



Powerful isotopic insights, elevated

Next-generation workflows for isotope ratio analysis

Orbitrap Isora Mass Spectrometers



thermo scientific

Advance isotope ratio analysis to the molecular level

Isotope ratios reveal origin, transformation, and formation mechanisms of compounds. They are central to research in geochemistry, environmental science, metabolism, food authenticity, and beyond.

IRMS analysis based on Thermo Scientific™ Orbitrap™ technology extends these insights by adding molecular context. By combining high-resolution accurate mass (HRAM) detection with electrospray ionization, structural information is preserved while obtaining isotope and isotopologue ratios directly from intact molecular ions.

Thermo Scientific™ Orbitrap™ Isora™ Mass Spectrometer (MS) and Orbitrap™ Isora™ Pro Mass Spectrometer (MS)—together with the Thermo Scientific™ Vanquish™ Duo UHPLC System and Thermo Scientific™ Isotope Discoverer™ Software—offer a fully integrated solution for isotope ratio analysis and data processing.

The result is a more comprehensive view of isotopic composition—connecting isotope ratios with molecular structure and enabling deeper analytical insights:



Measurement of isotope ratios of individual analytes at natural abundance and low-level isotopic enrichment



Position-specific isotope analysis (PSIA) through controlled fragmentation



Investigation of multiply substituted (clumped) isotopes



From acquisition to isotope ratios, streamlined

Orbitrap Isora MS transforms advanced isotope science into a streamlined, reproducible workflow—ready for today's research challenges and tomorrow's discoveries.



1

Vanquish Duo UHPLC System

for sample introduction and
fast sample/reference
measurement setup



2

Orbitrap Isora MS

with dedicated software for
acquisition strategies designed
for isotope ratio experiments



3

Isotope Discoverer Software

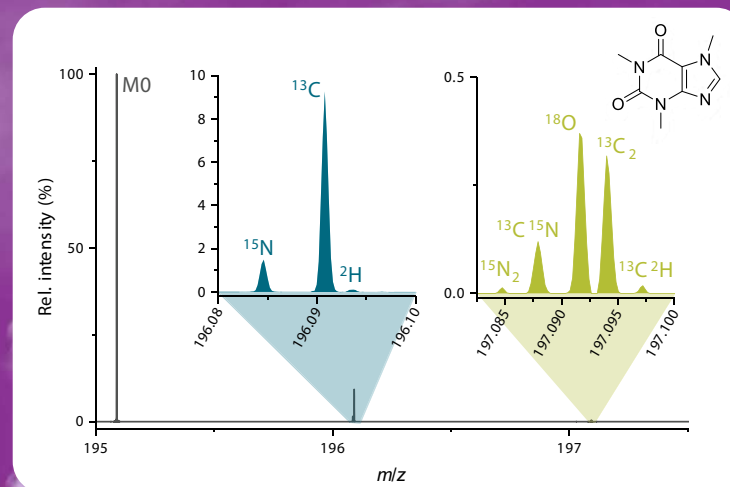
for integrated isotope ratio
data processing and
visualization in a single
environment

Multi-isotopic profiles in a single run

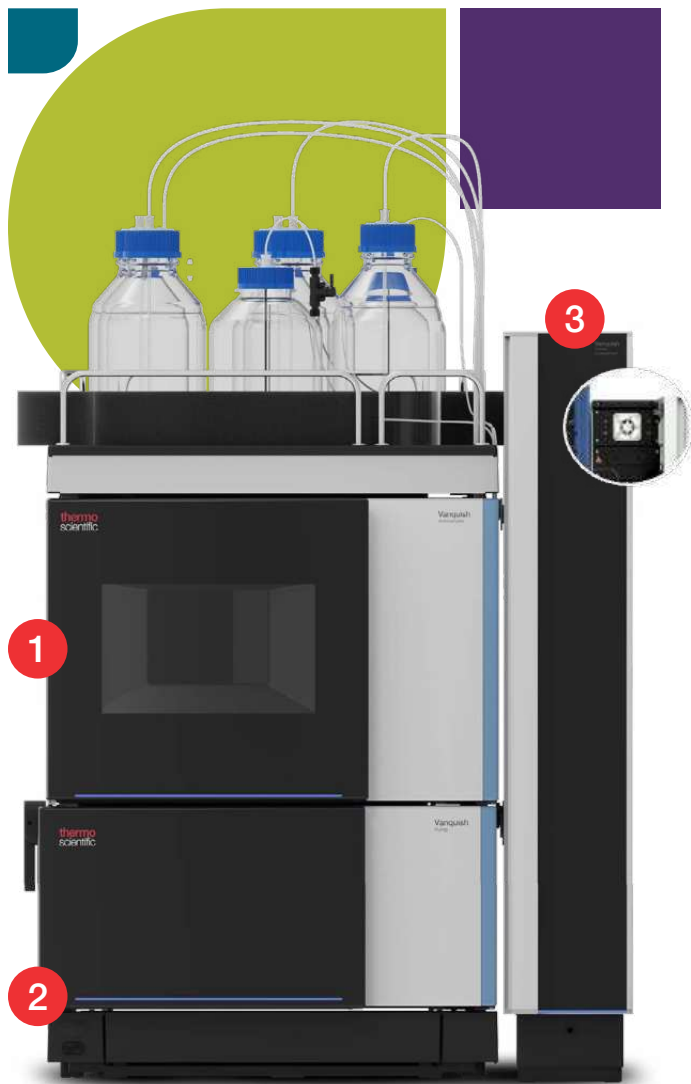
Using electrospray ionization, polar compounds are introduced directly from solution. Molecular integrity is preserved, allowing isotope ratios to be evaluated in their structural context.

