

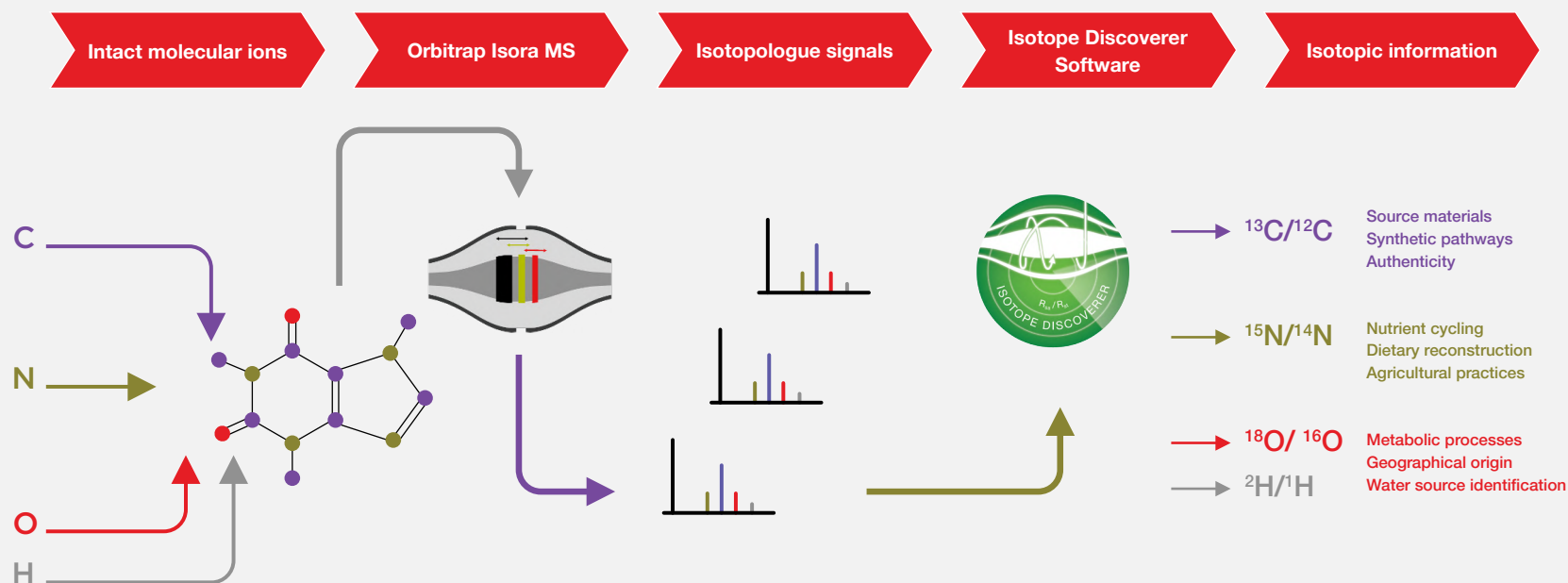
Isotope Discoverer Software
Streamline your isotope data processing

Reveal the story behind your samples using isotope ratios

Natural abundance isotope ratio measurements provide powerful insight into origin, transformation, and underlying processes in compounds across a wide range of applications. High-resolution analysis with Thermo Scientific™ Orbitrap™ Isora™ Mass Spectrometer (MS), combined with Thermo Scientific™ Vanquish™ Duo UHPLC Systems for sample/reference introduction, generates rich, information-dense datasets, capturing isotopologue distributions with exceptional detail. **Thermo Scientific™ Isotope Discoverer™ Software enables efficient and structured evaluation of isotope ratio data, translating complex datasets into reliable results.**

Built for isotope data processing

- Streamlined data evaluation for greater efficiency and ease of use
- Adaptable workflows to support diverse isotope applications
- Structured processing from raw spectra to calibrated delta values
- Visibility into data at each step of analysis



Transform Orbitrap IRMS data into reliable results

Isotope Discoverer Software provides structured, efficient isotope data processing for high-resolution measurements generated by Thermo Scientific™ Orbitrap™ technology. The software supports data analysis of multiple compounds and multiple isotopes within a single acquisition, enabling comprehensive evaluation of complex datasets.



