DiscoveryQuant™ 3.0.2 Software Release Notes

New Features and Enhancements in Version 3.0.2

The following TOF MS workflow features are included in version 3.0.2:

- The data file structure naming now allows the inclusion of subfolders from the import file.
- The Q1 Resolution, CES, and CE parameters can now be set from the table.

The following issues have been fixed in version 3.0.2:

- Peptide Editor: Users cannot double-click an amino acid and then add a peptide sequence.
- Analyze Review: When the **Sum Multiple Ions** option is selected, calibration curves do not generate.
- Users are unable to exclude water loss from product ion spectra for multiply charged species.
- Users must open and then close review settings to automatically integrate negative peaks.
- (TOF workflow) Negative polarity cannot be set correctly in the Product Ion scan type.

New Supported Mass Spectrometers

- SCIEX Triple Quad™ 5500+ system
- TripleTOF® 6600+ system. Users must select the TripleTOF® 6600 system in the hardware profile.

New Supported Software

- Analyst® 1.7.1 software
- Analyst® TF 1.8 software

New Autosampler Support

- CTC PAL3 autosampler

Fixes included from 3.0.1 HotFix 2

- Support for the Windows 10, 64-bit operating system. The Windows 7, 32-bit or 64-bit, operating systems continue to be supported. Cybersecurity support is included for the Windows 7, 64-bit operating system and the Windows 10, 64-bit operating system.

  Note: Cybersecurity support is not included for the Windows 7, 32-bit operating system.

- Support for Microsoft Office 2013, 64-bit, and Microsoft Office 2016, 64-bit. Microsoft Office 2010, 32-bit and 64-bit versions, continue to be supported.
- Support for the Analyst® software, version 1.7. All previously supported versions of the Analyst® software and the Analyst® TF software continue to be supported.
- Support for Analyst® Device Driver, version 1.3. This version of the Analyst® Device Driver replaces all previous versions of the Analyst® Device Driver. Previous versions are no longer supported.
- In previous versions of the software, when a ChromaTune batch containing 12 or more samples was submitted, occasionally the Status on the Queue tab of the Results Table was not updated from Unsampled to Sampled after the batch was completed.

Install the DiscoveryQuant™ 3.0.2 Software

1. If applicable, remove any currently installed versions of the DiscoveryQuant™ software.
2. If applicable, do the following:
   a. Back up the Optimize compound databases, CompoundDB21.mdb and CompoundDB30.md, found in C:\DiscoveryQuant\.
   b. Move the Analyze settings database, DiscoveryQuant-Analyze21.mdb, found in C:\DiscoveryQuant\Analyze\, to a new location.
   c. Back up the C:\DiscoveryQuant30 folder.
3. Download the DiscoveryQuant3.0.2Installer.zip from the SCIEX website and then extract the installation files.

   Note: To prevent potential installation issues, save the file to a location other than the computer desktop and disconnect any external USB storage devices.

4. Double-click **setup.exe** and then follow the on-screen instructions.
5. Click **Done**.

Notes on Use

- Analyze Review sessions saved in version 2.1 do not work in version 3.0 and any data must be acquired again. Contact sciex.com/request-support for help in converting the data.
- In DiscoveryQuant software version 2.1.x, users were warned if the files were locked and they were asked if they wanted to unlock them. In version 3.0, the software unlocks the files (configuration and database files) without asking.
- The scripts to create a Microsoft SQL server Global database are located in C:\Program Files\DiscoveryQuant30\Support Files. The scripts are only compatible with Microsoft SQL server 2014.
- When Analyze batches are submitted in a combined workflow with Optimize batches, the software uses only the first Q3 fragment found in the preceding Optimize batch to create the MRM method.
- When the combined workflow batches are submitted with cassetted Analyze samples, if one compound in the cassette fails the Optimize experiment, then the Analyze batch will terminate.
- ChromaTune batches cannot be submitted using conditions that exist only in the Global database.
- The Global database is designed to hold results. Optimize and ChromaTune experiment settings and ChromaTune review settings are not transferred to the Upload database using the Upload Data tool. To view ChromaTune results in the Global database, use the Compound Summary panel. The ChromaTune Review panel is designed to review data acquired to the local database.
- Although all of the compounds are in the database, the software only loads the most recent batch entry in the Review Analyze workspace under the following conditions:

  1. The user enters a set of compounds in the database using the **Edit Compounds** function with a batch name.
  2. The user enters a different set or subset of compounds with the same batch name.
     In the Analyze Setup workspace, the **Load From Database** function returns the latest set of compounds associated with the batch name.

- In previous versions of the software, if the autosampler and other peripherals were controlled by different software, such as the Analyst® Device Driver or the Analyst® software, then the DiscoveryQuant™ software might fail to recognize the correct autosampler and generate errors. For most configurations, this issue has been fixed. However, in rare instances this issue might occur. If the DiscoveryQuant™ software fails to recognize the correct autosampler, then contact sciex.com/request-support.

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