High resolving power enables clear separation of closely spaced isotopic species, including low-abundance substitutions. Optimized experiment setups and integrated data evaluation enable the collection of high-quality isotope ratio information.

The result is isotope ratio analysis with expanded analytical depth—combining isotopologue resolution with molecular specificity.

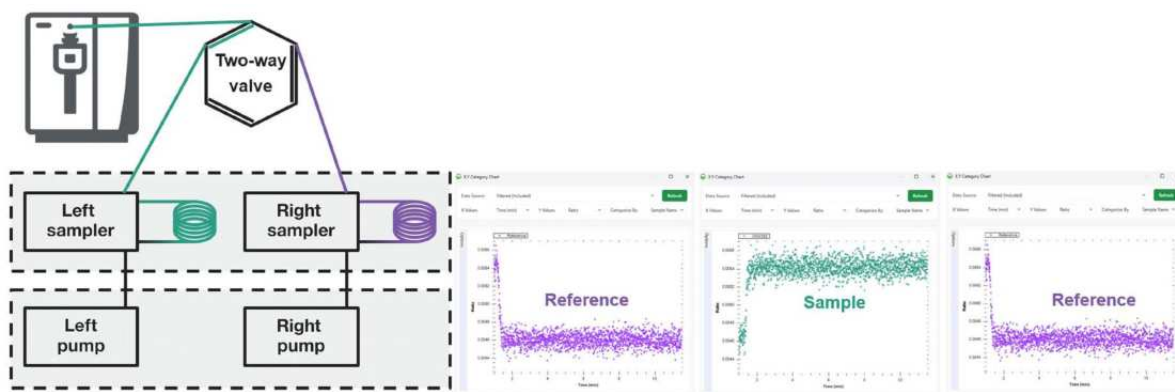


Configured for accuracy in isotope ratio analysis



Reliable isotope ratio analysis depends on comparing unknown samples to reference materials. Consistent sample/reference bracketing is essential for accurate results. The Vanquish Duo UHPLC System is configured to support these workflows using a dual pump and dual split sampler. The result is:

- ✓ Automated alternating sample/reference injections
- ✓ Consistent and reproducible measurement conditions
- ✓ Efficient high-throughput operation



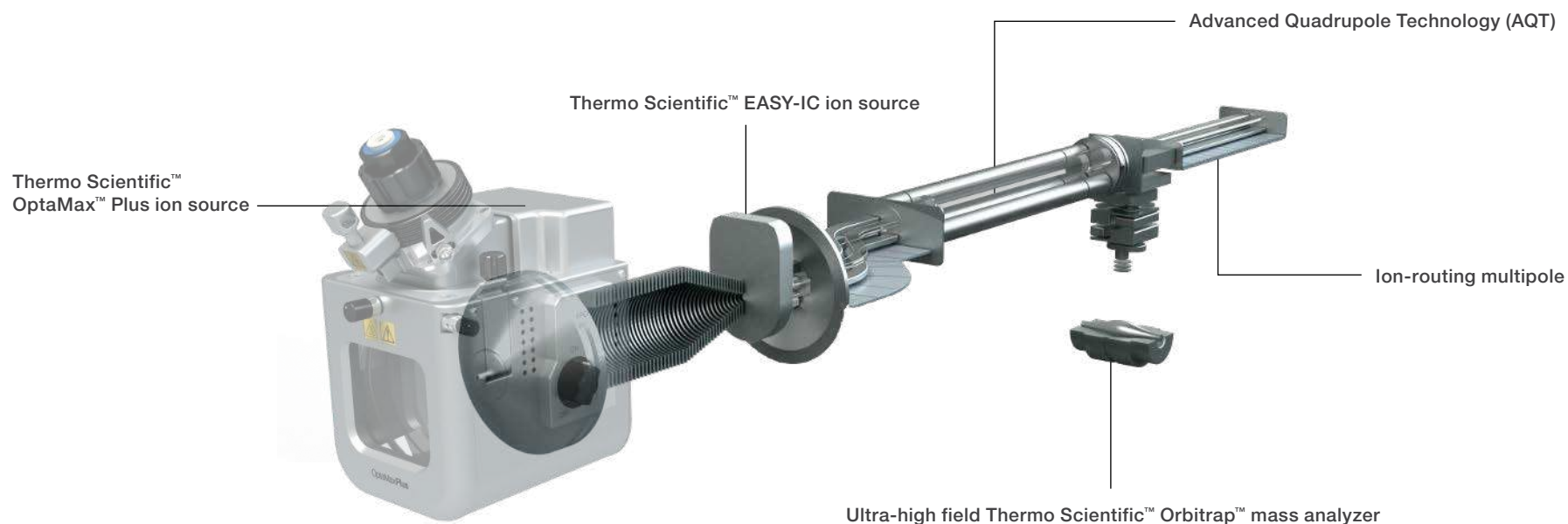
- 1 Thermo Scientific™ Vanquish™ Dual Split Sampler** holds two independently controlled injection units, including separate injection valves and injection needles.
- 2 Thermo Scientific™ Vanquish™ Dual Pump** merges two individual mixing pumps in one housing, enabling separate eluents and gradients for each pump. Operating across a wide flow range, from 1 $\mu\text{L}/\text{min}$ to 8 mL/min , they support isotope workflows at low flow rates as well as sample characterization at higher flow rates—with the flexibility to switch seamlessly between both.
- 3 Thermo Scientific™ Vanquish™ Column Compartment** helps ensure reliable matching of the eluent and column temperature for superior UHPLC performance and the flexibility to meet all your analytical needs for UHPLC applications. The column compartment also integrates the valve for sample/reference injections.

