

Biomarker and Omics Solutions

FOR DISCOVERY AND TARGETED LIPIDOMICS

Lipids play a key role in many biological processes, such as the formation of cell membranes and signaling pathways. They are a chemically diverse group of molecules that vary widely in size and structure.

The *lipidome* refers to all the lipids that exist in cells and how they affect diverse cellular processes. To understand the lipidome, it is important to characterize and quantify lipids, both collectively and individually. Mass spectrometry has emerged as a powerful analytical tool for lipidomics research.

AB SCIEX provides a powerful suite of electrospray mass spectrometry tools, and partners with other industry providers to enable systems-level lipidomics.

Starting with the right tools

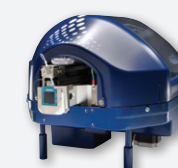
Powerful mass spectrometry systems combined with innovative software and reagents enable workflows that increase productivity, while saving time and money.

Lipidomics solutions

Hardware and software for non-targeted and targeted workflows



TripleTOF™ 5600
System Solutions



Advion TriVersa
NanoMate®



QTRAP® 5500
System Solutions



MarkerView™ Software



LipidView™ Software



MultiQuant™ Software

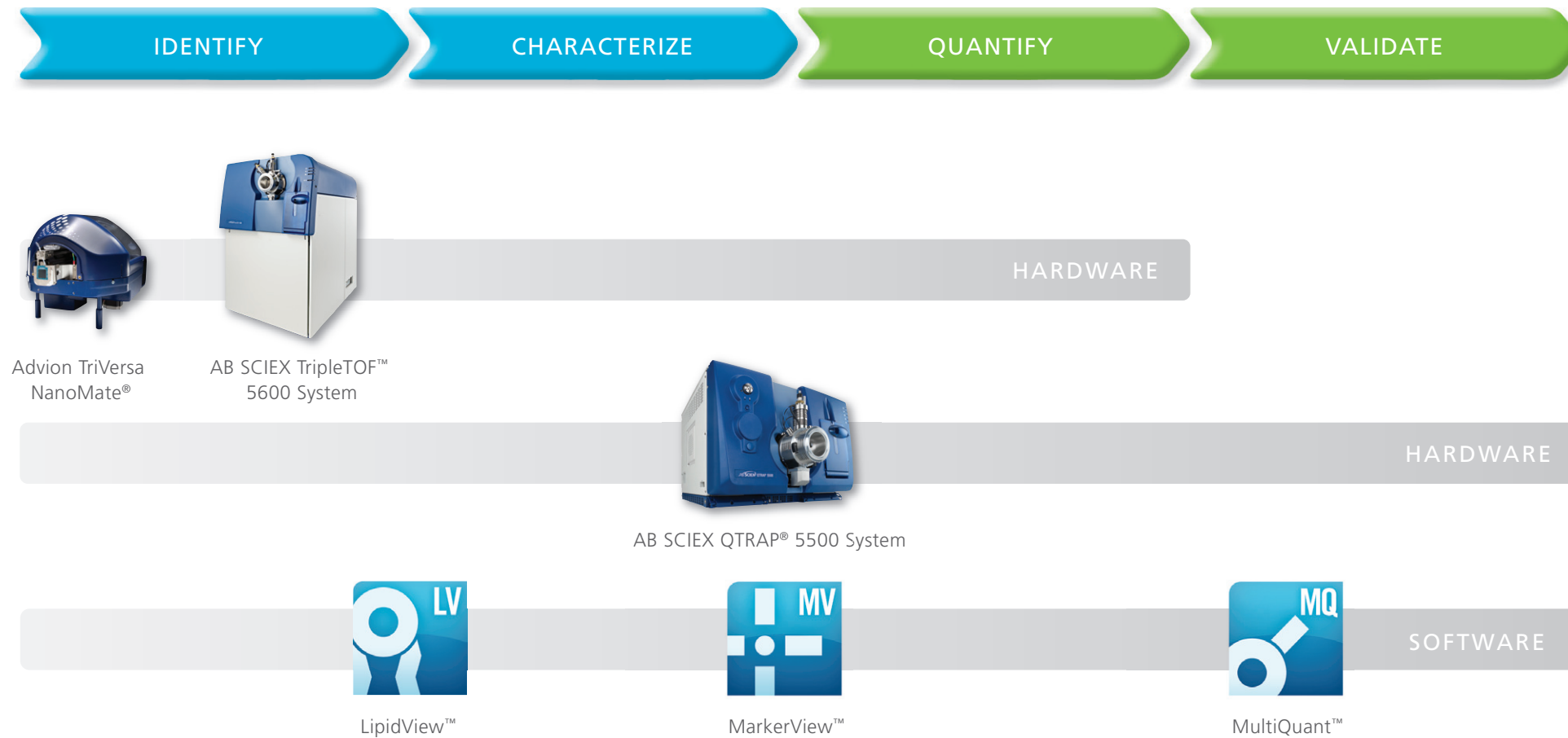
NON-TARGETED

TARGETED

Complete solutions for comprehensive lipid analysis

