MultiQuant™ MD 3.0.3 Software

Release Notes

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EC REP

AB Sciex Netherlands B.V.
1e Tochtweg 11,
2913LN Nieuwerkerk aan den Ijssel
Netherlands

AB Sciex Pte. Ltd.
Blk 33, #04-06
Marsiling Ind Estate Road 3
Woodlands Central Indus. Estate.
SINGAPORE 739256

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Release Notes 1

Changes from MultiQuant™ MD 3.0.2 HotFix 1 to Version 3.0.3

New Features

- MultiQuant™ MD 3.0.3 software supports Microsoft Windows 10 (64-bit) operating system.
- MultiQuant™ MD 3.0.3 software supports Microsoft Office 2016.
- The MultiQuant™ MD 3.0.3 software now shows the actual ratio and expected ratio of MRM2/MRM1 in the row for MRM1.
- The MultiQuant™ MD 3.0.3 software now supports transfer of additional columns to LIMS.
- The MultiQuant™ MD 3.0.3 software now remembers the sample being reviewed and the cursor stays on that sample when the user navigates to a different analyte.

Fixed Issues

Scheduled MRM Pro Polarity Switch Data Processing Issue

Issue MQ-2512 is fixed. Previously, users were unable to process *Scheduled* MRM Pro polarity switched data.

Summing Ions from an Unequally Spaced Full Scan Data not Working Correctly

Issue MQ-2513 is fixed. Summing ions from an unequally spaced full scan data was not working correctly. When performing the summed ion calculation for a data type such as TOF IDA or *Scheduled* MRM HR, the summed peak area might have been greater than the expected value.

Mouse cursor was flickering when upgrading the MultiQuant™ MD software

Issue MQ-2801 is fixed. When upgrading the software to MultiQuant™ MD 3.0.2 version or the MultiQuant™ MD 3.0.2 HotFix 1, the issue of flickering mouse cursor was experienced.

MultiQuant™ MD Software Features

The MultiQuant™ MD software is a quantitation package designed to process SCIEX instrument data. The MultiQuant™ MD software incorporates many additional new features not available in the Analyst® MD software Quantitation module.

- Ability to add samples from multiple batches and multiple wiff files.

- **Faster, Better: Speed Improvements:**
  - **Faster Navigation:** The design of the user interface for the MultiQuant™ MD software has been improved, resulting in faster navigation, including visual cues for row selection and faster sample assignment for multi-component samples.
  - **Faster Integration:** Integration using the latest version of the Analyst® MD 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 the MultiQuant™ MD 3.0 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 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™ MD Advanced Audit Trail Software**
  The MultiQuant™ MD 3.0 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.
  - **Searching:** The MultiQuant™ MD software provides users with 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 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. However, a QC reviewer can still log comments about the Results Table in the audit trail. This enforces separation of roles, and makes sure 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.

Installation Instructions

Prerequisites for Installing Using the DVD

The following are required to install and run the MultiQuant™ MD software. The logged on user must be an administrator on the computer to install the software. For Microsoft Windows 7 and Windows 10 operating systems, the User Account Control setting should be set to "Never notify".

- Windows 7 with SP1 (32- or 64-bit) or Windows 10 (64-bit) operating systems

- • Analyst® MD 1.6.1 software (on Windows 7 (32-bit) operating system)
  - Analyst® MD 1.6.2 software (on Windows 7 (32- and 64-bit) operating systems)
  - Analyst® MD 1.6.3 software (on Windows 7 ((32- and 64-bit) and Windows 10 (64-bit) operating systems)
- .NET Framework 3.5 (SP1 or higher)

Note: On Windows 7 operating system, .NET 3.5 SP1 is installed by default. On Windows 10 operating system, if .NET 3.5 SP1 is not already installed before the installation of the MultiQuant™ MD 3.0.3 software, then the user is informed that .NET 3.5 SP1 is not installed and should be installed after the installation is completed. Users should contact their IT department to install .NET 3.5 SP1. Refer to Figure 1-1.

Additional Software Requirements

- Only the English versions of the Windows 7 operating system with SP1 and the Windows 10 operating system are 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, 2013, or 2016 is required for generating or modifying reports.

