

Metabolomics

# GO BEYOND

## Harness the power of metabolomics



Translate your data into valuable discoveries

Through collaboration with the scientific community, we've developed metabolomics solutions powered by Thermo Scientific™ Orbitrap™ LC-MS instruments, innovative data analysis software and premier mass spectral databases. With unique, built-in intelligent data acquisition and flexible workflows, we deliver the total package needed to perform increasingly complex analysis from compound annotation to quantitative metabolomics, so you can go beyond faster to actionable outcomes.

Sample collection  
and preparation

Chromatographic  
separations

Mass spectrometry  
data acquisition

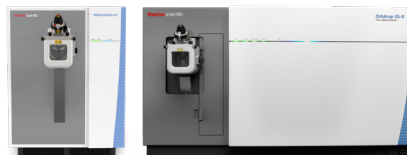
Data processing



QA/QC practices for  
sample preparation



Thermo Scientific™ Vanquish™ Horizon UHPLC system, Thermo Scientific™ Accucore™ C30 HPLC column, Thermo Scientific™ Hypersil GOLD™ C18 Selectivity HPLC column



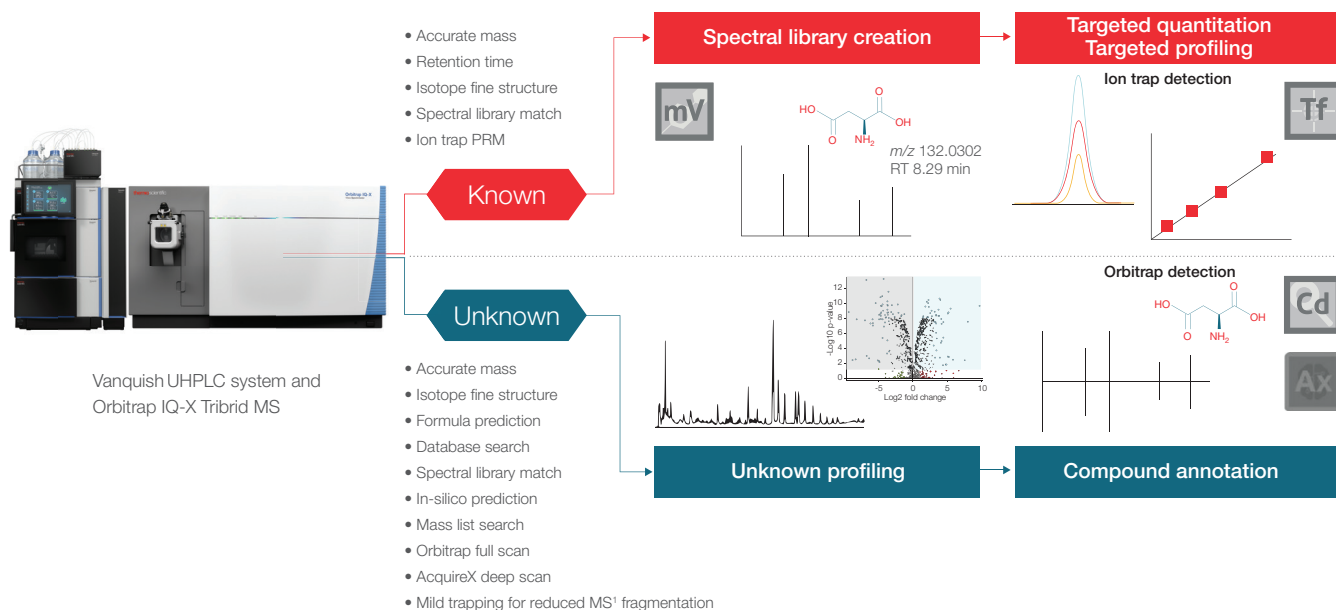
Thermo Scientific™ Orbitrap Exploris™ 240 mass spectrometer and Thermo Scientific™ Orbitrap IQ-X™ Tribrid™ mass spectrometer



Thermo Scientific™ Compound Discoverer™ software, Thermo Scientific™ TraceFinder™ Software, Thermo Scientific™ mzCloud™ mass spectral library

# Simultaneous Quantitation and Discovery (SQUAD) Analysis: the complete picture in one experiment

Traditionally, separate LC-MS instruments and methods are used for targeted analysis and untargeted profiling. Now, you can simultaneously measure known metabolites and discover unknown compounds in a single, workflow.

