

Drug Discovery and Development

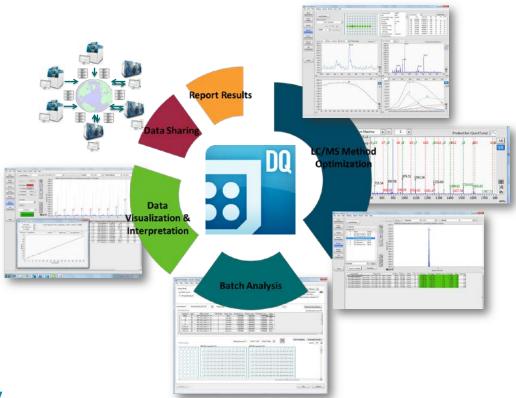


DiscoveryQuant™ Software

Better and Faster LC/MS Methods for New Chemical Entities (NCEs) and New Biological Entities (NBEs)

Suma Ramagiri, Ian Moore; SCIEX, Concord, ON

DiscoveryQuantTM Software reduces tedious LC/MS method development time with a fast, robust, and reliable process that optimizes methods for hundreds of small and/or large molecules. It expedites the method development process from existing database information, automates on-column optimization, and can easily analyze and process multiple samples at the same time. DiscoveryQuantTM 3.0.1 Software is supported on all AB SCIEX MS platforms and can seamlessly communicate with MultiQuantTM 3.0.2, ensuring success for everyone involved in drug discovery and development



Challenge Today

- Manual compound optimization can occupy significant amounts of time reducing lab output
- Emergence of complicated biotherapeutics makes method development challenges even bigger
- Huge need for automated software tools to navigate throught the complex LC/MS method optimization process for protein and peptide therapeutics

DiscoveryQuant™ Software was designed to address some of the key challenges in Pharma R&D and CRO bioanalytical workflows by providing

- Rapid and automated optimization of multiple MRM conditions for most sensitive quantitative assay development
- Support HT-LC/MS method building for HT-ADME screening studies to select new drug candidates with high potential for success in preclinical and clinical studies
- High quality data with fast turnaround results for screening 100s or thousands of compounds



Drug Discovery and Development



New Features in DiscoveryQuant™ 3.0.1 Software

Single Software Program - DiscoveryQuant Optimize and DiscoveryQuant Analyze in one unified software solution

ChromaTune - On-column MRM optimization to eliminate false positives

- Validate MRM's from QuickTune and FineTune on column
- Screen compounds based on chromatographic properties: sensitivity, retention time, peak width and peak tailing
- Performs linear response experiments across multiple plates
- Comprehensive compound summary panel for quick and easy review

Peptide MRM optimization

- Supports HT-ADME screening of emerging new biological entities (NBEs) along with new chemical entities (NCEs)
- Improve the workflow for tuning and analysis of small peptides and large protein digests
- Optimize and fine tune MRM conditions using real time labeling of y and b ions for extra confirmation
- Handle custom amino acid side chain modifications with new peptide editor
- Import Skyline MRM transitions to the DiscoveryQuant database for FineTune optimization
- Database searches for peptide sequence and charge state

Seamless Integration with MultiQuant™ Software

 for enhanced batch processing of 100's of samples with multiple MRM transitions

High Resolution Accurate Mass Support – All the great features of the DiscoveryQuant Analyze

workflow now available for high resolution accurate mass systems- TripleTOF® 4600, TripleTOF® 5600+ and TripleTOF® 6600 Systems

DiscoveryQuant Software Features and Benefits

Fast and efficient MRM method building using the DiscoveryQuant[™] global database

 Using the DiscoveryQuant[™] database you can build MRM methods containing multiple compounds with multiple transitions per compound eliminating tedious method building.

Automated batch building and time saving template design

 With a visual approach, templates can be made for frequently run studies that include sample assignment, quantitative information and internal standard assignment.

Easy peak review, data analysis and report generation

- All injections from a study can be visualized on a single plot to improve trend analysis.
- Customizable tables allow tailoring of DiscoveryQuant[™] Analyze to suit customer report formats.

Intuitive interface and concise plate review

- Provides a full-featured solution to the Discovery HT screening assay
- Plate-by-plate, compound-by-compound, allows the lab to meet its throughput objectives.
- Built for speed, with quick review screens for optimizations and assay results.

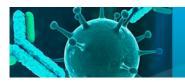
Enterprise-wide solution

- Import your results to your LIMS system for a final report
- Compound Library storage, sharing and retrieval
- DiscoveryQuantTM Software provides solution to multi-lab and multi-site labs and allows for a globally connected discovery environment



DiscoveryQuant[™] 3.0.1 Software Compatibility Matrix

Operating System	Windows 7 32-bit and 64-bit
Mass Spectrometers	API 3000 TM system Triple Quad TM 3500 system (new) 3200 QTRAP® system API 4000 TM and 4000 QTRAP® system API 5000 TM system QTRAP® 5500 and AB SCIEX Triple Quad TM 5500 system QTRAP® 4500 and AB SCIEX Triple Quad TM 4500 system QTRAP® 6500 and AB SCIEX Triple Quad TM 6500 system QTRAP® 6500+ and AB SCIEX Triple Quad TM 6500+ system QTRAP® 6500+ and AB SCIEX Triple Quad TM 6500+ system (new) TripleTOF® 4600 system (new) TripleTOF® 5600+ system (new) TripleTOF® 6600 system (new)
Analyst® Software	Analyst® 1.6.3 software (new) Analyst® TF 1.7.1 software (new) AnalystDeviceDriver 1.0 (required for use with Aglient Infinity II autosamplers G7167A and G7167B) (new)
LC Systems (Autosamplers)	Agilent 1100, 1200, 1260 (G1367E, New) and 1290 (G4226A, New) Shimadzu HTA, HTC, SIL10, SIL20, SIL 20 ACXR, SIL 30AC (New), SIL30ACMP (New) Waters Acquity (including iClass) CTC-PAL NanoMate MPX-2 High-Throughput System (New) Eksigent microLC 200, UltraLC 110, UltraLC 110XL, Ultra 110 HTC/HTS Aglient Infinity II autosamplers G7167A and G7167B (new) ExionLC TM AC and AD systems, and the ExionLC TM AD Multiplate Sampler (new)
Free Trial Download Link	http://sciex.com/licensing



Drug Discovery and Development



© 2015 AB Sciex. For Research Use Only. Not for use in diagnostic procedures.

The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners. AB SCIEX $^{\text{\tiny{M}}}$ is being used under license.

Document number: : RUO-MKT-02-3418-A



www.sciex.com