DiscoveryQuant™ 3.0.1 Software

Release Notes

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Contents

New Features and Enhancements in Version 3.0 1

New User Interface

- Version 3.0 of the DiscoveryQuant™ software combines the DiscoveryQuant-Analyze software and the DiscoveryQuant-Optimize software in one application.

- The single application allows combined Optimize and Analyze workflows.

- The new Compound Summary pane shows the complete tune history for Optimize experiments and ChromaTune experiments in a single view.

New ChromaTune Feature

- Users can validate MRMs from QuickTune and FineTune on column.

- Compounds can be screened based on chromatographic properties such as sensitivity, retention time, peak width, and peak tailing.

- Users can perform linearity response checks across multiple plate dilutions.

Support for TripleTOF Systems (TripleTOF 4600, 5600, and 6600)

- Analyze setup and Analyze review features are available using the Analyst® 1.7 software data acquisition.

- Supported TripleTOF® TOF method types: TOF MS and Product Ion.

- Connect to an existing DiscoveryQuant™ software database to use the mass information for data extraction.

- Optimize features are not supported.

New Peptide Optimization and Quantitation Features

- Improved workflow for the tuning and analysis of small peptides and large protein digests.

- Dynamic product ion start mass to focus on high mass product ions.

- y and b ion mass labels on product ion spectrum in Optimize Review.

- Ability to create custom amino acid side chain modifications with new peptide editor.

- Peptide sequence and charge state added to search.

- Import tool for peptide transitions from Skyline software (MacCoss Lab Software).

Improvements to Analyze Setup

- New cassetting user interface with options to set the mass interference to zero, automatically exclude errors and highlight mass interference errors, and include internal standards in interference checks.

- Users can create methods using polarity switching on 4500, 5500, and 6500 series of systems.

- The dwell time can be set through the Analyze experiment.

- Users can create custom comments for tables.

- Using LIMS import, casssetted compounds can have different concentrations.

Improvements to Analyze Review

- Individual standards from a calibration curve can be rejected without having to change the sample type.

- Ability to sum multiple Q3 ions.

- Peak processing can be done per MRM or per analyte.

Improvements to Optimize Setup

- **Original Submitters**, **Original Plate**, and **Plate ID** are new columns that are associated with a record. The columns are kept with **Compound ID** but are not searchable. The **User Name**, **Lab Name**, **Lab Group Name**, **Project Name**, and **Project Code** are searchable.

- In version 3.0, in batches with optimize experiments with **QuickTune** and **FineTune** experiments, if there are no passing conditions for the compounds after the **QuickTune** experiment, then the **FineTune** will not run.

Improvements with MultiQuant 3.0 Software Integration

- **Compound ID** from the DiscoveryQuant^{TM} 3.0 software database is now incorporated in the MRM method and the subsequent .wiff files.

- Analyte concentration information is written in the .wiff file as concentration (not weight-to-volume).

- MultiQuant^{TM} 3.0 software allows isomers in the same results table with the same MRM to be plotted on separate calibration curves, provided they have a unique compound ID (enabled through the DiscoveryQuant 3.0 software).

Improvements to Edit Compounds Workspace

Previously, only the Load from Database option was available to search when editing compounds. Now data can be searched and modified using saved searches.

Supported Mass Spectrometers

- API 3000™ system

- QTRAP® system

- API 3200™ and 3200 QTRAP® systems

- API 4000™ and 4000 QTRAP® systems

- API 5000™ system

- QTRAP® 5500 and SCIEX Triple Quad™ 5500 systems

- QTRAP® 4500 and SCIEX Triple Quad™ 4500 systems

- QTRAP® 6500 and SCIEX Triple Quad™ 6500 systems

- TripleTOF® 4600 system (new)

- TripleTOF® 5600+ system (new)

- TripleTOF® 6600 system (new)

Supported Software

- Analyst® 1.6 software

- Analyst® 1.6 with Components for 6500 software

- Analyst® 1.6.1 software

- Analyst® 1.6.2 software (new)

- Analyst® TF 1.7 software (new)

New Autosampler Support

- Agilent 1100 (G1367, G1377), 1200 (G1367B, G1367C, G1367D, G1377A), 1260 (G1367E), 1290 (G4226A)

- Shimadzu HTA, HTC, SIL10ADvp, SIL_20A/HT, SIL_20AC/HT, SIL_20ACXR, SIL_20AXR, SIL_30AC, SIL_30ACMP

- Waters Acquity (including Acquity iClass)

- CTC-PAL

- CTC-MPX, Shimadzu-MPX

  - The MPX™ driver software is compatible with the Microsoft Windows 7 32-bit operating system only.

