, for Results Tables that were created with an un-synced audit map and Quantsettings.sdb, the issue is still not fixed. To avoid this issue, update the currently used audit map for the project by clearing and selecting a feature and then saving it. Then create a Results Table. (AN-1089)

Notes on Use, Known Issues, and Limitations

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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 below. If you find additional issues, contact SCIEX at sciex.com/request-support.

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

Guidance for Antivirus and Backup Software

While it is a widely acknowledged good practice to employ antivirus and backup software, these applications might interfere with the real-time nature of the Analyst® software. Some antivirus and backup applications are configured by default to automatically scan and archive a file immediately after creation. Because the Analyst® software can perform multiple writes to a single data file during an acquisition sequence, it is important to disable these real-time features to prevent the antivirus or backup software from locking the data file while it is still needed by the Analyst® 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 files). Failure to do so 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 example, when configuring the Symantec Endpoint software, the following settings have been found to increase performance during data acquisition:

- **Antivirus and Antispyware Protection > File System Auto-Protect > File Types:** Choose "Selected" and then make sure that the Extensions list does not contain wiff, wiff.scan, or rdb file extensions.

- **Antivirus and Antispyware Protection > File System Auto-Protect > File Types > Advanced > Scan files when:** Scan when a file is modified.

For instructions on how to best configure your particular antivirus or backup software, contact your antivirus or backup software provider.

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. Failure to do so might result in failed acquisitions or corrupted data files.

Notes on Use

Settling Time field for *Scheduled* MRM™ algorithm experiments disabled for all mass spectrometer models except for 6500+ series of instruments

The Settling Time field for *Scheduled* MRM™ algorithm experiments has been disabled for all mass spectrometer models except for 6500+ series of instruments. For other mass spectrometer models, the values being used are defined in the software and not in the Method Editor user interface.

Do not modify the computer date and time after Analyst® 1.7 Software with HotFix 1 is installed

For both node-locked and server-based licensing, make sure that the computer date and time is correct on both the client computer and the server before installing the Analyst® software. After the Analyst® 1.7 Software with HotFix 1 is installed, manually modifying the date and time might invalidate the license and cause users to be unable to log into the Analyst® software.

Results Table's Audit Map has different "Modified" date-time from the "Modified" date-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-time from its "Modified" date-time shown with the project node (accessed under the Projects node) or in a Windows folder. This issue can happen with Results Tables created using 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 click the Settings tab. Select each factory installed Audit Map and then click Save. From this point on, the Audit Map date-times for Results Tables created with the Audit Maps will match the date-times shown with the project node.

This is applicable to all of the project folders that existed before upgrading to the Analyst® 1.7 Software with HotFix 1, and the customer-created project folders (project folders other than API Instrument, Default, and Example) on Analyst® 1.7 Software with HotFix 1 installation using an existing Analyst Data folder where no Analyst software is currently installed (Analyst software re-installation). The Analyst® 1.7 Software with HotFix 1 fresh installation using an existing Analyst Data folder and the three installed folders API Instrument, Default, and Example would not have this issue.

Delay Time behavior in an MRM scan is different from a *Scheduled* MRM™ scan

For a period that contains dynamic scans such as a *Scheduled* MRM™ 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 without being looped with a *Scheduled* MRM™ 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 is open, then opening the Analyst® Help will automatically close the LC Help. If the user needs both Help files to be open, then open the LC Help after opening the Analyst® Help.

Firmware and configuration table upgrade on 4500 QTRAP® instruments

After a firmware and configuration table are upgraded on a 4500 QTRAP® instrument, the instrument must be reset by pressing the red "Reset" button on the instrument or by turning off and then turning on the instrument.

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.

Use either the UPN or SAM format to log on to the Analyst® software if domain field is not shown on logon screen

If the Analyst® software is used in Mixed security mode, then log on to the Analyst® software using either the UPN (username@company.com) or the SAM (domain\username) format if the domain field is not shown on the logon screen.

Use the UPN format to log on to the Analyst® software in Mixed Mode if the network domain is not shown in the Domain field

For a computer with cyber security, a user might not be able to log on to the Analyst® software in Mixed mode using Domain\UserName format, and the network domain might not be shown in the Domain field. Either add the network domain as a trusted domain if it is allowed by the company policy or log on to the Analyst® software using the UPN format UserName@domain.com.

ExionLC™ Systems

The Analyst® 1.7 Software with HotFix 1 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 the LC device for the column oven.

If the WAIT TIME for the column oven is manually set to 0 on the hardware, then make sure to equilibrate the system and wait for 10 to 15 minutes after the column oven has reached the set temperature before submitting any samples. Alternatively, set the WAIT TIME to a value equal to any integer from 1 to 10 and then select 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 must be adjusted to be equal to or shorter than the MS method.

Acquisition will stop if missing vials are detected when ExionLC autosamplers are used

Within the Queue Options window (Tools > Settings > Queue Options), users are able to select the option **Fail whole batch in case of missing vial**. However, with ExionLC autosamplers, the batch will fail when a

missing vial is encountered, whether or not this option is set. The failed sample will include an error message stating that a missing vial was encountered.

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

(double-click ![icon] on the Status bar in the Analyst® software), these devices remain on even after the hardware profile containing these devices is deactivated. The user might think that the devices are switched 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 switched off manually.

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

The ExionLC 100 LC system switches 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 switch on the system again either from the Sciex LC Controller status dialog or from the LC system front panel.

Known Issues

This section describes the known issues in the Analyst® 1.7 Software with HotFix 1.

Audit Trail

Audit trail time stamp for 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 fresh installation of the Analyst® 1.7 Software with HotFix 1 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)

Audit trail wrongly records that the Analyst Classic algorithm parameters changed when in fact the MQ III algorithm parameters were 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)

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. Any subsequent users who log on to the Analyst® software at a workstation that is running RDP is 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

ß is shown as a superscript z

Avoid using the above characters in the audit trail.