Confidence in isotopic data by HRAM detection

Orbitrap Isora MS combines improved sensitivity, extended dynamic range, and exceptional mass accuracy with HRAM detection for comprehensive isotope ratio analysis. HRAM enables clear differentiation of isotopologues—including minor and multiply substituted species—while reducing interferences from complex matrices, supporting high-quality and reliable isotope data.

Resulting capabilities:

- ✓ Preserve intramolecular isotopic information
- ✓ Measure multiple isotopologues in a single run
- ✓ Detect low-abundance isotopologues with high sensitivity
- ✓ Reduce interferences through selective scan ranges
- ✓ Enable PSIA through controlled fragmentation



A dedicated toolbox for isotope method development

Orbitrap Isora MS control software provides a structured environment for developing and optimizing isotope ratio methods, combining visualization, tuning, and predefined workflows for efficient setup and consistent performance.



Visualize isotope data—isotope ratio and shot noise plots deliver direct insight into isotopologue signals, highlighting ion statistics and signal stability for confident evaluation of precision



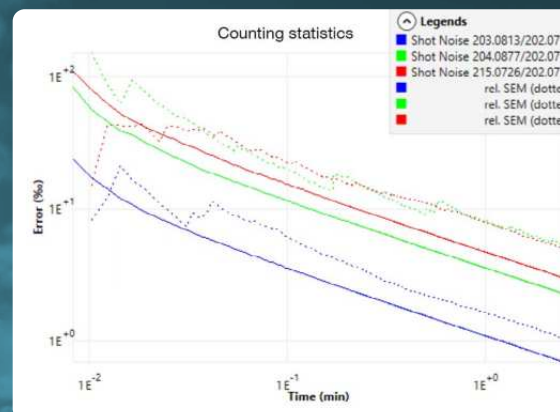
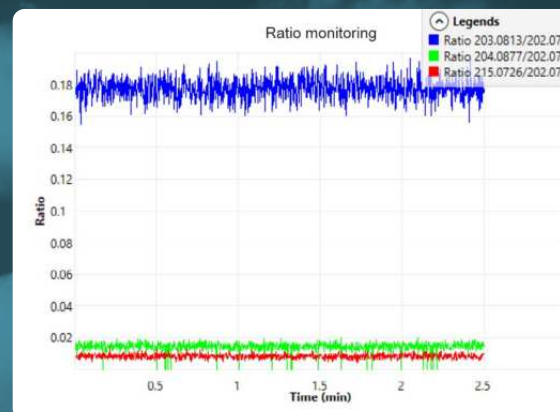
Optimize across dynamic range—Automatic Gain Control (AGC) and resolution scanning, combined with increased microscans, enable balanced performance across low- and high-intensity ions



Enable precise acquisition—dedicated trapping modes and integrated calibration procedures help ensure consistent, reproducible isotope measurements



