

Analyst[®] 1.6.1 Software

Release Notes



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Thank you for choosing AB SCIEX to supply your LC/MS/MS system. We are pleased to give you the Analyst® 1.6.1 software, the most comprehensive LC/MS/MS software package available.

The *Analyst® 1.6.1 Software Release Notes* describe the many new features introduced in the Analyst 1.6.1 software, as well as workarounds for possible issues. Use these release notes for reference as you become familiar with the software, and for future reference. For installation and software compatibility information, see the *Analyst® 1.6.1 Software Installation Guide*.

Support

At AB SCIEX, we are committed to providing the highest level of support for our Analyst software users. To obtain answers to questions about any of our products, report problems, or suggest improvements, visit www.absciex.com. For on-site service, support, and training, visit www.absciex.com/FAQ or www.absciex.com/training.

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 1.6.1 software 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 and Fixes in Analyst® 1.6.1 Software on page 7](#) of the release notes and then also read up to and including the section describing the software version you are upgrading from.

Everyone should read [Notes on Use, Known Issues, and Limitations on page 41](#), as this section applies specifically to issues that are known in the Analyst 1.6.1 software.



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



New Enhancements and Fixes in Analyst® 1.6.1 Software

New Features and Enhancements

4500 Series Instrument support

The Analyst 1.6.1 Software adds support for the following new instruments:

- AB SCIEX QTRAP® 4500 system
- AB SCIEX Triple Quad™ 4500 system

Shimadzu SIL-30ACMP and CTO-30AS

The Analyst 1.6.1 software adds support for the Shimadzu SIL-30ACMP autosampler and CTO-30AS column oven.

Method Converter for the 4500 Series of Instruments

The Method Converter script has been updated to allow conversion of existing methods to be used on the 4500 Series of instruments. In addition, several enhancements and improvements have been made to the script to address various issues. Refer to the [Fixed Issues](#) section for more information.

New firmware available for 5500 instruments

The firmware for the AB SCIEX QTRAP 5500 and AB SCIEX Triple Quad 5500 systems has been upgraded. The new firmware addresses an issue where some mass spectrometers would reset if the acquisition queue was aborted while the system was in the equilibration state. There are no changes that affect data or data quality. For information on how to upgrade the firmware of your mass spectrometer, refer to the *Installation Guide* for the Analyst 1.6.1 software.

Documentation Changes

Combined Hardware- and Software-Specific Information for 4500 Series of Instruments into a Single Guide

All the hardware- and software-specific information for the 4500 series of instruments has been combined into a single guide called the 4500 Series of Instruments System User Guide. The guide also contains basic information for setting up and using the Analyst software to create methods, acquire samples, and analyze data. This System User Guide replaces the Getting Started Guide for the 4500 series of instruments. The Getting Started Guide is still applicable to instruments other than the 4500 series of instruments.

Advanced User Guide

A new guide called the Advanced User Guide has been created. It contains all the advanced information needed to set up and use the Analyst software to create methods, acquire samples and analyze data. This guide replaces the Software Reference Guide.

Updated Reference Tables

The calibration reference tables have been updated in the Analyst 1.6.1 software. The changes are only applicable to the 4000 and 4500 series of instruments. Existing calibration reference tables will not be updated.

When installing a new 4500 series instrument, the FSE will install the new calibration reference tables.

Fixed Issues

Change to Quantitation Fix introduced in Analyst 1.5.2 HotFixes to February 2011 software

In the Analyst 1.5.2 HotFixes to February 2011 software, a fix was introduced to allow the use of the Sum Multiple Ions feature with compressed data. This fix has been improved upon. This change has no effect on quantitation results. (TT 31956)

Improved support for Agilent 1260 DAD

The Agilent 1260 G4212B DAD was introduced in the Analyst 1.5.2 software. However, users were not able to reliably activate the device or use it for acquisitions. This issue has been corrected. (TT 33318)

Shimadzu Nexera POST treatment is now supported

In the Analyst 1.6 software, it was recommended to ensure that post-injection wash cycles were completed before the end of the mass spectrometer acquisition to avoid errors. The Analyst 1.6.1 software allows users to use post-injection wash cycles of any length with the Shimadzu Nexera devices. Wash cycles no longer need to be completed before the end of acquisition. (TT 33825)

Corrected MRM Optimization script issue on the Windows 7 operating system

Occasionally when running the MRM Optimization script on the Windows 7 operating system, the script would stop responding during the optimization process. This issue has been fixed and the script now runs to completion. (TT 33878)

Unable to extract Multiple XICs to stacked panes

In the Analyst 1.6 software, if users attempted to extract multiple ion chromatograms to individual panes, only one pane would contain an XIC; the rest would be blank. This issue has been corrected and the Extract XIC functionality has been restored. (TT 34196)

Method duration may be calculated incorrectly

When calculating the expected duration of multi-period mass spectrometer acquisitions or acquisitions with polarity switching, there may have been a mismatch between the calculated number of cycles and method duration. As a result, acquisitions may have appeared to end early. There was no data lost as the number of cycles acquired was correct — the defect was graphical.

This has been corrected and the expected duration now matches the calculated number of cycles. (TT 34541)

Method Converter

Several defect fixes have been implemented in the Method Converter script for the Analyst 1.6.1 software:

- Users were unable to convert AB SCIEX Triple Quad™ 5500 system methods to the API 4000™ or API 5000™ system methods.(TT 34543)
- Various user interface corrections, such as spelling, punctuation, and so on.
- When converting MCA methods, the “Number of Scans to Sum” parameter was not transferred to the converted method. (TT 34788)

Column Oven Parameters Help topic updated

The Analyst Help topic for Column Oven Parameters has been updated for clarity. (TT 34730)

Maximum/Minimum DP values for the 5500 instruments in Compound Optimization was showing +/- 400 instead of +/- 300

When running the Compound Optimization routine, the reports were incorrectly showing the Declustering Potential (DP) for the 5500 series of instruments as +/- 400 instead of +/- 300. This issue has been corrected and the limits now show properly. (TT 34909)

No message displayed for source change when method editor active

The Analyst 1.6 software introduced a change that inadvertently removed the user message when the source was removed or replaced while an acquisition method was open. This issue has been addressed, and users will again see a message if the source is removed. (TT 34919)

Scheduled MRM™ Algorithm: Unable to save method if RT < Half Detection Window

The Analyst 1.6 software introduced a requirement that retention times for ions in *Scheduled* MRM™ algorithm methods had to be less than half of the user-set detection window. In response to customer feedback, this limitation has been removed. (TT 35095)

Text in Current Spectrum window may overlap in Instrument Optimization

When running Instrument Optimization, users may have seen overlapping text in the Current Spectrum window. This has been resolved. (TT 35177)

Agilent 1260/1290 DAD: Data mismatch with Agilent Instant Pilot

Recent firmware changes by Agilent have modified the scale used for absorbance data sent from the Agilent 1260 and 1290 DADs to the Analyst software. As a result, users may have seen a mismatch between the data shown in the Analyst software and the data shown on the Agilent Instant Pilot. This has been corrected and features have been implemented to ensure that scale changes will not affect the Analyst software data in the future. (TT 35191)



Note: The absorbance data as collected in the Analyst software was correct, but was scaled improperly. Because DAD data is relative, the data was internally consistent.

New Enhancements and Fixes in Analyst 1.6 Software

- Analyst[®] software splash screens and icons have been updated.
- Introduces support for Windows 7 (Professional Edition)
 - For users with Administrator privileges (Built-in Administrator or Protected Administrator Users), the following UAC level is recommended: “Default – Notify me only when programs try to make changes to my computer”.
 - For users without Administrator privileges (Standard Users), the following UAC level is recommended: “Default – Always notify me when”.
 - Added the ability to pin both the AnalystLauncher and Analyst software shortcuts to the Task bar. The shortcuts are consolidated into one button that launches the Analyst software.
 - Ability for the Analyst software to track recently or frequently used files using the Windows 7 jump list feature.
- *Scheduled* MRM[™] algorithm scan type enhancements
 - Two *Scheduled* MRM algorithm scan types are now supported in acquisition methods.
 - IDA acquisition methods can now include two *Scheduled* MRM algorithm scan types.
 - Introduces the ability to switch polarity during cycles that contain two *Scheduled* MRM algorithm scan types.
 - The 5500 series of instruments now supports the acquisition of 4000 *Scheduled* MRM algorithm transitions with four parameters (CE, DP, EP, CXP).
 - *Scheduled* MRM algorithm data containing more than 2500 transitions will be opened in TIC mode.
- Reporter 3.2 software is included with the Analyst 1.6 software
 - Reporter 3.2 software is now automatically installed during the installation of the Analyst software.
 - Users can edit the Reporter 3.2 templates found in the <drive>:\Analyst Data\Projects\API Instrument\Templates folder. User-created templates that were created using previous versions of the Reporter software must be updated using the Reporter Template Converter.
- Analyst software now supports CTC firmware version 4.2.
- Increased the mass range of the 3200 QTRAP[®] system to 2000 Da in RFDC mode. LIT scan types are still limited to 1700 Da. A new configuration file for the 3200 QTRAP system is included. To use the increased mass range, the configuration table must be updated using the ConfigUpdater.

New firmware for 5500 instruments is included

This firmware allows users to ramp the collision energy parameter using the CE values in the mass ranges table. (ST 29645)

Analyst Access Object subproject support

The Analyst Access Object supports projects that use subprojects. (ST 16999)

User-created audit map enhancements

You can now delete the Default audit map and select a user-created audit map that will be applied automatically when a new project is created. (ST 18933)

Users with the Administrator role can unlock the software

Users that have the Administrator role for the Analyst software can now unlock the Analyst software if the application is locked by the current user. (ST 27692)

Users can print Results Tables that have been changed but not saved

If users modified the peak review layout and attempted to print the Results Table without first saving it, they were prompted with a message stating that the Results Table has to be saved. This issue has been fixed and users can now print the Results Table after the peak review layout has been changed but not saved. (ST 27869)

Files in Cache folder are deleted

If you have confirmed that all data has successfully been uploaded to the server and files still remain in the cache folder, restart the PC, navigate to \Analyst Data\WIFF_CACHE_BACKUP (hidden folder) and delete the contents before re-launching the Analyst software. This issue has now been fixed. After network acquisition during which one sample file is saved per .wiff file has completed, the files in the Cache folder are now deleted. (ST 28260, ST 28323)

Acquiring data to a network location does not clear temporary (Cache) files

When using Network Acquisition, the local cache folder may not be emptied after successfully uploading the data file to the network. If this happens, users may see that the "Date Modified" date for some data (.wiff) files in Windows has changed to a more recent time than when the file was actually acquired. While the Windows timestamp of the file has been changed, the actual contents of the file are not modified, unless there are actual changes to the data file that have not yet been uploaded to the network.

Mapped drives are converted automatically

Previously network acquisition over mapped drives was not recommended. Now mapped drives are converted automatically to full UNC paths. Full network path lengths must be limited to 128 characters. (ST 29237)

Audit Trail Manager logs invalid checksum

If Data File Checksum is activated, at the end of batch acquisition, the Audit Trail Manager now logs any invalid checksum. (ST 31209)

Data discrepancy in quantitation

When performing an integration using the Analyst Classic algorithm, a discrepancy between the chromatogram in the peak review and the Results Table is observed if the sample is corrupted. The remaining samples were integrated incorrectly. This issue has now been fixed. (ST 16964)

Unable to open Wiff to MatLab files generated using the Analyst 1.5 software

Files generated using the Wiff to MatLab script and Analyst 1.5 software data cannot be opened in later versions of the Analyst software. This issue has now been fixed. (ST 21099)

During infusion Compound Optimization on the 5500 series of instruments, the preset syringe pump options are used

Previously, during infusion Compound Optimization, the preset syringe pump options were used; the syringe pump diameter and flow rate used were 4.61 mm and 7 μ L/min respectively and could not be changed. To use a different syringe pump diameter, start the syringe pump in Manual Tuning and then start Compound Optimization. (ST 9255, 24334)

Custom Injection program does not work for Agilent autosamplers

Previously, users could only create a basic custom injection program. This issue has been fixed and users can now also create a custom injection program. (ST 31036)

Data acquisition using DFT occasionally results in a loss of sensitivity during some DFT-enabled scans

When acquiring data using Dynamic Fill Time (DFT), in some rare instances users may experience a loss of sensitivity during some DFT-enabled scans. When viewing the DFT Tracker, they will also see that negative fill times are occasionally calculated during these scans. This issue has now been fixed. (ST 29880)

Shimadzu software stops responding during sample acquisition

The software stops responding during sample acquisition, either in pre- or post-run. This issue has now been fixed. (ST 29804)

Analyst[®] 1.5.1 Patch for AAO Batches

This patch corrects an issue found in the Analyst 1.5.1 software that prevents users from using the Quantitation option available within the Batch Editor when the selected quantitation method contains more than 150 transitions and control of any LC device is established through AAO (Analyst Access Objects). In this scenario, attempting to acquire the batch results in failed acquisitions. This patch functionality is included in the software.