Wrong audit trail information with manual integration

The information in the audit trail is incorrect when you choose to revert back to the manual integration results (that is, when Reject Manual Integration is set). It shows Change Reason and E-signature even though they are not set to prompt for input. (SCR 13761)

Audit event deselected unexpectedly

In the Audit Map Editor dialog, if you right-click the Audited column and click 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 you close an IDA data file, the event is not logged in the audit trail. (ST 9487)

The Analyst® software stops responding when performing print preview

When you select to print preview an audit trail that has more than 100 records using the All Pages menu option (right-click), the Analyst® software might stop responding. You can preview one page at a time using the Current Page menu option instead. (ST 4284)

Audit trail printout columns truncated

When printing 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)

Wrong module recorded in audit trail

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

Error when printing 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)

Audit events on 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

The Analyst® software toolbar user interface might not refresh properly on the Microsoft Windows 10 operating system

On the Windows 10 operating system, the Analyst® software toolbar might not refresh correctly and can cause some icons to 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 locking or unlocking the screen or 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)

Usernames should not contain spaces

Although Windows supports the use of usernames containing spaces, the Analyst® software does not. If in Mixed Mode security, a user attempts to log into the software with a username containing a space, the Analyst® software will show an error and fail the login. (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. This includes 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, refer to the Microsoft Management Console for configuration instructions. Alternatively, users can restart the computer.

Method editor access

You must have read and write permissions for the Project Information folder to access the method editor. If you have read-only permission and try to open the method editor, the system might stop responding. (SCR 8037)

Mapped network drives might not be visible in Mixed Mode

When setting 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 UNC (Universal Naming Convention) format (\\computer name\drive name) instead of the mapped letter. (SCR 11094)

The Analyst® software does not start if you have no file permissions

You cannot start the Analyst® software if the root directory is set to a network drive for which you have no file permissions set. If the person trying to log on is an Administrator, the Analyst® software prompts for an alternate root directory. (ST 9836)

Screen lock wait time incorrect in the audit trail

In the audit trail data, the wait time recorded for the Screen Lock in the Security Configuration is incorrect. There is also no audit record 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, remove all users assigned to this role. If you do not remove users, the results might not be shown properly.

Unlocking the Analyst® software using the UPN name format

When attempting to unlock the Analyst® software using the UPN format and a user (with unlocking rights) who was not logged on to the software when it was locked, the Analyst® software shows an error stating that the user is not recognized. This happens whether or not the new user is a legitimate user on the domain. To unlock the software, click OK on the error window and type the new user's 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" for Explore function is disabled for a user role, the user with this role can still modify the integration algorithm for retrieving the peak list.

Help Find

To activate the Find tab in the Help for the first time after installation, you need to be the Windows Local Administrator or have the equivalent rights. Otherwise, the message "Unable to display the Find tab (177)" is shown. (SCR 13792)

Screen lock settings not retained on reinstall

After the Analyst® software is installed, the Network Acquisition account screen lock settings are not retained. Type this information in the Security tab of the Security Configuration dialog.

Configure — Hardware Configuration

The Shimadzu SIL-30 MTP sample order specified in the hardware profile is ignored

Within the Analyst® software Hardware Configuration editor, when configuring the Shimadzu 30AC autosamplers, users can change the MTP Sample Order. However, changes in this interface are not reflected in the Batch Editor. Only the default order is allowed. (AN-462)

Possible issue activating Shimadzu hardware containing Nexera devices when upgrading from a previous version of the Analyst® software to Analyst® 1.7 Software with HotFix 1

In some rare cases, after upgrading to the Analyst® 1.7 Software with HotFix 1 from a previous version, users might be unable to activate a hardware profile containing Shimadzu Nexera devices. However, if the user edits the hardware profile and then sets the P.Max setting to Auto or Off, the profile activates properly. (AN-46)

Incorrect profile shown in the error message

The hardware profile dialog might show an incorrect profile in the error message when failing to activate a profile. (SCR 13820)

Incorrect 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 intermittently show 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, when removing the Analyst® software, a message asking the user to deactivate the hardware profile is shown even if the hardware profile has been deactivated. To clear this issue, restart the Analyst® software. (ST 16060)

Tune and Calibrate — Compound Optimization

Compound Optimization CE max value is 130 even though 180 is set in the Parameter Settings

For 3500, 4500, 5500, 6500, and 6500+ series of instruments, the maximum CE value is 130 in Compound Optimization even though 180 is allowed in the Parameter Settings. If a higher value than 130 is required, then optimize the CE manually in Manual Tune. (AN-1088)

Compound Optimization report wrongfully shows the CEP parameter (3200 series of instruments only)

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

Total sample volume does not update when the total number of injections are changed in the FIA (Flow Injection Analysis) source parameters in Compound Optimization when 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 remains 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, some parameters are not optimized correctly for the duplicate transition. (SCR 9450)

Use of Shimadzu and Tempo MDLC devices when performing infusion Compound 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 that you can use for infusion Compound Optimization.

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

On the 5500 series of instruments, the actual range for the DP ramp used during the optimization is 0 and 300 Volts. (ST 9248)

Compound Optimization does not start the integrated syringe pump for an API 3200™ LC-MS/MS system

Users can either 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 on the API Instrument\Instrument Optimization folder

Users who do not have the Delete privilege on 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 to this folder. (AN-593)

Unable to switch to Tune mode

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

Empty subfolders in 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 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

When in the Select the scan mode screen, clicking More Options allows you 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 Analyst® software stops responding if you press the Start Over button after you have run Instrument Optimization several consecutive times. Restart Instrument Optimization from the Analyst® Navigation bar instead of using the Start Over button. (ST 8029)

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

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

Instrument Optimization fails to run after installation

Occasionally, after removing and reinstalling the Analyst® software, 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 and then reinstall.

Correct masses are occasionally not selected when using the Alternate Tuning option

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

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

If this occurs after Instrument Optimization, you can 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 restart the Analyst® software. Use the Task Manager program to close Instrument Optimization and then restart Instrument Optimization. (ST 13044)

Typing a negative value for the IonSpray source voltage in Negative mode causes the optimization to fail

When running Instrument Optimization in Negative mode, type IonSpray™ source voltages as absolute (positive) values. (ST 3778)

Poor data quality during Instrument Optimization tuning

Occasionally, the Analyst® software scans less 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, restart the optimization process. (ST 13460)

Tune and Calibrate — Manual Tuning

Updating resolution on-the-fly when acquiring data using a *Scheduled* MRM^{TM} algorithm acquisition method in Manual Tune causes the Analyst® software to remain in acquisition

When running a *Scheduled* MRM^{TM} algorithm acquisition method without selecting the option of Q1/Q3 Resolution in Manual Tune, the sample acquisition or the queue cannot be stopped if the user changes the resolution settings on-the-fly under the Resolution tab. The computer must be started to regain the communication. To avoid the issue, do not change the resolution settings while running a *Scheduled* MRM^{TM} algorithm acquisition method in Manual Tune. (AN-1071)

