



MultiQuant™ 3.0.1 Software

Release Notes



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Changes from Version 3.0 to Version 3.0.1

Note: No additional license activation step is required when upgrading from version 3.0 to version 3.0.1.

The following issues have been fixed.

- When the administrator adds a user group to the Security Configuration and then connects that group to the software, those users cannot run the software. Only the users who are added to the Security Configuration as an individual user can run the software. This issue has now been fixed. (MQ-283)
- Users can now export the correlation coefficient (r value) as an additional column in the exported text file. (MQ-291)
- Support has been added for monochrome pictures in reports. (MQ-292)
- Previously, a created report was deleted when the discard changes option in Audit Trail was selected. This issue has now been fixed. (MQ-289)
- The axis labeling in the chromatogram report is too small and difficult to read. Now the user can specify a font size for axis and peak labeling in the template editor for each picture tag. (MQ-294)
- If there are compounds using the same MRM transition, then the Q1/Q3 transition for the first compound is used for the later compounds if, after creating a **Results Table**, the user updates the method using the **Edit Results Table Method** option and then resets the new typical sample. The new typical sample is a sample from another .wiff file with the same compounds acquired but in a different order. This issue has now been fixed. (MQ-342)
- In the previous release, incorrect data was shown in the **Results Table** if all of these conditions were met:
 - The **Cache Chromatograms for Faster Peak Review** check box was selected.
 - The data files used to create the results had identical file names and were stored in separate folders.
 - The user created multiple **Results Tables** simultaneously using the **Results Table** wizard. This release resolves this issue so that these conditions no longer result in incorrect data in the **Results Table**. (MQ-297)

Installation Instructions

Prerequisites for Installing Using the DVD

The following are required to install and run the software. The logged on user must be an administrator on the computer to install the software. For Microsoft Windows 7, the User Account Control setting should be set to "Never notify".

- Windows XP with SP3 (32-bit) or Windows 7 with SP1 (32- or 64-bit)
- 1.5.2 software or higher. (Only required for the Audit Trail and Security Features edition. If you are not using the Audit Trail and Security Features edition, then you do not need the Analyst software installed.)

Prerequisites for Installing Using the Web Site Download

If you are using the installer that was downloaded from the Web site, then the following prerequisite software must be installed manually. The prerequisite software can be downloaded from the Microsoft Web site. The logged on user must be an administrator on the computer to install the software. For Windows 7, the User Account Control setting should be set to "Never notify".

- Windows XP with SP3 (32-bit) or Windows 7 with SP1 (32-or 64-bit)
- .NET Framework 3.5 SP1
- .NET Framework 4.0

Additional Software Requirements

- Only the English version of the Windows XP operating system with SP3 or the English version of the Windows 7 operating system with SP1 is supported. The format for numbers, currencies, dates, and time must be set to English (United States). Setting the format to a different value might result in erroneous data.
- Microsoft Office 2010 or 2013 is required for creating or editing queries and for generating or modifying reports.

Note: Query functionality is not available if the version with the Audit Trail and Security Features is installed.

Installation Notes for MultiQuant™ 2.x Software Users

If the MultiQuant 2.1.1 software with the patches is installed and you want to upgrade to the MultiQuant 3.0.1 software, then you must manually remove all of the patches before installing the MultiQuant software.

If you are upgrading from the MultiQuant 2.x to the MultiQuant 3.0.1 software, you must first remove the current version of the MultiQuant software and then remove and re-install the Analyst Administrator Console (AAC)

software on the server, if you are using the AAC. Refer to [Install the Software Update on the Analyst Administrator Console \(AAC\) Server](#) for the information on how to upgrade the AAC server.

When using the AAC, only one version of the MultiQuant software with Audit and Security features (versions 2.x or 3.0.1) can be used in one organization because of the security settings.

When the MultiQuant software is installed again, the MultiQuant software security items are repopulated in the Analyst® software. Reconfigure the security settings after the installation.

Install the Software

A new license is required for the software to run after installation is finished.

