

Release Notes



Analyst® 1.5.2 Software with Hotfixes to February 2011

February 2011

AB SCIEX

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Chapter 1 Introduction	5
Support.	5
How to Use These Release Notes	5
Chapter 2 Enhancements and Fixes	7
New Enhancements and Fixes in the Analyst® 1.5.2 Software with Hotfixes to February 2011	7
AAO and Companion Software	7
Acquire — Acquisition and Batch Editor	8
Configure — Hardware Configuration	8
Explore	9
Explore — Library Search	9
Firmware Files	10
Help Files and Tutorials	10
Quantitation	10
Scripts	11
Program Shortcuts	11
Upgrading from the Analyst® 1.5.1 Software	12
Enhancements and Changes	12
Acquisition	12
Device Support	12
Quantitation	12
Security	12
Fixed Issues	13
Acquisition	13
Security	14
Quantitation	14
Upgrading from the Analyst® 1.5 Components for 5500 Systems	14
Enhancements in the Analyst® 1.5.1 Software	14
Configure — Hardware Configuration	16
Acquire — Acquisition and Batch Editor	16
Tune and Configure	17
Quantitate	17
Compatible Software	17
Enhancements in the Analyst® 1.5 Components for 5500 Systems	18
Audit Trail	18
Acquire — Acquisition and Batch Editor	18
Acquire — Information Dependent Acquisition (IDA) and IDA Method Wizard	20
Quantitate	21
Other	23
Upgrading from the Analyst® 1.5 Software	23

Acquire — Acquisition and Batch Editor	23
Other	24
Notes on Use	24
Chapter 3 Notes on Use, Known Issues, and Limitations	27
New in the Analyst® 1.5.2 Software with Hotfixes to February 2011	27
Peripheral Devices: Agilent	27
Peripheral Devices: CTC PAL	30
Peripheral Devices: Shimadzu	31
Acquire — Information Dependent Acquisition (IDA)	31
Network Acquisition	31
Quantitation	31
Reporter 3.0.1 Software	32
Applicable to All Versions of the Analyst® Software	32
Audit Trail	32
Configure — Administration/Security	33
Configure — Hardware Configuration	34
Configure — Report Template Editor	35
Tune and Calibrate — Compound Optimization	35
Tune and Calibrate — Instrument Optimization	36
Tune and Calibrate — Manual Tuning	37
Acquire — Information Dependent Acquisition (IDA) and IDA Method Wizard	39
Acquire — Method / Batch Editor	41
Acquire — <i>Scheduled</i> MRM™ Algorithm	43
Acquire — Network Data Acquisition	44
Explore	45
Explore — Library Search	48
Explore — WIFF Data File	49
Quantitate	49
Installer	53
Other	54
Compatible Software	54
Scripts	55
Peripheral Devices	57
Agilent Devices	57
CTC PAL / Leap Devices	58
DAD Devices	58
LC Packings Devices	58
PerkinElmer	59
Shimadzu Devices	59
Tempo™ MDLC System	60
Chapter 4 21 CFR Part 11 Compliance	61
Chapter 5 Programs and Utilities	63
Appendix A Technical Information Regarding Integration	65
Integration Issue Addressed in the Analyst® 1.4.2 Software	65
Changes Introduced in the Analyst® 1.5 Software	65

Thank you for choosing AB SCIEX to supply your LC/MS/MS system. We are pleased to give you the Analyst® 1.5.2 Software with Hotfixes to February 2011, the most comprehensive LC/MS/MS software package available.

The *Analyst® 1.5.2 Software with Hotfixes to February 2011 Release Notes* describes the many new features introduced in the Analyst 1.5.2 Software with Hotfixes to February 2011, 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® 1.5.2 Software with Hotfixes to February 2011 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 1.5.2 Software with Hotfixes to February 2011 release notes have been structured so that you only have to read the sections that are relevant to you.