Integrated, end-to-end isotope data processing—combine isotope ratio extraction, filtering, summarization, data correction, and calibration within a single structured workflow, transforming raw spectra into calibrated delta values while reducing manual steps and accelerating time to result.



Flexible workflow configuration—support diverse isotope workflows and laboratory setups with configurable processing steps, valve- and metadata-based data annotation, and compatibility with sample introduction techniques such as direct infusion, in-flow injection, and dual inlet. Reusable workflow templates enable consistent processing and simplify routine analysis across large datasets and multiple files.



Transparent and traceable data evaluation—access intermediate and final results at every stage of processing, helping ensure reproducible calibration workflows, simplified troubleshooting, and confidence in isotope ratio results.



Interactive data exploration and reporting—visualize isotope data through customizable plots and export results at any stage for reporting, further analysis, and documentation.

Data quality at a glance

Isotope Discoverer Software is a study-based application in which all data processing and evaluation is performed within a structured study environment. Raw data, processing results, and derived isotope ratio outputs are automatically organized and stored, enabling traceability, reproducibility, and efficient data management. Integrated visualization tools support method development and data quality assessment.

By combining structured data management with interactive visualization, Isotope Discoverer Software simplifies data evaluation and supports confident analysis of isotope results.

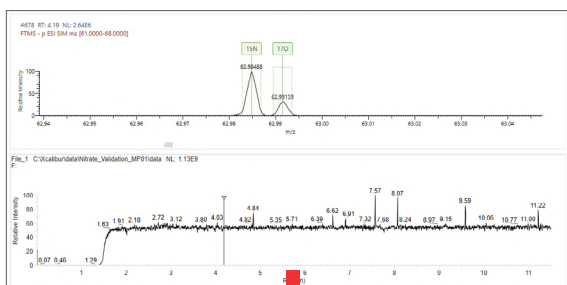


Integrated, end-to-end isotope data analysis

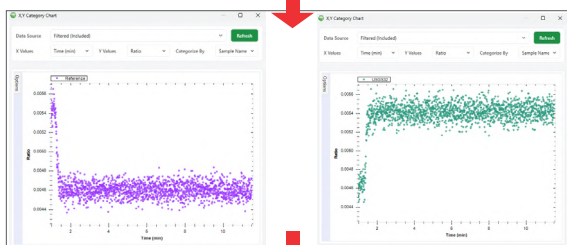
Isotope Discoverer Software provides an integrated approach to isotope data processing, transforming large, information-rich datasets into reliable and consistent isotope ratio results. This structured, end-to-end processing reduces data complexity and enables efficient extraction of meaningful isotopic information from high-resolution measurements.

“ Isotope Discoverer Software is a significant step forward in our ability to process the rich datasets generated by Orbitrap IRMS. Especially in bioscience research, where large numbers of sample replicates are required, automated workflows remove a major data processing bottleneck and accelerate discovery science. ”

-Professor Douglas Morrison,
SUERC, University of Glasgow



Long acquisition sequences generate thousands of high-resolution mass spectra, resulting in large, information-rich datasets that capture isotopologue signals across the duration of the experiment.



A key aspect of isotope ratio analysis is the comparison of sample and reference measurements to help ensure data accuracy. Isotope Discoverer Software assigns data to sample and reference, enabling accurate calculation of isotope ratios and subsequent calibration.



Isotope Discoverer Software integrates summarization, correction, and calibration into a unified workflow, delivering reproducible and traceable δ values as the final result.