  - The MPX™ driver software is supported in Analyze only, but not in Optimize or ChromaTune.

- Advion NanoMate

- Eksigent® microLC 200 Plus system (under CTC-PAL), Eksigent UltraLC 110 and UltraLC 110 XL, and the Ultra 110 HTC/HTS

OS Support

Supports Microsoft Windows 7 Professional, 32-or 64-bit operating system.

New Features and Enhancements in Version 3.0.1

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Fixed Issues

- The Live Plot feature now updates after every injection.

- Peptide transitions imported to the DiscoveryQuant™ software database now support side chain modifications using square brackets.

- Peptide transitions import supports more than one charge state per import and incorporates charge state labels in the compoundID column.

- Added Stream assignment import for the MPX™ driver software in LIMS Import.

- Fixed vial positions for well plates other than the 96 and 384 well plates in the DiscoveryQuant™ software queue.

- The autosampler states are now cached to speed up the loading of the program.

- The CTC-MPX LIMS and Template Import workflows in Analyze now use CTC plate location formatting in the import text files. Use wells 1 to 96 and plates 1 to 6 for a 3-drawer stack and plates 1 to 12 for a 6-drawer stack. Analyze will format to the corresponding CTC-MPX vial locations after batch submission.

- The error when building methods if the FineTune precursor was set to true and QuickTune was set to true is now fixed.

- The issue with cassetting negative only compounds with no internal standard on an instrument that does not support Pos Neg switching is now fixed.

- Compound ID is now maintained when building methods with the Keep Existing Transitions option selected.

- Retrieval of Compound Lot information is now on a per condition basis.

- The TOF negative product ion scan now subtracts the mass of the proton.

- The software now allows the import of charge states for TOF workflows.

- The issue that caused compounds to be missed when uploading from the 2.1 SQL database to the 3.0 SQL database is now fixed.

- The issue that caused the CAD gas to default to 0 for some scan types is now fixed.

New Supported Mass Spectrometers

- QTRAP® 6500+ system

- SCIEX Triple Quad™ 6500+ system

- SCIEX Triple Quad^{TM} 3500 system

New Supported Software

- Analyst$^®$ 1.6.3 software
- Analyst$^®$ TF 1.7.1 software

New Autosampler Support

- AnalystDeviceDriver 1.0 with Aglient Infinity II autosamplers G7167A and G7167B
- ExionLC^{TM} AC and AD systems, and the ExionLC^{TM} Multiplate Sampler

Installation Instructions 3

Install the DiscoveryQuant^{TM} 3.0 Software

Use this procedure if you are installing the DiscoveryQuant^{TM} software for the first time.

1. Download the DiscoveryQuant 3.0 Installer.zip from the Web site and then extract the installation files.

2. Double-click **setup.exe** and then follow the on-screen instructions.

   The installer will install Microsoft .NET 4.5.2 if it is not detected on the system. It will also install the LabView runtime if required.

   > **Note:** After Microsoft .NET 4.5.2 is installed, the .NET installer opens a dialog asking the user to restart the computer to complete the installation of .NET 4.5.2. **Click No. Do not restart the computer at this time.** Complete the DiscoveryQuant^{TM} software installation and then restart.

