Thermo Fisher SCIENTIFIC

Metabolomics

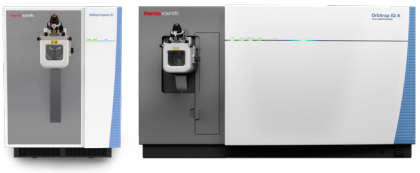
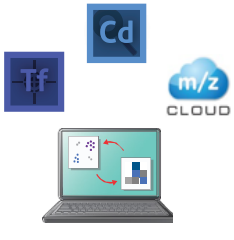
GO BEYOND

Harness the power of metabolomics

Translate your data into valuable discoveries

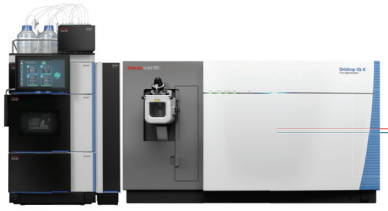
Through collaboration with the scientific community, we've developed metabolomics solutions powered by Thermo Scientific™ Orbitrap™ LC-MS instruments, innovative data analysis software and premier mass spectral databases.

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.

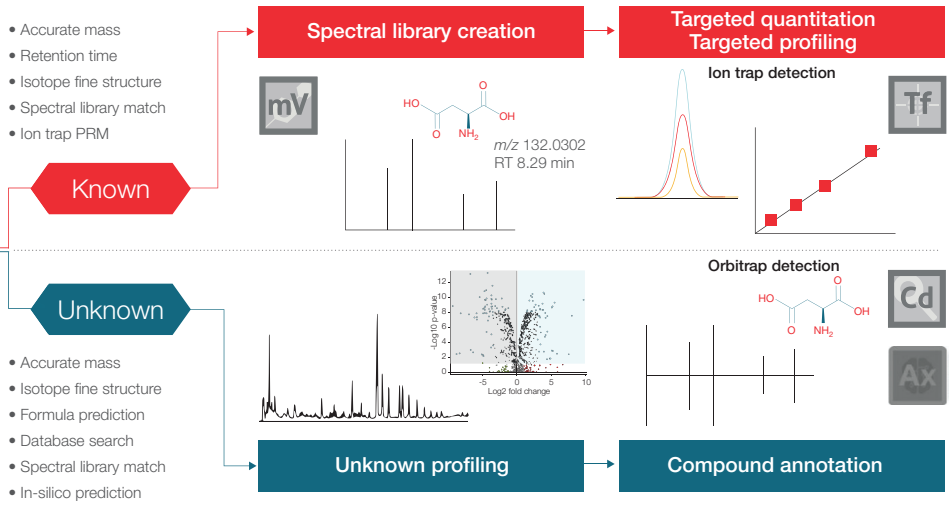
Sample collection and preparation	Chromatographic separations	Mass spectrometry data acquisition	Data processing
			
QA/QC practices for sample preparation	Thermo Scientific™ Vanquish™ Horizon UHPLC system, Thermo Scientific™ Accucore™ C30 HPLC column, Thermo Scientific™ Hypersil GOLD™ C18 Selectivity 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.