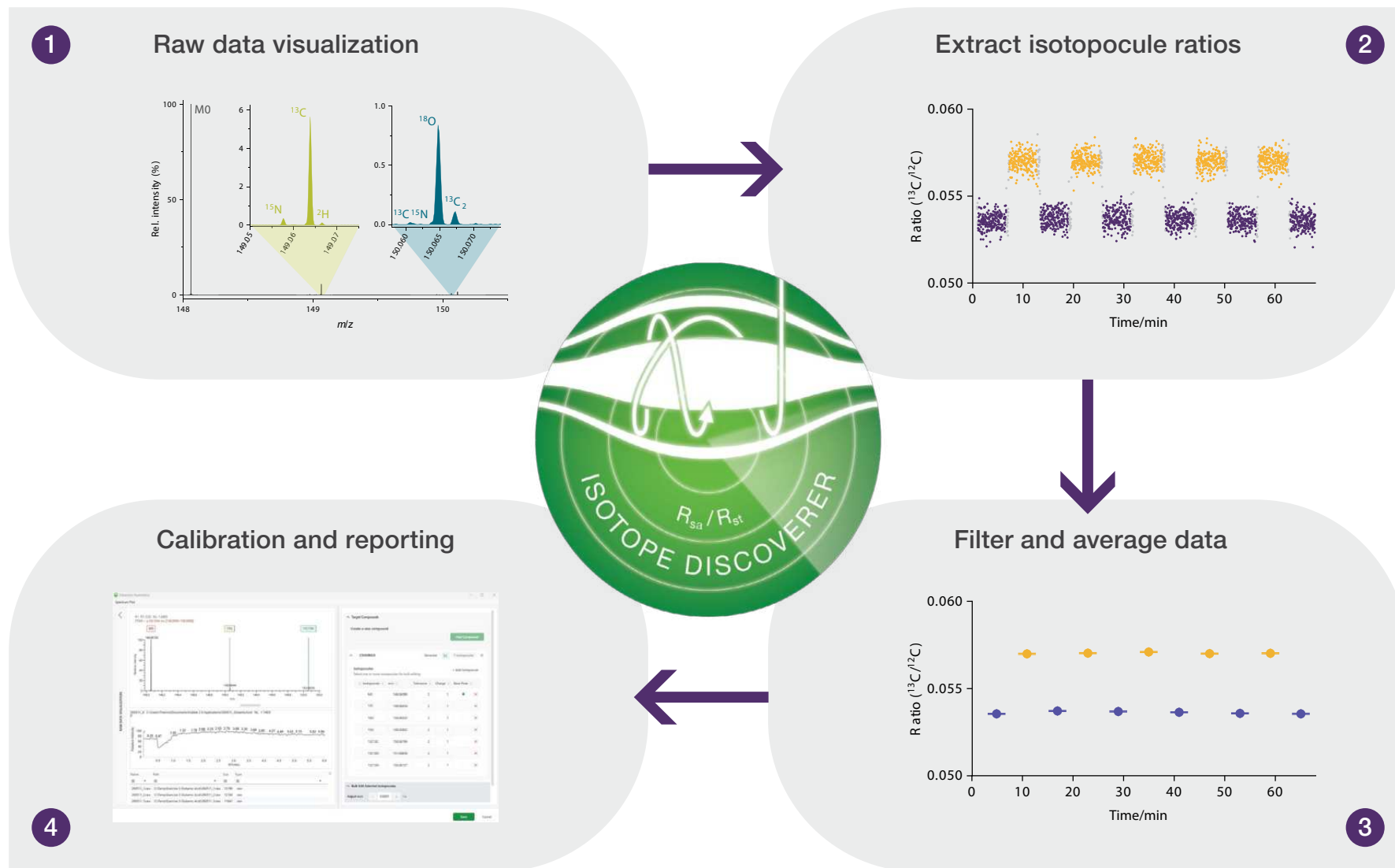
Simplify method setup—application-specific templates and structured workflows reduce complexity and support reproducible method implementation



Dedicated software for integrated isotope data processing

Orbitrap Isora MS delivers high-resolution isotope measurements with exceptional precision. Isotope Discoverer Software completes the solution by providing a dedicated platform for structured, efficient isotope data processing.

Designed specifically for isotope ratio analysis, Isotope Discoverer Software integrates isotope ratio extraction, filtering, summarization, data correction, and data calibration into one streamlined environment—enabling laboratories to process data faster, evaluate results more clearly, and report with greater confidence.



Transform Orbitrap IRMS data into reliable results

Integrated processing

From raw spectra to calibrated delta values within a single structured workflow.

