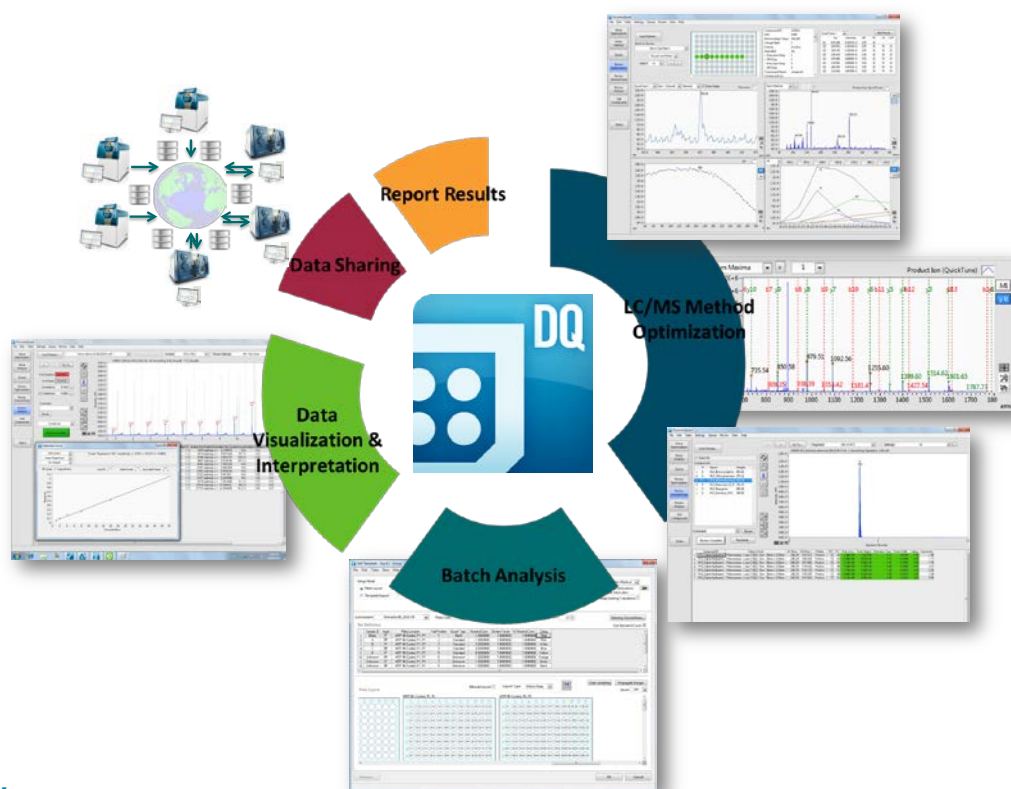


## DiscoveryQuant™ Software

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

Suma Ramagiri, Ian Moore; SCIEX, Concord, ON

DiscoveryQuant™ 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. DiscoveryQuant™ 3.0.1 Software is supported on all AB SCIEX MS platforms and can seamlessly communicate with MultiQuant™ 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 through 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

### 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**

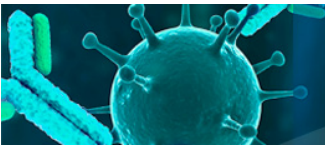
- Provides a full-featured solution to the Discovery HT screening assay
- Plate-by-plate, compound-by-compound, allows the lab to meet its throughput objectives.
- Built for speed, with quick review screens for optimizations and assay results.

#### **Enterprise-wide solution**

- Import your results to your LIMS system for a final report
- Compound Library storage, sharing and retrieval
- DiscoveryQuant™ 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	<p>API 3000™ system</p> <p>Triple Quad™ 3500 system (new)</p> <p>3200 QTRAP® system</p> <p>API 4000™ and 4000 QTRAP® system</p> <p>API 5000™ system</p> <p>QTRAP® 5500 and AB SCIEX Triple Quad™ 5500 system</p> <p>QTRAP® 4500 and AB SCIEX Triple Quad™ 4500 system</p> <p>QTRAP® 6500 and AB SCIEX Triple Quad™ 6500 system</p> <p>QTRAP® 6500+ and AB SCIEX Triple Quad™ 6500+ system (new)</p> <p>TripleTOF® 4600 system (new)</p> <p>TripleTOF® 5600+ system (new)</p> <p>TripleTOF® 6600 system (new)</p>
Analyst® Software	<p>Analyst® 1.6.3 software (new)</p> <p>Analyst® TF 1.7.1 software (new)</p> <p>AnalystDeviceDriver 1.0 (required for use with Agilent Infinity II autosamplers G7167A and G7167B) (new)</p>
LC Systems (Autosamplers)	<p>Agilent 1100, 1200, 1260 (G1367E, New) and 1290 (G4226A, New)</p> <p>Shimadzu HTA, HTC, SIL10, SIL20, SIL 20 ACXR, SIL 30AC (New), SIL30ACMP (New)</p> <p>Waters Acquity (including iClass)</p> <p>CTC-PAL</p> <p>NanoMate</p> <p>MPX-2 High-Throughput System</p> <p>(New) Eksigent microLC 200, UltraLC 110, UltraLC 110XL, Ultra 110 HTC/HTS</p> <p>Agilent Infinity II autosamplers G7167A and G7167B (new)</p> <p>ExionLC™ AC and AD systems, and the ExionLC™ AD Multiplate Sampler (new)</p>
Free Trial Download Link	<a href="http://sciex.com/licensing">http://sciex.com/licensing</a>



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## Drug Discovery and Development



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



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