Flexible workflow configuration

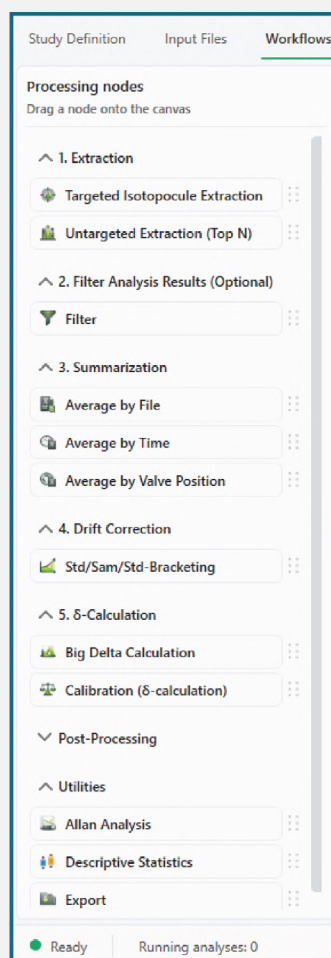
Isotope Discoverer Software enables configuration of data processing workflows for different sample introduction techniques and analytical objectives. Workflows can be defined for a variety of sample introduction techniques, including direct infusion, in-flow injection, and dual inlet, or to assist optimization and method development. Reusable workflow templates provide predefined configurations for common applications, while customizable workflows allow adaptation to specific isotope systems and measurement strategies, supporting consistent and reproducible data processing.

Workflows are built from processing nodes organized into six key steps:

- Extraction
- Filtering
- Analysis results
- Summarization
- Drift correction
- δ and Δ calculation

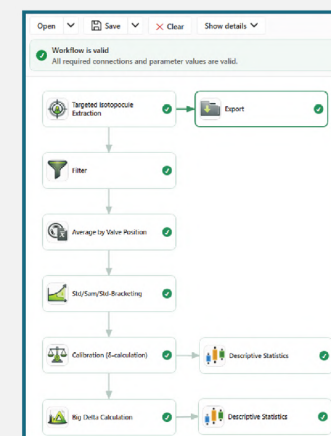
Users can assemble workflows using a drag-and-drop approach, selecting and connecting nodes to define the data processing sequence.

Built-in validation checks verify workflow completeness and parameter consistency before execution, helping ensure correct setup and reducing the risk of processing errors.



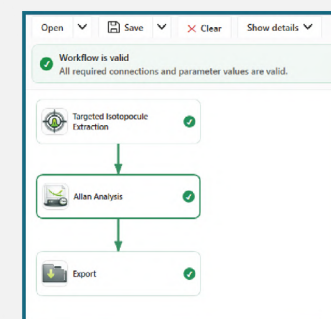
Data processing workflows

(Vanquish Duo UHPLC System setup example)



Optimization and method development workflows

(Allan variance analysis example)



Tailor isotope data processing to your experiments



Define which isotope signals are extracted from raw data

Extract isotope information directly from raw scans by selecting specific masses for the target compound. The list of target compounds and isotopologues can be custom created and modified by the user or automatically generated based on the chemical composition of a compound. This targeted approach focuses the analysis on relevant signals and reduces data complexity.

Assign scans to sample and reference measurements

Assign scans to sample and reference data based on acquisition conditions. For valve-based systems, valve positions are automatically read from raw files to distinguish sample from reference infusions. Alternative grouping methods support different sample introduction techniques, helping ensure correct pairing for downstream data processing.

Generate calibrated isotope ratio results

Convert isotope ratios into δ values using single- or two-point calibration. Calibration can be performed against defined reference materials, helping ensure results are reported on internationally recognized isotope scales. This step translates processed data into final isotope results ready for interpretation.