The Analyst® software closes unexpectedly and the Tunedata.tun file is truncated after entering an invalid search range in "Edit Tune Peak Parameters"

The Analyst® software closes unexpectedly after entering 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 for 3500, 4500, 5500, 6500, and 6500+ series of instruments

When the mass calibration of the mass spectrometer is significantly off, users might see effects such as the observed cycle time in the datafile is significantly different from the expected MRM method cycle time. (AN-411)

Application Event Log errors generated while operating QTRAP® 4500 LC-MS/MS system in Manual Tune

When the QTRAP® 4500 LC-MS/MS system is operated in the Manual Tuning mode, 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)

Unable to paste a mass table in Manual Tune for all scan types

Without the Method Editor open, the user is unable to paste copied cells or rows from an Excel sheet to the mass table in Manual Tune. The workaround is to keep the Method Editor open, and then paste the copied content in the mass table in Manual Tune. (AN-980)

GS2 is available when the APCI probe is in use (specific to the 3200 series of instruments)

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, the system might stop responding if one run is terminated and a new one started. Closing the Graph Information pane might prevent this. (SCR 8879)

Possibility of incorrect TIC data when ramping parameters using 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 API 3200™ LC-MS/MS System instrument

For the API 3200™ LC-MS/MS 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.

Syringe diameter does not change during acquisition

On the 5500 series of instruments, if you change both the syringe pump diameter and flow rate while the syringe pump is running and then click Set Flow Rate, the flow rate changes but the diameter does not. You must 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 less 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 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)

Syringe pump error not clearing if ignored

On the 5500 series of instruments, when the syringe pump reaches the stopper, a syringe pump error appears. If you ignore the error for an extended period of time, and you continue clicking through the Analyst software, the error will return but you might not be able to clear it as the Clear Error button might be unavailable. To clear the error and regain communication with the syringe pump, you can deactivate and reactivate the hardware profile. If the error is not cleared, then restart the computer. In rare cases, you will have to deactivate the hardware profile and then restart the computer and the instrument. (ST 9880)

Visible graphs might be slow to update when running the 12 000 Da/s scan speed in Manual Tuning mode

When running the 12 000 Da/s scan speed in Manual Tuning mode, 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 switches applications and then switches back. However, the data is collected successfully and the program updates when the scan stops.

On the QTRAP® 5500 LC\MS\MS system, masses greater than 1000 Da can be entered in the Isolation and Excitation tables

Although the mass range for the linear ion trap is 50 to 1000 Da, the software allows you to enter values for masses greater than 1000 Da in the Isolation and Excitation tables. The effect of entering additional rows for masses above 1000 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 the QTRAP® 5500 LC\MS\MS system, after performing 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

Manually created 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 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 EPIs in an IDA method, only the second EPI passes to the MS3 scan

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

Modifying 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, manually correct the produced method for the EMS mass ranges. (AN-705)

MS3 isolation always uses the new LIT resolution table

In the IDA (Information Dependent Acquisition) 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 and you want to set the Exclude Former Target Ions of IDA Criteria page to Never, select the For 0 secs option. (SCR 11762)

IDA not triggering on specific charge state

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

DP and CE values not stored in 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 you have created 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. (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, 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 1000 Da

When you create an IDA method with a quadrupole survey scan and a confirmation scan (Enhanced Resolution), you cannot have a survey quadrupole mass range greater than 1000 Da. You will be prompted to lower the mass range or remove the confirmation scan.

On the QTRAP® 5500 system, occasionally this message appears "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 you can ignore the message. (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)

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

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)

Mass shifts of up to 1 Da might be observed for data generated using the IDA Wizard for SCIEX Triple Quad™ 5500 system users only

When creating a method through the IDA Wizard, the scan speeds are not available for selection. However, the scan time is available and is editable and is populated in the final method. The final method defaults to 200 Da/s, however, the specified scan time may not necessarily 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, you can select a

different scan speed, or if you want to use the 200Da/s scan speed, select a different scan speed, switch 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 results in 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 check 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 the other IDA criteria. (ST 17045)

No dependent scans are performed for an IDA method which 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 selected for 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 over the ions that were satisfying all the IDA Criteria. To avoid this issue, set the Intensity threshold > 0. The IDA method works as expected. (ST 18941)

IDA acquisition fails if the hardware profile contains an ADC device

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

Acquire — Acquisition Method Editor

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 allowed to 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 when the compound-dependent parameters are in the mass table does not work

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)

Unable to 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 imported 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 switching 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)

Method Editor user interface (UI) issue when modifying scan type and polarity of a saved method

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 making changes to scan type or polarity, to refresh the method UI. (AN-48)

Filename is lost from the UI when resaving an existing method that fails validation

If after the user opens (or creates and saves) a method, modifies the method, and then tries to resave, 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 filename if they try to save the method again. (AN-78)

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

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 (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 set the Ionspray (IS) voltage to the same value for all experiments. If users select differing IS voltages, the voltages are not applied correctly during acquisition. (CBUFW-25)

Acquire — Method/Batch Editor/Queue Manager

Signal loss on negative EMC spectrum on the 4500, 5500, 6500, and 6500+ series of instruments

On the 4500, 5500, 6500, and 6500+ QTRAP® series of instruments, signal cutoff might be observed for some mass ranges in the negative EMC spectrum. (AN-1198)

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 <drive>:\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 checksum into wiff file if the file stays open in the MultiQuant™ or other compatible software

If a datafile (wiff) 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 is not working 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 Information shows 0.0 if Window field left blank in the method

When creating a *Scheduled* MRM^{TM} Pro method, users can enter 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), the File Information will show 0.0 in the Window column for that particular transition. (AN-270)

Users should not turn on the SelexION® system during an acquisition

If the user turns on the SelexION® system during acquisition, the currently acquiring sample is aborted and the system briefly goes to an Error status. When the system recovers to the Ready status, if users attempt to reacquire their sample, 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 on or off the SelexION® system during acquisition. If this happens, new acquisition batches should be submitted, rather than using the 'reacquire' function in the software. (AN-115)

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 Analyst 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)

Error is shown when using invalid characters in sample names

If the user enters a forward slash in a sample name within a batch, upon attempting to submit the batch the error: "Invalid character found in path (/)." If the user enters other invalid characters (:, ", <, >,?, |), then the error will be "Invalid character found in path (: "< >? |)" is shown. (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, they should manually expose all columns first, to make sure that data is pasted as intended. Alternately, the user must make sure that the data they are pasting in the Batch editor contains information for all columns, visible and hidden. (AN-216).