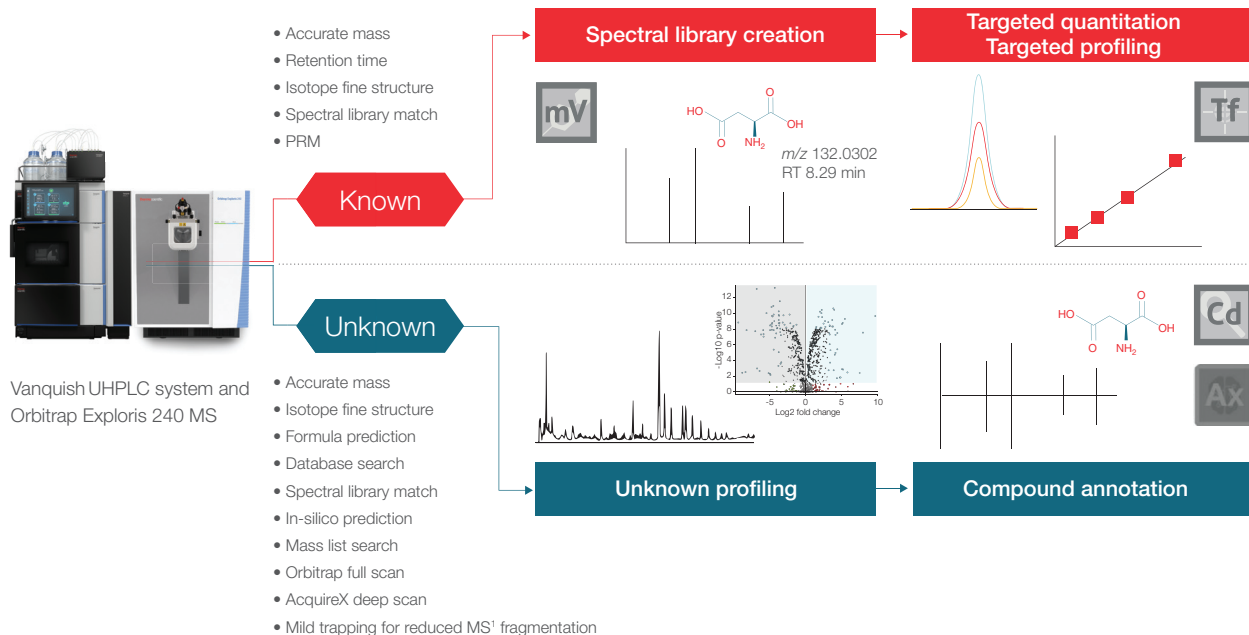


## Quantify known metabolites of interest

Individual reference standards, with or without stable isotope labels, establish retention time, mass measurement, isotopic fine structure, and MS<sup>2</sup> spectral confirmation against an in-house library for the identification and quantification of target metabolites. When stable isotope labels are used, absolute quantitation can be achieved.

## Discover novel metabolic signatures

As part of the same workflow, statistical analysis is applied to unknown compounds, focusing on relevant biological changes. The development of intelligence-driven data acquisition strategies, such as Thermo Scientific™ AcquireX™, enables scientists to dive deeper into the sample while providing an overview of known metabolites. Annotation tools, including formula prediction, database searches, spectral library searches, and in-silico prediction, are used to increase annotation confidence.



# GO BEYOND Harness the power of lipidomics

## Comprehensive lipidomics solutions

Lipidomics is a field of metabolomics that has evolved into a class all its own and aims to annotate and quantify lipid species to identify biomarkers and elucidate metabolism at the cellular level. Lipid species are diverse and complex, and the development of Thermo Scientific Orbitrap mass spectrometers has risen to the challenge of lipid analysis, offering an unprecedented level of resolution, sensitivity, selectivity, and precision.

## Designed for lipid analysis

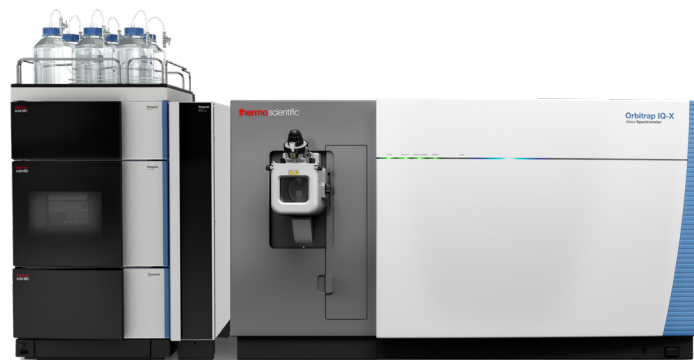
The Orbitrap IQ-X Tribrid mass spectrometer is designed to reveal complex chemical structures for compound identification and structural elucidation of lipids. The system combines industry-leading mass analyzer technology with intelligent automation with real-time decision making, intuitive software, and remote, hands-free calibration, to address the complexities of lipid identification and characterization so you can confidently collect more meaningful data.