Vanquish UHPLC system and Orbitrap IQ-X Tribrid MS

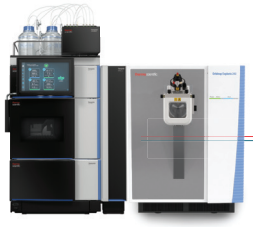


Quantify known metabolites of interest

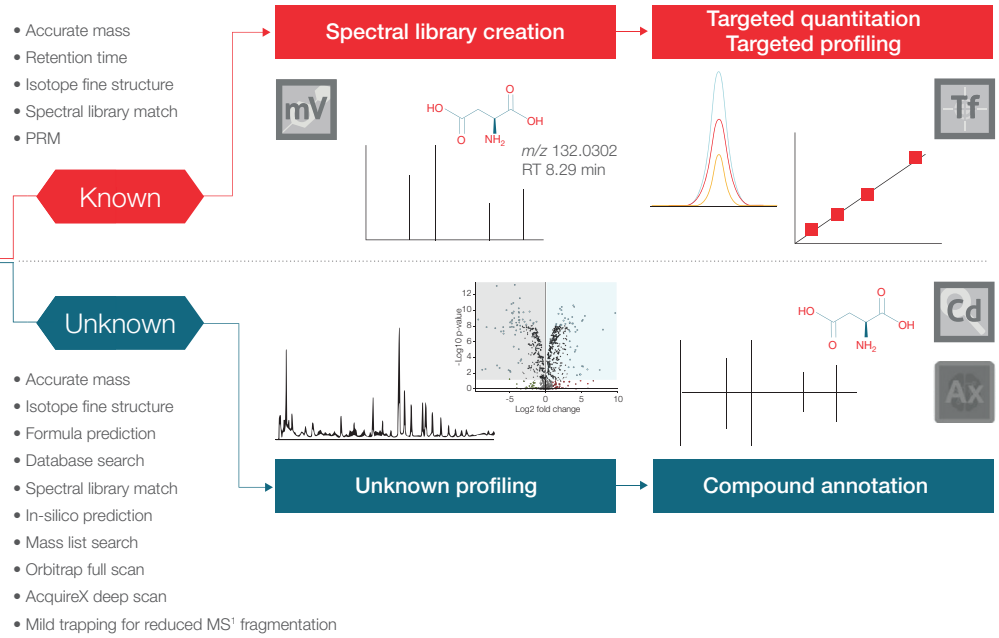
Individual reference standards, with or without stable isotope labels, establish retention time, mass measurement, isotopic fine structure, and MS^2 spectral confirmation against an in-house library for the identification and quantification of target metabolites. When stable isotope labels are used,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

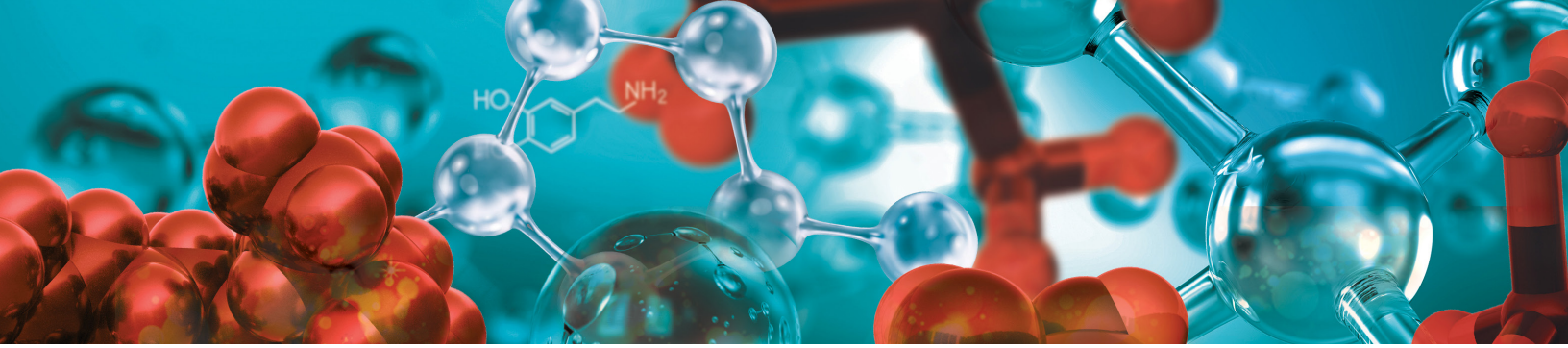
Discover novel metabolic signatures

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 software, 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.



Vanquish UHPLC system and Orbitrap Exploris 240 MS





Go beyond
Harness the power of lipidomics

Comprehensive lipidomics solutions

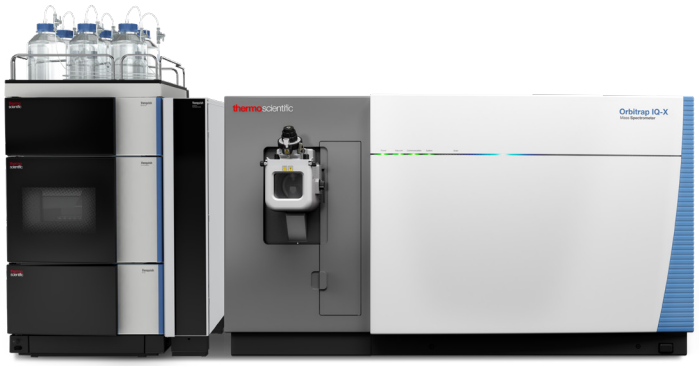
Lipidomics is a field of metabolomics that has evolved into a class all its own and aims to annotate and quantify lipid species to identify biomarkers and elucidate metabolism at the cellular level. Lipid species are diverse and complex, and the development of Thermo Scientific Orbitrap mass spectrometers 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^n and UVPD for structural elucidation