TDF Scans removed for the 5500 instruments

TDF scans are no longer supported for the 5500 series of instruments. The 4500 series of instruments do not support this scan type either. If users attempt to submit a batch in the Analyst 1.7 Software with HotFix 1, which uses methods containing TDF scans (created in a previous version of the software), the acquisition will fail and an error will be logged in the Event Log.

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)

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)

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 cycling between tabs

When users switch tabs in the Acquisition Method Editor, fields are recalculated. As a result, if the user sets a method duration and then cycles 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)

Analyst® software might stop responding if external valve is in hardware profile but is not used in 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, the Analyst® software might stop responding during acquisition. If the valve will not be used during acquisition, 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 switches 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 testing new methods and so on), 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 running an experiment containing a single MRM transition, 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, these waiting samples might be deleted from the queue. To avoid this, increase the number of completed samples shown in the queue. (TT 35286)

Queue: 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 right-click menu show 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)

Unable to delete the last row when there are more than the maximum limit of MRM transitions in the acquisition method

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

Note: For systems other than 4500, 5500, 6500, and 6500+ series of instruments, 300 MRM transitions are the limit when acquiring MRM data and 1000 MRM transitions are the limit when acquiring *Scheduled* MRM™ algorithm data. For the 4500, 5500, 6500, and 6500+ series of instruments, 1250 transitions are the limit when acquiring MRM data and 4000 per method is the limit when acquiring *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 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

Refer to the Help for instructions when copying and pasting to the mass ranges table from one acquisition method to another or from an external file to an acquisition method.

Unable to modify and save number of cycles

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

Scans unexpectedly set to sum to 1

If you set the scans to sum to greater 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)

Missing column headers in previous versions of batch files

If you 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 defaults in parameter settings

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

Unable to save or submit batch with long file path

You cannot save or submit an acquisition batch if the project path is longer than 126 characters. When you submit this type of file, the following error message: "Failed to set Header data" is received. When you save this file, the following error message: "Failed to save BatchName" is received.

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 value might not always work. You must copy and paste the whole Excel sheet with updated dependent parameter values.

Pasting rows in mass ranges table

Pasting more than 300 lines into an MRM mass table could 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 you are importing. (ST 2717)

Error message is shown when importing a text file into an MRM or *Scheduled* MRM^{TM} acquisition method

When importing a text file into an MRM or *Scheduled* MRM^{TM} algorithm method, a message: "Invalid value entered into table. Make sure only numeric values are entered" might be shown. Although this message might be shown, the file is imported correctly. This issue is not observed when importing csv files or when copying and pasting 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 pasting into a mass ranges table during acquisition, the Analyst® software could stop responding. You can only copy and paste into an MRM or *Scheduled* MRM^{TM} algorithm table either before or 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 when creating a quadrupole experiment after switching 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, 1000 to 1250 Da and then switch 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 you create a batch, if you go to the last row in the Batch Editor and then press the Tab button, 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 your batch are shown before this one. When you submit your batch, 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 button to add rows to the batch. Use the Add Samples button instead. (ST 14024)

Samples in a batch remain suspended after instrument error is corrected

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

Invalid ion energy 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^{TM} Algorithm

Scheduled MRM^{TM} algorithm experiment limit

For mass spectrometers other than 4500, 5500, and 6500 series of instruments, to maintain optimum system performance, a *Scheduled* MRM^{TM} algorithm, non-IDA experiment should not exceed 1000 transitions and three dependent parameters. A *Scheduled* MRM^{TM} algorithm, IDA experiment should not exceed 1000 transitions and two dependent parameters. If the experiment exceeds these limits, then the Analyst® software might stop responding

and you must restart the instrument and reactivate the hardware profile. You can reduce the number of transitions if you want to increase the number of dependent parameters.

For the 4500, 5500, and 6500 series of instruments, the limit is 4000 transitions with four parameters (CE, DP, EP, CXP).

Multi-period *Scheduled* MRM^{TM} algorithm experiments not supported

Multiple period *Scheduled* MRM^{TM} algorithm experiments are not supported in the Analyst® software. You cannot create these methods.

In certain cases there might be a decrease in sensitivity on the API 5000^{TM} instrument when using *Scheduled* MRM^{TM} algorithm as compared to MRM

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^{TM} algorithm functionality on the API 5000^{TM} instrument. (ST 15149)

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

Batches containing the maximum number of *Scheduled* MRM^{TM} 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^{TM} algorithm parameters cannot be changed on-the-fly

Compound-dependent parameters for an acquisition method using the *Scheduled* MRM^{TM} algorithm might not be applied when changed in real-time in Manual Tuning. When changing parameters for a *Scheduled* MRM^{TM} algorithm method in Manual Tuning under Tune and Calibrate mode, the method should be stopped between adjustments and then restarted. (ST 9436)

Modifying *Scheduled* MRM^{TM} algorithm mass ranges table can take several minutes

Modifying a *Scheduled* MRM^{TM} algorithm mass ranges table with 1000 MRM transitions can take several minutes. (ST 5251)

Acquire — Network Data Acquisition

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, it is possible that the Analyst® software will stop responding or will result in a failed checksum. This is because network interruptions might cause a delay in writing the full file to the network and require the AnalystService and client to be restarted. Alternately, the file itself might become corrupted. Users should make sure that the file has been fully copied to the network location before attempting to validate the checksum. (AN-202)

Potential loss of data when acquiring from multiple instruments to same data file

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

The Analyst® software prompts you to re-enter root directory path

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.

Network data security mode

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

Cannot access current data

If you are using network acquisition, you cannot see the acquired data from a remote workstation until the sample is finished.

