Release Notes

DiscoveryQuant™—Optimize Software

Version 2.1.1

New Features and Changes

- Table settings are now saved with the Save to Dataset option.
- Annotations now shown in each CE spectra for review.
- Upload Data time window defaulted to be two weeks upon first open.
- Edit Experiment now provides readouts for polarity, tune types, and saturation control in use.
- All peaks now appear in the Precursor Ion graph.
- Can now export the results of selected tune, QuickTune, or FineTune data.
- QTRAP® Product Ion scan types now limit the Product Of values to QTRAP limits.
- 5500 instruments with Q3 scan types only sum one scan.
- Review table now shows appropriate values in the center table for Precursor, Product, and Fragment items.
- When using large retention widths on the Timing tab on the Edit Experiment dialog, the cycles are now correctly calculated.
- Submitted Batches are now saved to file for inspection and cataloging.
- Edit Results allows fragments greater than 999 full resolution to be edited to three decimal places.
- On the Results tab, the CE/CXP graph legend now shows fragments greater than 999 with more than one decimal place.
- Switching the database on review with previously loaded data no longer removes the previous results being shown.
- Initial drawing of the results for the first well now appears correctly.
- Backslash in the compoundID name is now supported.
- Support for alphanumeric characters when using the Nanomate system.
- Edit Experiment no longer asks to save a configuration when nothing has changed for settings.
- Submitting a positive only run, then a negative run using the positive results no longer removes the positive information.
- Submitting a positive only run no longer enters both positive and negative .wiff file paths into the database.
- Entire file path is now available in the review experiment.
- If a Negative Only tune fails, it is no longer marked as Positive.
- Review Experiment no longer shows 0 for QuickTime CE dwell time when the setting is 0.5.

- Collision energy data from the AB SCIEX Triple Quad™ or QTRAP® 5500 systems can now be processed using the Analyst® 1.5.1 software.
- Polynomial Fit is no longer empty when using 5 values or less.
- All methods are now stored in the methods folder.
- When QuickTune fails with no Product Ion, FineTune will now also fail.
- Upper limit of the mass range now set to 1250 Da for the AB SCIEX Triple Quad or QTRAP 5500 instruments in triple quad mode.
- In QuickTune only polarities with passing results will be used when comparing intensities.
- Alpha Numeric types for Vial Numbers are no longer off by one.
- Resolved the issue where processing was incorrect for molecules where charge state was 3 or greater.
- Using the Precursor Peak Finding 'Closest Peak to m/z' with a charge state >1 now excludes the precursor ion from selection.
- Review of Charge State is no longer off by one.
- Automaton database conversion and uploading has been improved.
- Now able to modify the Compound ID using the Edit Compound DB tool.
- Resolved issue with the Edit Compound Database where Compound ID changes where not saved.
- Ion Source length greater than 5 characters no longer results in error adding or modifying.
- Uploading results to the same database from multiple workstations at the same time no longer causes loss of data.
- When uploading, the cancel button no longer becomes unresponsive.
- Exporting All Tune data to file now only includes tested tune types.
- Large added datasets now show the proper number of compounds on the Setup Tab table and the Review Tab Load Dataset table.
- Adding by File no longer results in mismatched batch results and maintains the acquisition times from the file.
- Universal Data Link files now encrypt passwords for security.
- If Date/Time is not included or N/A, the Date/Time is not included.
- Loading Data with a SQL Server Database first load no longer produces an error.
- Application no longer locks up upon closing after a batch submission.

Where to Get Help

Support

For support, contact AB SCIEX.

- Email: support@absciex.com
- Web: www.absciex.com

Requirements

The DiscoveryQuant™—Optimize 2.1 software must be installed.

Installation Instructions

DiscoveryQuant—Optimize Software.exe extracts three (3) files in the “C:\ DiscoveryQuant—Optimize Software” folder by default: DiscoveryQuant—Optimize 2.1.1.msi, UpdateInfo.exe, and HowToUseUpdateInfo.doc.

- Double-click **DiscoveryQuant—Optimize 2.1.1.msi** file and then follow the instructions.

Updated files

C:\Windows\System32

fpimage.dll

C:\Program Files\FarPoint Technologies\Spread70\Bin

FPSPR70.ocx
fpSpru70.ocx
spr32d70.dll
spr32du70.dll
SS70PP.dll

C:\Program Files\DiscoveryQuant\Optimize

ABSciex.LRAM.dll
ABSciex.LRAM.tlb
DiscoveryQuant-Optimize.aliases
DiscoveryQuant-Optimize.exe
DiscoveryQuant-Optimize.ini
DiscoveryQuant-Optimize.tlb
Lmgr10.dll
Lvanlys.dll
Lvinput.dll
Lvwutil32.dll
Lvzlib.dll
ProcessHandles.dll
Rscoree.dll
ScxMSSW0.dll

Removing the Software

1. Open the Control Panel and then double-click **Add/Remove Programs**.
2. Select **DiscoveryQuant—Optimize 2.1.1** from the list and then click **Remove**.

Uninstalling this software restores the original DiscoveryQuant—Optimize 2.1 software files.

AB SCIEX

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Printed in Canada.