3. Click **Done** on the Migrate 2.1 Databases dialog, if there are no existing DiscoveryQuant 2.1 software databases to migrate.
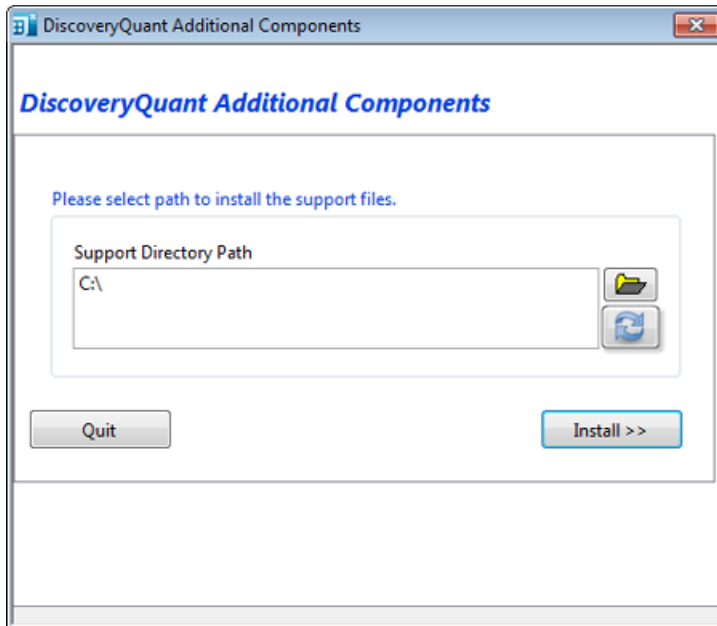
Upgrade the Software from Version 2.1.2

1. Back up the Optimize compound database, CompoundDB21.mdb, found in C:\Program Files\DiscoveryQuant\ and the Analyze settings database, DiscoveryQuant-Analyze21.mdb, found in C:\ProgramFiles\DiscoveryQuant\Analyze\ to a new location.

2. Upgrade the operating system to Microsoft Windows 7 Professional.

3. Download the DiscoveryQuant_3.0.zip file from the Web site and then extract the installation files.

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

   The prerequisite software is automatically installed.

5. Specify the location where the support directory will be created and then click **Install**.

Figure 3-1 Support Files Directory Selection

6. In the **Migrate DiscoveryQuant 2.1 Databases** dialog, select the existing databases and then click **Start**. Refer to step 1.

Figure 3-2 Database Migration
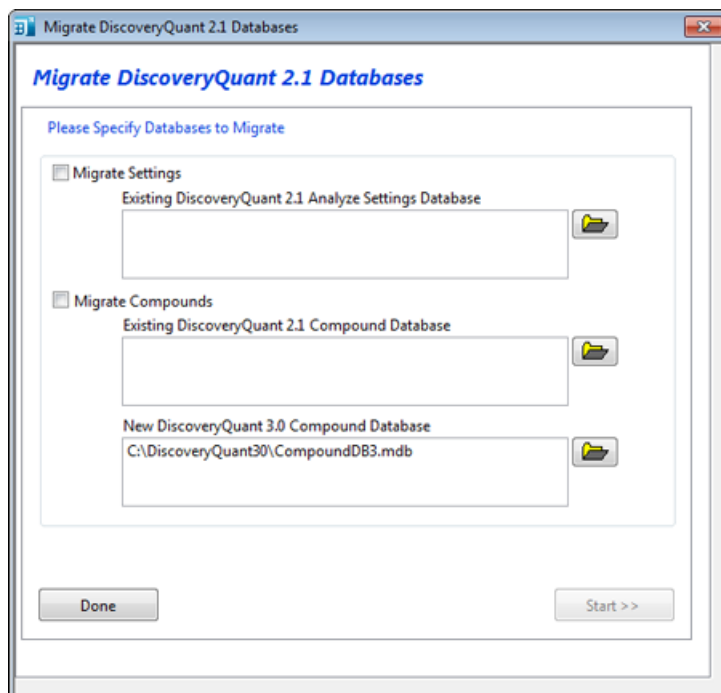
7. Click **Done** to migrate the settings and compounds.

Upgrade the Software from Version 2.1.3

1. Back up the Optimize compound database, CompoundDB21.mdb, found in C:\DiscoveryQuant\ and the Analyze settings database, DiscoveryQuant-Analyze21.mdb, found in C:\DiscoveryQuant\Analyze\ to a new location.

2. Remove the DiscoveryQuant™-Optimize software and DiscoveryQuant-Analyze software version 2.1.3 and associated patches.