No audit trail record 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. You can add steps to your standard operation procedures (SOP) to check with your IT department regularly if there has been any network interruption during previous data acquisition processes and to avoid data acquisition during network maintenance work. You can also review the Windows application event log to check 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)

Slight time delay due to file transferring

When data files are acquired to the network, the time reported in File Info in Explore mode for Last Sample Finished is the actual 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 file transfer complete

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

Long wait period if you have no write access

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

File transferring fails due to limited space on the network

When acquiring to the 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. (SCR 11420)

Spectral arithmetic output file not saved

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

Explore

Simplified CAD gas setting shown incorrectly in file information

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 averaging and stepping through the XIC (Extracted Ion Chromatogram) 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 5500, 6500 (low mass mode), and 6500+ (low mass mode) series of instruments in the calibration peak list

On 5500, 6500 (low mass mode), and 6500+ (low mass mode) series of instruments, additional ions 1254, 1545, and 1952 are shown in the calibration peak list. This has no impact on the calibration of the mass spectrometers. (AN-500)

Processing large data while performing long data acquisition

Avoid processing (for instance, performing XIC) 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. If you need to open the currently acquiring data, 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 Processing Options / Integration screen (Tools > Settings > Processing Options, Integration tab), allows you to enter decimal values between 0 and 100. However, once the screen is closed and reopened, these values truncate to their integer values.

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

When right-clicking on a chromatogram, the feature seems to be enabled whether or not it actually is. To see whether or not 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.

Unable 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.

Cursor 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.

Missing data when exporting to 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 saving a processed data file (PDT) with a Contour plot shown, the saved file shows a different time range from the original Contour Plot.

X-axis not extended

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

DAD margin for negative absorbance not functioning

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

Performance impacted due to 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 you open an IDA experiment data file 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 you open the data file 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. You can open the sample in the IDA Viewer if you reopen the file. (SCR 9805)

Integrated Harvard syringe pump 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 Information

Opening the File Information pane using the Show File Information 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 occurs, 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 Information 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 in File Information

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

Delay in displaying sample list

On the 5500 series of instruments, it takes more than 90 seconds to populate the sample list for a data file acquired with more than 1000 samples. Allow for at least 90 seconds to populate the entire sample list. If you acquire more than 1000 samples into a wiff file, 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 you acquire the samples into different data files, if possible.

Syringe pump method information missing from the File Info

On the 5500 series of instruments, the syringe pump details used to collect the data are not displayed in the File Information pane for data where a syringe pump was used. You should 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 information by right-clicking on the file information to select Save Acquisition Method. You are required to have the same devices in your hardware profile to recreate the method completely. (ST 7861)

Explore History file is not shown correctly

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 offset in History pane not being shown

You must reopen the History pane to show changes to the offset. (ST 9486)

Reviewing MRM data changes the active XIC

When opening 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, 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 you expand data 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 you expand data from the IDA Viewer during the acquisition of a second sample to the same wiff file. (ST 18228)

Undocked 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 is often the case 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, you can look into a data file acquired in Q1 negative mode. (ST 13331)

Sections of ions appear to be missing in EPI scans

On the 5500 series of instruments, when you use Q0 trapping, 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, you can 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 opening 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 field is populated with "NA" instead. To overcome this issue, it is recommended that the user save the original database into two separate databases in order to be able to view all entries and then populate future entries in a new database. For example, delete the last 10000 entries and save this database as "Part 1" and then reopen the original database, delete the first 10000 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 you click View Manager from the Search Results window and add a new field, the results for this new field might seem to be blank. Clicking on 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 you edit the name of a compound in the library, click OK, and then attempt to edit the compound again, the Analyst® software stops responding. To avoid this, after clicking OK to change the compound name, close and re-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 you upgrade acquisition computers to the newer Analyst® software, you should also upgrade 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

Results table may get overwritten when it's being modified by multiple users at the same time

When two users are processing the same data file from the same network location at the same time, the results table saved by the first user gets overwritten if the second user clicks Save and then click Yes to the message that this results table already exists and do you want to replace it, even though the second user gets another message after that: "the result table that you have chosen is already opened by another user or you're in a ready-only environment. Any change cannot be saved back to the result table". Moreover, the audit trail for that results table does not have the log for the changes made by the second user even though the changes were saved to the results table. The workaround is to click "No" to the warning that the result table already exists and do you want to replace it, and then enter a different file name to save. (AN-32)

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

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 receiving 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)

Sum Multiple Ions option might produce results that are slightly incorrect

When using the Sum Multiple Ions option within 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 Quantitation audit trail incorrectly adds the word Samples to the change descriptions

In the Quantitation audit trail, the word "Samples" is incorrectly added before the text, "The concentration/calculated concentration units were changed to…" in the change description when the concentration or calculated concentration units are changed for either the Analyte or Internal Standard. (AN-430)

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

When performing regression in the Analyst® software (Quantitation module) and saving 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 when the file is closed and reopened. (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)

Accuracy values might be different between different versions of the Analyst® software

In the Results Table, the Accuracy values might be different between Analyst® software versions 1.5.x and 1.6, for the results created using same samples – data files. In the Analyst® 1.6 software, accuracy values are rounded to 13 decimals. In some cases, the difference on the 10th decimal might be observed. (ST 33935)

Zero Accuracy values display as N/A in previous versions of the software

Zero Accuracy values 0.00 were displayed as "N/A" in previous software versions. In the Analyst® 1.6 software, if the calculated accuracy value is 0.00 (up to 13 decimals), that value will be displayed as a number (0.00). (ST 33935)

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)

Formula columns are not validated by the Analyst® 1.7 Software with HotFix 1

The formula columns in the quantitation module of the Analyst® 1.7 Software with HotFix 1 allow users to design custom calculations for their specific needs. We strongly recommend that users verify and validate results of these custom formulas before use. (AN-59)

Incorrect printouts if manual integrations are not accepted

If the user performs a manual integration and attempts 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. For more information, refer to Technical Information Regarding Integration on page 64. 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.

- The Quantitation wizard cannot create a quantitation method for a data file that contains more than 94 transitions. Before you can use the Quantitation Wizard to generate a Results Table, you must first 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 <drive>:\Program Files\Analyst\Scripts\All Mass Spectrometers folder.

- You cannot add *Scheduled* MRM™ algorithm 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 that you use IntelliQuan - MQ III as the default integration algorithm, as the peak is sometimes not found in the retention time window when using *Scheduled* MRM™ algorithm with IQA ll.

IntelliQuan - IQA ll parameter-free integration algorithm not set by default

For regular MRM data, IntelliQuan - IQA II is the preferred default algorithm. For fresh Analyst® 1.5 software installations, this must be set manually, as the MQ III algorithm is set by default. For instructions, see the Help.