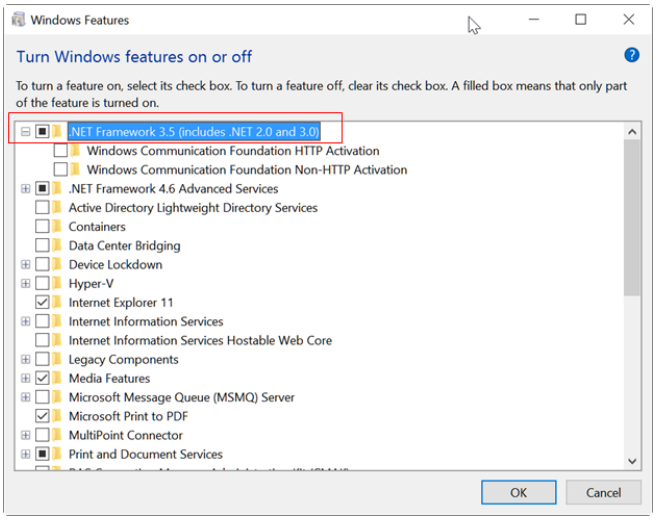
Install the Software

Note: If you are upgrading to the MultiQuant™ MD 3.0.3 software from the MultiQuant™ MD 3.0.2 software with HotFix 1, then first remove the hotfix before installing the MultiQuant™ MD software. Refer to the *Remove the HotFix* section in the *MultiQuant™ MD 3.0.2 HotFix 1 Release Notes*.

1. Run the **setup.exe** file.
2. Activate the licence.
3. On Windows 10 operating system, if .NET 3.5 is not already installed on the computer, then in **Control Panel > Program and Features**, select **Turn Windows features on or off**.

   The Windows Features dialog opens.
4. Select the **.NET Framework 3.5** option to enable the install of .NET 3.5. You might need IT permission to do this.

Figure 1-1 Windows Features Dialog



5. After the installation, confirm the presence of .NET 3.5 in the Windows Features dialog. If it is installed, then the **.NET Framework 3.5** option will be selected.

Remove the Software

Remove the MultiQuant™ MD software before removing the Analyst® MD software.

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

Windows 7 or Windows 10 Operating System
Click **Programs** or **Programs and Features** and then click **Uninstall a program**.
Click **MultiQuant MD 3.0.x**.
Click **Uninstall**.

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

Notes on Use

- The MultiQuant™ MD software only integrates peaks within the detection window defined in the Analyst® MD software *Scheduled* MRM algorithm acquisition method. For *Scheduled* MRM Pro data using dynamic window extension, MultiQuant™ MD software integrates peaks from where the detection windows starts to where it stops, that is, from RT - 0.5 DetectionWindow to where the extended window stops, which is up to RT + 1.5 DetectionWindow. The detection window start and stop for each transition might not be where the acquisition starts and stops.
- Intermittently, the MultiQuant™ MD software might stop working when a Results Table with more than 100 000 rows is processed. To avoid such a situation, we recommend processing fewer samples to create a Results Table containing less than 100 000 rows.
- 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.
- 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 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.
- 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 the 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 users change the active project in theMultiQuant™ MD software and then return to the Analyst® MD software, the new active project must be selected from the **Project** list. The Analyst MD software project list is not automatically updated when the project is changed using the MultiQuant MD software.

Known Issues and Limitations

- The fill down function Ctrl + D does not work on editable columns such as Actual Conc. and Dilution Factor. To avoid this issue, switch the position of the Actual Conc. column with Outlier Reason and the position of the Dilution factor column with the Retention Time column. (MQ-2305)
- Calibration equation is not recalculated when the internal standard (IS) is reintegrated and the changes are applied for the first time. When the same changes are done and applied the next time, the calibration equation is recalculated. This issue only affects the calibration equation shown in the UI of the Calibration curve. The result is always updated when the internal standard is reintegrated. (MQ-2782)

- On Windows 10 operating system, the Installation Verification report does not open and a message about pdfFactory not being installed is shown when the user attempts to print the report. To avoid this issue, make sure that the computer is connected to the network. This issue does not affect the Installation Verification feature. (MQ-3204)
- The MultiQuant™ MD software shows an error message that the operation cannot be completed when an attempt is made to generate a report, using the **Create Report and Save Results Table** menu item, from a locked Results Table that was copied from another computer. As a workaround, unlock the locked Results Table on the current computer and then lock it again. Then create the report.

  Note: A report cannot be created using the Analyst® MD software in such a scenario because the Analyst® MD software users do not have the required permission to unlock a MultiQuant™ MD software Results Table.