1. Remove any previous versions of the software and all of the patches.
2. Run the **setup.exe** file.
3. Run the software.
4. Activate the licence.

Install the Software Update on the Analyst Administrator Console (AAC) Server

If your organization is using the software with Audit Trail and Security Features and uses the AAC, then you must update the AAC Server to add the software security items. The software update file (**AACUpdateSetup.exe**) is located on the software installation DVD in the **InstallerAdminConsole** folder.

1. In Control Panel, remove any previous versions of the "Administrator Console Server - Update for MultiQuant X.x", if applicable.
2. (Only applicable for Windows 7 64-bit operating systems.) Copy and paste the **securitydb.odt** file from the C:\Program Files (x86)\Administrator Console Server folder to the same folder and then rename it to **MQBackupSecurityDB.odt**.
3. Double-click **AACUpdateSetup.exe** and then follow the on-screen instructions.

Install the Software on a Workstation Connected to the AAC

This procedure is only applicable if your organization is using the software with Audit Trail and Security Features and the AAC .

Note: If the workstation is connected to the AAC, then you must first disconnect the workstation from the AAC before you can install the software.

1. In the software, in **Configure** mode, click **Tools > Settings > Administrator options**.
2. Clear the **Use Server Based Security** check box.

3. Close the software.
4. Install the software.
5. If required, activate the licence.
6. Use the AAC client to check if the MultiQuant software security items exist. Click **Roles > Administrator > Properties**.

Make sure that **MultiQuant** is present as a top-level security item. If it is not, then the update must be installed on the AAC server. Refer to [Install the Software Update on the Analyst Administrator Console \(AAC\) Server](#).

7. Start the software.

Note: The software security must be set to Mixed Mode or Integrated Mode.

8. Reconnect the workstation to the AAC. Refer to the *Laboratory Director's Guide*.
9. Start the software from the software navigation bar.

Because the software is connected to the AAC, the software includes the security permissions from the AAC security database.

Revert the Security Database

Use this procedure to remove the software security items from the software security database. This procedure must only be performed on the AAC server by a user with administrator privileges.

CAUTION: The database is reverted to the last version of the database that was saved prior to the installation of the AACUpdateSetup.exe. All security changes and all audit changes made after the installation of the AACUpdateSetup.exe are lost if you revert the database.

1. Click **Start > Run** and then type **CMD** in the **Open** field.
2. Type **net stop Poet** in the command window. (Do not close the command window.)
3. Open the <drive>:\Program Files\Administrator Console Server folder where the AAC server is installed.
4. Rename the **securitydb.odt** file to **securitydb.bak**.
5. Rename the **MQBackupSecurityDB.odt** file to **securitydb.odt**.
6. Return to the command window and then type: **net start Poet**.

The database is reverted.

Remove the Software

Remove the software before removing the software.

1. Open **Control Panel**.
2. Proceed as follows, depending on the operating system:

Windows XP	Windows 7
Double-click Add or Remove Programs .	Click Programs and Features and then click Uninstall a program .
Click MultiQuant 3.0.x .	Click MultiQuant 3.0.x .
Click Remove .	Click Uninstall .

During removal, you are prompted to remove the MultiQuant software configuration files. If you intend to reinstall the MultiQuant software on this computer at a later date, then keep the configuration files.

3. Remove the software.

Notes on Use

- When opening a quantitation method created using the previous the MultiQuant™ software versions in MultiQuant 3.0.1 software, the **Outlier Settings** is automatically filled with a default value. Users can adjust the settings manually. The embedded quantitation method in the **Results Table** created from the earlier version is not affected.
- The MultiQuant 3.0.1 software uses an updated WiffReader. This might have a slight impact on integration, especially for MS3 and EMS data, most likely at the sixth or seventh digit of peak area and height.
- Processing data files while they are being acquired using network acquisition can cause conflict errors. To avoid these errors, it is recommended to use a single injection per .wiff file.
- For processing TOF data, Results Tables that contain over 10 000 rows might require a computer with more than 4 GB RAM.
- Results Tables that contain over 100 000 rows might require a computer with at least 4 GB RAM.
- The license file becomes corrupted if users change the date on their computer to a date after the expiry date of the license and then try to change the date back to the current date.
- English-only operating systems are supported.
- If Microsoft Office is not installed on the workstation, then the reporting functionality is hidden.
- Reporter queries must reside in the same folder as the Reporter templates.
- When creating reports in the CSV format, templates must not contain any picture tags.