Default integration algorithms

Newly created projects always copy the default integration settings from the Default project. For fresh Analyst® 1.5 software installations, this preset is now IntelliQuan - MQ III. If you are reusing your Analyst Data folder from a previous version, the preset from that Default Project will carry forward to the Analyst® 1.5 software.

Large signal-to-noise values 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. Readjust 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 the IntelliQuan Parameters dialogs opened by right-clicking in a data list. (SCR 12984)

Exporting with Sum Multiple Ions produces 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 not removed

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

Analyte mass range column contains N/A

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

Peak asymmetry error

When you create a Results Table and display Peak Asymmetry, the column shows 0.00 if no peak is found. (SCR 10688)

Inconsistent last decimal digit

When opening a Statistics table 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), the last digit for some of the statistical results (Mean) could be different depending on the order of opening the data files. The same issue is also seen in mean calculations as well. (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.

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 2500 transitions can take about three minutes. (ST 9944)

- Creating or saving a quantitation method using *Scheduled* MRM™ algorithm data that contains 2500 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)

Cancel button unresponsive when closing an unsaved quantitation method

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

Analyst® software stops responding when you export a Results Table to a non-existent directory

This 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)

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 were 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 increasing the RT window beyond 40 seconds

When you use the IQA II algorithm, RT windows larger than 40 seconds are ignored. When the user sets a window larger than this, 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, switch to the MQ III algorithm. (ST 17676)

Error when quantitating using TIC as Q1/Q3 selection

If you use the Quantitation wizard and specify the TIC as the Q1/Q3 selection, the Analyst® software shows an error when you advance 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 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, you cannot open it. Quick Quant works as expected with all other scan types. It is recommended that you 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 through the Quant Method Editor Settings dialog. (SCR 6997)

An intensity drop might be observed if running a *Scheduled* MRM™ algorithm experiment with masses greater than 1000 Da

Avoid using masses above 1000 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 building a quantitation method 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 building 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, refresh the window by saving it. (SCR 11282)

Analyst® Software Reporter

Delete privileges are required to create a report using the Reporter Software

Users need the delete privileges to a specific data folder to create a report using the Reporter software or save the report to that folder. (AN-358)

Report cannot be generated when using Library search template in the Reporter 3.2 software

When trying 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)

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

When editing the Blank Template in Reporter, 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 creating a Reporter template, 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)

Reporter Template Converter: 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 using the Reporter 3.2 software 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, after generating the report, 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 the user specifies 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)

Generating a PDF report might be slower for Microsoft Windows 7 users

On Windows 7, if you are not an Administrator then the report takes longer to run. (ST 033975)

Installer

Message about DCOMPerm.dll might be shown during Analyst® software installation

During the installation of the Analyst® 1.7 Software with HotFix 1, a message "Cannot move DCOMPERM.dll while installing DCOMPerm. Win32 errrorcode 262272. Please contact your software manufacturer." might be shown. Click **OK** in the message to continue with the software installation. If you plan to use the CTC PAL autosampler, then test if 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)

Unable to upgrade or re-install the Analyst® software 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 re-installing it. This might result in the user losing their instrument tuning files. The issue is caused by the Waters driver and Waters support has been advised.

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

Smart Services runtime error

Occasionally, a Smart Services runtime error appears when installing or uninstalling the HotFixes. 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

Screen flickering

There might be some flickering when switching between modes and between windows in the Analyst® software. The flickering does not indicate a serious issue or potential shut down and does not affect data. (ST 3614)

Changing power management settings on the Optiplex 960 is not recommended

Long delays (up to five hours has been observed) between samples in the batch might be seen on the Optiplex 960 if the power management settings (C-State control) in the BIOS are changed. This has not been observed for all scan types. (ST 18017)

Nebulizer Current status is not displayed correctly in the Detailed Status window

On the 5500 series of instruments, 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 appears but this does not accurately reflect the actual applied current. Contact your FSE if no change in performance is observed when you change the nebulizer current in the method or if you suspect a problem with your nebulizer current.

Compatible Software

Administrator Console audit trail records does not record the log out events

In an AAC environment, the Administrator console audit trail records when the user logs into AAC Client, but it does not record the log out event. (AN-314)

Automaton support 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

LightSight software for metabolite identification is unable to create GSH precursor ion IDA methods when the molecular weight of the molecule is above 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. LightSight software can create GSH Prec methods for molecules with a molecular weight above 550 Da only if you do not create an IDA method.

AAO Development Kit

For third party developers to develop with this version of AAO, they can find the AAO Development Kit on the Analyst® 1.6.2 software DVD in the \Extras\AAO folder. The kit contains a User's Guide, Release Notes, Source Files, Sample Code, and so forth.

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

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

Method Converter script may change the CAD gas setting on the converted method

When converting a method in which the CAD gas setting will be changed from a numerical value to Simplified settings or vice versa (such as from 6 to Low), the CAD gas setting will be changed to the default CAD setting in the Parameter Settings of the instrument to which the method is converted. After the method is converted, review the method for the CAD setting and then update it if it is incorrect. (AN-1283)

A longer settling time may be set in a *Scheduled* MRM™ algorithm polarity switch method that is converted from a non-6500+ series of instrument using Convert Methods script

When converting a *Scheduled* MRM™ algorithm polarity switch method from a non-6500+ instrument to a 6500+ series of instrument using the Convert Methods script, a longer settling time from the non-6500+ instrument might be retained in the new method. Make sure to review the method and update the settling time if a shorter settling time is preferred before using the converted method for acquisition. (AN-1281)

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

Convert Methods script does not generate an error message when it is unable to convert an acquisition method with Q1/Q3 above 1250 for a 6500 High Mass or 6500+ High Mass series instrument into a method for a 5500 series instrument. 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

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)

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 Windows Explorer

Notes on Use, Known Issues, and Limitations

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).