Analyst[®] 1.5.1 Patch for DiscoveryQuant[™] Software

This patch corrects the following issue: DiscoveryQuant — Optimize 2.1 software is not able to successfully process certain product ion spectra (CE), and returns the error—2147467259 to the user. The issue occurs randomly and is not always for the same sample. This patch functionality is included in the software.

New Enhancements and Fixes in the Analyst 1.5.2 Software with HotFixes to February 2011

AAO and Companion Software

ChemoView Software Reports with large numbers of samples would intermittently fail

When using the ChemoView™ software to create reports with large numbers of samples, users would intermittently see reporting fail for some samples. This was only seen for large (typically over 100 samples) report batches, and re-running the report would often work properly. This has been corrected. (ST 24863)

Submission of a batch fails if the user selects a Quantitation method with more than 150 transitions

When creating an acquisition batch through an AAO application, if the user selected a Quantitation method with more than 150 transitions, the batch submission would fail. This has been corrected. (ST 21398)

Reporter 3.0.1 Software Integrated into the Analyst Software Installer

Previously, the Reporter 1.0 software was installed by default, and the Reporter 3.0.1 software was included in the installation DVD as an optional software. The Reporter 3.0.1 software is now integrated into the Analyst 1.5.2 Software with HotFixes to February 2011 and installed along with this software. If users have older Reporter 1.0 reports and wish to use them with the Reporter 3.0.1 software, there is a conversion utility available from Start > Programs > AB SCIEX > Reporter 3.0.1. (ST 24738)



Note: *If the standalone Reporter 2.0 software is installed on the computer, it should be uninstalled before installing the Analyst 1.5.2 Software with HotFixes to February 2011. If the Reporter 3.x software is installed on the computer, it will be automatically removed and replaced with the integrated Reporter 3.0.1 Software during the installation of the Analyst 1.5.2 Software with HotFixes to February 2011. Any custom queries and templates will be preserved. If a default query has been modified, a new unmodified version will also be installed with the suffix “_new”.*



Note: *If the standalone Reporter (2.0 or 3.x) software is installed after installing the Analyst 1.5.2 Software with HotFixes to February 2011 and is later uninstalled, the Analyst 1.5.2 Software with HotFixes to February 2011 may lose reporting capabilities. In this scenario, the Analyst 1.5.2 Software with HotFixes to February 2011 should be reinstalled.*

Users were required to log-in twice when using certain Companion Software

When a user logged into the Analyst software with Mixed Mode security enabled and then launched certain companion software (for example, MPX™ driver software), they may have been required to enter their logon credentials when launching the Analyst software as well as when

launching the companion software. This has been changed, and users will be required to provide their credentials only upon launching the Analyst software. (ST 25713)

DiscoveryQuant — Optimize software would fail during acquisition

When using the DiscoveryQuant™ — Optimize software, data acquisition would fail for certain samples and report the error - 2147467259. The Analyst software has been corrected to prevent this issue from occurring in future versions of the DiscoveryQuant — Optimize software that support the Analyst 1.5.2 Software with HotFixes to February 2011. (ST 26055)

Acquire — Acquisition and Batch Editor

Some *Scheduled* MRM algorithm scans would result in lower intensities than the corresponding MRM scans

In rare situations, users would see that a *Scheduled* MRM algorithm scan would show lower intensities than the corresponding MRM scan if the line obtained by plotting Resolution offsets against Mass passed through (or near to) the origin. This has been corrected, and now the corresponding *Scheduled* MRM algorithm scans will show proper intensities. (ST 24728)

Configure — Hardware Configuration

Included support for the following Agilent 1260 devices (ST 24294):

- G1310B Isocratic Pump
- G1311B Quaternary Pump
- G1312B Binary Pump
- G1316A Thermostatted Column Compartment (TCC)
- G1367E Autosampler
- G4212B Diode Array Detector (DAD)

Included Support for the following Agilent 1290 devices (ST 25922):

- G4220A Binary Pump
- G4226A Autosampler
- G4212A Diode Array Detector (DAD)
- G1316C Thermostatted Column Compartment (TCC)

Added support for barcode reading with CTC PAL autosamplers

Users are now able to enable or disable reading and recording the barcode information on vial labels during acquisition, when using a CTC PAL autosampler that supports this feature. The information will be stored and visible in the data file (File Info). Also, when data containing scanned barcodes is quantitated, a “Scanned Barcode” column will automatically be added to the Results Table. (ST 26786)

RFID tags supported for 1290 TCC switching valve

The Agilent 1290 TCC (G1316C) supports switching valves with RFID tag. When data is acquired with an RFID tagged switching valve, the valve type and serial number will be added to the File Info of the sample.

RFID tags supported for DAD Flow Cell and Lamp

The Agilent 1290 DAD (G4212A) supports RFID-tagged flow cells and lamps. When data is acquired using an RFID tagged flow cell or lamp, the serial number of the part will be added to the File Info of the sample.

Analyst 1.5.2 Software with HotFixes to February 2011 supports the most recent Agilent devices firmware

The Analyst 1.5.2 Software with HotFixes to February 2011 has been tested with the latest (at time of release) released firmware versions for supported 1100, 1200, 1260 and 1290 devices. For a list of supported firmware, see the *Software Installation Guide* for the Analyst software.

Explore

The Calibration Tables timestamp shown in File Info may be incorrect if a non-US time format is used

If data was acquired on a computer using a non-US date format, and if the users view the File Information on a different computer, they might see that the “Last Modification Date” for the Calibration Tables was the same as the Sample Acquisition timestamp. This has been corrected, and the data acquired on a computer using a non-US date format will display the correct timestamp for the Calibration Tables’ Last Modification Date. (ST 22722)

Checksum Verification may fail even though the data file is intact and not corrupted

In rare instances, when verifying the Checksum information embedded within a .Wiff file, the Analyst software would incorrectly report that the verification had failed. The Analyst 1.5.2 Software with HotFixes to February 2011 corrects this issue and will now correctly report that the verification has succeeded when the data is intact. This does not affect the verification results of corrupted/modified files, which will continue to fail checksum verification. (ST 26701)

Explore — Library Search

Printed Library Search results do not match the on-screen results

When printing the results of library searches, users would see the following formatting errors in the printed output: the font size of the printed text would be too large; in single-page printing, the second library match would always be printed even when not requested; and in multi-page printing, UV spectra would not be printed even when requested. The Library Search printing functionality now works properly; the text is printed in a reasonable font size, and only the requested elements are printed. (ST 23330)

Firmware Files

New firmware available for AB SCIEX QTRAP 5500 and AB SCIEX Triple Quad 5500 systems

The firmware for the AB SCIEX QTRAP[®] 5500 and AB SCIEX Triple Quad[™] 5500 systems has been upgraded. The changes made in this firmware revision are not customer facing. For information on how to upgrade the firmware of your mass spectrometer, see the *Software Installation Guide* for the Analyst software.

Help Files and Tutorials

Contents of Ion Optics Tutorial revised

The Ion Optics Tutorial (available at Start > Programs > AB SCIEX > Analyst > Tutorials) has been revised for content and accuracy. (ST 25565)

“Library Search Results” Help topic updated

The topic “Search Results: Print Options Dialog” has been updated to more accurately reflect the various printing options. (ST 28211)

Obsoleted Help files removed

Two help files, ENDURANCEAS.hlp and PALAS.hlp are no longer required and have been removed from the \Program Files\Analyst\Help folder. (ST 23351)

Quantitate

Quantitation fix to prevent rounding errors with IntelliQuan Algorithm (addendum to fix in the Analyst 1.4.2 software)

In the Analyst 1.4.2 software, a change was implemented for the IntelliQuan algorithm to reduce the likelihood of rounding errors causing a discrepancy between the Results Table and Peak Review due to an improper selection of the Noise Threshold. The Analyst 1.5.2 Software with HotFixes to February 2011 builds upon this fix by further reducing the likelihood of these discrepancies being created. The IntelliQuan algorithm has not been changed. (ST 27614)

Quantitation fix to prevent rounding errors with Analyst Classic Algorithm

When using the Analyst Classic algorithm to create Results Tables, there was a rare possibility that users might see a discrepancy between the values shown in the Results Table and in Peak Review. Depending on the Peak Separation Width selected, a small rounding error could affect the baseline calculation and cause the Peak Review pane to calculate areas differently than in the Results Table. The likelihood of users experiencing this discrepancy has been significantly reduced without changing the Analyst Classic algorithm. (ST 21863)



Note: For details on the original solution implemented in the Analyst 1.4.2 software, see [Appendix B](#) (reprinted from the Analyst 1.4.2 Software Release Notes).

Record Modified flag stays on even though the entire quantitation method was updated

If the user changed some integration parameters in Peak Review and then selected the option to Update the Method, the Record Modified flag would not always be cleared for the updated peaks. This has been corrected and the Record Modified flag will now be cleared when the method is updated. (ST 26582)

Sum Multiple Ions may produce incorrect results

Previously, when the Sum Multiple Ions option was used to create a quantitation method, the Results Tables produced with this method may have shown visible artifacts when the peaks were viewed in Peak Review. This issue has been fixed. (ST 21831)

Accept Changes dialog may not be shown for manual integrations

If the user performed a manual integration in Peak Review and navigated to a different sample or the Results Table, they may not have been prompted to accept the change before it was committed. This has been corrected, and the Accept Changes dialog will be displayed when navigating away from an uncommitted change. If the Audit Map is configured to require either a Reason or E-Signature for a manual integration, the Accept Changes dialog will not be presented to the user. (ST 22745)

Scripts

MRM3 Optimization Script replaces MS3 Quant Optimization script and is installed by default

The MS3 Quant Optimization script has been replaced by the MRM3 Optimization Script. This script provides the functionality of the MS3 Quant Optimization script and adds the ability to work with peptides and multiple charged ions. Users who upgrade from a previous version of the Analyst software will retain the previous MS3 Quant Optimization script and also receive the new MRM3 Optimization script. Users who perform a fresh installation of the Analyst software will see only the MRM3 Optimization Script in the Script menu within the Analyst software. (ST 22752)

Program Shortcuts

New documentation is available in Start > Programs > AB SCIEX > Analyst > Site Planning Guides

- *API 2000™ System Site Planning Guide*

New documentation is available in Start > Programs > AB SCIEX > Analyst > Qualified Maintenance Guides

- *API 2000™ Qualified Maintenance Guide*

New documentation available in Start > Programs > AB SCIEX > Analyst > Ion Source Guides

- *Turbo V™ Ion Source Operator's Guide*

- *NanoSpray® Ion Source Operator's Guide*
- *DuoSpray™ Ion Source Operator's Guide*
- *API 2000™ Source Operator's Guide*
- *NanoSpray III Head and Emitter Tip Assembly*
- *PhotoSpray® Ion Source Operator's Guide*
- *Ion Source Specifications*

Device Support

Support for Agilent G1367D Autosampler

Analyst® 1.5.1 HotFixes to June 2010 adds support for the Agilent 1367D model Autosampler. (ST 18976)

Support for Agilent 1200 G1329B Autosampler

Analyst® 1.5.1 HotFixes to June 2010 adds support for the Agilent 1200 1329B model Autosampler. (ST 18976)

New Enhancements and Fixes in the Analyst 1.5.1 HotFix



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

Acquire

Default scan speed for ER scans on the 3200 QTRAP system changed to 1000 amu/s

The default scan speed for ER (Enhanced Resolution) scans on the 3200 QTRAP system has been changed to 1,000 amu/s. The option for 250 Da/s still exists and can be selected by users who want to use the slower speed. (ST 21519)

Quantitate

Prevent exporting or saving Results Tables containing unsaved changes

Users will now be forced to save a results table before they export or print from it. This new workflow feature is designed to help customers adhere to operating procedures that prohibit the practice of printing or exporting unsaved results tables. However, it remains the responsibility of the customer to ensure that SOPs are created and followed to prevent users from taking actions in the software that may be possible, but not desirable. (ST 19788)