3. Download the DiscoveryQuant_3.0.zip file from the Web site and then extract the installation files.

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

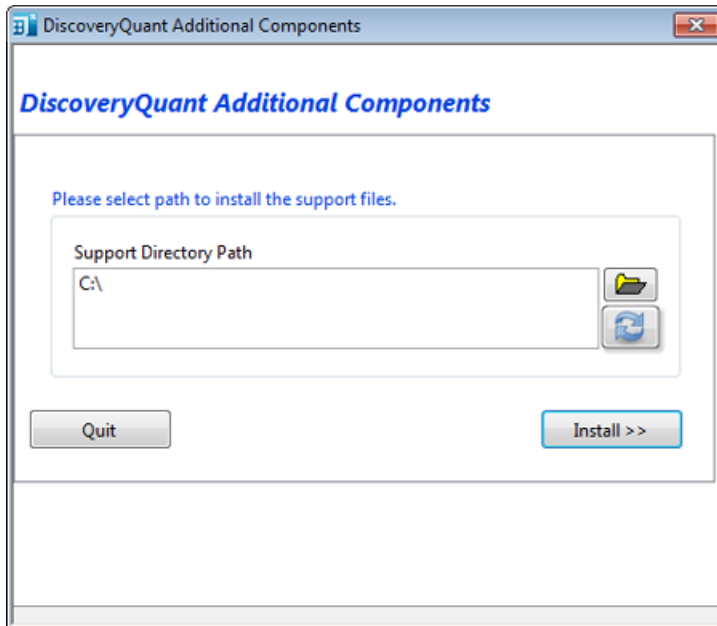   The prerequisite software is automatically installed.
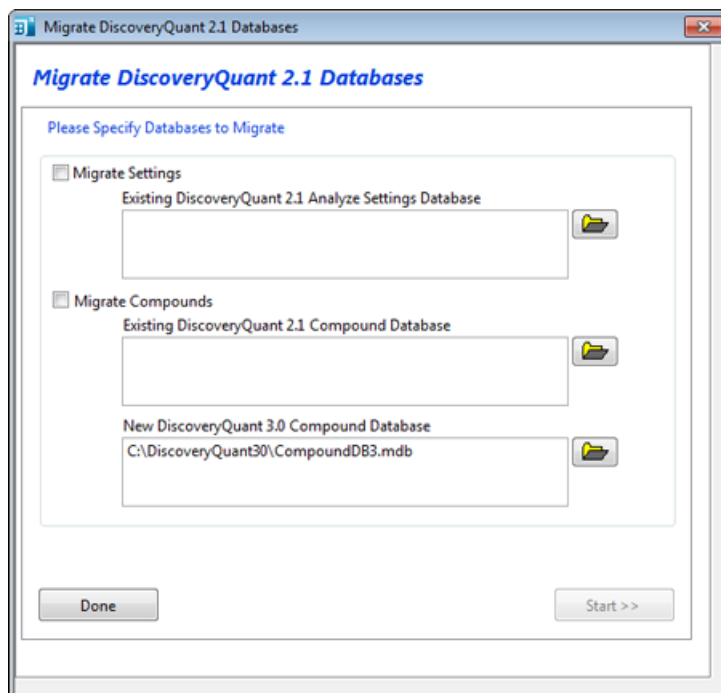
5. Specify the location where the support directory will be created and then click **Install**.

Figure 3-3 Support Files Directory Selection

6. In the **Migrate DiscoveryQuant 2.1 Databases** dialog, select the existing databases and then click **Start**. Refer to step 1.

Figure 3-4 Database Migration

For DiscoveryQuant 2.1.3 software, the paths are C:\DiscoveryQuant\CompoundDB21.mdb and C:\DiscoveryQuant\Analyze\DiscoveryQuant-Analyze21.mdb.

7. Click **Done** to migrate the settings and compounds.

Notes on Use

• Analyze Review sessions saved in version 2.1 will not work in version 3.0 and any data must be acquired again. Contact sciex.com/support/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 will only use the first Q3 fragment found in the preceding Optimize batch to create the MRM method.

• When submitting the combined workflow batches 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 to 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.