Read the [New Enhancements and Fixes in the Analyst® 1.5.2 Software with Hotfixes to February 2011](#) section 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 the [Notes on Use, Known Issues, and Limitations](#) section of the release notes, as this section applies specifically to issues that are known in the Analyst 1.5.2 Software with Hotfixes to February 2011.



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



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

AAO and Companion Software

ChemoView 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™ scans would result in lower intensities than the corresponding MRM scans

In rare situations, users would see that a *Scheduled* MRM™ 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 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 Analyst Software Installation Guide.

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, refer to the Analyst Software Installation Guide.

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 Box” 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)

Quantitation

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. (ST27614)

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. (ST21863)



Note: For details on the original solution implemented in the Analyst 1.4.2 software, see [Appendix A—Integration Issue Addressed in the Analyst® 1.4.2 Software](#) (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 corrected. (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
- Ion Source Specifications

Upgrading from the Analyst® 1.5.1 Software

If you are upgrading from the Analyst® 1.5.1 software, the following features and enhancements have been added. This is in addition to the features and enhancements in [New Enhancements and Fixes in the Analyst® 1.5.2 Software with Hotfixes to February 2011 on page 7](#).



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

Enhancements and Changes

Acquisition

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)

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 G1329B Autosampler

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

Quantitation

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

Acquisition

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)

Quantitation

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)

Upgrading from the Analyst® 1.5 Components for 5500 Systems

If you are upgrading from the Analyst® 1.5 Components for 5500 Systems, the following features and enhancements have been added. This is in addition to the features and enhancements in [New Enhancements and Fixes in the Analyst® 1.5.2 Software with Hotfixes to February 2011 on page 7](#) and [Upgrading from the Analyst® 1.5.1 Software on page 12](#).



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

Enhancements in the Analyst® 1.5.1 Software

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

- ◆ 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 Analyst 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 Cliquid® 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™ 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 box

Previously, users had to select the autosampler in the Select Autosampler dialog box 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™ instrument, AB SCIEX Triple Quad™ 5500, and AB SCIEX QTRAP® 5500 system) 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)

Enhancements in the Analyst® 1.5 Components for 5500 Systems

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™* 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 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 box. (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 box. (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™* 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)

Upgrading from the Analyst® 1.5 Software

If you are upgrading from the Analyst® 1.5 software, the following features and enhancements have been added. This is in addition to the features and enhancements in [New Enhancements and Fixes in the Analyst® 1.5.2 Software with Hotfixes to February 2011 on page 7](#), [Upgrading from the Analyst® 1.5.1 Software on page 12](#) and [Upgrading from the Analyst® 1.5 Components for 5500 Systems on page 14](#).

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.

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 in the Analyst® 1.5.2 Software with Hotfixes to February 2011

Peripheral Devices: Agilent

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.