Class-leading solutions for both lipid identification and quantitative profiling

The lipidomics profiling pipeline



Accurate mass, high-resolution lipid analysis can be achieved on the AB SCIEX TripleTOF™ 5600 System for lipid identification in both positive and negative modes.

The AB SCIEX QTRAP® 5500 System offers a more targeted quantitative approach to lipid analysis, with fast multiplexed scanning by MRM, precursor ion, or neutral loss scanning.

Data types from either approach are fully supported by dedicated software and algorithms that enable you to:

- Automate deciphering of lipid MS and MS/MS spectra
- Identify lipid species by database searching
- Correct isotopes
- Perform semi-quantitation analysis against lipid-class internal standards

You can also visualize and quantify data with advanced statistical tools in MarkerView™ Software and seamlessly process targeted lipid assays with MultiQuant™ Software.

When used with the Advion TriVersa NanoMate®, these systems provide reproducible, long stable spray times, for deeper interrogation and consistent profiling, with no sample to sample carryover.

TripleTOF™ 5600 System for lipidomics

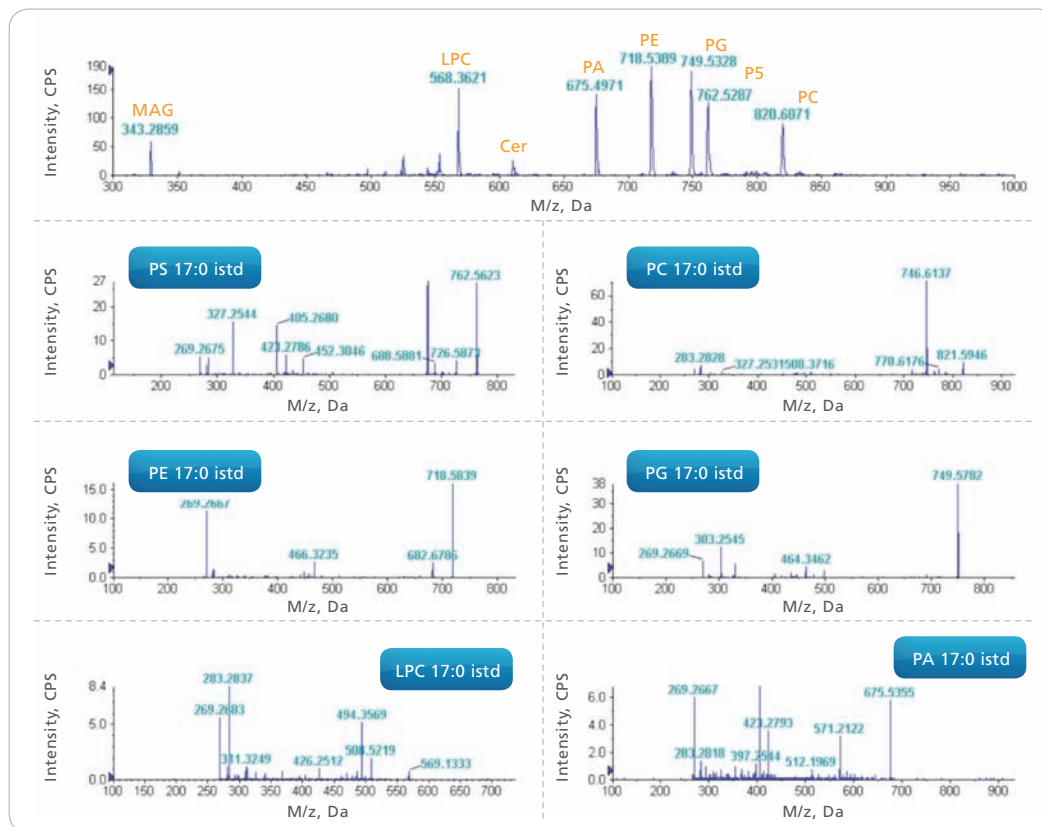
High resolution and accurate mass discovery with sensitive triple quad-like quantitation