Security

Project Level Security enhancement when using AAC

Analyst 1.5.1 software introduced changes to the way in which project-level security is managed when using AAC (Analyst Administrator Console). The Analyst® HotFixes to June 2010 introduces the ability for users to choose between strict project-level control (as in Analyst 1.5.1 software) and the previous (pre-1.5.1) project-level control. Administrators have the option to enable or disable enhanced project-level security on a client-by-client basis, allowing some users to operate in a relaxed environment while tightly controlling the project-level security of other users. No changes were made to the AAC Server for this enhancement. (ST 20497)

Fixed Issues

Acquire

IDA Experiments with an ADC Card in the active hardware profile are now possible

If an ADC (Analog-Digital Conversion) card was active in the Hardware Profile, users were unable to run IDA experiments. Doing so caused the ADC card to fail and turn red in the Instrument Status area, which in turn caused the acquisition to fail. (ST 16102)

Users can now control Agilent 1100 or 1200 Hardware in a CAN configuration over Ethernet

Users were unable to connect Agilent LC hardware in a CAN configuration if the first device was connected to the computer via Ethernet. Users can now use both Ethernet and RS-232 connections for the first device in a CAN configuration. (ST 16108)

Peak Hopping scans missing first data point

When performing acquisitions using the Peak Hopping scan mode, the data list would begin above the requested start mass. This has been corrected and when performing Peak Hopping scans, users will see all non-zero data points. (ST 16866)

Mass Defect not applied uniformly during Peak Hopping scans

When performing acquisitions using the Peak Hopping scan mode, if the number of measurements (or spectrum data points) was less than or equal to 97 users would see the entered Mass Defect only applied to the first data point. Subsequent points would then be incremented solely based on the step size. However, if the mass range was greater than 97 Da, the Mass Defect would be applied correctly, but data points would be shifted as described above. (ST 22642)

Dynamic Fill Time was occasionally calculated incorrectly for ER scans

When an ER scan using DFT was included in a method that uses LC, occasionally, the required fill time was improperly estimated and defaulted to the maximum fill time value regardless of ion intensities. This sometimes resulted in ER scans that were of poor spectral quality due to space charge. This issue applied only to non-AB SCIEX QTRAP 5500 systems, but is now fixed. (ST 17281)

IDA methods using two EMS scans of opposite polarities now properly triggers dependent scans

If an IDA method contained two EMS survey scans of opposite polarities, the dependent scan would not be triggered even if the IDA criteria were satisfied. (ST 17045)

Security

Analyst software now supports long domain names in Mixed Mode

If a network domain contained more than 15 characters, users were unable to use Audit Trails. Users would find that upon entering their credentials for an e-signature, the password would be rejected and an error message would be presented. (ST 20279)

Quantitate

Area Ratio columns containing Div/0! would be exported as “-7”

When exporting Results Tables to text files, if an Area Ratio column containing Div/0! entries was exported, the Div/0! fields would be exported as “-7”. They will now be exported as “N/A”. (ST 18919)

Quantitation Methods with multiple decimal places may be modified if the user switches between tabs

If the user was building or viewing a quantitation method that includes transitions specified to 2 or 3 decimal places, switching between the Components and Integration tabs in the full method editor may have caused similar transitions to be modified or switched. Users would notice that the decimal components of the transitions were rounded or changed upon returning to the Components tab and the chromatograms may have become mismatched with their respective analytes in the Integration tab. (ST 22277)

New Enhancements and fixes for the Analyst 1.5.1 Software



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

Merged two software platforms into a single version of the software

This release combines the Analyst 1.5 software and the Analyst software 1.5 5500 Components, providing one software version that supports all our currently supported QTRAP and triple quadrupole instruments. For a list of supported instruments, see the *Analyst® 1.5.1 Software Installation Guide*. In addition, previously released HotFixes and patches have been included.

Added support for the following Microsoft products

- Microsoft Office 2007

- Microsoft Windows XP SP3

New software and hardware documentation available

In **Start > Programs > AB SCIEX**, the following new documentation is available:

- *Standard Quantitation Tutorial*
- Hardware Guides for all systems
- Safety Guides in the following languages: French, German, Italian, Japanese, Spanish, and English
- Protein and Peptide Quantitation Tutorial
- Ion Optics Tutorial for the 5500 series of instruments
- Qualified Maintenance Guides
- Site Planning Guides

Integrated support for GPIB driver version 2.5

GPIB driver version 2.5, including USB.

Script enhancements

- Improved IDA Trace Extractor script to allow the ability to select polarity per fragment or neutral loss specified or fragment and neutral loss specified.
- Improved Dynamic Background Subtraction™ (DBS) algorithm to add more control over the DBS functionality embedded in methods created in the Analyst software. Users now have access to the number of background spectra that they want to average as well as access to the number of points for smoothing the current spectrum.
- Improved Merge MRM methods script to allow the option to populate the Compound ID column in the final MRM method with the compound name used in Compound Optimization.
- Improved the Regression calculator by resizing the form, text boxes, and labels to enable the display of values smaller than 0.001. (ST 16959)
- Convert Methods script enhancements. The following Convert Methods script issues have been fixed:
 - Convert Methods script incorrectly converted *Scheduled* MRM algorithm methods to MRM methods. This script now allows the user to automatically carry over the retention time information and all other *Scheduled* MRM parameters without having to enter them manually. (ST 15463)
 - The Compound IDs were not carried over to the newly created method when running the Convert Methods script. The Compound IDs are now carried over automatically. (ST 15464)
 - When users converted IDA methods, the IDA criteria and dependent scan experiments were lost. This script now carries over the IDA Criteria and dependent scans automatically. (ST 15326)
 - The Convert Methods script did not optimize the mass ranges for LIT scan types when converting methods for use between QTRAP systems. This script now automatically optimizes the mass ranges for the new method. (ST 18670)

Configure — Hardware Configuration

Included support for the following Shimadzu devices for the 5500 series of instruments

- Included support for the Shimadzu High Pressure LC devices: LC-20ADXR pump and the SIL-20ACXR and SIL-20AXR autosamplers. (ST 15748)
- Integrated Shimadzu LC MIMIC 5.4 SP1 driver (version 5.4.1.7). (ST 17947)

Agilent 1200 DAD G1315 C and D models acquire at the set rate

Agilent 1200 DAD G1315 C and D models acquire at the set rate when in Spectral Mode. All frequencies can be acquired now. (ST 12696)

A new entry has been added to the autosampler database to support the MPX™-2 High Throughput System

The autosampler database has been updated to include MPX-CTC as an option on the Location tab in the Batch Editor. (ST 16742)

Invalid parameter Access Ranges are now corrected

After installing the Analyst® 1.5 HotFixes to March 2009, the parameter Access Ranges were replaced by the firmware ranges, atypical behavior may have been observed and it may not have been apparent that the parameter settings were the cause. Because the firmware range for each parameter is typically much wider than the Access Range appearing in the originally installed software, switching a positive mode polarity method to the negative mode polarity, or vice versa, causes opposite polarity lens values to be applied and used in a method without any software error messages appearing. Consequently, a user may not have been able to see any data being collected when running such methods. During installation of the Analyst 1.5.1 software, these ranges are checked and the user is prompted if they need correcting. (ST 15063) (Analyst® 1.5 Patch for ParamSettings Access Ranges.)

Acquire — Acquisition and Batch Editor

The Target Scan Time for 5500 systems is now optimized

The actual scan time calculated from the Target Scan Time in *Scheduled* MRM algorithm experiments is now calculated differently for the 5500 systems because of the superior performance of these systems. As a result, users may notice a decrease in the dwell time used in their methods. Also, a greater number of MRM transitions in a single window can now be acquired. (ST 13970)

Autosamplers are now automatically selected in the Select Autosampler dialog

Previously, users had to select the autosampler in the Select Autosampler dialog when they imported a batch. Now when you import a batch, the autosampler that is automatically selected is the same one used in the active hardware profile. (ST 15747)

Charge state now optimized when switching polarity at the dependent scan level

In previous Analyst software versions, when the charge state of a peak at the survey or confirmation level was undetermined, the mass assignment for that peak was not changed as expected in subsequent experiments. The polarity switching is now working correctly when switching polarity at the dependent scan level in an IDA method regardless of the assigned charge state for the survey peak. (ST 14702)

Improvements to the MS/MS/MS scan type for the 3200 QTRAP systems

Improved the intensity for MS/MS/MS scan types. Users may notice an increase of 30.5 ms in their acquisition methods. (ST 17882)

Issue applying Source/Gas parameters to opposite polarity experiments in a single method now corrected

If the acquisition method had two experiments with different polarities and the user applied source and compound parameters to all other experiments, the Analyst software may have stopped responding. This issue is now resolved. (SCR 14299)

Tune and Configure

DP values used during optimization are now within range

Instrument Optimization now addresses the issue where the DP values used during optimization were out of range for some systems (API 5000™, AB SCIEX Triple Quad 5500, and AB SCIEX QTRAP 5500 systems) causing Instrument Optimization to stall in some instances. For these cases, optimization is expected to be more successful. (ST 17937, ST 9982)

Quantitate

Quantitation methods distinguish between MRM transitions

The quantitation method now distinguishes between MRM transitions where masses are at least 0.001 Da apart. This limit was previously 0.1 Da. (ST 14231)

Compatible Software

Analyst software menu option and icon now automatically opens the Reporter software

The Tools > Report menu option, including the icon in the tool bar, will open the Reporter software found in the Companion Software section in the Navigation bar. (ST 15755)

Analyst Administrator Console support improvements

When users log on to the Analyst software, they will only see projects for which their workgroup has access. Now users will be forced to re-authenticate their credentials if they change root directories. As a result, users may not have access to local projects such as the API Instrument project. These local projects must be shared and then added to Workgroups if access to these

folders is required at the Workgroup level. The local projects are still available when logging in locally. (ST 14015)

Improvements to the Translate.exe utility

You can now translate NETCDF files to .wiff files and .wiff to NETCDF files for all data files. (ST 14018)

Audit Trail

Screen lock and auto logout Wait Times recorded correctly in the Audit Trail Manager

The wait times for screen lock and auto logout were reversed in the Audit Trail records when the features were enabled. These fields are now recorded correctly. (SCR 5014) (Analyst[®] 1.5 HotFixes to March 2009)

Actual Lockout and Auto Logout Wait times can be entered correctly

The actual Lockout and Auto Logout Wait times within the Security Configuration options were reversed relative to the entered values. This issue has now been fixed. (Analyst[®] 1.5 HotFixes to March 2009)

Acquire — Acquisition and Batch Editor

The mass range has been increased to 1250 Da for quadrupole scan types on the 5500 series of instruments

This change is for quadrupole scan types only (Neutral Loss, Precursor Ion, Product Ion, MRM, Q1 MS, Q1 Multiple Ions, Q3 MS, Q3 Multiple Ions). The mass range for LIT scan types remains at 50 to 1000 Da. (ST 13316) (Analyst[®] 1.5 Software Components for 5500 Systems HotFixes to April 2009)

A new scan speed has been introduced for quadrupole scan types on the 5500 series of instruments

A new scan speed of 12000 Da/s is now available for the following scan types: Neutral Loss, Precursor Ion, Product Ion, Q1 MS, Q3 MS. (ST 11711) (Analyst[®] 1.5 Software Components for 5500 Systems HotFixes to April 2009)

Mass range for the API 3200 LC/MS/MS System has been increased to 2000 Da

An updated Configuration Table is included for this enhancement. The feature is optional and will not be activated until the updated Configuration Table (B9633002.FW) has been installed on the API 3200™ instrument. This mass range extension only applies to the triple quadrupole system and does not apply to the 3200 QTRAP system. (TT 10436) (Analyst[®] 1.5 HotFixes to March 2009)

The pause time is maintained for Q1, Q3, MS2, Precursor, and Neutral Loss scan types for the API 5000™ system

The user can now toggle between tabs without the pause time doubling when the average mass entered in the mass ranges table is equal to or exceeds 1000 Da. (ST 11465)

Diverter valve fixes

- The diverter valve on the 5500 series of instruments now switches correctly in MS/MS/MS experiments. (ST 14521) (Analyst® 1.5 5500 Components Patches - August 2009)
- Acquisition is now successful when the diverter valve on a 5500 instrument is included in a method containing a *Scheduled* MRM algorithm experiment type, when the method is an IDA method, or if the acquisition method is being collected with Dynamic Fill Time (DFT). (ST 13730) (Analyst® 1.5 5500 Components Patches - August 2009)
- Users can now switch the integrated diverter valve on a 5500 instrument when using an LC stack during MRM acquisition. (ST 12157) (Analyst® 1.5 Software Components for 5500 Systems HotFixes to April 2009)
- Running a batch with over 200 samples will no longer cause the batch queue to stall at about sample 210 when the acquisition method contains a diverter valve method for the internal diverter valve on a 5500 instrument. (ST 17168) (Analyst® 1.5 5500 Components Patches - August 2009)

