DiscoveryQuant™ 2.0 Software: The Definitive Solution for LC/MS/MS Early-ADME Workflows

Key Features

- Cassetting Wizard makes setup of pooled samples fast and simple
- Multiply injected assay support allows maximum autosampler speed (Shimadzu, CTC, Agilent, or Acuity) while continually acquiring data for increased throughput
- LIMS connections enabled through easily configurable output column mapping to take full advantage of your established enterprise-wide systems
- Global database support allows compounds optimized in one lab to be used at another without re-optimizing, improving efficiency and productivity across your organization

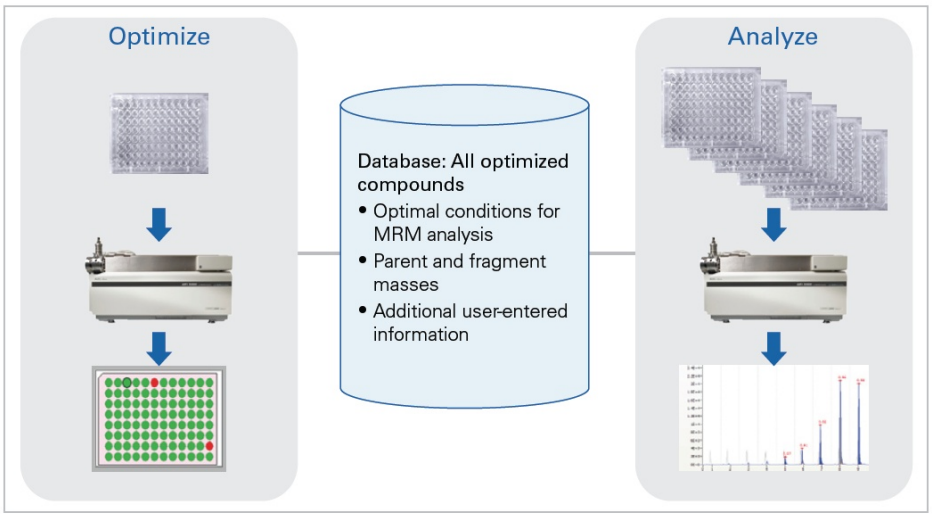

Figure 1. The Optimize module in DiscoveryQuant™ Software maximizes compound-dependent parameters and populates a database with these parameters. The Analyze module allows users to create quantitative methods for their analytes based on the stored values in the DiscoveryQuant™ software database. Analyze is also used to create batches, run studies, integrate data, and generate final reports.

Overview

Today's high-performance discovery lab performs many different assays on an increasing number of novel compounds. To improve the discovery pipeline, drug discovery labs must gather more information on a greater number of new chemical entities. Plate-based technologies, shared conditions information, and pooling strategies are often used to increase throughput in the lab. New software tools can also greatly improve the situation through automation, information sharing, and monitoring functionality.

DiscoveryQuant™ 2.0 software has been designed specifically for early-ADME workflows in a drug discovery environment. With a simple and elegant workflow, DiscoveryQuant™ 2.0 software is a very powerful and comprehensive software solution that streamlines the drug discovery process by providing better efficiency and productivity.

With the Optimize and Analyze modules, you can work in parallel on multiple MS systems. The Optimize module will automatically determine the optimal ion path parameters (DP and CE) for maximum quantitative sensitivity for your compounds and then populate a database with this information. At the same time, the Analyze module can use the same database to access MS methods for use in your assays. With a database that can be shared among labs around the world, you can seamlessly collaborate with your colleagues, work in parallel, and avoid duplicating effort.

Intuitive Interface

The graphical user interface has been designed to be intuitive and obvious. The main workflows in the software are set out on tabs at the top of the page that you progress through to set up your method optimization. You can easily import data when possible to avoid manual re-entry, and the information can all be saved and recalled as needed.

Concise Plate Review

See the results of your entire plate graphically. The color-coded display gives you immediate and clear visualization of the result and quick access to assess individual problem samples with a single click.

Express Cassetting Wizard

Group the compounds for dosing directly within the software to facilitate straightforward analytical setup. The intelligently designed DiscoveryQuant™ 2.0 software will warn you if there are any conflicts in polarity or if the masses of parents or fragments will interfere with each other during the analysis.

Multiply Injected Assay Support

Maximize costly instrument time by keeping your MS instrument acquiring over multiple injections, and improve your throughput and productivity. When the run is done, the software deconvolutes the analysis into individual compound results. This cuts down on a significant amount of instrument calibration and delay overhead during device communication and synchronization.

Rapid Review Capability

Review multiple concentrations of a single compound across many injections. The software stitches your runs together automatically to give you a clear and concise picture of your results.

Time-Saving Templates

Choose your plate layouts from pre-defined templates that you can build and share. Spend less time entering sample locations. Enter a few samples for a new plate and click “Propagate Groups” to auto-fill the rest based on the current pattern you have defined. When you have plate after plate of samples to run, easy sample entry reduces the tedium typically associated with large-batch analysis.