The AB SCIEX TripleTOF™ 5600 System combines our leadership in high sensitivity triple quadrupole quantification with high resolution and accurate mass for comprehensive lipid characterization. This new hybrid time-of-flight platform offers in-depth lipid profiling by molecular compositions at high speeds without compromising resolution or sensitivity. Whether the experimental approach benefits from LC fractionation or could simply be carried out by a direct infusion shotgun approach, a novel MS/MS^{ALL} workflow with high resolution TOF MS and MS/MS is a powerful toolset for lipid systems analysis.



Key benefits of the TripleTOF™ 5600 System:

- Accurate mass and high resolution full scan TOF MS and MS/MS at the detectable dynamic range achieved on 4000 QTRAP® System
- Up to 100 MS/MS per second, 50 in data dependent mode
- Resolution > 30,000 in both MS and MS/MS
- Mass accuracy of 2 ppm across mass range
- Dynamic range is approximately 4 orders
- Multiple precursor ion scanning simultaneously while storing all TOF product ions
- Novel workflows for acquiring data; MS/MS^{ALL} and neutral loss dependant MS/MS scanning

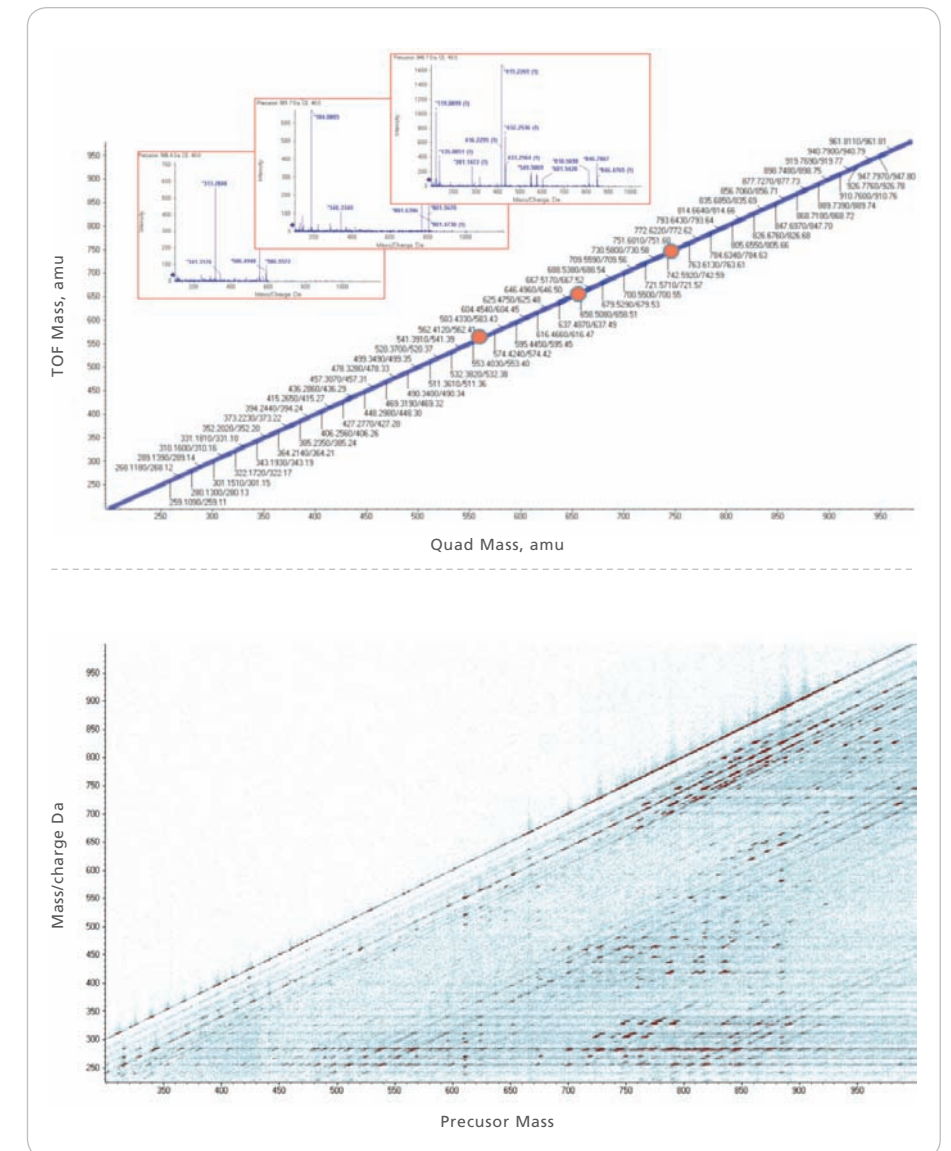


MS/MS^{ALL} on the TripleTOF 5600

A data-independent approach offers advantages when profiling lipids in complex biological extracts by providing MS/MS data for all lipid species in a given sample.

In an MS/MS^{ALL} workflow, Q1 steps through the mass range at unit-mass resolution, fragmenting all precursors and storing all product ions. This enables the recall of any precursor ion spectrum and post-acquisition lipid-class specific profiling.

Additionally, a high resolution TOF MS scan is looped within the acquisition to supplement the precursor profile with high mass accuracy measurements for optimal lipid identification.