- To make sure that reports are generated correctly, in the **Components** table of the quantitation method, list all of the analytes at the top of the table and all of internal standards at the bottom of the table. Analytes from the same group must be listed together and in the correct order. Groups cannot be mixed in the method. If groups are mixed, then the columns in the report will be misaligned. The mixture of grouping and non-grouping of analytes in the quantitation method is not supported. All the analytes are assigned to groups or all the analytes are not assigned to groups.
- If you change the active project in the MultiQuant software and then return to the Analyst[®] software, you must select the new active project from the Project list. The Analyst software project list is not automatically updated when the project is changed using the MultiQuant software.
- To make sure that the page up and down feature is working properly in the **Side- by-Side Sample Review** pane, it is recommended that the number of rows in the pane are a multiplier of the number of components in a group.

Upgrade from the MultiQuant 2.x Software

When viewing a version 2.1 .qmap file in the **Audit Trail** manager (viewing audit maps, editing audit maps, or creating a **Results Table**), the software will set the **Audited** column to ON for every event that was not ON previously. For all the other columns and predefined reasons, they will remain as is in the **Audit Map Editor**. In the **Audit Map Editor**, the new 3.0.1 software events are added and the **Isotope Correction** is removed.

When opening a MultiQuant 2.1 software qSession file, the previously unaudited events are now audited silently and the events are shown when the user clicks **View Session Audit Map**, but the **Isotope Correction** is not displayed in the map. If this event was triggered before in the **Results Table**, it is shown in the **Audit Trail Viewer**.

When creating a new **Results Table**, the active map used is upgraded. The previously unaudited events are now audited silently and the new 3.0.1 software events are added.

Known Issues and Limitations

- If the Analyst Administrator Console (AAC) is used to manage people, then projects, and workstations, the MultiQuant[™] software allows users to access all projects regardless of the AAC workgroup settings. (ST032639)
- Users should not browse to a folder called Analyst Data unless it is the Analyst Data root folder created by the Analyst software.
- Avoid using the same name for a custom column in the acquisition file and a column in the **Results Table**. If the same name is used, then the information in the custom column is not read in the **Results Table**. In addition to the columns listed in the *Reference Guide*, the **Barcode** and **Scanned Barcode** are also used exclusively by the software and must not be used in the acquisition method. The column name is not case sensitive. (MQ-345)

Support

Additional Documentation

Refer to the documentation that comes with the software.

Contact Us

AB SCIEX Support

- support@absciex.com
- www.absciex.com

Customer Training

- NA.CustomerTraining@absciex.com

Customer Documentation

- techpubs@absciex.com

Technical Support

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

Changes from Previous Versions

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Changes from Version 2.1.1 to Version 3.0