Support for new autosampler layouts

The Analyst software autosampler database has now been updated to support new autosampler layouts from the device vendors: (Analyst® 1.5 HotFixes to March 2009)

- Dionex TSP AS3000/AS3500 (SCR 15521)
- Dionex ACC-3000 (SCR 15521)
- Jasco AS-1555 (SCR 15522)
- Jasco AS-1550 (SCR 15522)
- Jasco AS-1559 / AS-2059 / AS-2059-SF / X-LC3059AS (SCR 15522)
- Jasco AS-2050 / AS-2051 (SCR 15522)
- Jasco AS 2055 / AS-2057 (SCR 15522)
- Shimadzu: control rack for SIL-20A, 20AC, 20AXR, and 20ACXR (SCR 15319)
- Waters Acquity (SCR 15524)

Sample peak in the MS no longer delayed when acquired with the Shimadzu UV detector

When the Shimadzu UV detector was used in acquisition, the sample peak in the MS was delayed 30 seconds even though no delay was specified. This issue has been fixed. The delay is no longer observed. (SCR 15534) (Analyst® 1.5 HotFixes to March 2009) (ST 12316) (Analyst® 1.5 Software Components for 5500 Systems HotFixes to April 2009)

Support for Shimadzu autosampler injection volumes of less than 1 µL

Acquisition methods with injection volumes down to 0.1 µL are now supported. Previously, users could only use injection volumes equal to or greater than 1 µL. (ST 10763) (Analyst® 1.5 HotFixes to March 2009)

Included support for the following Shimadzu devices

Support for the Shimadzu High Pressure LC devices, LC-20ADXR pump and the SIL-20ACXR and SIL-20AXR autosamplers, has been implemented for the following systems: 2000 series of instruments, API 3000™ instrument, 3200 series of instruments, 4000 series of instruments, and the API 5000 instrument. (ST 15748) (Analyst® 1.5 HotFixes to March 2009)

Autosampler name appears correctly in the Batch Editor Autosampler layout list

The LC Packings WPS-3000 autosampler now appears as Dionex WPS-3000. The autosampler layout is correct and has not been changed. (SCR 15551) (Analyst® 1.5 HotFixes to March 2009)

Injection volume can now be entered in the Method Editor

In the Method Editor, when attempting to enter the injection volume for CTC PAL autosamplers, users received an error for every digit they entered. Now users can enter the injection volume without any errors. (ST 14016) (Analyst® 1.5 Patch for CTC PAL Autosampler Injection Volumes)

Batch submission speed increased when using multiple methods

Previously when using a CTC PAL autosampler, batches with multiple methods slowed the submission speed of the batches. Batches using multiple methods submit successfully now with no delays. (ST 14016) (Analyst® 1.5 Patch for CTC PAL Autosampler Injection Volumes)

All valid injection volumes can now be used with CTC autosamplers in both the Method and Batch editors

With systems using the CTC PAL autosampler, when users attempted to enter an injection volume in the Method and Batch editors, they received an error when trying to enter valid volumes. All valid injection volumes can now be used in the Method and Batch editors. (ST 14016) (Analyst® 1.5 Patch for CTC PAL Autosampler Injection Volumes)

Injection volume now validates against specified syringe size for the CTC PAL autosampler

The injection volume can now be validated against the installed syringe, and the selected method syringe. (SCR 12931) (Analyst® 1.5 Patch for CTC PAL Autosampler Injection Volumes)

Acquire — Information Dependent Acquisition (IDA) and IDA Method Wizard

Long IDA batches containing an ER scan type now acquire successfully

Long (about 25 hours) Information Dependent Acquisition (IDA) batches that contained an ER scan type with DFT enabled are now acquired successfully. (ST 13718) (Analyst® 1.5 5500 Components Patches - August 2009)

Correction of calibration shifts

Calibration shifts of up to 1 Da or more were observed when two or more precursor ion scan types, two neutral loss scan types, or a combination of these two scan types was used either inside or outside an IDA experiment. This issue has now been fixed. (ST 12749) (Analyst® 1.5 5500 Components Patches - August 2009)

Correct DAC value applied for negative precursor ion scan type or neutral loss scan type

If a user ran an experiment that contained a negative precursor ion scan type or a neutral loss scan type, a calibration shift for the negative ions was observed. This issue has now been fixed. (ST 13636) (Analyst® 1.5 Software Components for 5500 Systems HotFixes to April 2009)

Calibration shift no longer observed when looping two precursor ion or two neutral loss experiments (or a combination of the two experiments)

If a user used any two precursor ion scans, two neutral loss scans, or a combination of those two scan types, a calibration shift of approximately 1 Da was observed. This issue is now fixed. (ST 12749) (Analyst® 1.5 5500 Components Patches - August 2009)

Quantitate

All Results Tables from previous versions of the Analyst software open successfully

If a user tried to open a Results Table created in a previous version of the Analyst software, the software occasionally closed unexpectedly without logging any errors in the event log. This issue did not affect data integrity. This issue has now been fixed. (ST 15562) (Analyst® 1.5 Software Components for 5500 Systems HotFixes to April 2009) and (ST 12870) (Analyst® 1.5 HotFixes to March 2009)

'Apply to All Rows' check box added to query for Results Tables

You now have the option of applying a query to only those rows that are currently visible in the Results Table or to all the rows in the Results Table. To use this feature, select the Apply to All Rows check box in the Query Editor dialog. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

Nested queries and group/ungroup logic fixes added to Results Table queries

You can now group or ungroup queries. You can also nest queries within other queries as long as they do not share the same start or end item. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

'One click' peak review available in Calibration plot

You can now open the peak review pane by clicking a data point on the calibration plot. Click another data point to refresh the peak review pane and show the peak associated with that point. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

Analyte names field expanded in the calibration pane

The Analyte list field containing the names in the calibration pane has been modified to allow for a greater number of Analytes to be displayed. Previously, the box showed a maximum of three analytes. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

Filter Results Table by Sample Type now available

In addition to filtering the Results Table rows by Analyte and Analyte Group, you can now filter a Results Table by Sample Type and view only a specific type at a time. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

New 'contains' Operator for custom Formula column available

You can now create a formula for a custom Formula column in the Results Table using the new "contains" operator. This operator performs a string comparison of two fields and then returns either a TRUE value, if one string is contained within the other, or FALSE, if one string does not contain the other.

The custom Formula column can then be queried to show only those that are TRUE or FALSE, depending on preferences. (SCR 15543) (Analyst® 1.5 HotFixes to March 2009)

Expected Retention Time appears correctly in the Results Tables

If you used the Quantitation Wizard to create a new Results Table using the Automatic Method option on the Select Method page, the Analyte Expected Retention Time was incorrectly reported as "0" for the first compound and Expected Retention Time values were shifted to the next compound. The Analyte Expected Retention Time is now correctly populated. (TT 9401) (Analyst® 1.5 HotFixes to March 2009)

ADC data can be quantified by the Analyst Classic algorithm

When quantifying ADC data with the Analyst Classic algorithm, the user received the message "The method cannot be used because it is not compatible with all of the selected samples." You can now quantitate ADC data using the Analyst Classic algorithm. (TT 6978) (Analyst® 1.5 HotFixes to March 2009)

Quick Quant method uses the customer-selected IntelliQuan values

After the preset parameters were modified using the IntelliQuan global settings, those preset values were not used when creating Quantitation methods using the Quick Quant feature in the Batch Editor. Instead, parameters in the Quantitation method creation dialog were reset to zero. Now, the Quantitation methods using the Quick Quant feature in the Batch Editor use the preset values that were set in the IntelliQuan dialog. (TT 6997) (Analyst® 1.5 HotFixes to March 2009)

IS Quality no longer displays unknown characters

When no peak was found, the IS Integration Quality in the Integration Quality displayed "-1.J#" instead of the correct value of zero. Now, the IS Integration Quality reports correctly as zero. (TT 7388) (Analyst® 1.5 HotFixes to March 2009)

Custom Columns updated in the Results Table

When Custom Columns were added in the acquisition Batch Editor, only the first compound was updated in the Results Table after quantitation. The remaining compounds displayed N/A. This

issue has been fixed. All compounds are updated in the Custom Columns. (SCR 15535) (Analyst® 1.5 HotFixes to March 2009)

Quantitation of *Scheduled* MRM algorithm data file

An internal change has been made to the way in which Analyst® software handles data layouts in the Results Table. Now the summary columns are handled in a more consistent fashion. This change is transparent and will have no functional impact to this feature. (ST 8250) (Analyst® 1.5 HotFixes to March 2009)

Expected RT and RT Window values no longer set to zero in the Results Table

When a Results Table was created and a peak was not found for a particular sample, the associated Expected RT and RT Window values were set to zero in the Results Table. Changing the integration parameters to correctly integrate these peaks would populate the correct Expected RT and RT Window values. This issue has been fixed. The Expected RT and RT Window values are now populated whether or not a peak is found. (TT 5447) (Analyst® 1.5 HotFixes to March 2009)

Other

4000 QTRAP instrument compatible with DuoSpray and PhotoSpray ion sources

With the previous Configuration Table, the 4000 QTRAP instrument (AR series) did not recognize the DuoSpray and PhotoSpray ion sources. An updated Configuration Table has been included in this release. To fix this issue, update the Configuration Table (B9609031.FW) on the 4000 QTRAP instrument. (SCR 15548) (Analyst® 1.5 HotFixes to March 2009)

Resolution settings saved after copying

When you copy experiments in the acquisition method, the resolution settings were not saved. Re-enter this information. This issue is now fixed. (SCR 13080)

New Enhancements and Fixes in the Analyst 1.5 Components for 5500 Systems

With the exception of the last item in this section, the following information describes support for the AB SCIEX QTRAP 5500 System and the AB SCIEX Triple Quad 5500 System.



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

Acquire — Acquisition and Batch Editor

Faster Linear Ion Trap (LIT) scan rates

The system performs LIT scans in all modes at up to 20000 Da/s, as well as 1000 and 10000 Da/s. In addition, Enhanced Resolution scan types are available at 50 and 250 Da/s.

Pre-set quadrupole scan rates

Quadrupole scanning is now done at fixed scan rates (up to 2000 Da/s), which simplifies operation for the customer while ensuring good data quality.

Better Quadrupole and LIT sensitivity relative to the 4000 QTRAP system:

- Better quadrupole sensitivity means increased MRM sensitivity resulting in lower limits of quantitation.
- Better LIT sensitivity means better qualitative and quantitative data.

Faster polarity switching

The system is capable of switching polarity in only 50 ms, which is more than 10 times faster than our existing systems.

Quadrupole MRM improvements

Shorter transit times across the improved LINAC[®] collision cell allow lower dwell and pause times to be used for multiple MRM experiments. Up to 1250 MRM transitions are now supported in a single experiment, and up to 2500 MRM transitions using the Scheduled MRM algorithm.

Quadrupole scanning improvements

The improved LINAC collision cell also leads to better precursor and neutral loss scanning, with scan rates up to 2000 Da/s at unit resolution.

Other

Communication via Ethernet now available

The communication between the system and the acquisition computer is now provided through an Ethernet connection instead of a GPIB connection.

Integrated syringe pump and integrated diverter valve available

The system is equipped with an integrated syringe pump and integrated diverter valve. You can start these devices manually or control them through the Analyst software.

Notes on Use

- In the DFT Method Options, the target TIC values are optimized for the 10000 Da/s scan speed with the exception of the Enhanced Resolution target TIC, which is optimized for the 250 Da/s scan speed. These values are suitable for all other scan speeds.
- By design, if the integrated syringe pump is configured in a method, the syringe pump will remain running after completing a run until the Max Idle Time is reached. You must manually stop the syringe pump after you have completed Instrument Optimization if you want to stop the flow from the syringe pump. Instrument Optimization will not turn off the syringe pump.



Tip! You can adjust the Max Idle Time in the Queue Options by clicking **Tools > Settings > Queue Options**.

- The Analyst software operation may be slow in the areas of the Method Editor, Explore, and Quantitation when dealing with a large number of MRM transitions.
- Make sure that you have a printer configured before running Instrument Optimization.
- The Queue must be in Ready state before you start the syringe pump: If the Queue is in Standby mode, put the queue in Ready state before starting the syringe pump.