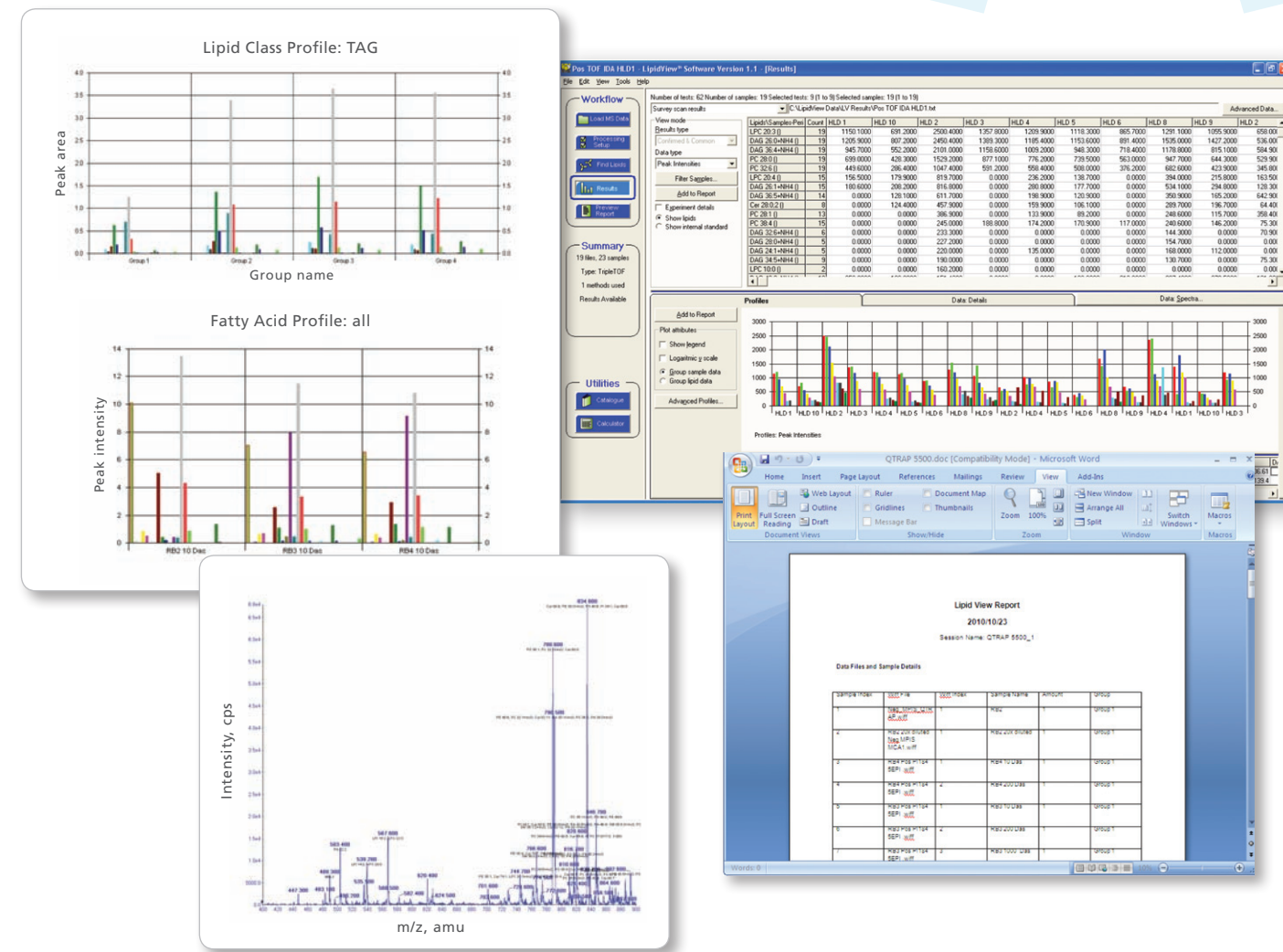


Graphical representations of a single cycle of MS/MS^{ALL} acquisition technique on the TripleTOF™ 5600 system. TOP: Ordered MS/MS acquisition of every precursor mass from 200 to 1000 m/z at 1 Da Q1 steps, resolved at UNIT resolution. A full product ion spectra is acquired at each step in as little as 10 ms producing 800 high resolution MS/MS collected across the mass range. BOTTOM: Three-dimensional plot of product ion m/z (y-axis) against precursor mass (x-axis) shown as peak intensities (blue to red). Data shown is negative mode cycle MS/MS^{ALL} workflow of a rat brain lipid extract.

LipidView™ Software for lipid molecular species identification and quantitation

LipidView™ Software is a unique application that hosts a data processing suite of tools and algorithms which identifies and quantifies lipid species from ESI-MS data. The software enables identification and characterization of lipid species through database searching of precursor and fragment ion masses, and provides numerical and graphical outputs for profiling various lipid classes by lipid head groups, fatty acid and long chain base characteristic fragments and neutral losses.

With a new user-friendly workflow driven format, LipidView™ software implements a simple 4-step workflow for automated data processing to obtain lipid species identification, isotope contribution removal of species with close lower m/z , multiple internal standards-based quantification, graphical visualization and reporting of the results. LipidView™ Software supports all data types from AB SCIEX Triple Quad™, QTRAP® and TripleTOF™ systems and complements to provide a full solution for mammalian lipid profiling research.



A few of the many numerical and graphical outputs provided by LipidView Software. TOP LEFT: Advanced Lipid Profiles View showing the class-specific and fatty acid profiles. TOP RIGHT: Results workspace providing confirmed lipid identifications aligning peak intensities or peak areas across all samples processed. BOTTOM LEFT: Displaying the Spectral Viewer with automatic peak labelling. BOTTOM RIGHT: Automatic report generation with customizable reporting.

