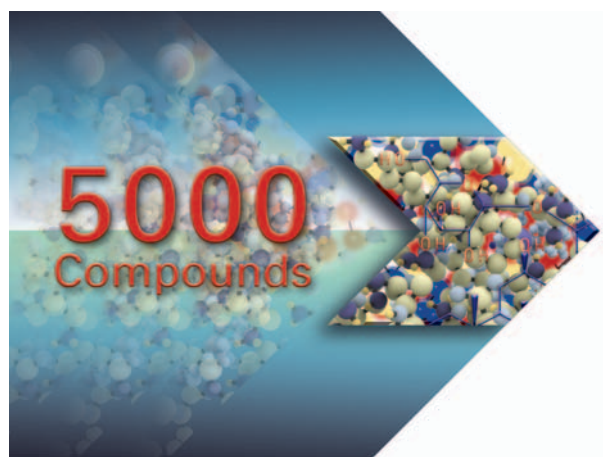


QuickQuan™ software speeds the pace of LC-MS/MS analysis in drug discovery through intelligent automation.

QuickQuan Software

A fully automated, high-throughput solution for early drug discovery applications



Challenge

A vital part of the drug discovery process is the assessment of drug properties for New Chemical Entities (NCEs). This evaluation requires determining compound properties such as metabolic stability, solubility, protein binding, and preliminary pharmacokinetics, often using assays such as PAMPA and CACO-2.

LC-MS/MS is routinely used to determine time course and concentration for drug metabolism and bioanalytical studies. Because LC-MS/MS is a highly specific and sensitive analytical platform, it has become an integral part of high-throughput compound assessment strategies in ADME.

However, the analysis of compounds that have not been characterized previously by LC-MS/MS may take many hours of valuable time for a trained specialist. High-throughput drug screening laboratories require specialized software for automated optimization of LC-MS/MS analysis to ensure the acquisition of accurate quantitative data for each compound being assessed.

The Thermo Scientific Solution

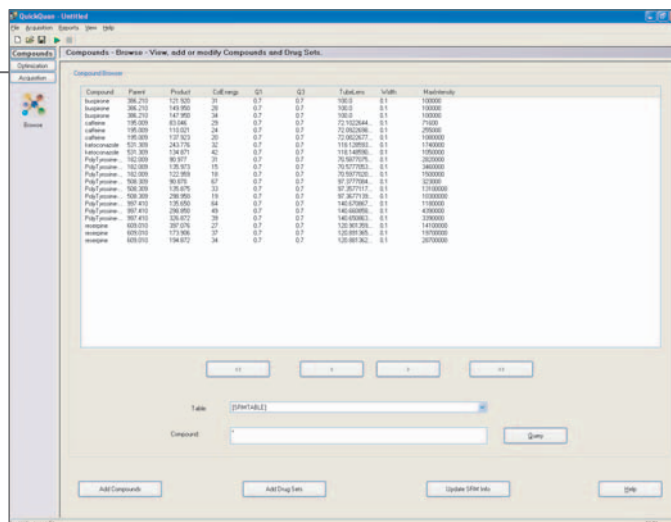
QuickQuan software was developed in partnership with multi-national pharmaceutical companies to provide a total solution for automated quantification in drug discovery. Combined with TSQ Quantum™ triple quadrupole mass spectrometers, QuickQuan allows automated LC-MS/MS analysis of chemically diverse compounds.

QuickQuan manages the data acquisition and processing for all compounds in the analytical run and generates quantitative results automatically. Data generated by QuickQuan is stored in a central Microsoft® Access or Oracle® database. This database allows fast and efficient retrieval of information about a specific compound and allows the method to be used in multiple assays as well as multiple TSQ Quantums, eliminating the need to re-optimize the LC-MS/MS tune conditions.

Network Method Transfer

Instrument methods can be seamlessly transferred from one TSQ Quantum to other TSQ Quantums across a user network.

All essential compound information for LC-MS/MS analysis is stored in a central database. Any TSQ Quantum on the network can access the database to perform sample analysis without individual instrument optimization of MS parameters.

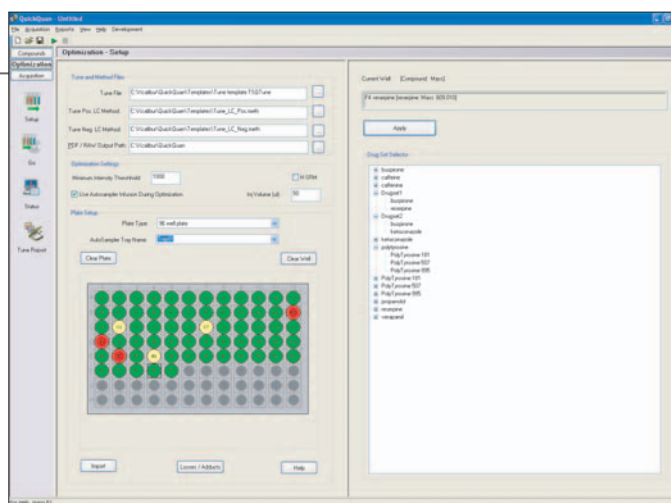


Essential compound information for LC-MS/MS analysis is stored to a central database for automated method creation.