- Compatible with the Analyst® 1.6.2 software and supports the processing *Scheduled* MRM™ Pro Algorithm data.
- Compatible with the Analyst TF 1.6 software.
- Compatible with data acquired with the AB SCIEX Triple Quad™ 6500 system and the QTRAP® 6500 system.
- Supports Microsoft Office 2010 and 2013 for reporting.
- Outlier Flagging flags the outliers for Accuracy for STDs & QCs, Ion Ratio, and Calculated Concentration.
- Enhanced Peak Review shows the indication of the Ion Ratio acceptance on an overlaid chromatogram. Users can magnify single chromatograms.
- Side-by-Side Sample Review allows the user to choose up to six samples to compare the peak responses across the samples.
- Includes the following Results Table columns: Asymmetry Factor, Tailing Factor, Slope of Baseline, Ion Ratio, Expected Ion Ratio, Outlier Reasons, Start Time at 5 %, Start Time at 10%, End Time at 5%, End Time at 10%, Width at 5%, Width at 10%, Points Across Baseline, and Points Across Half Height.
- Enables the processing of UV, DAD, and ADC data.
- Supports an audited LIMS transfer to Watson using an Analyst software digital link.
- Supports an audited LIMS transfer through middle vendor.
- Supports the Analyst software .wiff file checksum.
- User receives a the License Expiry notification prior to 30 days of license expiry when starting the MultiQuant 3.0.1 software.
- Provides report tags to improve report functionality. (MQ145, ST035016)
- Corrects the issue where the "IS PeakReview" picture tag works only in the loop for the "ForEach Internal Standard" instead of working with each chromatogram without the loop. (MQ102)
- Corrects the issue where the Metric Plot image report is not showing. (MQ105)
- Includes the Iterate field in the MultiQuant software exported text file for the Fit text line. This fix is also applicable to the "MacQuan" and "Analyst" formats. (MQ106)

Changes from Previous Versions

- The MultiQuant software data provider was updated to incorporate the current LIMS xml schema to address parsing issues during transfer. (MQ119)
- Corrects the issue where users without delete privileges for the Project folders cannot save Result Tables. (MQ142)
- Corrects the issue where the Analyst 1.6 software and the MultiQuant 2.1.1 software view data differently for looped experiments with *Scheduled* MRM™ algorithm data. (MQ124)
- Corrects the issue where the data cannot be read under corrupted admin account in the Windows XP system. (MQ163)
- Introduces secured report templates for the version with Audit Trail and Security features.
- For functionality available in the MultiQuant 3.0.1 software with Security and Audit Trail features, refer to the *Software Reference Guide*.

Changes from Version 2.1 to Version 2.1.1

- Ensures compatibility with 4500 instrument series data.
- Updated LIMS communication module.
- MultiQuant™ 2.1.1 installs Microsoft .NET Framework 4 Reliability Update 1 (KB2533523), that solves the 64-bit simple query calculation issue (TT 34311).

Notes on Use

To be able to generate reports on Windows 7, 64-bit, make sure that on the target computer, Microsoft Word 2007 or 2010 64-bit version is installed.

Changes from Version 2.0.2 to Version 2.1

- Improved flexibility:
 - software without the audit trail and security features activated allows users to browse outside the Analyst Data folder structure to access and store data.
 - If the software is installed, the Analyst software data structure is supported.
 - Per Sample Report, a new reporting option to accommodate large reports, is available.
- The MultiQuant 2.1 software can now generate and save very large Results Tables (up to 250 000 rows), which fixed the memory issues reported in previous versions.

- In addition to supporting Microsoft Windows XP with SP3 operating system, the MultiQuant software now provides support for the Microsoft Windows 7 with SP1 (32-bit) Professional operating system, and a Windows 7 (64-bit) operating system for the MultiQuant software version that does not include audit trail and security features.
- Includes the ability to perform a 'file-less' transfer of data with LIMS software.
- Speed of query execution is now 10 times faster. (ST 029790)
- Query flexibility: if a custom column in a query starts with an underscore, the column will be hidden by default in the Results Table. (ST 032075)
- The column order in the exported Results Table is now consistent with the column order in the user interface. (ST 018829, ST 029512)
- The MultiQuant 2.1 software allows users to re-select a representative sample for quantitation methods. (ST 023725)
- Printing from the Audit Trail is now fixed by using the letter paper size. (ST 33654)
- In the Audit Trail, the Full User Name is now displayed and printed correctly. (ST 33654)
- The MultiQuant software is now integrating peaks correctly after the first peptide group in cases where all transitions in the group were identical. (ST 032596)
- Upon opening Peak Review for the current .qSession file, the MultiQuant software verifies if the .wiff file used to display the XIC from is the same as the .wiff file used initially to create the qSession file; if there is a mismatch in the time stamp, the software will display an error message. (ST 033527)