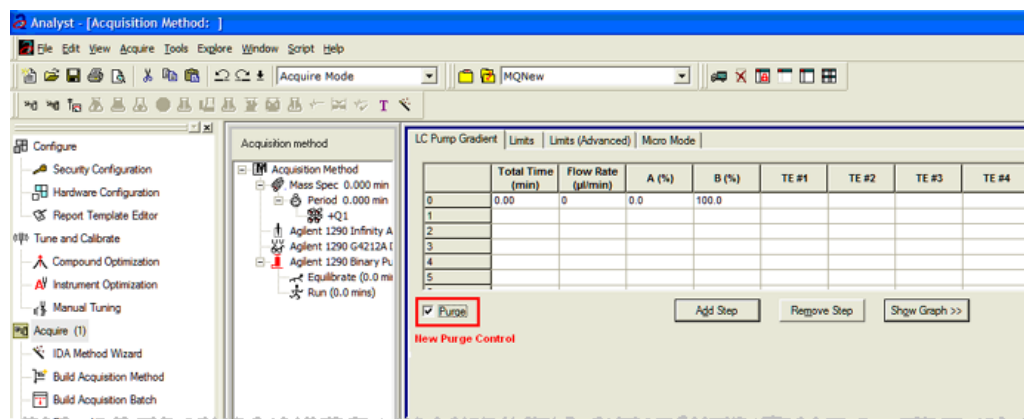


Figure 3-1 New Purge option in the Acquisition Method editor

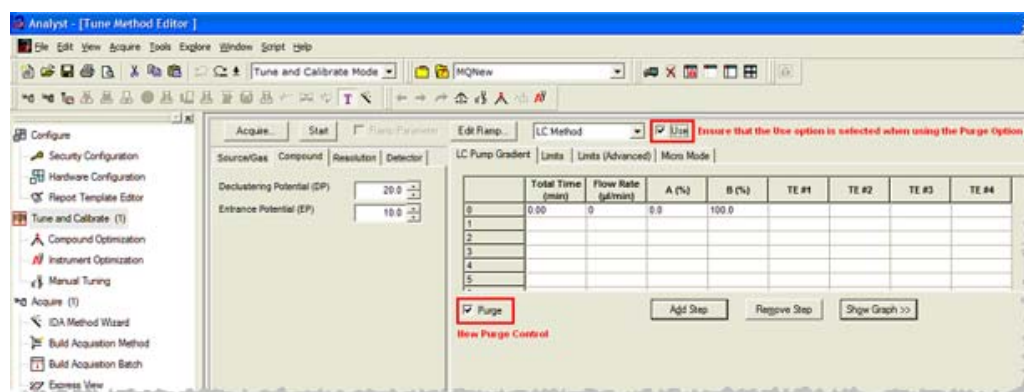


Figure 3-2 New Purge option in Manual Tuning

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.

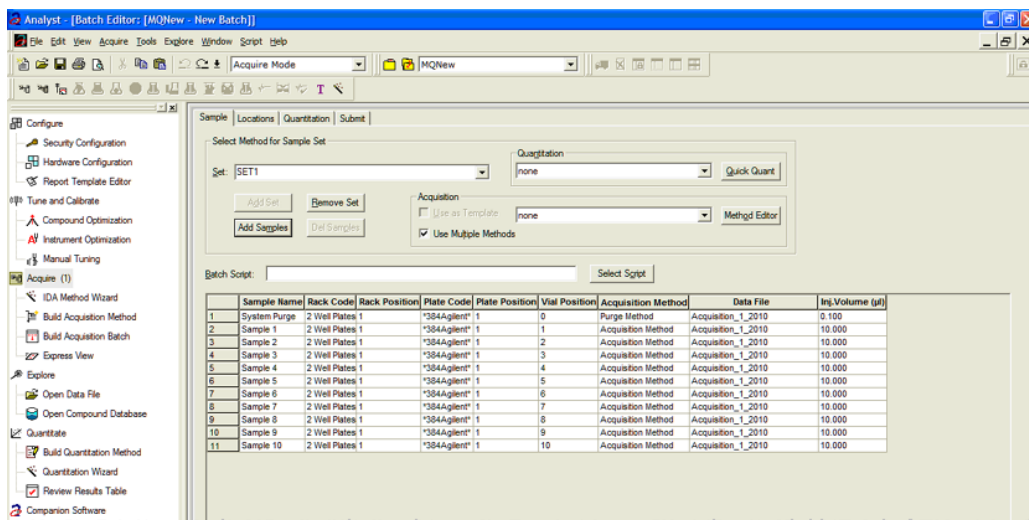


Figure 3-3 Example acquisition batch with a purge method before acquisition

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 19200.

DAD acquisitions at data rates > 40Hz are not recommended

It is currently recommended to acquire DAD data for both the G4212A and G4212B detectors at acquisition rates of 40Hz and below. Using higher acquisition rates will cause the acquisition to take much longer than expected. (ST 25396)

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)

Peripheral Devices: CTC PAL

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. Deselecting this check box will disable barcode reading.