Interactive data exploration

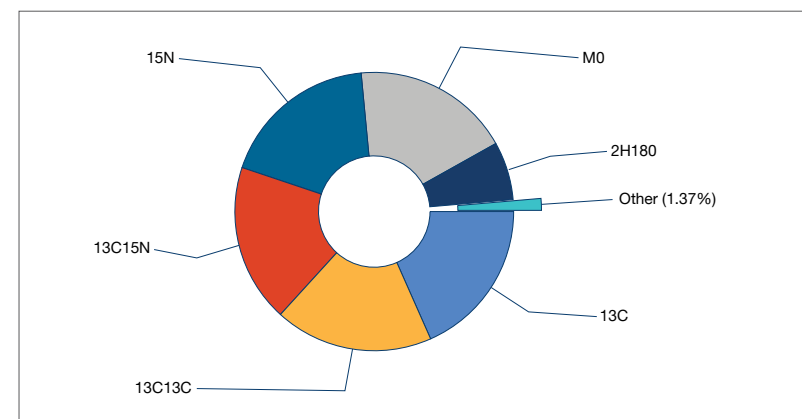
Inspect and compare your data

Isotope Discoverer Software enables interactive exploration of processed data to assess data quality and support scientific interpretation. Each processing step is represented as a separate node, with corresponding results stored and accessible throughout the analysis. This structure allows users to inspect how data evolves from extraction to final results, providing transparency and traceability.

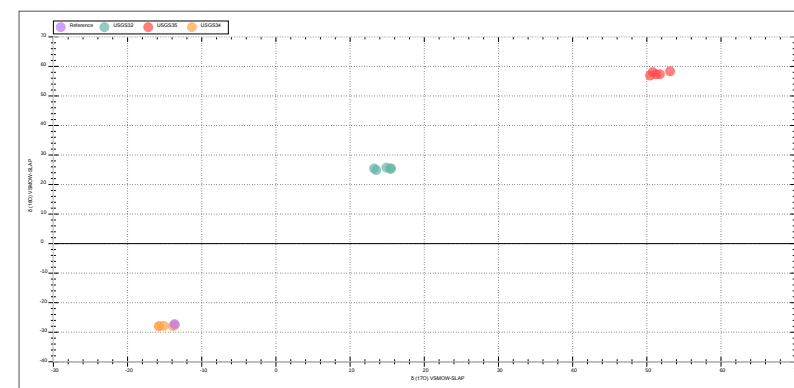
Results can be visualized at different processing stages, including extracted, filtered, drift-corrected, summarized, and calibrated data. Users can plot parameters flexibly and select from multiple chart types, such as scatter plots, histograms, bar charts, and pie charts, to compare isotope ratios, delta values, and metadata.

Interactive visualization also supports troubleshooting. Time-resolved signal plots, such as TIC traces, allow comparison of sample and reference data to reveal mixing effects or signal carryover, enabling refinement of analytical methods and experimental setup.

Assess data quality by visualizing multiple extraction results and isotopologue occurrences across the dataset.

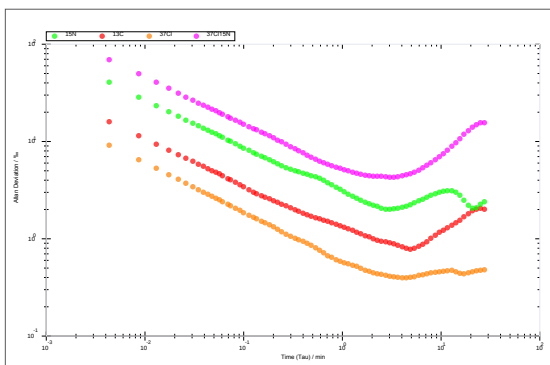


Compare isotope ratios, δ values, and metadata across samples using flexible x-y parameter selection and multiple chart types.



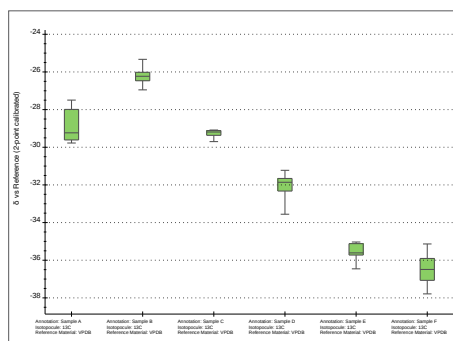
Advanced tools for method development and customization

Isotope Discoverer Software includes advanced features for method development, statistical evaluation, and customized data processing. These tools extend standard workflows and enable users to refine analytical methods, assess data quality, and adapt processing to specific research needs.