IntelliQuan parameters now selected in peak list tab for data acquired using the Scheduled MRM algorithm

When data acquired using the *Scheduled* MRM algorithm are opened, the corresponding peak list will now correspond to the recommended integration algorithm. Previously the Analyst Classic algorithm was being applied instead of the IntelliQuan algorithm to data when the first sample in the data file was not a *Scheduled* MRM sample. (ST 6981)

New Enhancements and Fixes in the Analyst 1.5 Software and the Analyst 1.4.2 HotFixes



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

Audit Trail

Actions logged to the correct Audit Trail*

It has been noted that if a user changes the active Project while data is being acquired, the Audit Trail will show data being added to the newly selected project rather than the original one. This issue has been resolved, and now changing the active project while data is being acquired will not affect which Audit Trail information is logged to. (SCR 15270) (Analyst® 1.4.2 HotFixes to July 2007)

**These actions require that the Audit Trail is set to record the described actions*

Record Modified flag now clears

If a user manually integrated a sample and accepted the changes but then manually cleared the “Manual Integration” check box and accepted that change, the Results Table reverted to the original (automatic) integration, but the Record Modified flag still remained. This has been corrected and now manually clearing the “Manual Integration” box and accepting the changes clears the Record Modified flag. (SCR 15161) (Analyst® 1.4.2 HotFixes to July 2007)

Canceling a manual integration no longer flags a sample as modified

When e-Signatures were required as per the Audit Trail settings, and if a user manually integrated a sample but clicked “Cancel” when prompted for an e-signature, the sample reverted to its original (automatic) integration, but the Record Modified flag remained. This has been corrected and now clicking Cancel when prompted for an e-signature now clears the Record Modified flag. (SCR 15338) (Analyst® 1.4.2 HotFixes to July 2007)

Updating the method now clears the check box

If a user manually changed a method parameter on a sample and accepted the change, then right-clicked on the chromatogram and selected “Update the Method” the user was asked if he/she would like to update all peaks, as opposed to only those which have not been manually integrated. If the user selected “No” (Update only those not manually integrated), the Record Modified flag was cleared for all manually integrated samples but the Manual Integration box remained checked on the chromatogram. Analyst® 1.4.2 HotFixes to July 2007 corrects this issue and the Record Modified flag remains checked for all manually integrated samples. (SCR 15160) (Analyst® 1.4.2 HotFixes to July 2007)

Record Modified flag now accurately reflects the modification status of the sample

Incorrect behavior of the record modified flag was found in the following scenarios:

- The Record Modified flag for a manually integrated Analyte Peak is set to “off” when the integration parameters for its Internal Standard peak are modified and globally updated.
- The Record Modified flag remains checked “on” for some Analyte peaks even after the integration method for all samples is reset using the “Update Method” operation.

This behavior has been corrected and the record modified flag is now set properly for these scenarios. (SCR 15506) (Analyst® 1.4.2 HotFixes to May 2008)

Audit Trail archives correctly

For quantitation Results Tables, this issue cannot occur. However, for project and instrument audit trails, in rare cases where the audit trail exceeded 1000 records (for instance, when there are a large number of subprojects), and the user has been denied “modify” permissions for the audit trail folder, a situation could have occurred where these audit trails became unpopulated of archive events.

The audit trails for the project and instrument automatically archive after 1000 records are written. The audit trail is saved in the Project Information folder with a name indicating the type of audit trail and the date and time. A new audit trail is then created with the first record giving the path of the previously archived audit trail.

In the Analyst software version 1.4.2 and earlier, if the user both did not have Windows “modify” permissions and was not explicitly given “delete” permissions, an empty archive file was created that did not show the audit trail records. With this release, neither “modify” nor “delete” rights are required to successfully archive audit trail files. However, Windows read and write access is still required. (SCR 15516) (Analyst® 1.4.2 HotFixes to May 2008)

Acquire — Acquisition and Batch Editor

Scheduled MRM™ algorithm now available

Scheduled MRM algorithm provides the ability to monitor up to a thousand potential analytes in a single chromatographic run. This can be accomplished by supplying a list of MRM transitions and their corresponding retention times and compound IDs, a time window, and a target or desired cycle time such that the system can automatically acquire only the necessary MRM transitions at any given time during a run. On QTRAP instruments, this method can service screening applications with triple quadrupole MRM selectivity and LIT MS/MS simultaneously by focusing on only a few analytes at a time, allowing extra time for MS/MS scans.

The *Scheduled* MRM algorithm functionality can also be used in an Information Dependent Acquisition (IDA) experiment to maximize screening and confirmation capabilities.

DBS (Dynamic Background Subtraction™) functionality now fully integrated

DBS functionality improves the ability of the mass spectrometer to find more analytes in a chromatographic run while using IDA. By subtracting predicted analyte signal from the analyte(s) of focus during the course of an IDA run, DBS dynamically filters new analytes from the background noise. This functionality is now fully integrated into the software as a check box on the First Level Criteria tab of an IDA experiment.

Methods for Agilent 1100 devices are compatible with Agilent 1200 devices

Methods created with an Agilent 1100 stack will now open or run when a functionally equivalent Agilent 1200 stack is configured. For example, if the 1100 method contained an isocratic pump and wellplate autosampler, this method did not open or run when connected to a 1200 isocratic pump and 1200 wellplate autosampler. Upon installation of this release, users who have created methods on their Agilent 1100 stack are able to use them on a functionally equivalent Agilent 1200 stack without having to recreate the methods. [Please note that the Agilent 1200 high-pressure devices (G1312 B pump, G1367C autosampler, G1316 C column oven) are not considered functionally equivalent to any Agilent 1100 device. Therefore, a user will still not be able to use their 1100 methods when a 1200 high-pressure device is configured.] (SCR 15141) (Analyst® 1.4.2 HotFixes to November 2006)



Note: The information for Agilent 1100 devices which is available in the Help is also valid for Agilent 1200 devices.

Delay times now properly applied

When a method was created with a delay time greater than 30 seconds and was run in a batch, the delay times were occasionally longer or shorter than what was specified. This issue has been resolved. Acquisition Delay Times now reflect the times specified in the method. (SCR 15142) (Analyst® 1.4.2 HotFixes to November 2006)

Improved data capacity

To accommodate the larger data size introduced by the *Scheduled* MRM algorithm functionality, .wiff data file compression has been introduced. As a result, the data capacity of files is now improved.

Dynamic Fill Time (DFT) improvements

Improvements have been made to the DFT to better control the number of ions in the linear ion trap. This can result in improved spectral quality.

QTRAP data available for EPI scans in IDA methods

In a small number of cases, an issue was observed on the QTRAP series of instruments involving Enhanced Product Ion (EPI) scans in IDA methods occasionally failing to fragment the parent ion. Analyst[®] 1.4.2 HotFixes to July 2007 resolves this issue and EPI scans in IDA methods will collect data properly. (SCR 15360, SCR 15298) (Analyst[®] 1.4.2 HotFixes to July 2007)

Tune and Calibrate

Tune enhancements

A fully automated Instrument Optimization tuning function, formerly offered as a script called "AutoTune" has been fully integrated into the Analyst 1.5 or later software. The instrument optimization feature automatically tunes your instrument for you in minutes, saving time and effort formerly used in the mass calibration process. Because Instrument Optimization includes the optimization of the resolution of the instrument, Resolution Optimization has been removed from the Tune and Calibrate module. In addition, Quantitative Optimization has been renamed Compound Optimization and the Tune mode as a whole has been renamed Tune and Calibrate.

Explore

XIC no longer shows empty graphs

In rare cases, selecting the XIC in Explorer could result in an empty graph. The HotFix corrects this issue, and the XIC shows the appropriate data. (SCR 15198) (Analyst[®] 1.4.2 HotFixes to November 2006)

Quantitate

Several updates have been made to the peak integration in the Analyst 1.5 software. These updates have been made with the following principles in mind:

- Updates apply to the IntelliQuan peak integration mode; that is, the IQA and MQII algorithms. The Analyst Classic peak integration mode remains unaffected.
- The updates are well-documented in the software; quantitative results that use the updated algorithms are labeled **IQA II** and **MQ III** in the Results Table.
- Previous Results Tables (created in versions of the Analyst software earlier than version 1.5) will continue to use the non-updated peak integration in the Analyst 1.5 and later software (as opposed to the updated IQA II and MQ III). This is true even if such Results Tables are opened with the Analyst 1.5 and later software, modified and re-saved. To use the new algorithms, create a new Results Table from scratch.
- All new Results Tables in IntelliQuan peak integration mode are created using the updated IQA II and MQ III algorithms.

A full technical explanation of the changes is included in [Technical Information Regarding Integration on page 85](#).

For faster review of peaks in Quantitation mode, a measure has been added to indicate the quality of integration of peaks. This new feature is available through the addition of two new columns in the Results Table named "Analyst Integration Quality" and "IS Integration Quality". Values closer to 1 indicate well-integrated peaks and values closer to 0 indicate that the peak is not well-integrated. This indicator makes reviewing manual peaks easier because operators can focus on the lower values to guide manual review of substandard peaks.

Quantitation Optimization above mass 998 is successful

When the Quantitation Optimization wizard was run on an API 5000 instrument (or in API 5000 system simulation mode) with a mass above 998 resulted in the message: "Quantitation Optimization Failed", followed by an "Unspecified Error" window. This issue is now fixed and optimization proceeds correctly. (SCR 14889) (Analyst[®] 1.4.2 HotFixes to November 2006)

Results Table Saving action logged in audit trail during QA Review*

When a user assigned the QA Reviewer role opened a Results Table and then attempted to close it, they were prompted "Do you want to add an annotation about your QA Review to the audit trail for this results table? Yes / No / Cancel". Even if the user selected "No" they were prompted for an e-signature and a saving action was logged in the Audit Trail. With this release, there is no prompt for an e-signature, and no saving action is logged unless an annotation is added. (SCR 14911) (Analyst[®] 1.4.2 HotFixes to November 2006)

Results Tables deleted on overwrite now logged in the Audit Trail*

With a Results Table active, a user could click File > Save As, and choose to overwrite an existing table. If the auditing capabilities were enabled, the user was prompted to input a reason for this action. Selecting "Cancel" at this point resulted in the deletion of the existing Results Table. No action was logged in the Audit Trail. After installing this release, the existing Results Table is neither deleted nor modified in the case described above. (SCR 15081) (Analyst[®] 1.4.2 HotFixes to November 2006)

*These actions require that the Audit Trail is set to record the described actions.

Discrepancy Between Results Table and Chromatogram is now corrected

If a user built a Results Table based on samples that were still being acquired, the Analyst software built the Results Table based on the information available at the time. This could lead to the Results Table showing results that did not agree with the associated chromatograms as shown in the Peak Review window. The Analyst software did not automatically update the Results Table after acquisition is complete.