- Unified data evaluation environment
- Reduced manual processing steps
- Faster turnaround from acquisition to result

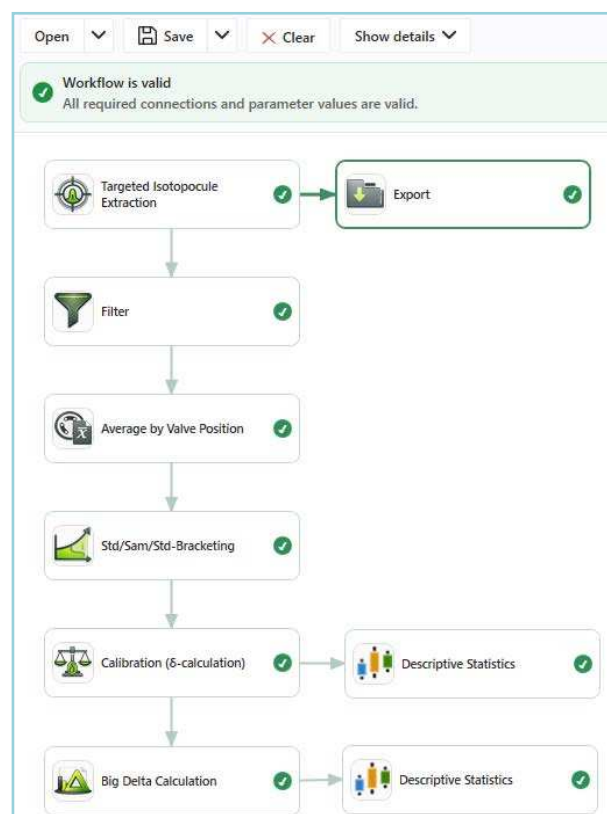
Flexible workflow configuration

Supports diverse isotope workflows and laboratory setups.

- Adaptable to sample introduction methods such as dual split sampler, dual syringe inlet, or in-flow injection
- Ability to calculate delta values from large datasets across multiple files
- Configurable processing steps for different isotope systems
- Valve- and metadata-based data annotation

Transparent and traceable results

- Full visibility into every stage of data evaluation
- Access to intermediate and final results
- Reproducible calibration workflows
- Simplified troubleshooting and quality control



Designed for confidence in isotope ratio data

Isotope ratios at natural abundance often differ by very small amounts, and detecting these subtle variations requires high precision. Orbitrap Isora MS enables high-precision isotope ratio measurements by combining HRAM detection with controlled acquisition strategies.



Extended signal acquisition

Isotopologue signals are measured over defined time windows—typically 8–10 min—supporting robust isotope ratio determination.



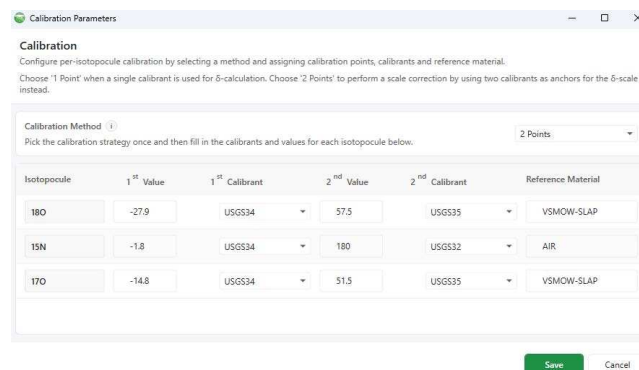
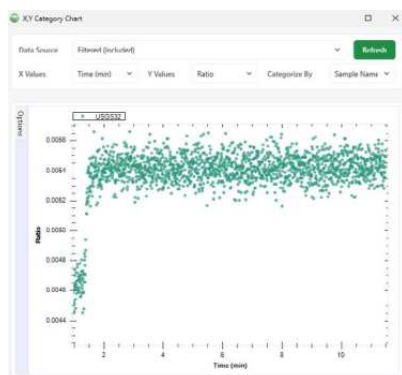
Sample/reference bracketing

Automated alternating measurements of samples and reference material helps ensure accurate ratio determination.

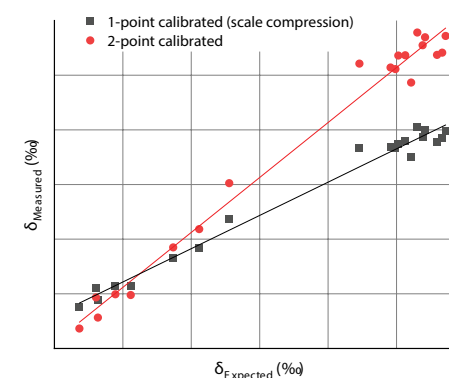


Two-point calibration

Isotope Discoverer Software enables seamless application of two-point calibration across datasets for consistent, reproducible, and comparable isotope ratios.

A screenshot of the 'Calibration Parameters' window in Isotope Discoverer Software. It shows the '2 Points' calibration method selected. The table below lists the calibration points for three isotopocules: 18O, 15N, and 17O. Each row includes the 1st and 2nd values, the corresponding calibrants (USGS34, USGS35, and USGS32), and the reference material (VSMOW-SLAP and AIR).