Reporting

- Reporter 3.2 software is integrated in MultiQuant 2.1 software.
- All Reporter templates installed by the MultiQuant 2.1 software are in the new file format .docx, which is supported by the Reporter 3.2 software.
- To use an existing template that is not included in the list of installed templates, convert the template using the ConverUI.exe utility located in the C:\Program Files\AB SCIEX\MultiQuant 2.1\TemplateConverter folder.
- To create or edit queries and generate or modify the report templates, then you need Microsoft Office 2007 or Microsoft Office 2010 software.
- If you are using Microsoft Word 2003 on the target computer, then the reporting functionality requires that the Office Compatibility Pack be installed. The Office Compatibility Pack can be downloaded at: www.microsoft.com/download/en/details.aspx?id=3&WT.mc_id=MSCOM_EN_US_DLC_MODULE_121LSUS007870.

Notes on Use

- Improvements to the smoothing algorithm may produce slightly different results when data is compared with MultiQuant 2.0.2 software data.
- The license file will become corrupt if users change the date on their computer to a date after the license will expire and then try to change the date back to the current date.
- Processing data files while they are being acquired using network acquisition can cause conflict errors. To avoid these errors we recommend use a single injection per .wiff file.
- English-only operating systems are supported.
- If Microsoft Office is not installed on the workstation, then the reporting functionality is hidden.
- Results Tables that contain over 100 000 rows may require a computer with at least 4 GB RAM.
- Reporter queries need to reside in the same folder as the Reporter templates.
- When creating reports in the CSV format, templates must not contain any picture tags.

Known Issues and Limitations

- If the Analyst Administrator Console is used to manage people, projects, and workstations, the MultiQuant software allows users access to all projects regardless of the AAC workgroup settings. (ST 032639)
- Reporting to secure .pdf format takes more time on Windows 7 than on Windows XP (ST 033918)
- The query functionality only supports .xls file format, it does not support .xlsx files.
- Users should not browse to a folder called "Analyst Data" unless it is the Analyst Data root folder created by the Analyst software.
- Creating reports in HTML format is restricted to workstations that have Microsoft Word 2007 SP2 or Microsoft Word 2010 installed. Microsoft Word 2003 does not support creating reports in HTML format.

Changes from Version 2.0.1 to Version 2.0.2

MultiQuant™ 2.0.2 Installer

- If you are upgrading from a previous version of the MultiQuant software, the installer will automatically uninstall that version before installing version 2.0.2. No data is lost during the installation. For more information, refer to the MultiQuant™ 2.0.2 *Software Installation Guide*.

Licensing

- Licensing support required to enable MultiQuant 2.0.2 software to register and activate licenses using the new AB SCIEX licensing subsystem is now available. (ST 028212)

Reporting

- Support for MRM Ratio reporter queries. (ST 027697) Improvements to the smoothing algorithm may produce slightly different results when data is compared with MultiQuant 2.0.2 software data.
- Creating reports in Word format when using the base or *Scheduled* MRM™ algorithm license is now available. (ST 028201)

External Calibration

- External calibration is now applied correctly when using the Area metric. This is applicable in cases where an external calibration for an analyte that does not use an internal standard is applied to one that does use an internal standard. (ST 27516).

Known Issues and Limitations

Group analytes and standards to ensure reports are generated correctly.

To make sure that reports are generated correctly, in the components table of the Quantitation method, list all analytes at the top of the table and all internal standards at the bottom of the table as shown in the following screen capture. Analytes from the same group should be listed together.

Notes on Use

Previously, opening *.wiff files from network drives and from projects containing large numbers of *.wiff files in the Results Table took several minutes. This issue has now been resolved.