Following installation of this release, when a user runs the Quantitation Wizard, samples which are in the process of being acquired will not be displayed in the wizard. This prevents users from selecting them and potentially generating incorrect results. If a user runs the Quantitation Wizard during acquisition, he/she will need to build a new Results Table or manually add the samples to the Results Table after the acquisition has completed in order to include samples which were not added because they were still being acquired at the time of the table's creation. (SCR 12842) (Analyst[®] 1.4.2 HotFixes to July 2007)

Area discrepancy between the Results Table and peak review is now fixed

In the Quantitation module, in rare cases, small discrepancies were reported between the Results Table peak area and the peak review peak area. In sites that reported experiencing the issue, fewer than 1 in 2000 integrations were affected. The issue has been addressed. See [Technical Information Regarding Integration on page 85](#). (SCR 15517) (Analyst® 1.4.2 HotFixes to May 2008)

Smoothing Value on reports is now printed

When a Quantitation report was printed for a manually integrated report, the smoothing value used was not printed on the report. This has been corrected and the smoothing value used is now shown. (SCR 14974) (Analyst® 1.4.2 HotFixes to July 2007)

Quantitation Parameters prints correctly when using IntelliQuan

When printing a Quantitation report for which the Integration Algorithm was set to IntelliQuan, the Integration Parameters shown on the report was actually the settings for the Analyst Classic Algorithm. This issue is fixed and now IntelliQuan reports will properly show the integration parameters used. (SCR 14340) (Analyst® 1.4.2 HotFixes to July 2007)

Peripheral Devices

The Analyst 1.5 software provides additional support for the following:

- Autosampler layout database for the Spark Holland Alias autosampler controlled through the Analyst Access Object (AAO) interface. (SCR 15523)
- Autosampler layout database for the Agilent autosampler AS G1367C Hip-ALS SL.
- Agilent DAD 1315D. (ST 17089)

Support for the following Shimadzu LC-20A Prominence devices:

- Controllers: CBM-20A
- CBM-20A Lite
- Pumps: LC-20AT
- LC-20AD
- LC-20AB
- Detectors: SPD-20A
- SPD-20AV
- RID-10A
- RF-10A
- RF-10Axl
- AutoSamplers: SIL-20A
- SIL-20AC
- Rack Charger
- Ovens: CTO-20A

- CTO-20AC

(SCR 14795, SCR 15282) (Analyst® 1.4.2 HotFixes to November 2006)

Support for Agilent 1200 DAD is now included

Support for the Agilent 1200 G1315 D Diode Array Detector. (SCR 15296) (Analyst® 1.4.2 Patch for Agilent 1200 G1315 D DAD)

Shimadzu FIA Quantitation Optimization Isocratic Method now recognized

Following the installation of Analyst® 1.4.2 HotFixes to July 2007, attempting to perform FIA Quantitative Optimization with Shimadzu devices configured natively within the Analyst software caused a message to appear informing the user that an isocratic method was needed. This occurred even when an isocratic method was provided. This issue is resolved and users can once again use Shimadzu devices to perform FIA Quantitative Optimization. (SCR 15516) (Analyst® 1.4.2 HotFixes to May 2008)

Other

Displaying File Information may have caused Analyst software to stop responding

In a rare number of instances, displaying the File Information for certain files caused the Analyst software to stop responding. This issue has been fixed. (SCR 15195) (Analyst® 1.4.2 HotFixes to November 2006)

The list of devices contained in an Analyst method is now returned

Program level access to Analyst method components (through use of the Analyst software SDK) would not return the list of devices contained in the Analyst software method. This issue is fixed and the full list of devices in a method is returned. (SCR 15240) (Analyst® 1.4.2 HotFixes to November 2006)

AAO batch acquisition error

LC and other peripheral device vendors (excluding Agilent, Shimadzu, and CTC) use the Analyst Acquisition Object (AAO) interface to run their device drivers. When running long batches with a driver using the AAO, the batches intermittently fail. This issue has been fixed. (SCR 14842) (AAO Development Kit for Analyst® 1.4.2 HotFixes to November 2006)

Calling ConfigureBatch() in AAO with more than one template mass range caused issue with column names

When using the AAO, the ConfigureBatch() command would result in erroneous column names being used if more than one template mass range was specified. This has been corrected with this release and calling ConfigureBatch() with more than one template mass range now results in the proper column names being created. (SCR 15187) (AAO Development Kit for Analyst® 1.4.2 HotFixes to November 2006)

Quantitation method reference included in .wiff files acquired by submitting batch through AAO

When submitting a batch through the Analyst software, a reference to the Quantitation Method used in the batch is created in the .wiff file. However, when submitting a batch via AAO, the

reference to the Quantitation method was missing from the resulting .wiff file. This error has been corrected in the HotFixes to November 2006, and now batches submitted via AAO which contain a reference to a Quantitation Method will have the Quantitation Method included in the resulting .wiff file. (SCR 15169) (AAO Development Kit for Analyst[®] 1.4.2 HotFixes to November 2006)

Added AAO event to notify client of change in the Analyst software project

When a new active project is selected within Analyst software, a new ProjectChange event containing the name of the newly selected project is fired from AAO, allowing the client application to be programmatically synchronized. (SCR 12965) (AAO Development Kit for Analyst[®] 1.4.2 HotFixes to November 2006)

Added AAO event to notify client of changes to Analyst software method file

In the Analyst software, on saving of a method file containing the AAO client application method, a new MethodRequested event is fired from AAO to notify the application of the save. The client application can then respond by calling a new method IAAO_Method::SendXMLMethodData() with the latest XML method data corresponding to the Analyst software method, which will then be passed back into the Analyst software and then saved into the method file, ensuring the methods in the Analyst software and in the client application are synchronized. (SCR 12963) (AAO Development Kit for Analyst[®] 1.4.2 HotFixes to November 2006)

Added ability to store Analog Detector information to Analyst software data file

DAD (Diode Array Detector) and ADC (Analog-to-Digital Converter) data acquired from peripheral devices controlled by AAO client applications can now be stored in real-time into the Analyst software .wiff data file via interface methods in IAAO_Acquire. (SCR 12958) (AAO Development Kit for Analyst[®] 1.4.2 HotFixes to November 2006)

Support for ADC Card PCI-6289 and NI-DAQmx 8.3

The Analyst software now supports the National Instruments PCI- 6289 ADC card as well as NI-DAQmx driver version 8.3. The new driver is required for the new ADC card, but also supports the existing model PCI-6032E. Therefore, this driver change will be transparent to the user, and will not affect any existing functionality. (SCR 15442) (Analyst[®] 1.4.2 HotFixes to July 2007)



Note: The existing driver for the ADC Card must be replaced if this release is installed on a PC where an ADC Card is currently installed.

Quantitation Optimization for AAO applications

Previously, Quantitative Optimization (Infusion) could not be performed with AAO-controlled devices, as the mass spectrometer would wait indefinitely for an injection to take place. This has been resolved and the mass spectrometer will no longer wait for an injection as methods are now configured in the NO SYNC mode. As a result, Quantitative Optimization will proceed as expected. (SCR 14921) (Analyst[®] 1.4.2 HotFixes to July 2007)

FIA Quantitation Optimization for AAO applications

When performing Quantitative Optimization with FIA, the wizard checks the method for an isocratic LC pump method and if an autosampler is present, will set up the display for the user to pick the rack, sample position, and so forth. With Software Applications using the AAO, this did not work and the wizard thought the method is a mass spectrometer-only method. This is now fixed and support for external AAO applications is implemented. AutoSamplers controlled via

AAO can now be configured (including rack/plate/vial selection) during the FIA Quantitative Optimization wizard. (SCR 12956) (Analyst® 1.4.2 HotFixes to July 2007)

Manual Tune now works with AAO controlled devices

Previously, during manual tune the user was not allowed to build methods for devices controlled by the AAO. This has been corrected and LC Pumps controlled via AAO can now be used to build a method as part of the Analyst software manual tune operation. (SCR 12977) (Analyst® 1.4.2 HotFixes to July 2007)



The following is a list of known issues, limitations, and important notes on using the software. There may be other issues or limitations with the Analyst® 1.6.1 software in addition to those listed below. If you find additional issues, email support@absciex.com.

In general, if the Analyst software is not responding, restarting the software may help. If this does not work, restart the computer to make sure the Analyst Service software 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 may 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 application. 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 may 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 will disable 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 may result in failed acquisitions or corrupted data files.

Audit Trail

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

We do not recommend that you access the Analyst software using RDP. Users who access the Analyst software using RDP are logged in the Analyst software audit trail. Any subsequent users who log in to the Analyst software at a workstation that is running RDP will be 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 will not appear properly even following the installation of the Analyst 1.5.1 software. Audit trail records will display correctly, but these special characters will appear differently in the record. (ST 14394)

For example:

∏ will appear as a box

Ñ will appear as a G

ß will appear 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 may be deselected. Do not use Fill Down over these events. (SCR 14266)

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

If you close an IDA data file, the event is not logged in the audit trail. (ST 9487)

Mass range extension and scan speed are not audited events

On the 5500 series of instruments, the mass range extension and scan speed addition are not audited events. Make sure that you update your maintenance log after updating the software.

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 may 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 may be truncated. In some cases, this issue may 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) may 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 will use the network server clock time instead of the local computer time. This is expected behavior. (SCR 12390)

Checksum events not recorded in the audit trail

After performing Verify Checksum activated in the Open File Dialog, the software does not record this event in the audit trail. (ST 24177)

Configure — Administration/Security

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 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, see 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 may 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 may not appear 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 into the software when it was locked, the Analyst software displays 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) appears. (SCR 13792)

Screen lock settings not retained on install

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

Configure — Hardware Configuration

Incorrect profile shown in the error message

The hardware profile dialog may 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 may 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 may 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 appearing during uninstall

Occasionally, when uninstalling the Analyst software, a message asking the user to deactivate the hardware profile appears even if the hardware profile has been deactivated. To clear this issue, restart the Analyst software. (ST 16060)

Configure — Report Template Editor

The report template created through the Report Template Editor may sometimes not be applied

Although a saved report template is selected in the Print dialog, the template is occasionally not applied to the printouts. This may be related to the rights of the user on the computer network.

Tune and Calibrate — Compound Optimization

Transitions with the same name may 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 will not optimize 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™ 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

Unable to switch to Tune mode

After performing Instrument Optimization, the Analyst software may not be able to switch to Tune mode. The Tune button on the toolbar may be disabled. If this occurs, deactivate and then reactivate 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 highly recommended that you use the approved tuning solution. If you use an unapproved solution, some masses may 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 will scan less than the number of MCA scans selected in an acquisition method. For example, the software will only return 3 scans for a Q1 scan when 10 MCA scans are specified. This MCA issue may affect Instrument Optimization. If this occurs during Instrument Optimization, restart the optimization process. (ST 13460)

Tune and Calibrate — Manual Tuning

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)

Display 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 Tune

If the Graph Information pane is open in Manual Tune, the system may stop responding if one run is terminated and a new one started. Closing the Graph Information pane may 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, may yield incorrect TIC data.

Offset drop from unit resolution for the API 3200 instrument

For the API 3200™ instrument, 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 will scan less than the number of MCA scans selected in an acquisition method. For example, the software will only return 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 Tune

In Manual Tune, the user interface is not refreshed when the Resolution table editor is moved. Click between the tabs to refresh the user interface. (SCR 9327)

Changing the Resolution Table can cause a loss of communication

Changing the Resolution Table on-the-fly in Manual Tune during a *Scheduled* MRM™ algorithm acquisition causes communication to be lost with the instrument. You must restart the Analyst software and AnalystService to regain communication. (ST 9771)

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 may not be able to clear it as the Clear Error button may 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)

Display graphs may 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 displayed graphs can be slow to update and the Analyst software may appear to stop responding. This is especially true if the user switches applications and then switches back. However, the data is collected successfully and the program will update when the scan stops.

On the AB SCIEX QTRAP[®] 5500 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 AB SCIEX QTRAP 5500 system, after performing a fresh installation of the Analyst software, reference tables may 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

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 may be added to the survey scan

Refreshing the UI by clicking in a different field, switching between the experiments, or saving the method will delete the added mass ranges. (ST 17047)

On the AB SCIEX 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 AB SCIEX 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 AB 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 may be observed for data generated using the IDA Wizard for AB 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 may 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 dependent 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 will work as expected. (ST 18941)

IDA acquisition fails if the hardware profile contains an ADC device

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

Acquire — Method / Batch Editor/Queue Manager

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 1.6.1 software, 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.

Method duration may 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 may 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 may 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 proper switching method in the acquisition method. If users submit a method that does not contain a valid valve switching method, the Analyst software may 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 may 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 may 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 may fail to maintain targets

In some cases, users may 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 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 will see the field updated. (TT 34884)

Simulation mode: Some methods may not end at expected times

When running acquisitions in the simulation mode (for testing new methods and so on), some methods may not end at the expected time. The mass spectrometer should never be simulated for real LC data acquisition. (TT 34893)

Dynamic Fill Time may not work in Manual Tune

When users run Manual Tune with DFT enabled, changes to compound parameters may not trigger DFT to recalculate fill times. Therefore, when running Manual Tune, 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, Dynamic Background Subtraction (DBS) 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 may 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 not available

The Pause Sample Now icon on the Queue toolbar is inactive and will not affect acquiring samples. (TT 35287)

Queue: Next Period button not available

The Next Period icon on the Queue toolbar is inactive and will not affect acquiring samples. (TT 35288)

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 031088)

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 will stop 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 non-5500 systems, 300 MRM transitions is the limit when acquiring MRM data and 1000 MRM transitions is the limit when acquiring *Scheduled* MRM algorithm data. For the 5500 series of instruments, 1250 is the limit when acquiring MRM data and 4000 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 may 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/or errors might result.

Copying and pasting to mass table

See 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 may 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 may disappear in the Batch Editor. (SCR 11578)

Source/gas information may 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 its project path is longer than 126 characters. When you submit this type of file, you will receive the following error message: "Failed to set Header data". When you save this file, you will receive the following error message: "Failed to save BatchName".