Isotopocule	1 st Value	1 st Calibrant	2 nd Value	2 nd Calibrant	Reference Material
18O	-27.9	USGS34	57.5	USGS35	VSMOW-SLAP
15N	-1.8	USGS34	180	USGS32	AIR
17O	-14.8	USGS34	51.5	USGS35	VSMOW-SLAP

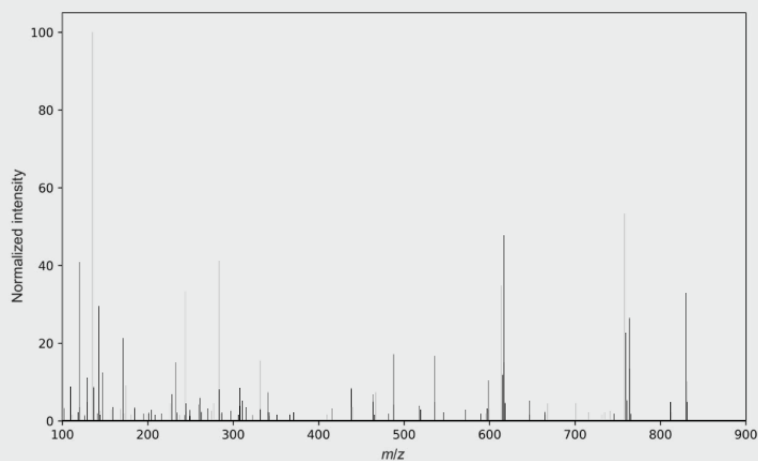


Two analytical dimensions. One platform.

Orbitrap Isora MS integrates isotope ratio workflows into a high-resolution Orbitrap MS environment. Perform classical MS analysis and isotope-focused experiments on the same technological platform, connecting molecular information with isotopic information—within a single analytical system.

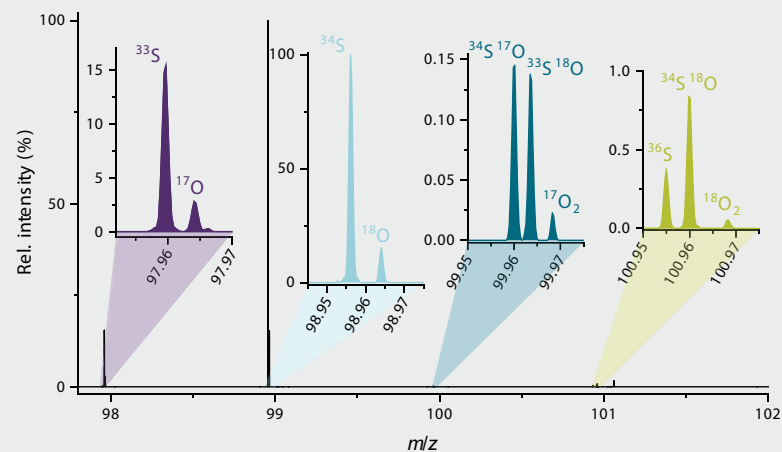
Dimension one

Access detection and quantification of compounds by high-resolution mass spectrometry.



Dimension two

Extract isotopologue information from mass spectra and calculate the isotope ratios.



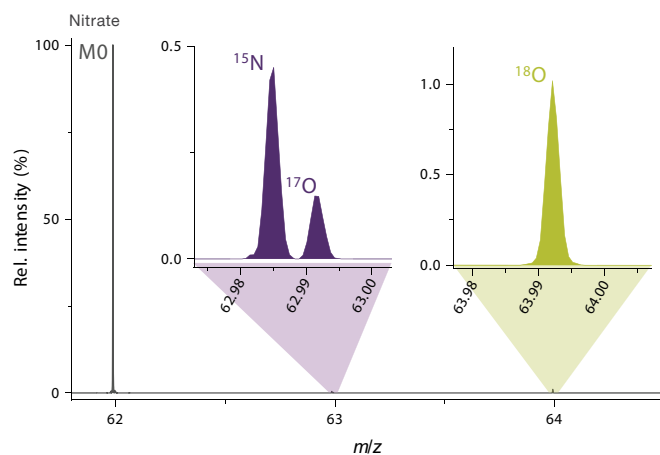
Expanding the scope of isotope research

Orbitrap Isora MS enables isotope ratio analysis across a broad range of applications—from environmental and geochemical studies to metabolism research and food authenticity. By combining molecular-level information with isotope ratios, new analytical questions can be addressed with greater depth and specificity.



Biogeochemistry research

Investigation of biogeochemical cycles using multiple isotopologues of CNSOH bearing species, e.g., in nitrate, sulfate, phosphate, acetate, and a wide range of common organic compounds and biomarkers.