On Microsoft Windows 7 operating system, the Mascot script does not populate the file name automatically

On Windows 7 with Internet Explorer 8, the Mascot script does not populate file name automatically. Users will need to select the file name manually using the Browse button. (ST 33797)

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

When running the BatchScriptDriver Script, if you select a *Scheduled* MRM™ algorithm data file to be processed with the AutoQuant with Automatic Reports.dll script, an error message indicating that samples are not compatible with the quantitation method appears. You can process MRM data successfully. (ST 9052)

Label XICs script labels traces with zeroes

If you run the LabelXICs script using Scheduled MRM algorithm data, 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)

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. On the Explore menu, click 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)

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 make this work, you must enter headers in the list in the format provided by the returned error message. (ST 2027)

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. An error message appears indicating the mass ranges that can be extracted can provide further guidance. Reopening the data file and restarting the script may also correct this issue. (ST 9646)

Subsequent integrated area not appearing

When running the Manually Integrate Script 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 run the script again to see the integrated area. (ST 9650)

Incorrect ramp information given for AF2 parameter

On the 5500 series of instruments, 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)

AF2 graph is not always legible

Occasionally, the AF2 graph produced while running 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)

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 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 avoid this issue, make sure the hardware profile activated in the Analyst software matches the active hardware profile for the MRM methods being merged. (ST 17455)

Merge MRM methods script does not merge the Compound ID

Enter the Compound ID manually. (ST 2474)

Error when selecting "Subtract Control Data from Sample Data" on the Scripts menu

Hold down the Shift key while selecting the script. An About dialog displays 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 avoid 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 over 1000 Da cannot be converted to QTRAP® 5500 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 you have created your method using this script, review the new method to make sure that the method has been converted to your satisfaction.

Peripheral Devices

ExionLC™ Series Devices

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 the Manual Tune mode. (AN-644)

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)

When using the Analyst® software Remote Instrument status feature, the detailed status for a connected ExionLC™ devices stack is not shown

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

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 other windows. This happens after installation or after the computer is restarted. To bring the ConfigUIDialog in the foreground (after clicking on Configure button), minimize all of the open applications until the ConfigUIdialog is visible. After this, every time the Configure button is clicked, the Configuration UI dialog will always open in the foreground. (AN-717)

Acquisition using the ExionLC PDA Detector in 2D mode might stop occasionally

When using the ExionLC PDA Detector, acquisition might stop occasionally. When this happens, the Analyst software will abort the acquiring sample and then stop the queue. This issue has occurred when using the PDA Detector in 2D mode. As a result, it is currently recommended to use the PDA Detector in 3D mode to minimize the likelihood of this occurring. Users who encounter this issue should contact SCIEX support at sciex.com/request-support to enquire about a solution. (AN-718)

ExionLC™ configuration of a newly created or edited hardware profile is being applied to all existing hardware profiles containing ExionLC™ devices

If the configuration of a hardware profile containing an ExionLC™ device is modified 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™ 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)

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

When a batch that contains a sample whose vial location is missing a vial is submitted and if the Queue option "Fail whole batch in case of missing vial" is not selected, then the sample experiences an acquisition error and the rest of the samples in the batch are suspended. (AN-965)

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

When the ExionLC™ devices are used, in rare cases, while auto-configuring the devices in the ExionLC™ stack during hardware profile creation, the "Devices in use" list in the SCIEX LC Configuration window might show the ExionLC™ 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™ devices, if 1, 2, or 3 rinse solvents are selected in the **Internal Rinse settings** section, then the internal rinse does not take place. Workaround is to select 4 solvents to start the internal rinse. However, 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)

CTC PAL / Leap Devices

Batch fails to continue on a missing vial error for a CTC PAL autosampler with the DLW (Dynamic Load and Wash) feature

If a CTC PAL autosampler is used with the DLW feature, then the batch fails to continue when 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)

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 Software with HotFix 1 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, trays and sample locations can be selected on the Sample tab in the Batch Editor. (AN-381)

CTC software update

If you have applications that are using CTC SDK (for example, CTC Cycle Composer or CTC Cycle Editor) that are older than version 1.6.0.3, they 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 3-1 Enable Barcode Reading check box
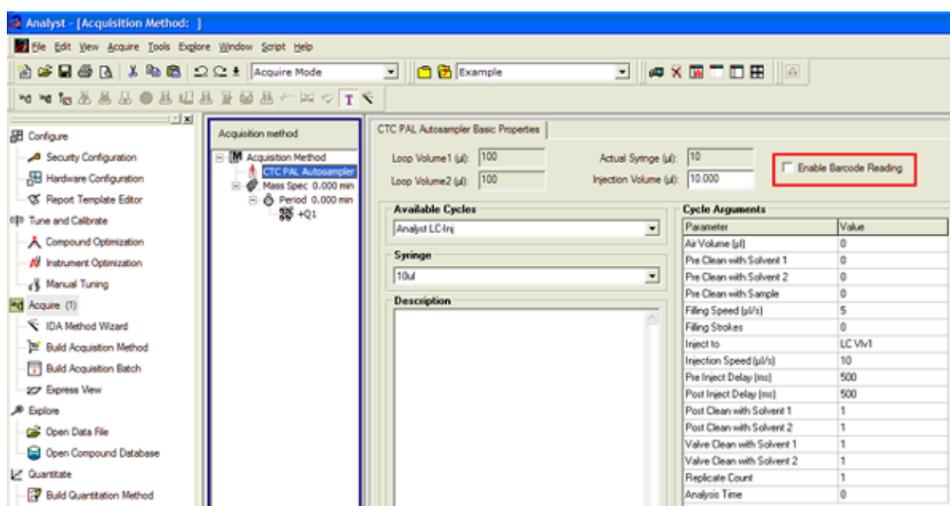
Failed barcode readings

If a barcode reading is attempted but fails (due to torn, misplaced or missing labels and so on), the barcode information for that particular sample is shown and stored as "N/A".

Barcode reading disabled

If the user disables the barcode reading feature, 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, 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)

Message is shown when removing CTC cycle editor (version 2.0.7)

When removing the CTC Cycle Editor, the message Remove Shared Files? is shown. Click No. If you click Yes, 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.

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)

Injection valve switches when CTC method is stopped

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

Terminal unlocks when 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, the hardware profile does not activate. (SCR 11665)

Shimadzu Devices

Shimadzu stack does not go into the standby mode when Standby is selected during equilibration

The Shimadzu stack does not go to standby when Standby is selected during the equilibration period. The mass spectrometer goes to standby but the pump and oven continue to run. As a workaround to put the Shimadzu devices in the stack in standby mode is to first press ready and then press Standby during equilibration. (AN-663)

Shimadzu: AutoConfig shows 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. There is a defect in this driver that 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, the File Info for acquired data reflects the correct serial numbers. (TT 35101)

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 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)

IP address must be typed to establish an Ethernet connection

For Windows 7 users, 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, the Shimadzu AAO might stop responding

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

Batches can fail if 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)

Loss of queue functionality

Performing an abort when a Shimadzu device is in the Equilibrate mode (by manually putting the device in the Standby or Ready mode 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 as you might not be able to activate the hardware profile.