MarkerView™ Software for principal component analysis

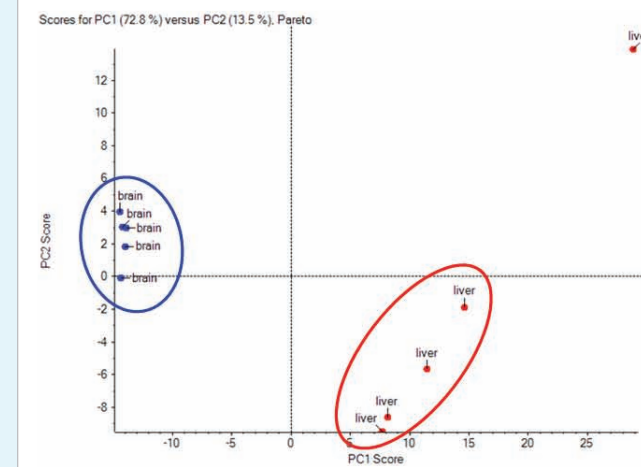
The ability to acquire data using information dependant acquisition (IDA), targeted MRM, or MS/MS^{ALL} workflow modes makes it possible to generate a myriad of complementary data sets for use in lipid profiling experiments across multiple samples. After lipid identification and relative quantitation, statistical multivariate analyses help in understanding the differences between lipidomes and the significance of the quantified lipids that give rise to these differences.

Principle component analysis

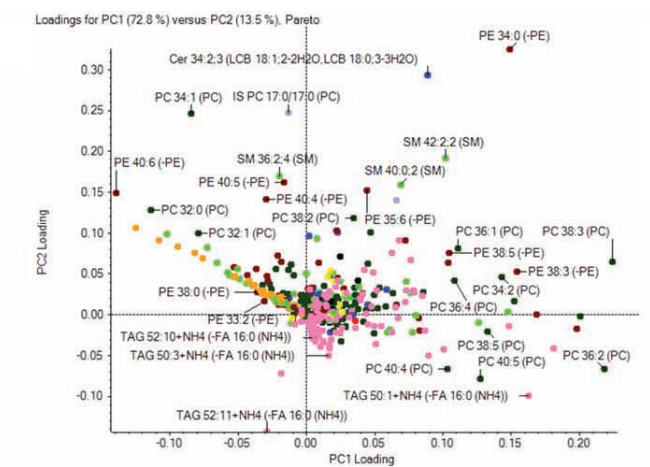
LipidView™ Software results can output the lipid identifications and quantitative data in a format suited for a direct import into MarkerView Software. There, you can visualize the abundance of lipid molecular species across batches of biological extracts using principle component analysis (PCA).

PCA starts with a scores plot to reveal sample grouping. Principle component variable grouping analysis on the PCA loadings plot highlights the lipids that share similar trends. This combination of lipid identification linked to PCA provides a powerful workflow to distill meaningful biological information from complex data sets.