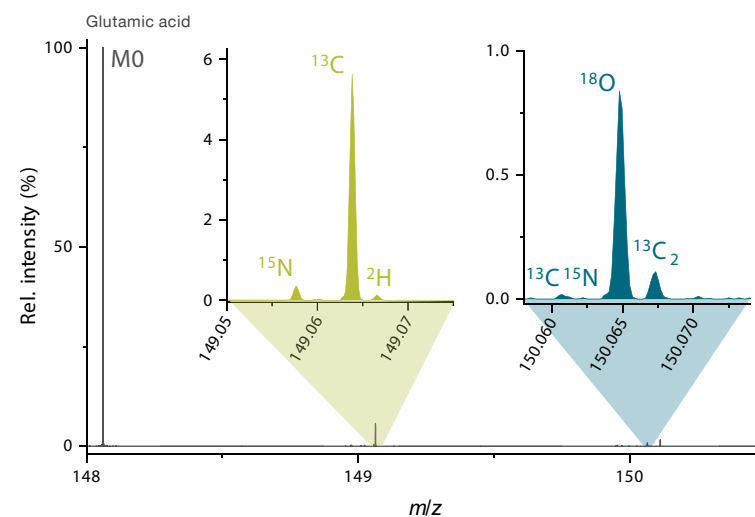


Instrument	Material	Ratio	Expected value (‰)	Measured value (‰)	Precision (SD)	Number of injections
Orbitrap Isora MS	Nitrate, USGS35	$\delta^{15}\text{N}$	2.7	3.5	0.3	5
	Nitrate, USGS32	$\delta^{18}\text{O}$	25.7	25.0	0.5	5
	Nitrate, USGS32	$\delta^{17}\text{O}$	13.2	14.0	0.8	5



Metabolism and physiology studies

Deconvolution of complex metabolic pathways by tracing metabolite transformations using, e.g., amino acids.



Instrument	Material	Ratio	Expected value (‰)	Measured value (‰)	Precision (SD)	Number of injections
Orbitrap Isora MS	Glutamic acid, USGS41	$\delta^{13}\text{C}$	36.6	35.4	0.6	5
		$\delta^{15}\text{N}$	49.5	49.1	1.8	5
		$\delta^2\text{H}$	—	1.1	3.1	5

Deepen your insights with PSIA

PSIA reveals how isotopes are distributed within individual molecular positions—providing insight into formation pathways, reaction mechanisms, and origin.

Using controlled fragmentation, Orbitrap Isora MS enables the measurement of isotope ratios from specific functional groups and molecular fragments, complementing whole-molecule analysis. This approach allows:



Identification of site-specific enrichment or depletion



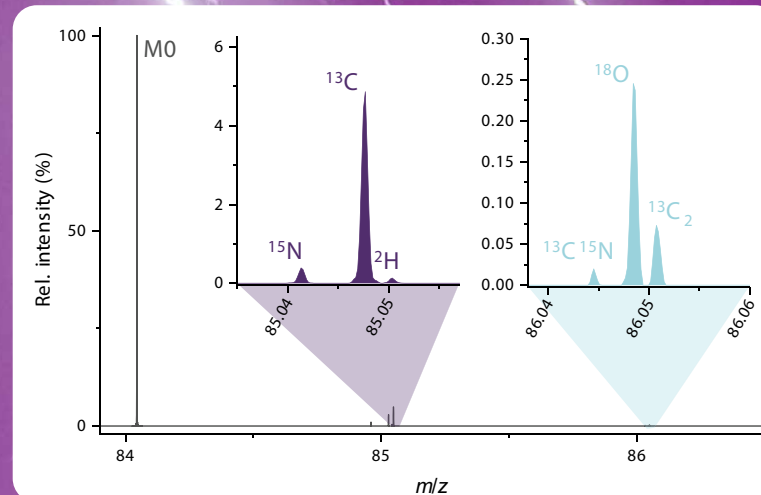
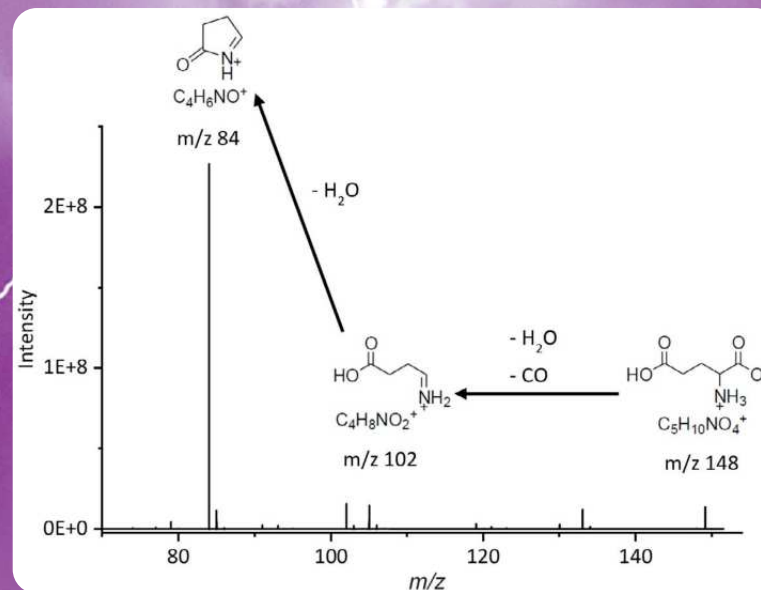
Detection of non-stochastic isotope distributions



Development of new isotopic proxies

Material	Structural information	$\delta^{13}\text{C}$ (‰)	Precision (SD)	Number of injections	Propagated error for C1 position
Glutamic acid, USGS41	Full molecule	35.4	0.6	5	—
	Immonium ion fragment	-24.3	1.1	5	—
	C1 position	274.5*	—	—	2.3

*Calculated from the measured $\delta^{13}\text{C}$ values of the full molecule and the immonium ion fragment.