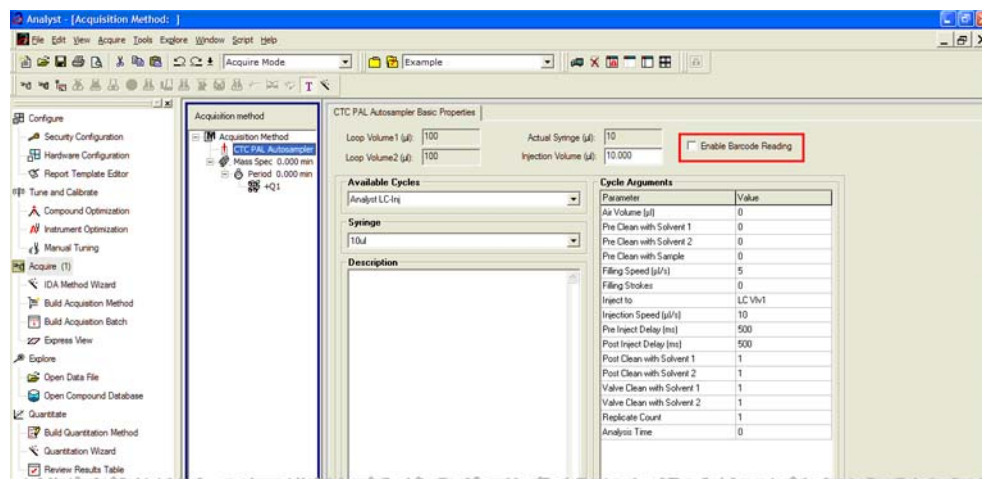


Figure 3-4 Enable Barcode Reading check box

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

The changes 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.

Peripheral Devices: Shimadzu

Incompatibility with Previously Created Methods

When upgrading from the Analyst 1.5.2 software, users may not be able to activate previously created Shimadzu methods. If this happens, recreate your hardware profile. You will then be able to use any old methods created with the Analyst 1.5.2 software.

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 Analyst Service and power-cycle the Shimadzu stack. (SCR 9588)

Acquire — Information Dependent Acquisition (IDA)

Poor data when performing EMS triggered IDA scans with Dynamic Fill Time (DFT) enabled

In very rare instances, performing an EMS triggered IDA scan can result in poor data being acquired if DFT is enabled. In this scenario, the DFT Tracker will show negative fill-time values being calculated. If this occurs, disable DFT for this particular experiment.

Network Acquisition

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.

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. (ST 28323)

Quantitation

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.

Reporter 3.0.1 Software

Requirements for the PDF only option with MS Word 2003

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.

Applicable to All Versions of the Analyst® Software

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® 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.

Audit Trail

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.

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 1.5.2 Software with Hotfixes to February 2011. Audit trail records will display correctly, but these special characters will appear differently in the record. (ST 14394)

For example:

Д will appear as a box

Ñ will appear as a G

β 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 box, 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.

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)

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)

Configure — Administration/Security**Managing Windows operating system file permissions**

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

Stopping the Analyst® Service software

Only local administrator group members are allowed to stop the Analyst® Service software (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 box 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 box is lost.

Configure — Hardware Configuration

Incorrect profile shown in the error message

The hardware profile dialog box 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)

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 indeed 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 box, 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)

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

During infusion compound optimization, the preset syringe pump options are used; the syringe pump diameter and flow rate used are 4.61 mm and 7µL/min respectively and cannot be changed. Use a 4.61 mm diameter syringe for infusion Compound Optimization. (ST 9255)

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 the 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 12000 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 lonspray™ source voltage in Negative mode causes the optimization to fail

When running Instrument Optimization in Negative mode, type lonspray 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 Analyst service 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 12000 Da/s scan speed in Manual Tuning mode

When running the 12000 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 — Information Dependent Acquisition (IDA) and IDA Method Wizard**MS3 isolation always uses the new LIT resolution table**

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

Set to never exclude former target ions from IDA

If a quadrupole mass spectrometer profile is activated in the IDA wizard 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)

Incorrect ions selected for confirmation scan

An IDA method with a *Scheduled* MRM™ 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)

Acquire — Method / Batch Editor

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 data. For 5500 systems, 1250 is the limit when acquiring MRM data and 2500 is the limit when acquiring *Scheduled* MRM 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™ 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™ 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™ experiment limit**

To maintain optimum system performance, a *Scheduled MRM™* algorithm, non-IDA experiment should not exceed 1000 transitions for non-5500 series instruments and 2500 transitions for 5500 series instruments, and three dependent parameters. A *Scheduled MRM* algorithm, IDA experiment should not exceed 1000/2500 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.