Quick View Calibration Curves

No need to send your data to an external package for regression. Do it all here and even view the graphical result.

Custom Column Mapping

Define the column headers and order in which the results appear in a .CSV output. This allows you to import the file directly to your legacy LIMS system for a final report, without any intervention or manual modification of the results.

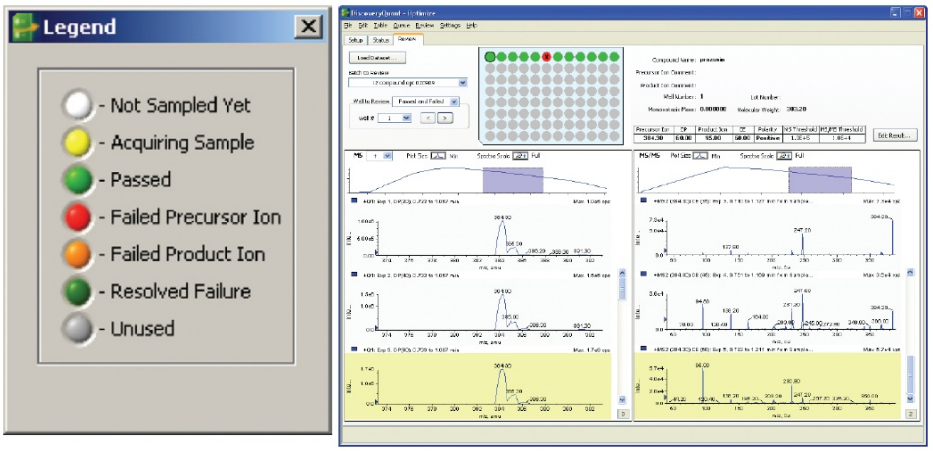

Figure 2. Intuitive software interface makes plate review simple and fast.

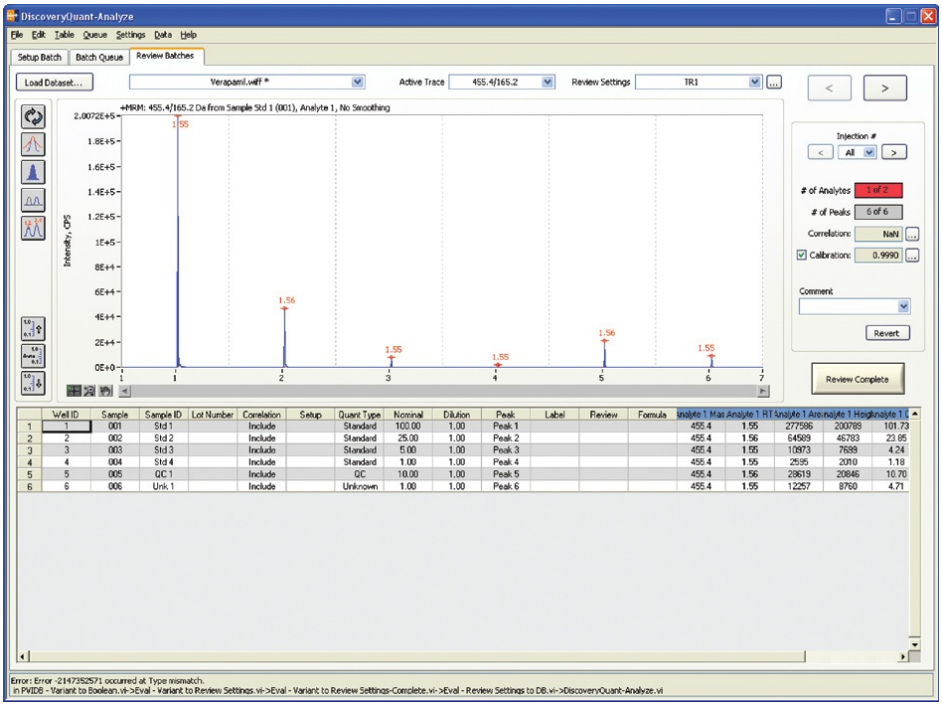

Figure 3. Peak Review in DiscoveryQuant™ software allows you to quickly check injection and integration in one interactive window.

Global Database Setup

Use the global database support in DiscoveryQuant™ 2.0 software to store and share your mass spectrometry methods. Leverage the size of your organization to create greater sample capacity and productivity by drastically reducing redundant work. When enabled, the software will automatically look for a method in the database before acquiring data to build a new one. Use methods from your colleagues around the globe, and share your own methods with them to keep your labs running consistently and efficiently.

Summary

DiscoveryQuant™ 2.0 software has been designed by experts in early-ADME drug discovery who understand the intricacies and needs of this area. This software has been carefully designed to deliver high-throughput analysis, without compromising on the quality of the results—you no longer have to sacrifice one for the other.