Rapid, Accurate Optimization

QuickQuan works with the CTC Autosampler to perform optimizations by automated infusion. The autosampler delivers a consistent stream of compound to the TSQ Quantum for accurate optimization results. To prevent carryover into sample analysis, an isolated injection port is used for the optimization infusions.

The optimization of product ions and respective collision energies, tube lens values, and polarity are all determined in 70 seconds per compound.

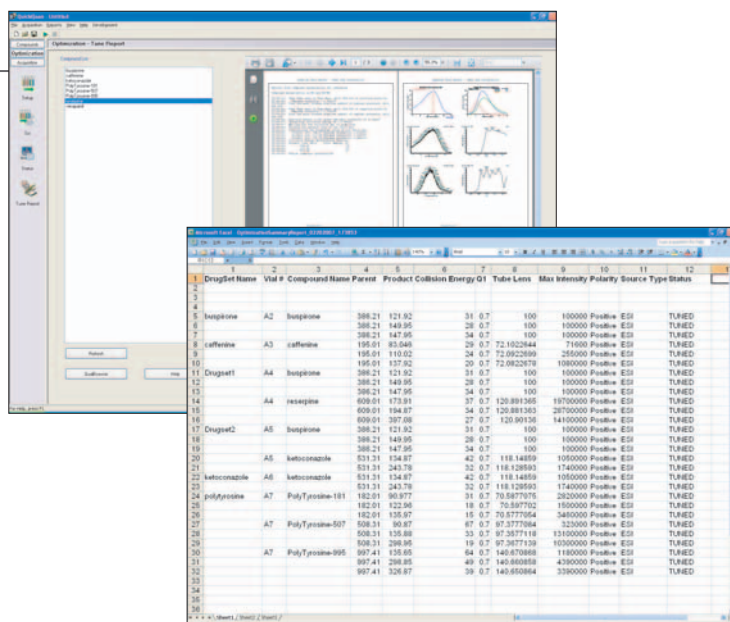


The tune plate interface is color coded for easy review of the compound optimization status.

Simplified Optimization Results Review

When optimizations are completed, tune reports are generated in PDF file format. These can be reviewed in the QuickQuan tune report browser.

For larger batches of compound optimizations, an optimization summary report can be generated in Microsoft Excel® format.



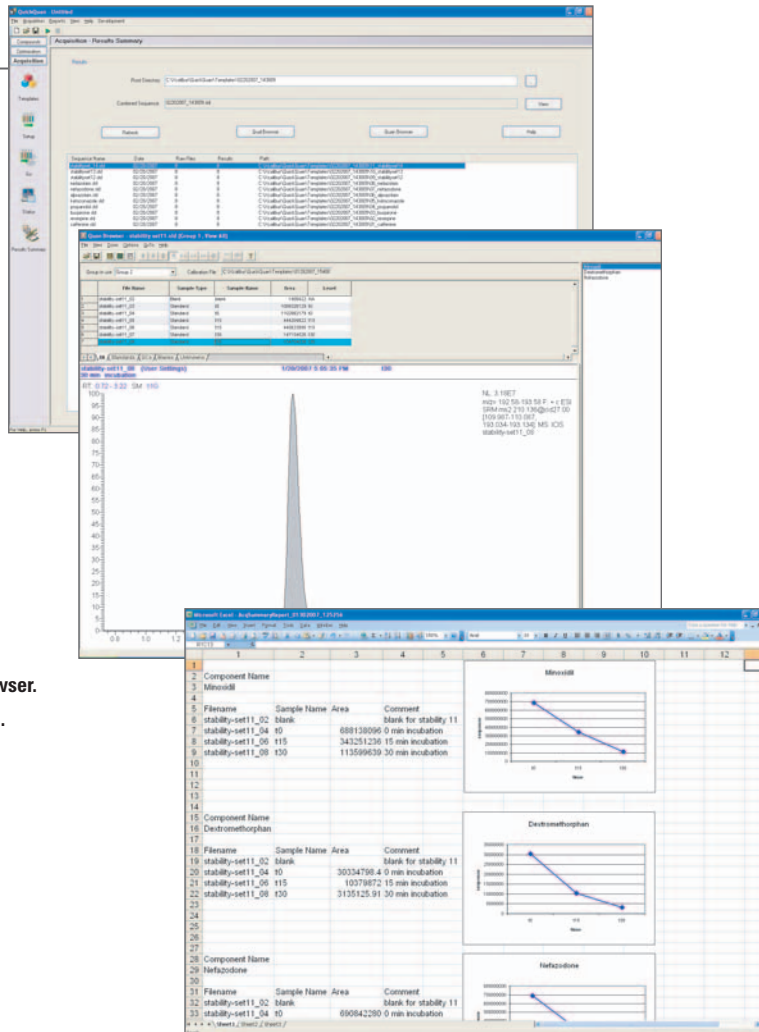
Top: The tune report in PDF format can be reviewed in the QuickQuan tune report browser. Bottom: The optimization summary report contains all essential optimization information.