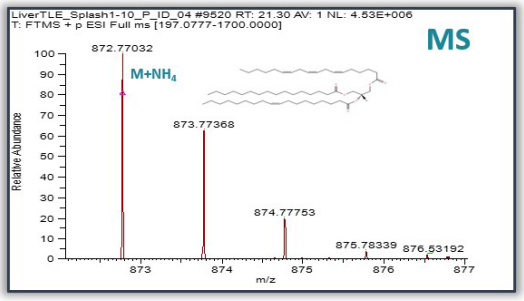
A fundamental issue in lipid identification is that lipids dissociate in a very predictable way to give relatively few product ions, and thus structural details are often incomplete. Obtaining more complete lipid structural information can be addressed in several different ways including MS^n analysis 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.

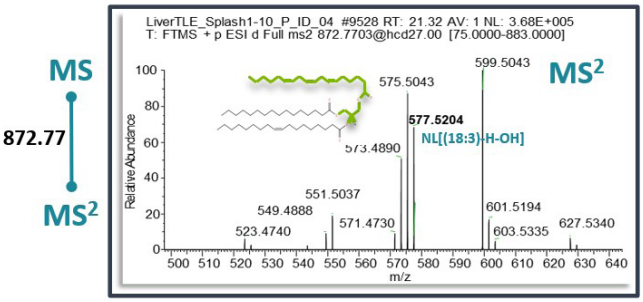


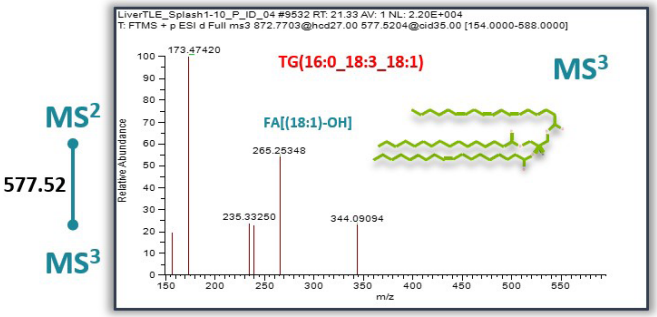
Vanquish UHPLC System and Orbitrap IQ-X Tribrid MS

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^n data acquisition and increases profiling efficiency to help you obtain a higher number of compounds with distinguishable fragmentations to empower deeper analysis.



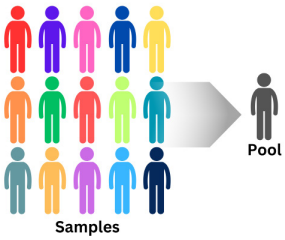


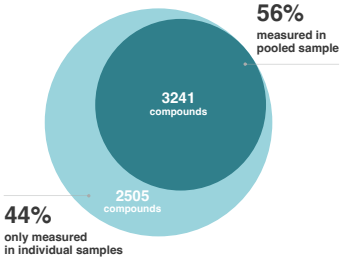


Orbitrap Astral mass spectrometer: New era of metabolomics & lipidomics

Metabolomics and lipidomics

Large-scale metabolomics studies commonly use full scan MS analysis on every sample to emphasize discovery data quality. This approach increases the number of compounds found, improves precision and quantitation. The identity of these compounds is then determined by using a study pool, which contains a small aliquot from each sample, as a surrogate to perform fragmentation analysis. While AcquireX can then be used to provide iterative data dependent fragmentation and gain insight into even the less abundant species in the sample, this data acquisition workflow methodology still relies on a surrogate sample that masks the inherent sample heterogeneity and often omits differentiating compounds from fragmentation due to their dilution during pooling. Typically, one must compromise over high quality MS1 profiling data and comprehensive compound fragmentation





Sample Pooling masks heterogeneity

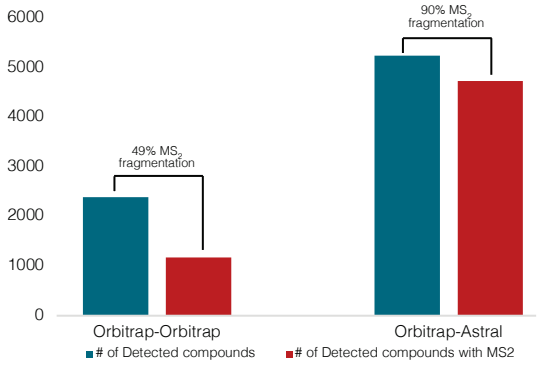
Key Applications

Orbitrap Astral Mass Spectrometer for Metabolomics and Lipidomics

With two high resolution accurate mass detectors run in parallel, the Thermo Scientific™ Orbitrap™ Astral™ mass spectrometer is uniquely poised to yield the complete metabolome in a sample in a single injection. The two HRAM detectors enables accurate and precision quantitation with MS1 scan but also unknown compound identification confidence with MS2 spectra.