Scores Plot



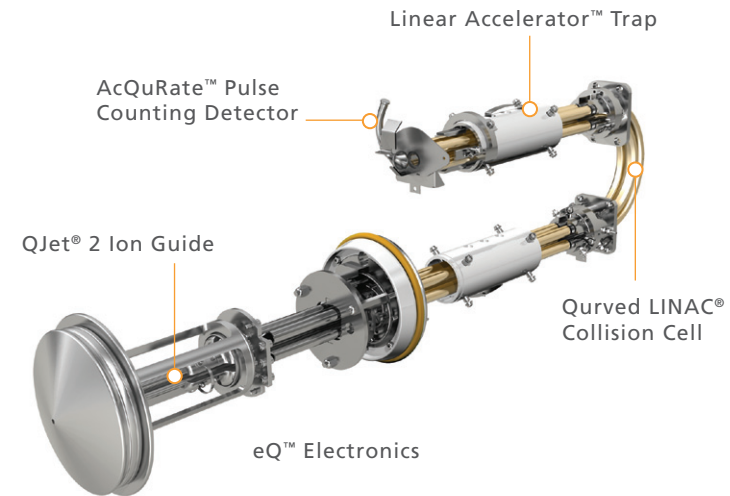
Loadings Plot



PCA starts with a scores plot to reveal sample grouping. Principle component variable grouping analysis on the PCA loadings plot highlights the lipids that share similar trends. This combination of lipid identification linked to PCA provides a powerful workflow to distill meaningful biological information from complex data sets.

QTRAP® 5500 System for lipidomics

Global lipid profiling strategies using TripleTrap™ scanning

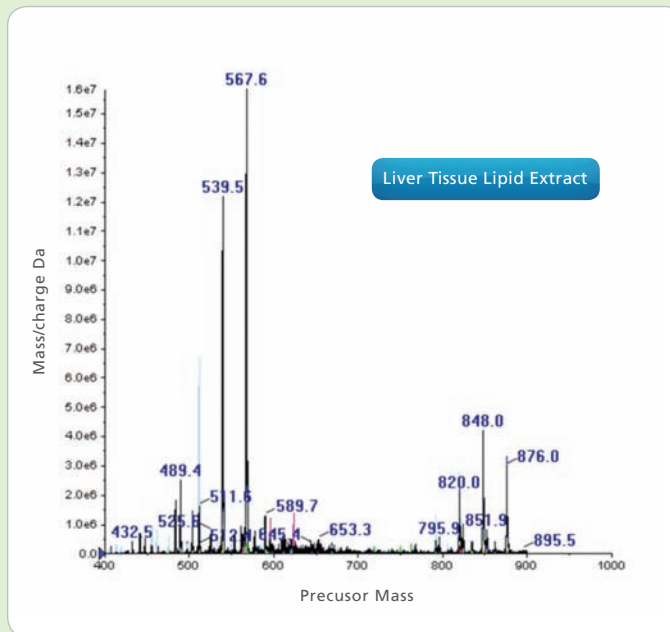


Targeted lipid quantitation

Targeted quantitation of lipid species

Targeted quantitative approaches represent a highly robust, sensitive and reproducible mode for lipid quantitation. Using LC methods suitable for the intended lipid class targets, targeted acquisitions can be collected on either the TripleTOF™ or QTRAP® system and then processed automatically using MultiQuant™ Software. On the TripleTOF System, a set of lipids can be analyzed using the MRM^{HR} workflow and high quality quantitation data is derived from the post-acquisition extraction of product ions collected at high resolution.

Scheduled MRM™ acquisition experiments on the QTRAP 5500 system benefit from the highest MRM sensitivity enabling high speed acquisition with high multiplexing to cover a wide range of lipid species with specific fatty acid compositions. With a proper internal standard strategy, reference ions are measured in the same fashion for lipid-class normalization or signal correction by the quantitative detection of common fragments. Such experiments can couple a series of specified fragment ions representing a unique lipid species, representing a value-added benefit to refining quantitation methods even after the data is acquired.