Changes from Version 2.0 to Version 2.0.1

Data Processing Support

MultiQuant™ software now supports processing of the AB SCIEX TripleTOF® 5600 system data. (ST 024542, ST 024040)

Fixed Issues

- MultiQuant 2.0.1 software can now be installed on non-English operating systems; however, MultiQuant software is not officially supported on non-English operating systems. (ST 024466)
- MultiQuant 2.0.1 software can now be installed on the Analyst® 1.4.2 software. (ST 025359)

MultiQuant 2.0 Software Features (All Users)

- Ability to Add Samples from Multiple Batches and Multiple .wiff Files.
- **Faster, Better: Speed Improvements:**
 - **Faster Navigation:** The user interface for MultiQuant™ software has been improved resulting in faster navigation, including visual cues for row selection and fast sample assignment for multi-component samples.
 - **Faster Integration:** Integration using the latest version of the Analyst® software integration algorithm, MQ4, is significantly faster for large MRM datasets, allowing users to review and edit the data more quickly.
- **Introduction of the SignalFinder™ Integration Algorithm**
 - The **SignalFinder integration algorithm** is a new integration algorithm introduced with MultiQuant 2.0 software. By using peak modeling capabilities using a reference spectrum, this algorithm is able to achieve impressive results, minimizing the need for manual integration of the data, or even for tweaking data parameters.
 - **Dynamic Range Extension** is achieved within the SignalFinder™ integration algorithm to extend the upper dynamic range of a sample set by up to 30 times during cases where detector saturation predominates.

MultiQuant 2.0 Software Features (Regulated Users)

For customers operating in a regulated environment, for example a 21 CFR Part 11 or GLP Environment, MultiQuant software incorporates many additional new features over the Analyst® software Quantitation module.

MultiQuant software redefines the audit trail experience for quantitation. It provides fast navigation tools and same-screen integration difference comparisons along with the audit trail entries.

- **MultiQuant Advanced Audit Trail Software**
 - **Searching:** MultiQuant software provides users the ability to filter through the audit trail quickly and effectively.
 - **"Before and After" Review of Integration Data:** By clicking on a sample in the audit trail, users will immediately see the integrated chromatograms from both before and after the change was made.
- **Results Table Lockdown and Fast E-Signatures**
 - After integrating the peaks, the user can lock down the Results Table. Only a user with the correct role-assignment can unlock the Results Table after it is locked down. However, a QC reviewer can still log comments about the Results Table in the audit trail. This enforces separation of roles, and ensures that changes are not made in the review process without appropriate approval.
 - E-Signatures on changes to integrations are consolidated, so that a single E-Signature signs off on the set of events that changes a chromatogram, rather than performing multiple E-Signatures for each change.

Notes on Use

Previously, opening *.wiff files from network drives and from projects containing large numbers of *.wiff files in the Results Table took several minutes. This issue has now been resolved. The date format in the Audit Trail Viewer is mm/dd/yyyy. The time format uses the 24 hour clock. This format is not configurable.

If you change the active project in the MultiQuant software and then return to the Analyst[®] software, you must select the new active project from the Project list; the Analyst software project list is not automatically updated when the project is changed using the MultiQuant software.

Known Issues and Limitations

Files must be saved following the Analyst[®] Software file structure

In previous versions of MultiQuant[™] software, files could be saved to any location. Now you must save your files following the Analyst[®] software file structure. All *.mquan files must be in the Results folder and all *.qmet files must be in the Quantitation Methods folder.

Selecting samples may be slow if the Analyst[®] software root directory is on the network

Selecting samples using the Create Results Table wizard may be slow if the Analyst software root directory is on the network. (ST 19035)

MultiQuant software may close when users click inside message box

MultiQuant software may stop responding and close when users click inside the Save Quantitation Session, Save Quantitation Method, or the audit trail message boxes. If this issue occurs, go to **Control Panel > Regional and Language Options > Languages Tab > Details Button > Advanced Tab** and then select the **Turn off advanced text services** option. (ST 19868)

Revision History

Revision	Reason for Change	Date
A	First release of document.	September 2013
B	Added "Changes from Version 3.0 to Version 3.0.1". Added issue MQ-342.	August 2014