  (MQ-1369)
- Avoid using the same name for a custom column in the acquisition file and a column in the MultiQuant™ MD software **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 MultiQuant™ MD software *Reference Guide*, the **Barcode** and **Scanned Barcode** are also used exclusively by the MultiQuant™ MD software and must not be used in the acquisition method. The column name is not case sensitive. (MQ-345)
- When only Upper Limit concentration for flagging outliers in the quantitation method is used, any samples with no peak found and shown as N/A in the Results Table are incorrectly flagged for Concentration. (MQ-548)
- Local users who are assigned to the analyst role in the Analyst® MD software cannot export and save Results Tables to a folder that has delete permissions denied. If users want to export and then save the Results Tables, they have two options: They can either export the Results Tables to another location on the hard drive, or they can select the same location and use the same file name and then save the files again. (MQ-600)
- If a quantitation method containing empty fields for the concentration units is exported as a text file and then imported as text, then the concentration units are populated using the value specified in the Units and Calibration Defaults dialog. It is recommended that the user confirms that all of the information contained in the method is correct before saving. (MQ-614)

Changes from Version 3.0.2 to MultiQuant™ MD 3.0.2 HotFix 1

The MultiQuant™ MD 3.0.2 HotFix 1 addresses the following issues:

Sum Multiple Ions Issue

Issue MQ-2009 is fixed. Previously, the summed peak area for some samples was greater than the sum of the actual values of the peak areas for the individual ions. The summed peak area is now aligned with the sum of the actual peak areas.

Improvements to the processing speed operation

Issue MQ-1895 is fixed. Previously, manual integration operated at a slower speed in the MultiQuant™ MD 3.0.2 software when compared to the speed of the manual integration in the MultiQuant™ MD 3.0.1 software. When this HotFix is installed, the performance speed is now similar to the performance speed of version 3.0.1.

Manual Integration Issue

Issue MQ-549 is fixed. Previously, an incorrect manual integration occurred when an analyte chromatogram was shown in overlay mode with the "percentage y-axis" option selected for the intensity axis of the chromatogram. The manual integration is now correct.

Changes from Version 3.0.1 to Version 3.0.2

New Features

- The software now shows the Ion Ratios in Chromatogram for all sample types, including standards.
- The software now shows the Expected Ion Ratio and Calculated Ion Ratio for all sample types in the Results Table. The software also flags samples that are outside of the specifications for the Expected Ion Ratio.
- Enabled support for reports containing queries.
- Enabled support for reports in Word, csv and HTML formats.
- Added two new reporter tags: query name and report template name.
- Enabled the import of quantitation method as text.
- Enabled the export of quantitation method as text.
- Added new report and associated query: Sample Report With Concentration Threshold.

Fixed Issues

- After a Results Table is created, users should not remove a standard from the Results Table because the results are not recalculated after the deletion. If users want to remove a standard, then save the Results Table after deleting the standard and then close and open the Results Table again. (MQ-382/493) This issue has now been fixed.
- Do not use the Export Calibration and Save Results Table or the Import External Calibration features found under the Process menu. (MQ-387) This issue has now been fixed.
- When the user creates a report after external calibration is applied, the "Calculated Concentration" column should not change. The column should retain the same values that were present before the report is generated. (MQ-379) This issue has now been fixed.
- The quantitation method can be exported but the same method cannot be imported. Quantitation methods containing an upper concentration limit that exceeds 100 cannot be imported into the software. (MQ-389) This issue has now been fixed.

- For Results Tables that were created in version 3.0.1 or earlier, the previous behavior for Gaussian smoothing for values below 0.3 is still applied even if the results are reprocessed. The scaling factor was incorrect for all Gaussian smoothing values below 0.3. (MQ399) This issue has now been fixed for new Results Tables created in theMultiQuant™ MD 3.0.2 software. If Gaussian smoothing values below 0.3 were applied during processing, then it is advised to create a Results Table using MultiQuant™ MD software and reprocess the data.
- Ion Ratio outlier flagging is not applied to QC samples. (MQ-282) This issue has now been fixed.

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 MultiQuant™ MD software, those users cannot run the MultiQuant™ MD software. Only the users who are added to the Security Configuration as an individual user can run the MultiQuant™ MD 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 monocolor 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)

Support

Additional Documentation

Refer to the documentation that comes with the software.

Contact Us

SCIEX Support

- sciex.com/contact-us
- sciex.com/request-support

Customer Training

- In North America: NA.CustomerTraining@sciex.com
- In Europe: Europe.CustomerTraining@sciex.com
- Outside the EU and North America, visit sciex.com/education for contact information.

Online Learning Center

- SCIEX**University**

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

Technical Support

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

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
C	Added "Changes from Version 3.0.1 to Version 3.0.2". Updated Known Issues and Limitations. Removed references to the Analyst Administrator Console.	January 2015
D	Changed AB SCIEX to SCIEX where required. Updated the copyright page. Changed the company logo to Sciex Diagnostics. Added Changes from Version 3.0.2 to MultiQuant™ MD 3.0.2 HotFix 1". Added Changes from MultiQuant™ MD 3.0.2 HotFix to Version 3.0.3". Updated the Prerequisites for Installing Using the DVD, Additional Software Requirements, Install the Software, Remove the Software, and Known Issues and Limitations sections.	June 2017