When used in a SQUAD analysis, researchers can yield accurate and precision quantitation via Orbitrap full scan with near complete compound fragmentation simultaneously and in a single injection.

While intelligent DDA and rolling exclusion lists have been extremely helpful for common metabolites, the approach presents challenges for rare chemicals that only occur in a subset of samples. The capability to generate MS/MS data for nearly all compounds in a single, short run on an Orbitrap Astral MS is a huge step forward in metabolomics. It will be particularly important for characterizing exposure chemicals, such as drugs and certain food components

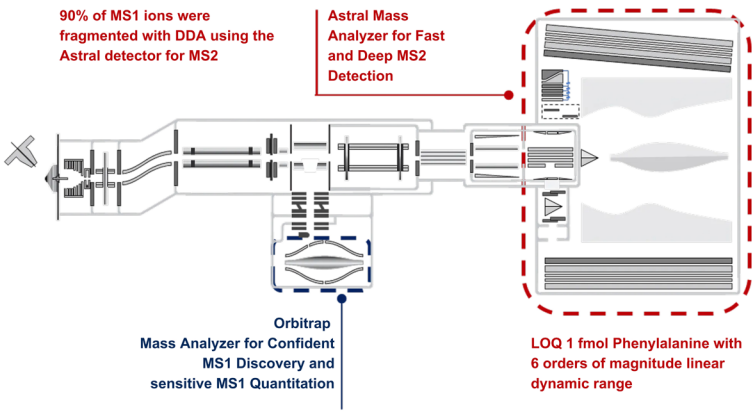


The percentage of compound fragmentation in data-dependent MS2 analysis (DDA) on Orbitrap Astral (Orbitrap-Astral) mass spectrometer and traditional DDA on Orbitrap mass analyzer only (Orbitrap-Orbitrap). The presented data represent plasma metabolites analyzed using a reversed-phase 15 min LC method.

SQUAD Analysis: the complete picture in one experiment on every sample!

Liquid chromatography-ultra-high resolution mass spectrometry (LC-UHRMS)

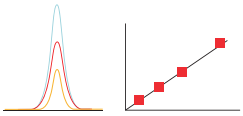
Vanquish HPLC system and Orbitrap Astral Mass Spectrometer



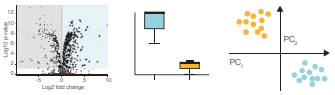
Streamline your path to metabolomics insights

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.

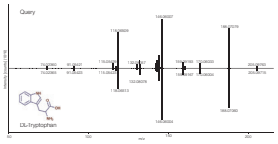
Thermo Scientific™ TraceFinder™ software
Rapidly detect targeted knowns for QA/QC, profiling, and absolute quantitation



Thermo Scientific™ Compound Discoverer™ software
Ultimate toolbox for complete analysis of untargeted metabolomics data

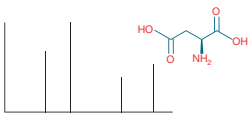


Thermo Scientific™ mzCloud™ mass spectral library
MS^n reference spectra for confident unknown annotation and identification

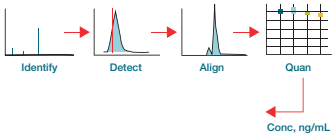


Thermo Scientific™ AcquireX™ intelligent data acquisition
intelligent acquisition for real-time precursor selection

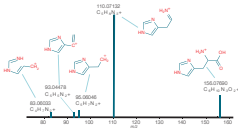
Thermo Scientific™ mzVault™ library
Create mass spectral libraries for metabolite annotation and identification



Thermo Scientific™ LipidSearch™ software
Lipid-specific untargeted analysis for confident lipid annotation and quantitation



Thermo Scientific™ Mass Frontier™ spectral interpretation software
MS^n spectral tree searching, interpretation and in-silico fragment ion prediction



Learn more at **thermofisher.com/metabolomics**