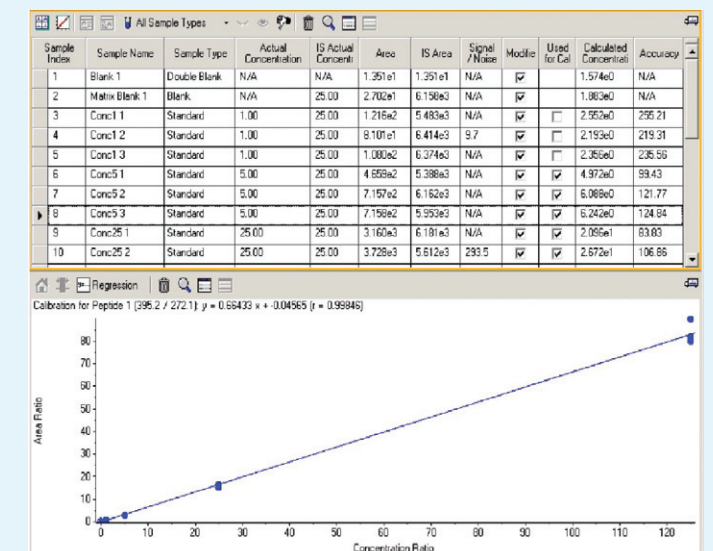
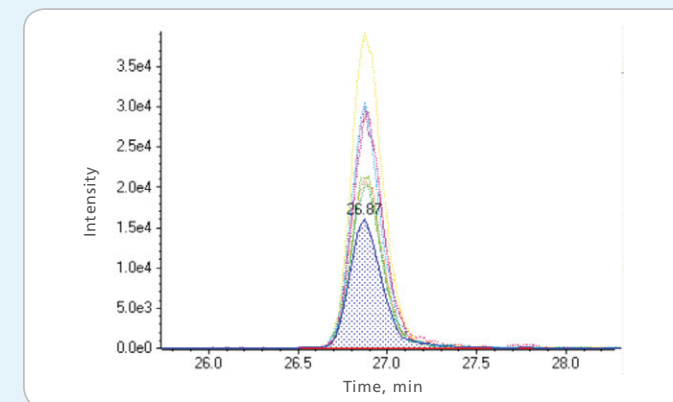


The AB SCIEX QTRAP® 5500 System is a triple quadrupole (QqQ) and linear ion trap (LIT) hybrid platform with unique scanning functions that provides the selectivity to deal with lipid species diversity within lipid classes and the sensitivity needed to characterize lipid structures in samples of wide dynamic range. Highly multiplexed MRM, Precursor Ion, and Neutral Loss scanning shows a 5x improvement in sensitivity compared to similar acquisitions carried out of the 4000 QTRAP® System and a 30-100 times sensitivity improvement in LIT MS/MS modes (enhanced product ion). This hybrid QqLIT design therefore enables class-specific lipid quantitative measurements combined with full scan MS/MS for lipid species molecular confirmation.

Multiplexed precursor ion and neutral loss scanning in negative mode on the QTRAP® system enables up to 60 targeted lipid class-specific scans in a single acquisition method. Liver tissue lipid extract data is shown where 57 precursor and neutral loss scans are overlaid providing fatty acid profiles for the targeted glycerophospholipids.

MultiQuant™ Software—Automation drives productivity

Built upon years of experience in MRM quantitative processing, MultiQuant™ Software was designed to enhance and automate the processing of MRM datasets in an intuitive, user-friendly workspace. It supports all internal standard strategies for both relative and absolute quantitation and provides query tools to minimize manual data review and data integration. Flexible reporting capabilities are available to create user-specific reports, and the data can be easily exported to Microsoft Excel®.



You invest in our technology. We invest in your success.

As the world leader in mass spectrometry, AB SCIEX creates solutions that are backed by the industry's most extensive service and support organization. With a network of service professionals, experienced compliance specialists, and over 150 PhD application scientists worldwide, we are dedicated to supporting your technical needs and helping you get the most out of your AB SCIEX systems.

AB SCIEX service professionals are recognized as the most highly qualified in the industry. They are certified on our instrument platforms through a rigorous 4-step certification program, with re-certification occurring every two years. This award-winning program helps to ensure that you receive the most efficient, highest-quality, and most up-to-date service available for AB SCIEX products and technology. Choose from flexible service plans and a variety of services for the right level of support for your laboratory's needs and budget.

Our customer support network is available to provide expert assistance in the use and application of AB SCIEX products through a comprehensive range of services, including application support, technical service, and training.

Whether you access our service and support team by phone, email, on-site visits, or through our innovative remote monitoring technology, you can be confident that the AB SCIEX organization will be there for you.

For more information, visit www.absciex.com

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Headquarters

500 Old Connecticut Path | Framingham, MA 01701 USA
Phone 508-383-7700
www.absciex.com

International Sales

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