Pasting columns in mass ranges table

Pasting of individual column of values for compound dependent parameters in MRM and *Scheduled* MRM algorithm methods from an external .csv or .txt value may 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 revealed 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 appears when importing a text file into an MRM or *Scheduled* MRM acquisition method

When importing a text file into an MRM or *Scheduled* MRM algorithm method, a message may appear reading: "Invalid value entered into table. Please ensure only numeric values are entered". Although this message appears, 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 019141)

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 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 will stop responding and you will have to 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 switches 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 will appear before this one. When you submit your batch, this phantom row will not be submitted. If a user creates a batch with this extra row, the sample specified in this row will not be 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)

Real time data display is delayed when using Agilent 1200 DAD D model

The real time data display between TWC and TIC is delayed when using Agilent 1200 DAD D model. Data written to the file is not affected. Reopen the file after it is acquired to see the entire data file. (ST 16524)

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 Algorithm

***Scheduled* MRM algorithm experiment limit**

For the non-5500 series of instruments, to maintain optimum system performance, a *Scheduled* MRM algorithm, non-IDA experiment should not exceed 1000 transitions and three dependent parameters. A *Scheduled* MRM algorithm, IDA experiment should not exceed 1000 transitions

and two dependent parameters. If the experiment exceeds these limits, the Analyst software may stop responding and you will need to restart the instrument and reactivate the hardware profile. You may reduce the number of transitions if you want to increase the number of dependent parameters.

The limit for the 5500 series of instruments, the limit is 4000 transitions with four parameters (CE, DP, EP, CXP).

Multi-period Scheduled MRM™ algorithm experiments not supported

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

In certain cases there may be a decrease in sensitivity on the API 5000 instrument when using *Scheduled* MRM algorithm as compared to MRM

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

Batches containing the maximum number of *Scheduled* MRM 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 algorithm transitions and 3 mass dependent parameters, DP, CE, and EP, causes the system to stop responding. To avoid this occurring, do not include EP as one of the mass dependent parameters. (ST 16066)

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

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

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

Modifying a *Scheduled* MRM algorithm mass ranges table with 2500 MRM transitions could take several minutes. (ST 5251)

Acquire — Network Data Acquisition

Potential loss of data if reacquiring samples using the same .wiff file name

If you must reacquire a batch, then submit all samples using a new .wiff file name per sample.

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.

Windows reporting Delayed Write Failed

On Windows XP, while the Analyst software is acquiring data to a network computer, Windows may display an error dialog stating Delayed Write Failed at the bottom right corner of the screen when there is a network interruption. This error does not prevent files from eventually being transferred. Do not restart your computer at this time because Windows is still transferring files.

For more information, see the Microsoft Web site at:

<http://support.microsoft.com/default.aspx?scid=kb;en-us;330174>.

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. Now 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/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 down

When the network is down, 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 Process (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 down. (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 may 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 may intermittently fail if the data file transfer to the network is in progress. Checksum will work after the transfer is complete. (SCR 11419)

Invisible subset file

When you make a subset of a sample file on the network, the file name may not be visible until after you restart the Analyst software. (SCR 11729)

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 may 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 may not be able to detect the remaining space available. As a result, the data transfer process may fail, but acquisition is not impaired. The data remains on your 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 may not be saved. (SCR 11746)

Explore

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 may 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 appears to be active; menu item in the right-mouse menu does not update

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

Unable to sort Peak Lists properly

In rare instances, the Peak List does not sort properly. To restore functionality, close the Peak List (deleting the pane) and re-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 may 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 displays a different time range from the original Contour.

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 degradations 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 while acquiring, it displays 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 displays 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 appear 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 may cause the software to stop responding or to omit information from the display. This is an intermittent display problem and no data is lost. If this occurs, configure the Audit Trail Manager settings to No Audit Map or alternatively deselect 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 has the privilege to configure the audit trail settings.

Overlay on plot for isotopic distribution in calculator

Occasionally, this feature does not function as expected, however, the text will still be 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 not displaying properly

The Explore History File does not display properly. The description of all the changes is sometimes merged into one cell but it is often still legible. In some instances, some information may be missing. (ST 9481)

Changes to offset in History pane not appearing

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 displayed data is the overlaid XICs but reviewing the changes will change 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 this occurs, open the previous or any subsequent sample and use the forward and back arrows to navigate to the sample that will not open. (ST 13169)

If you expand data in the IDA viewer while a sample is acquiring to the same data file, data from an acquired sample is not displayed

No data is displayed in Explore mode for an acquired sample if you expand data from the IDA Viewer while a second sample is being acquired to the same .wiff file. (ST 18228)

Undocked Graph Information Window may cause the software to stop responding

Occasionally when the Graph Information Window is opened and undocked the software stops responding. This is especially 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 may 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 display full information

When opening Compound Library databases that have over 20 000 entries, the individual fields will not display the full information used to populate the original database; "NA" is populated instead. The recommendation to overcome this issue is to re-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 10,000 entries and save this database as "Part 1" and then reopen the original database, delete the first 10,000 entries and save this database as "Part 2". **Note:** Deleting entries and then adding new ones is not recommended. (ST 19297)

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 appear blank. Clicking on the field a few times, will cause the results to appear. 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 may 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 may 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)

New version of library database

If you have an old library database, you will receive an error when the Analyst software tries to connect to the library. To update your library, contact AB SCIEX technical support at: support@absciex.com.

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

If this occurs, 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, Analyst 1.5 software data files, for example, do not consistently open in Analyst 1.4.2 software or older versions. 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 display data in the flat file (.WIFF.scan) for files up to 2 GB in size. Any data stored beyond this limit may not display properly. In addition, larger file sizes may degrade overall performance. Begin acquiring data to a new data file if your file size nears this limit (for example at 1.5 GB).

Quantitate

Accuracy values may be different between different versions of the Analyst software

In the Results Table, the Accuracy values may 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 may 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 may be larger than in the previous version of the Analyst software. (ST 33496)

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 may be incorrect. The user will see 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 will function as intended.

Algorithm compatibility

Scheduled MRM algorithm data cannot be analyzed with Analyst Classic or previous versions of the IntelliQuan (IQA/MQ II) algorithms. For this reason, the IntelliQuan integration algorithms have been improved to support *Scheduled* MRM algorithm data, and have been renamed IQA II and MQ III. For more information, see [Technical Information Regarding Integration on page 85](#). Due to this change, several behaviors will be observed in the software:

- When creating a new quantitation method with Analyst Classic as the preset algorithm, the software warns about algorithm incompatibility and the new method uses IntelliQuan-MQ III instead. This operation has no effect on 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 re-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 Analyst Classic or older IntelliQuan algorithms.

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

For *Scheduled* MRM algorithm data, it is highly 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 II.

IntelliQuan - IQA II 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 appear under incorrect headers and the text file may 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 displays N/A

If an automatic quantitation method is used to build a new Results Table, the Analyte Mass Ranges column displays 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 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:

- **Analyst 1.4 software:** The first transition ordered from lowest to highest for which both the Q1 and Q3 masses are within a tolerance of 0.1 Da is selected. For example, given two separate transitions, one with Q1 140.0 and Q3 of 134.0 and another transition with Q1 of 140.1 and Q3 of 134.1, a quantitation method will not be able to distinguish between the two transitions. Since the algorithm finds the first transition within the 0.1 tolerance, the 140.0/134.0 transition will be selected both times.
- **Analyst 1.4.1 software:** This was changed to use a smaller tolerance of 0.0001 Da. The reason for the change in the Analyst 1.4.1 software was to allow two transitions with both Q1 and Q3 masses within 0.1 Da, but more than 0.0001 Da, of one another to be quantitated. If you use the same example as in the previous version, 140.0/134.0 and 140.1/134.1 are now valid. This allows two close transitions to be distinguished; however, this did not take into account the mass tolerance values used by users who apply the same quantitation method across instruments, each with their own unique calibration.
- **Analyst 1.4.2 and newer software:** 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 will appear 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 nonexistent 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 where the data file was located instead of the Quantitation Methods folder. Browse to the appropriate folder before saving the quantitation method. (ST 16129)

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

When you use the IQA II algorithm, RT windows larger than 40 seconds are ignored; even if the user sets a window larger than this, a window of +/-20 seconds is effectively 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)

Older versions of Quantitation methods may cause the software to stop responding

When selecting a Quantitation method in a batch that was created with the Analyst 1.4.2 software, the Analyst software stops responding. To use quantitation methods from previous versions of the Analyst software, save the methods using the Analyst 1.5.1 software and then select them. (ST 18026)

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 displays 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 may 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, we recommend using the MRM scan type. (ST 11772)

Some items unavailable under the Administrator role for the Quantitate module are not honoured

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)

Correct data displayed in the calibration window

The data in the calibration window may 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

Adobe Acrobat may stop responding after printing to PDF

If the user selects both options to Print to PDF and Print Automatically, after generating the report, Adobe Acrobat will launch but will stop responding. If the user manually closes Adobe Acrobat, the report will open 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 may cause the Reporter to crash

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 will cause an error to be generated: “Failed to process the report file. Unsupported format requested.” For example, specifying a report as “report 1.2.3” will cause a crash; whereas, specifying “report 1.2.3.docx” will generate the report as intended. Note that the extension must match the format selected in the Reporter software. (ST 35636).

Generating a PDF report might be slower for Windows 7 users

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

MS Office Requirements

For the Analyst 1.6 software, MS Office 2007 or 2010 is required. For earlier versions of the Analyst software, MS Office 2003 is required.

During the installation of the Analyst[®] 1.5.2 Software with HotFixes to February 2011, if the PDF only option is selected and MS Word 2003 is installed, then the FinePrint pdfFactory software (version 2.x or 3.x) is required to generate reports. If the pdfFactory software has not been installed, upon attempting to launch the reporter, the user will receive an error stating that the pdfFactory software is not installed, and the Reporter 3.0.1 software will not be usable.

To correct this issue, re-install the Analyst 1.5.2 Software with HotFixes to February 2011 and select the option to allow printing reports in all formats or contact support@absciex.com.

Installer

Message appears during installation advising users to downgrade the firmware on the 5500 series of instruments

If you have the 5500 Components Patch installed and you are installing Analyst 1.5.1 software, you will receive a message instructing you to downgrade the firmware. Ignore this message and continue with the installation procedure. Follow the instructions in the installation guide to upgrade your application firmware. The installer will automatically uninstall the 5500 Components Patch for you.

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

File Translator utility

The File Translator utility does not support the translation of Agilent MSD data to .wiff.

Copy/paste to Microsoft Office 2003 applications

If you copy and paste to a Microsoft Office 2003 application in Meta file format, do not edit the final graph. Doing so might distort the graph.

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 may 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

Automaton support discontinued

The Analyst 1.5.1 software release does not support the Automaton software. The Automaton software package is now replaced by the DiscoveryQuant™ software.

LightSight software for metabolite identification does not support the 1.5 mL vial for the Shimadzu Rack Changer

When submitting methods or creating new acquisition methods in the LightSight® software for metabolite identification with the Shimadzu Rack Changer as the autosampler, an extra window appears when in the Acquire MS Wizard. The window indicates the 1.5 mL Vial for the Rack Changer is a custom plate type, it is not. The 1.5 mL Vial is not a supported plate type. For the LightSight software to function properly, select any actual plate type for the 1.5 mL Vial in the extra window, and then select the appropriate Plate Type for your configuration, except for the 1.5 mL Vial, in the Acquire MS Wizard.

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.

MIDAS Workflow Designer software limits the maximum number of transitions to 200

These limits are suitable for all systems except for the 5500 series of instruments. For these instruments, you can change the settings in the MIDAS™ Workflow Designer.txt file to allow non-Scheduled MRM algorithm transitions up to 1000. The file is found in the following directory:
<drive>:\program files\MIDAS TRAQ\

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 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

Make Subset Script: Decompose function does not work

The Make Subset script has an option to decompose a file with multiple samples into individual samples. This feature no longer works. (TT 35062)

On Windows 7, 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)

Moving the cursor over the graph can cause the MRM3 Optimization script to stop responding

If you move the cursor over a graph that is not displaying correctly, the MRM3 Optimization script stops responding. To avoid this issue, do not move the cursor until the script has finished running. (ST 33987)

The MRM3 Optimization script is not supported on Windows 7

For Windows 7 users, using the MRM3 Optimization script causes the AnalystService to stop responding. This script is not supported for Windows 7. (ST 33878)

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.