## MS<sup>n</sup> and UVPD for structural elucidation

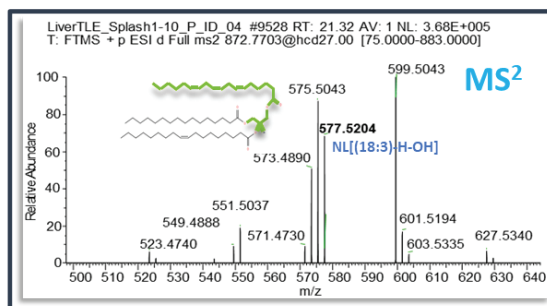
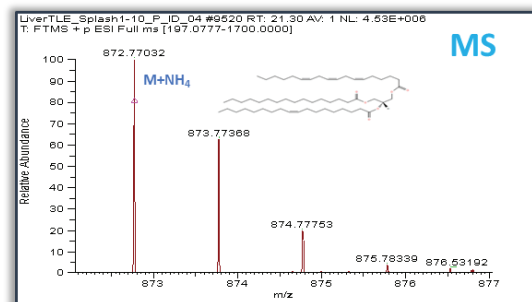
A fundamental issue in lipid identification is that lipids dissociate in a very predictable way to give relatively few product ions, and thus structural details are often incomplete. Obtaining more complete lipid structural information can be addressed in several different ways including MS<sup>n</sup> analysis to obtain a series of selective transitions revealing structure or using alternative dissociation techniques such as UV photodissociation (UVPD) to yield fatty acid regioisomer location. All fragmentation mode capabilities are available on Thermo Scientific™ Orbitrap™ Tribrid™ mass spectrometers such as the Orbitrap IQ-X Tribrid mass spectrometer.

## Intelligent acquisition to collect more meaningful data

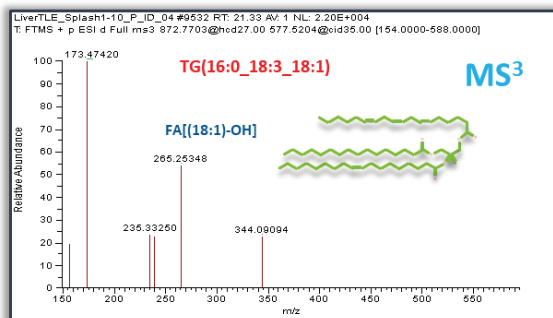
The intelligent Real-Time Library Search acquisition tool on the Orbitrap IQ-X Tribrid mass spectrometer automates MS<sup>n</sup> data acquisition and increases profiling efficiency to help you obtain a higher number of compounds with distinguishable fragmentations to empower deeper analysis.



Vanquish UHPLC System and Orbitrap IQ-X Tribrid MS



MS  
872.77  
MS<sup>2</sup>



MS<sup>2</sup>  
577.52  
MS<sup>3</sup>

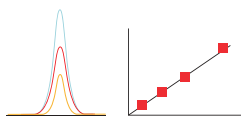
**Software**

**Streamline your path to metabolomics insights**

Thermo Fisher Scientific has invested heavily in developing metabolomics and lipidomics software that lives up to the high standards set by our leading instrumentation, promising the same standards of quality, usability, and data integrity. Now you can have the total package needed to perform increasingly complex analysis and lead the way to high-impact discoveries. Our suite of integrated applications is built to take you quickly from data acquisition to interactive analysis and interpretation of results. Customize your workflow with flexible solutions and simplify analysis of large-scale data.

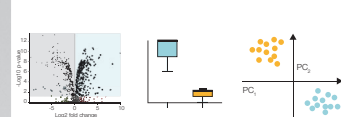
**TraceFinder software**

Rapidly detect targeted knowns for QA/QC, profiling, and absolute quantitation



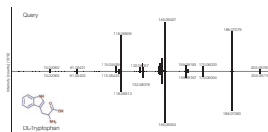
**Compound Discoverer software**

Ultimate toolbox for complete analysis of untargeted metabolomics data



**mzCloud mass spectral library**

MS<sup>n</sup> reference spectra for confident unknown annotation and identification



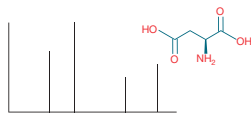
**AcquireX intelligent data acquisition**

Intelligent acquisition for real-time precursor selection



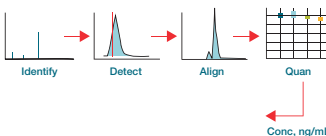
**Thermo Scientific™ mzVault™ library**

Create mass spectral libraries for metabolite annotation and identification



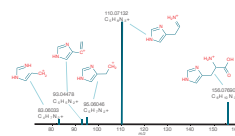
**Thermo Scientific™ LipidSearch™ software**

Lipid-specific untargeted analysis for confident lipid annotation and quantitation



**Thermo Scientific™ Mass Frontier™**

spectral interpretation software  
MS<sup>n</sup> spectral tree searching, interpretation and in-silico fragment ion prediction



Learn more at [thermofisher.com/metabolomics](https://thermofisher.com/metabolomics)