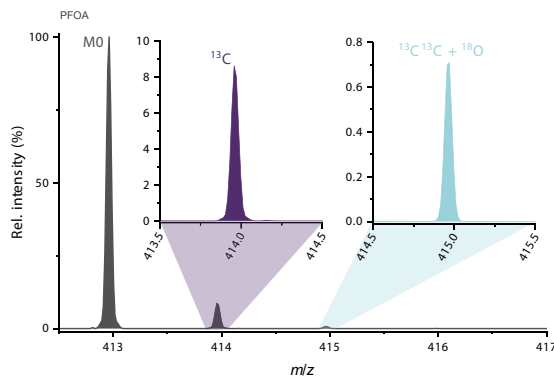


Expanding the scope of isotope research



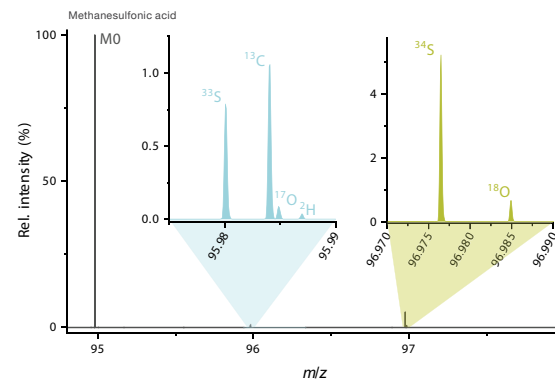
Environmental research

Using stable isotopic analysis, it is possible to trace the sources of pollution and track environmental change across space and time, e.g., identifying the sources and pathways of PFAS.



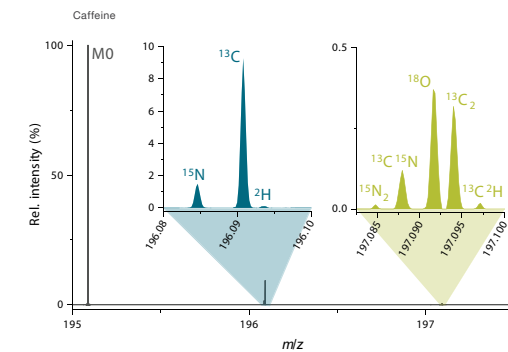
Geology, climatology, and archaeology

Study of redox states in the geological past, e.g., different oxygen reservoirs in geological records, presence of microbial activity, atmospheric conditions, and atmosphere hydrosphere interactions.



Food authenticity

Verification of food and beverage authenticity using multi-element isotope ratio analysis and PSIA, e.g., to distinguish between synthetic and natural flavors and ingredients, such as caffeine.





To reduce carbon footprint and overall maintenance, Orbitrap Isora MS and Orbitrap Isora Pro MS come standard with a single rough dry pump instead of two oil pumps.



Dry pump = no oil

Orbitrap Isora MS	Orbitrap Isora Pro MS
Equal sensitivity	
Equal mass accuracy	
Equal linear dynamic range	
Equal intra-scan dynamic range with eDR scan	
Same mass range m/z 40–6,000	
Scan rate up to 40 Hz	Scan rate up to 70 Hz
240K maximum resolution	480K maximum resolution
Entry-level model for molecular characterization and isotopic analysis of small molecules	For advanced molecular characterization and isotopic analysis of small molecules
Operation mode: Isotope ratio, small molecule	Operations mode: Isotope ratio, small molecule, peptide
	Thermo Scientific™ TMTpro™ 35-plex
	Bent trap pre-accumulation
	Hybrid-DIA with adaptive RT routine



Vanquish Duo UHPLC System

Designed with sustainability in mind—portfolio certified with the My Green Lab™ ACT™ Ecolabel 2.0 and polyvinyl chloride/polystyrene-free secondary and tertiary packaging.

Support and service, simplified

Choosing Orbitrap Isora MS or Orbitrap Isora Pro MS means more than just acquiring advanced technology; it means partnering with Thermo Fisher Scientific, a leader in scientific innovation and support. Our Unity™ Lab Services team delivers world-class service solutions to support your instruments. Our comprehensive service portfolio includes instrument service plans, on-demand services (compliance, maintenance, and installation), and education support. Services Central allows you to easily request, manage, and view services via a centralized online platform. You can also check service plan or warranty coverage, access manuals, and more.



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