Connect with your colleagues in other ADME areas around your organization. Store your methods in the database and share them globally. In an environment where efficiency is vital, you can avoid duplication of effort and get the most out of your mass spectrometry systems.

With DiscoveryQuant™ 2.0 software, the LC/MS/MS early-ADME workflow is completely covered—no more partial solutions or manual data transport to other systems. DiscoveryQuant™ software provides a total solution that takes you from beginning to end and everywhere in between. Your early-ADME workflows have never seen anything like this.

For a free 90-day trial of this software, visit www.absciex.com/discoveryquant

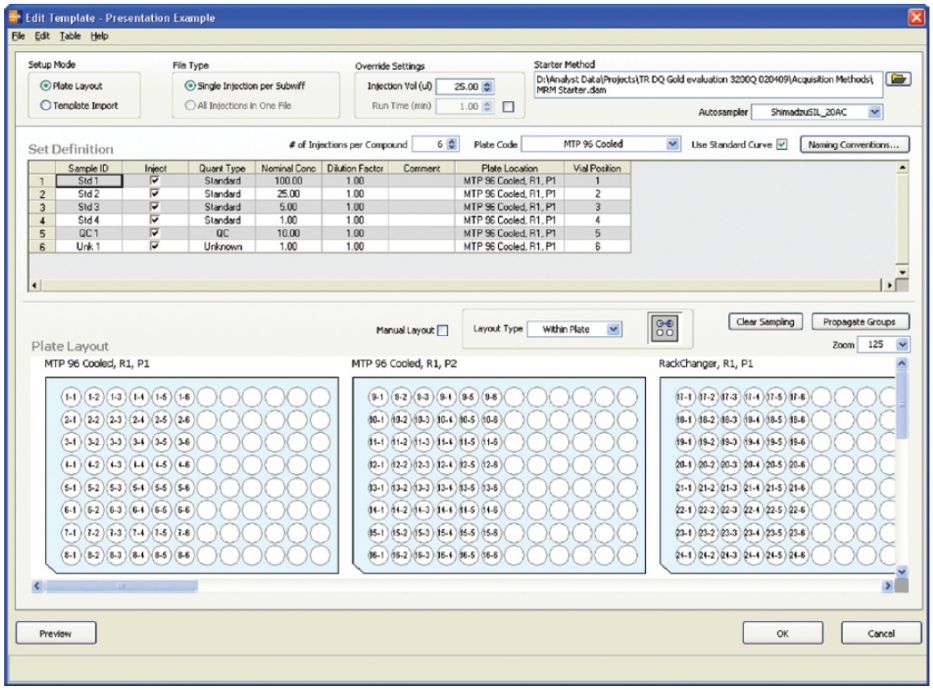

Figure 4. Plate templates make large-batch sample entry efficient and easy.

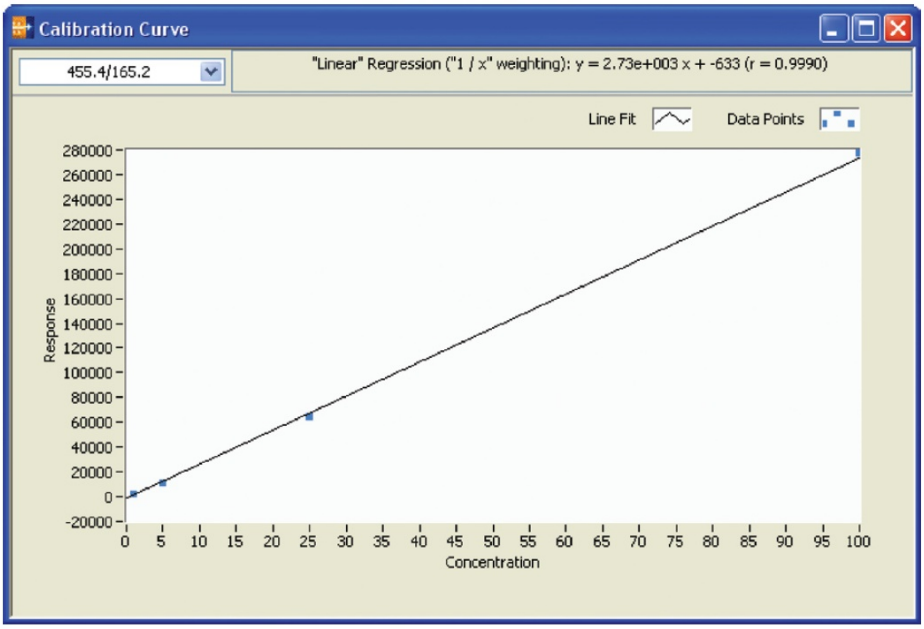

Figure 5. The calibration curve window displays the calibration data and the linear regression for each MRM transition.

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