Multi-period Scheduled MRM™ experiments not supported

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

Looped experiments not fully supported

Looped *Scheduled MRM™* experiments are not fully supported by the Analyst® 1.5 software. The software does not prevent you from creating such experiments, however, the acquisition may fail when trying to run 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™* functionality on the API 5000™ instrument. (ST 15149)

Batches containing the maximum number of *Scheduled* MRM™ 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™ transitions and 3 mass dependent parameters, DP, CE, and EP, may cause 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 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 box 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. If you use a mapped drive, the Analyst® software may not be able to determine the proper network path in the subsequent sessions and prompts you to re-enter the path.

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™ 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, after 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 box. 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)

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 12000 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 resave 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 or older software 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

Algorithm compatibility

Scheduled MRM™ 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 data, and have been renamed IQA II and MQ III. For more information, see [Appendix A—Changes Introduced in the Analyst® 1.5 Software](#). 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 affect on the preset algorithm. (ST 5388)

- IntelliQuan Results Tables from versions of the Analyst® software earlier than 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 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 data to Results Tables using Analyst Classic or older IntelliQuan algorithms.

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

For *Scheduled* MRM™ 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 dialog boxes 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)

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 box points to incorrect folder

When users save a quantitation method that required a data file to open, the Save As dialog box 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 1.5.2 Software with Hotfixes to February 2011 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 box. (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)

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 the 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.

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 delay (up to five hours has been observed) between samples in the batch may be seen on the Optiplex 960 if the power management settings 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® 1.5.2 Software with Hotfixes to February 2011 does not support the Automaton software. The Automaton software package is now replaced by the DiscoveryQuant™ software.

LightSight® software 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 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 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 can not create GSH Prec IDA methods and in version 2.2, the software can not 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™ 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® 1.5.2 Software with Hotfixes to February 2011 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)

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

When running the BatchScriptDriver Script, if you select a Scheduled MRM™ 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™ 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)

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™* 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**Agilent Devices****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)

CTC PAL / Leap Devices

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)

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.

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)

PerkinElmer

Missing last decimal number in the status dialog box

The flow rate of a PerkinElmer pump reported in the status dialog box 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)

Shimadzu Devices

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.

Problem when restarting Analyst® Service software

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)

Problems 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 after the mass spectrometer has finished scanning. Press Run on the controller to stop the run or change the default Shimadzu run duration to match the MS duration in the Shimadzu method editor. (SCR 9515)

Deselecting "Fail whole batch in case of missing vial" does not work

Deselecting 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)

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® 1.5.2 Software with Hotfixes to February 2011 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 1.5.2 Software with Hotfixes to February 2011 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 1.5.2 Software with Hotfixes to February 2011 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 1.5.2 Software with Hotfixes to February 2011 is 21 CFR Part 11 compliant is dependent on the actual usage and configuration of the Analyst 1.5.2 Software with Hotfixes to February 2011 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 5-1 Utilities

Program	Description
FileBundler.exe	Standalone utility that combines the data file .wiff and .wiff.scan into one file.
Translat.exe	Utility to convert Agilent data files to the Analyst® software data format and Macintosh Library files to the Analyst 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.
RackBuilder.exe	Adds new plates and trays to the Analyst software. See Analyst Autosampler Utilities User's Guide.doc in the C:\Program Files\Analyst\Help folder.
AutosamplerAddIn.exe	Adds new plates and trays to the Analyst software. See Analyst Autosampler Utilities User's Guide.doc in the C:\Program Files\Analyst\Help folder.



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 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%.