Data Processing and Review

The sequence for sample acquisition can be created in QuickQuan or imported from Excel spreadsheets and Xcalibur sequence templates.

Data and reports are automatically generated, allowing review of results on a compound-by-compound basis.

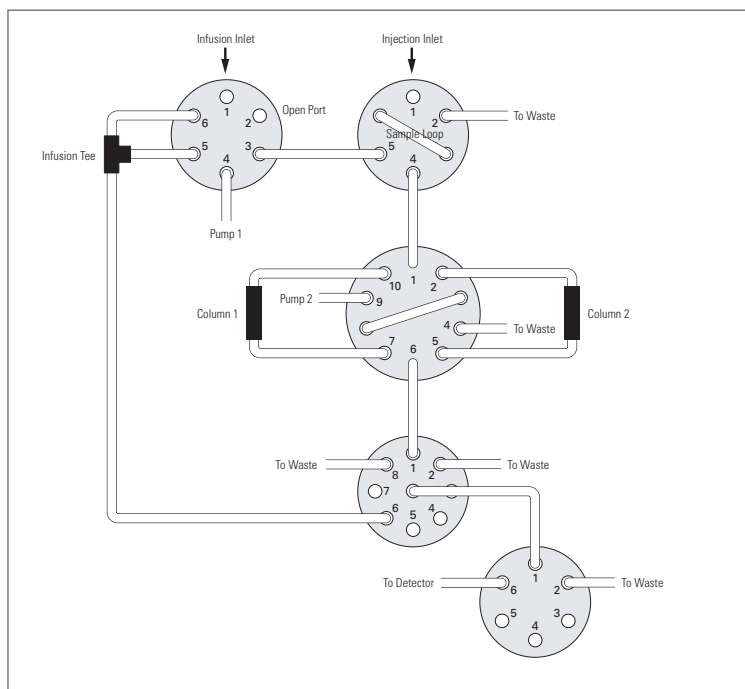
Customized reports can be generated in Excel or Xreports, customizable Thermo Scientific reporting software. Specialized macros can accommodate calculations in Excel sheets to automate result processing.



Top: Acquisition sequence is created or imported.

Middle: Compounds are reviewed in the Quan browser.

Bottom: Data can be reviewed in Xreports or Excel.



QuickQuan Total Solution option valve diagram

QuickQuan Total Solution Option

The QuickQuan Total Solution option includes a pre-configured CTC Autosampler with Trio SV Valve Stack (valve diagram shown at left). The option includes prewritten macros for the infusion-optimization procedure, as well as template instrument methods for hassle-free column switching capabilities.

With the QuickQuan Total Solution option, optimization and sample analysis can be performed sequentially in a true high-throughput fashion. After compounds are optimized on the left injection port, the software can proceed immediately into sample analysis. If sample optimization for a compound fails in the first step, QuickQuan skips analysis to avoid wasting time and samples.

When incorporating column switching, the column equilibration time is removed from the analytical run, increasing sample throughput.

Time Savings Evaluation: Average Time per Step for a New Compound Analysis

MS Procedure Step	Average Time per Step Without QuickQuan	Average Time per Step With QuickQuan
Compound optimization through infusion	10 minutes per compound	1.1 minutes per compound
MS instrument method setup	2 minutes per compound	Automated; no time required
Data processing method setup	5 minutes per compound	Automated; no time required
Data processing and report generation	10 minutes per compound	Automated report generation; 2-3 minutes for data review
Total time per compound (excluding acquisition)	27 minutes per compound	4.1 minutes per compound

QuickQuan Provides:

Scalability

To meet future demands for increased capacity, QuickQuan's ability to seamlessly drive the experiment from a central data-base enables "plug-and-play" installation of additional instruments.

Speed

Individual compounds can be fully auto-optimized in approximately one minute due to the infusion-based, valve switching auto-tuning procedure. This capability makes QuickQuan the fastest commercially available software solution for high-throughput LC-MS/MS.

Sensitivity

High sensitivity is achieved using Highly Selective Reaction Monitoring (H-SRM) and Heated Electrospray Ionization (H-ESI), enabling QuickQuan to successfully analyze a wide range of difficult-to-ionize compounds. In addition, new techniques such as Reversed Energy Ramp (RER) scanning used during the MS/MS analysis help to identify the optimal SRM transition. The use of breakdown curves enables an accurate determination of the optimum collision energy setting, ensuring the highest possible sensitivity for quantitation.

QuickQuan Ordering Options:

QuickQuan is available in three options: **Software Only**, **QuickQuan Basic**, and the fully-automated column switching option called the **QuickQuan Total Solution**. Please contact your local sales office for further details.

ORDERING OPTIONS	DESCRIPTION
QuickQuan Software Only	Software only; for use with installed CTC Autosampler, TSQ Quantum, and pumps
QuickQuan Basic	Software, CTC Autosampler, TSQ Quantum, and pumps
QuickQuan Total Solution	Software, CTC Autosampler, TSQ Quantum, pumps and Trio SV Valve Stack

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