Optimize measurement precision

Evaluate signal stability over time using Allan variance analysis. The evaluation identifies the optimal acquisition length required to achieve target isotopic data precision, enabling efficient method development.



Summarize and assess data

Utilize statistical tools to summarize individual parameters from processed data, calculate statistical error, and visualize distributions.

This figure is a screenshot of the 'Node Parameters' dialog box for a 'Scripting Node'. The dialog box contains several sections: 'Scripting Node' (with a green checkmark indicating 'All 5 visible parameters are valid'), 'Executable and Parameters' (with a dropdown for 'Path to Executable' and a button 'Open editor'), 'Command Line Arguments' (with a text field '%NODEARGS%' and a button 'Open editor'), 'Requested Tables and Columns' (with a dropdown and a button 'Open editor'), 'Use R-Friendly Columns' (with a checked checkbox), and 'Archive Datafiles' (with an unchecked checkbox).

Extend data processing capabilities

Perform custom data processing through a scripting node. Users can integrate external scripts (e.g., R and Python) into the workflow to perform specialized calculations and extend standard functionality.

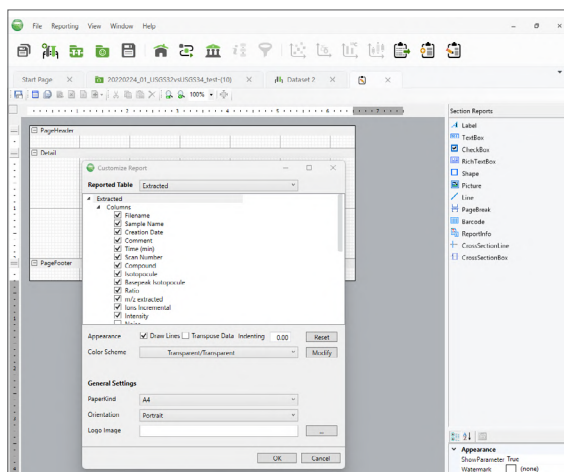
From analysis results to ready-to-share reports

Isotope Discoverer Software generates structured reports directly from processed data, enabling clear presentation of analysis results. Reports are created from user-defined templates and include key outputs such as calibrated δ values and associated data.

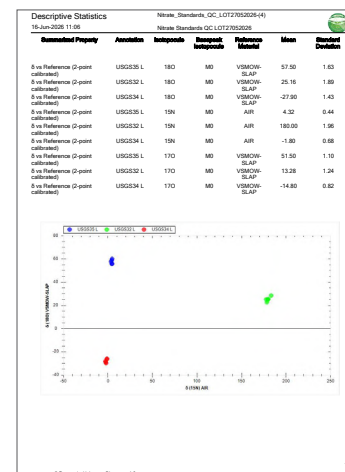
Results can be exported at different stages of the workflow, from intermediate processing steps to final analysis outputs. Tables can be filtered, customized, and formatted before export, supporting flexible reporting and data sharing.

Reporting and export options

- ✓ **Export intermediate results during workflow execution** using export nodes to generate .csv files
- ✓ **Customize results tables** by filtering data and selecting visible columns before exporting to MicrosoftTM ExcelTM software
- ✓ **Generate structured reports** using configurable templates for consistent output
- ✓ **Export polished .pdf reports** for presentation and documentation of analysis results



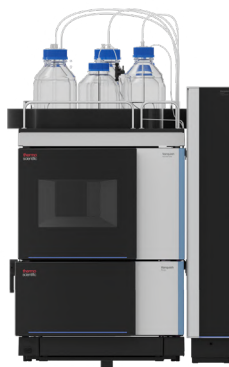
Define report structure and content using customizable templates.



Generate comprehensive reports with calibrated results and structured data.

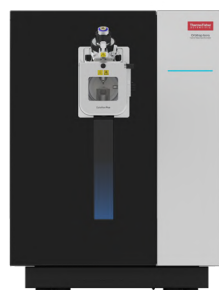
Powerful isotopic insights, elevated

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

Learn more at thermofisher.com/isotope-discoverer

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