Multiple scripts appearing

Two copies of the IDA Trace Extractor script are available. Use the executable found in the <drive>:\Program Files\Analyst\Scripts \Triple Quad and Trap Only\IDATraceExtractor folder.

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)

Opening data created with Make Subset File script occasionally causes the Analyst software to stop responding

Opening data created with the Make Subset File script occasionally causes the Analyst software to stop responding when attempting to subset large data files. This is especially an issue when trying to subset a data file with many samples and many MRM transitions. Do not use this script with files acquired at the acquisition limits of 100 samples per data file and 1000 transitions in a *Scheduled* MRM algorithm data file. (ST 6849)

Occasionally, error messages appear when running the Make Subset File script

Close the error messages if they appear; the script will still run correctly. (ST 18961)

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 AB SCIEX 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

CTC PAL / Leap Devices

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 1.6.0.3, they may not work after the Analyst 1.6 software is installed. Contact the manufacturer for the latest versions of the CTC software. (ST 32245, ST 33375)

Enabling/disabling barcode reading

The CTC PAL Autosampler Method Editor now contains an “Enable Barcode Reading” check box. Selecting this check box (flag ON) will activate the barcode reading/storing feature. Clearing this check box will disable barcode reading.

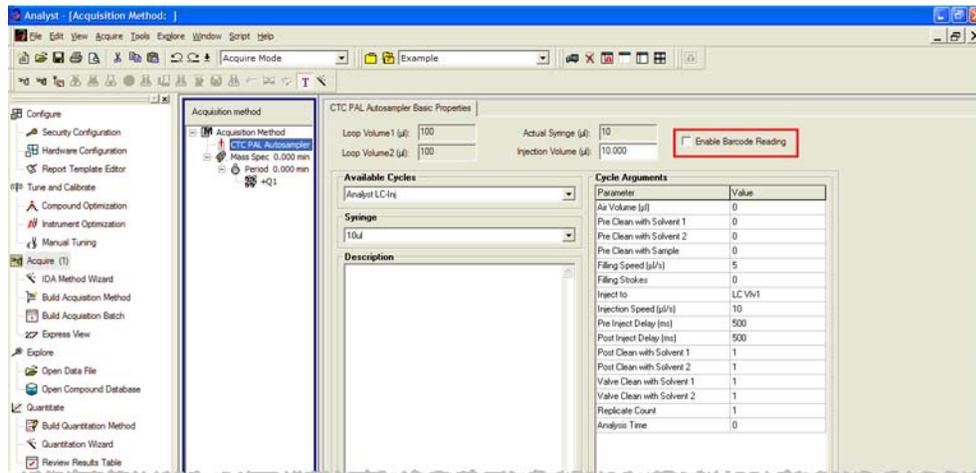


Figure 3-1 Enable Barcode Reading check box

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 will be displayed and stored as “N/A”.

Barcode reading disabled

If the user disables the barcode reading feature, no barcode information will be added to the data file and results tables created from these files will 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 will display “N/A” in the “Scanned Barcode” column.

Backward and forward method compatibility

Methods created using the Analyst 1.6 software have not been fully tested with previous versions of the Analyst software. All methods created with previous versions (1.5.x) can be used in the Analyst 1.6 software.

The changes introduced in the Analyst 1.5.2 Software with HotFixes to February 2011 to the CTC PAL Autosampler Method Editor are transparent to previous versions of the Analyst software. That is, if an acquisition method is created with the Analyst 1.5.2 Software with HotFixes to February 2011 and opened with a previous (supported) version of the Analyst software, the user will not see the Enable Barcode Reading check box. Users will be able to modify, save, and use these methods in previous (supported) versions of the Analyst software. Conversely, if users create and save a CTC PAL method in a previous version of the Analyst software and open it in the Analyst 1.5.2 Software with HotFixes to February 2011, they will see the Enable Barcode Reading check box added to the method, defaulted to OFF. Users will then be able to enable barcode reading, save the method, and use that method to scan and store barcode information.

Problem with multiple trays assignment

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

Message appears when uninstalling CTC cycle editor (v 2.0.7)

When uninstalling the CTC Cycle Editor, a message Remove Shared Files? appears. 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 Cycle Editor. (SCR 13501)

Injection valve switches when CTC method is aborted

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

Terminal unlocks when CTC method is aborted

The CTC PAL terminal unlocks when the CTC method is aborted. To re-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: AutoConfig shows same serial number for all pumps

The Shimadzu driver included in the Analyst 1.6.1 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 will cause all connected pumps to show the serial number of the first pump. However, if the devices are configured using the integrated device driver in the Analyst software, the File Info for acquired data will reflect the proper 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 entered manually 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 manually enter the IP address. (ST 29400)

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

In Mixed Mode, if a different user logs on to the Analyst software, the Shimadzu AAO may 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)

No forward compatibility of Shimadzu hardware profiles created before Analyst® 1.4.2 HotFixes to November 2006

All profiles containing Shimadzu devices created before Analyst 1.4.2 HotFixes to November 2006 need to be recreated. However, all previously created methods will work with re-created hardware profiles.

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 may 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 may 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 may occur if the acquisition time specified is shorter than the time necessary for the autosampler to complete its rinse washes. Make sure your Mass Spec acquisition method is at least 1 to 2 minutes long.

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

The default pump pressure maximum limit may be too low and lead to pressure errors on the hardware and subsequent acquisition errors. Therefore, the default limit may 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 may 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. When the Analyst software is installed, previously existing Shimadzu profiles will not be usable until a Windows Local Administrator activates the profile. (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)

Loss of queue functionality

Performing an abort during Shimadzu Equilibrate results in a loss of queue functionality. To regain control of the queue, stop the Analyst Service software. (SCR 9588)

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 will not be able to stop the tune run using the Analyst software once 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 as 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 may 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 > 20Hz are not recommended

Previously, it was recommended to acquire DAD data for both the G4212A and G4212B detectors at acquisition rates of 40Hz and below. With the Analyst 1.6.1 software, this guidance is lowered to 20Hz and below. Using higher acquisition rates will cause the acquisition to take much longer than expected. (ST 25396, ST 35524)

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

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 device(s) 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: In order 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 will show 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 resave it (or save as a new method and use the new method for acquisition).

Purging and Priming using the Analyst software

The 4220A Binary Pump now uses an integrated software-controlled purge valve. Previously, users were responsible for manually purging and priming via a manual valve.

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

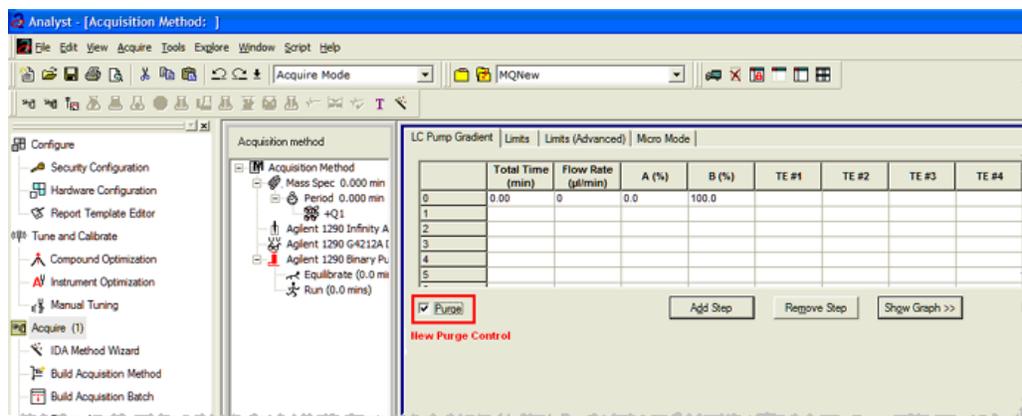


Figure 3-2 New Purge option in the Acquisition Method editor

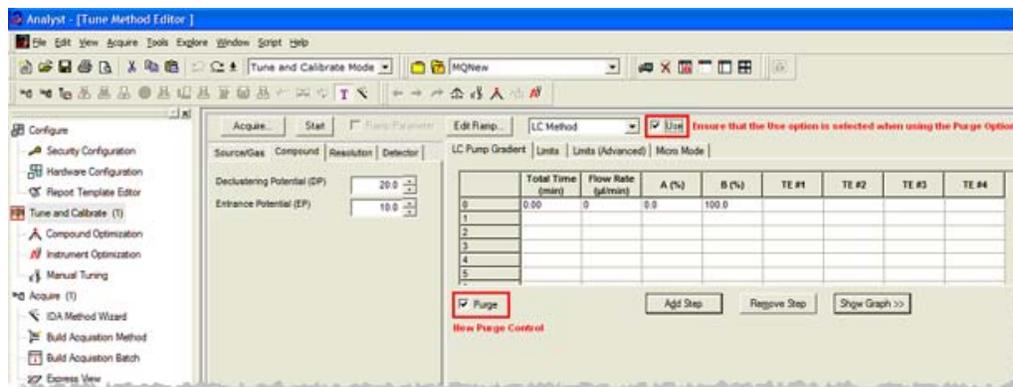


Figure 3-3 New Purge option in Manual Tuning

When the Purge option is activated, the Agilent 1290 Binary Pump will open 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 will be ignored.

Users can either use Manual Tuning to purge or prime their system, or they can create an acquisition method that will be used exclusively for purging. This method can be submitted via the Acquisition Batch Editor in the same manner as acquisition methods. Note that in this scenario, the mass spectrometer will acquire data to the specified .wiff file.

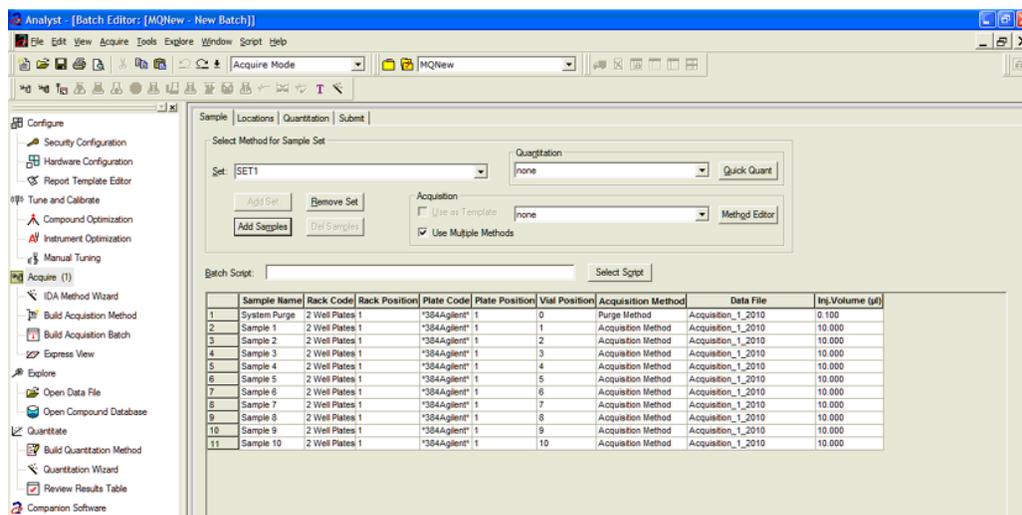


Figure 3-4 Example acquisition batch with a purge method before acquisition

Changes to DAD acquisition

The Agilent 4212A and 4212B DADs have a single lamp source, rather than two lamps as in previous DAD models. As a result, the usable wavelength range has been changed to 190–640 nm. Additionally, the 4212A DAD supports slit widths up to 8 nm, and the 4212B has a fixed slit width of 4nm.

Baud Rate for Serial communication

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

Incompatibility with hardware profiles created with previous versions of the Agilent devices patch

Any hardware profiles created with previous versions of the Analyst[®] 1.5.1 Patch for Agilent Devices or the Analyst[®] 1.5.1HF Patch for Agilent Devices may have to be re-created, as they may be incompatible with this release. Acquisition methods created with these patches will continue to function as intended.

Fractional injection volumes are not supported for Agilent autosamplers

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

Hardware profile containing an Agilent DAD 1315 D

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

Agilent wellplate

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

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)

Agilent 1100 and 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)

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.

You can use the Analyst[®] 1.6.1 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 1.6.1 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 1.6.1 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 1.6.1 software is 21 CFR Part 11 compliant is dependent on the actual usage and configuration of the Analyst 1.6.1 software in the lab.

Validation services are available through AB SCIEX Professional Services. For more information, contact softwarevalidation@absciex.com.



The following utilities are installed with the Analyst[®] software. They can be found in the \Program Files\Analyst\Bin\ folder.

Table A-1 Utilities

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



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 affect 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%.