Enabling additional devices in the Shimadzu Prominence 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 make sure that a hardware profile can be successfully activated in the Analyst® software.

Loss of synchronization when specifying short acquisition times with 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 necessary for the autosampler to complete the rinse washes. Make sure your MS acquisition method is at least one to two minutes long.

Pump pressure maximum limit might need to be increased when creating Shimadzu methods

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

No error message when missing Shimadzu deep-well plate

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

Issue when restarting AnalystService

If you reboot the computer or restart the AnalystService.exe (through the Windows Services screen), 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)

Need Windows local Administrator rights to modify hardware profile

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

Wrong vial number

When you use Shimadzu devices, the wrong vial number is sent to the autosampler when 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 due to 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), you are not able to stop the tune run using the Analyst® software after the mass spectrometer has finished scanning. Press Run on the controller to stop the run or change the default Shimadzu run 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)

LC Packings Devices

Problem locating reagent vial positions

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

Define pressure in bar units

When using the UltiMate Integrated System, select the pressures in bar units. (SCR 9257, SCR 13863)

Missing vials

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

DAD Devices

Single wiff file for large data

Acquiring a large amount of data with a DAD (Diode Array Detector) device to a single wiff file might result in file corruption. To prevent this from happening, always acquire DAD data to multiple wiff files if you have a large number of samples.

Agilent Devices

DAD acquisitions at data rates > 20 Hz are not recommended

With the Analyst® software, the guidance is 20 Hz and below. 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, the File Information shows that the acquisition method was created with a 1200-series device. To avoid this, 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 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 3-2 Purge option in the Acquisition Method editor
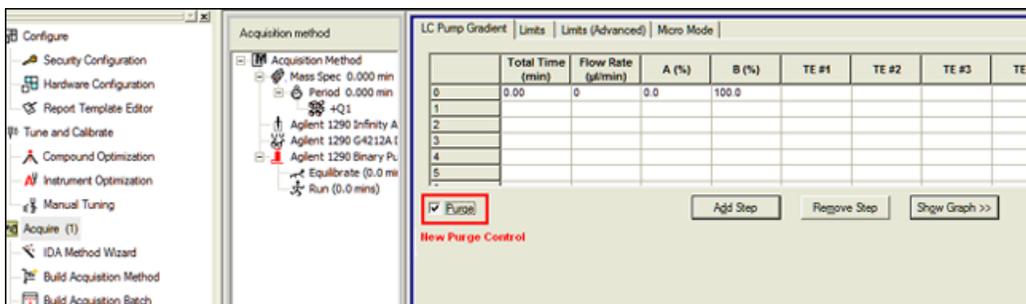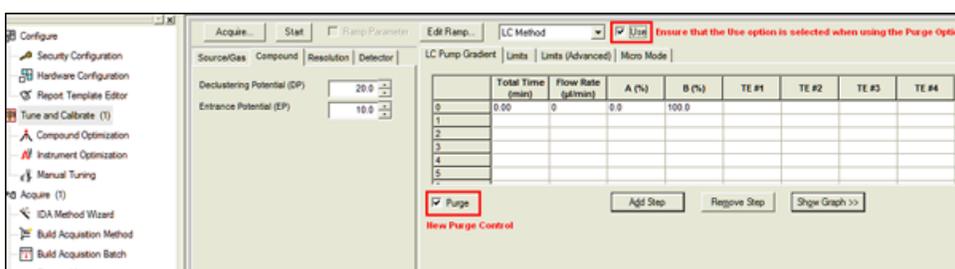

**Figure 3-3 Purge option in Manual Tuning**

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

When creating a purging method, only the Total Time, Flow Rate, and A/B(%) fields are used. Anything entered into the Limits, Limits (Advanced), and Micro Mode tabs are ignored.

Users can either use Manual Tuning to purge or prime their system, or they can create an acquisition method to be used exclusively for purging. This method can be submitted via 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 3-4 Example acquisition batch with a purge method before acquisition
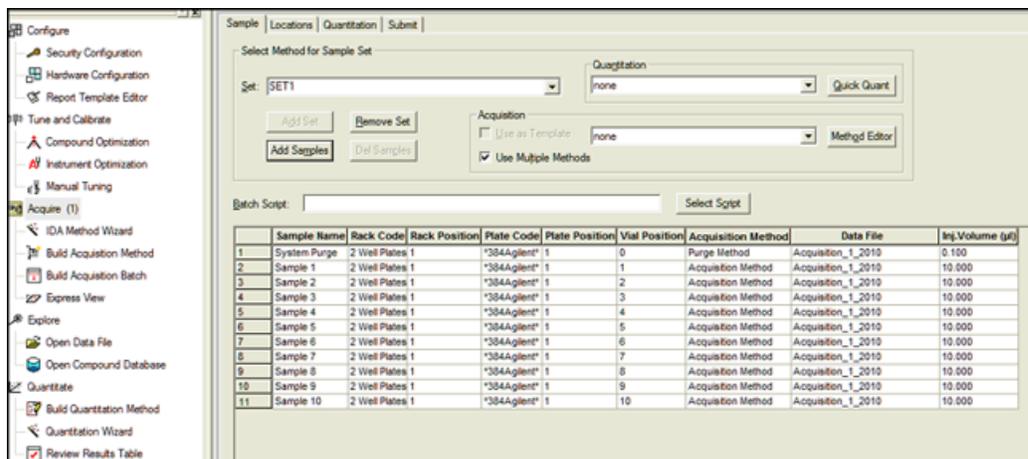
Changes to DAD acquisition

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)

Hardware profile containing an Agilent DAD 1315D

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)

PerkinElmer

Missing last decimal number 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, the report shows 70 µl/minute instead of 75 µl/minute. (SCR 11370)

Tempo MDLC System

Acquisition with 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, resubmit the remaining samples.

21 CFR Part 11 Compliance 4

You can use the Analyst® software to make sure that your site complies with the 21 CFR Part 11 Electronic Records and Electronic Signatures regulations. This compliance relies on an administrator's 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 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 or not the usage of the Analyst® 1.7 Software with HotFix 1 is 21 CFR Part 11 compliant is dependent on the actual usage 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® 1.7 Software with HotFix 1 in the \Program Files (x86)\ Analyst\Bin folder.

Table A-1 Utilities

Program	Description
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%.