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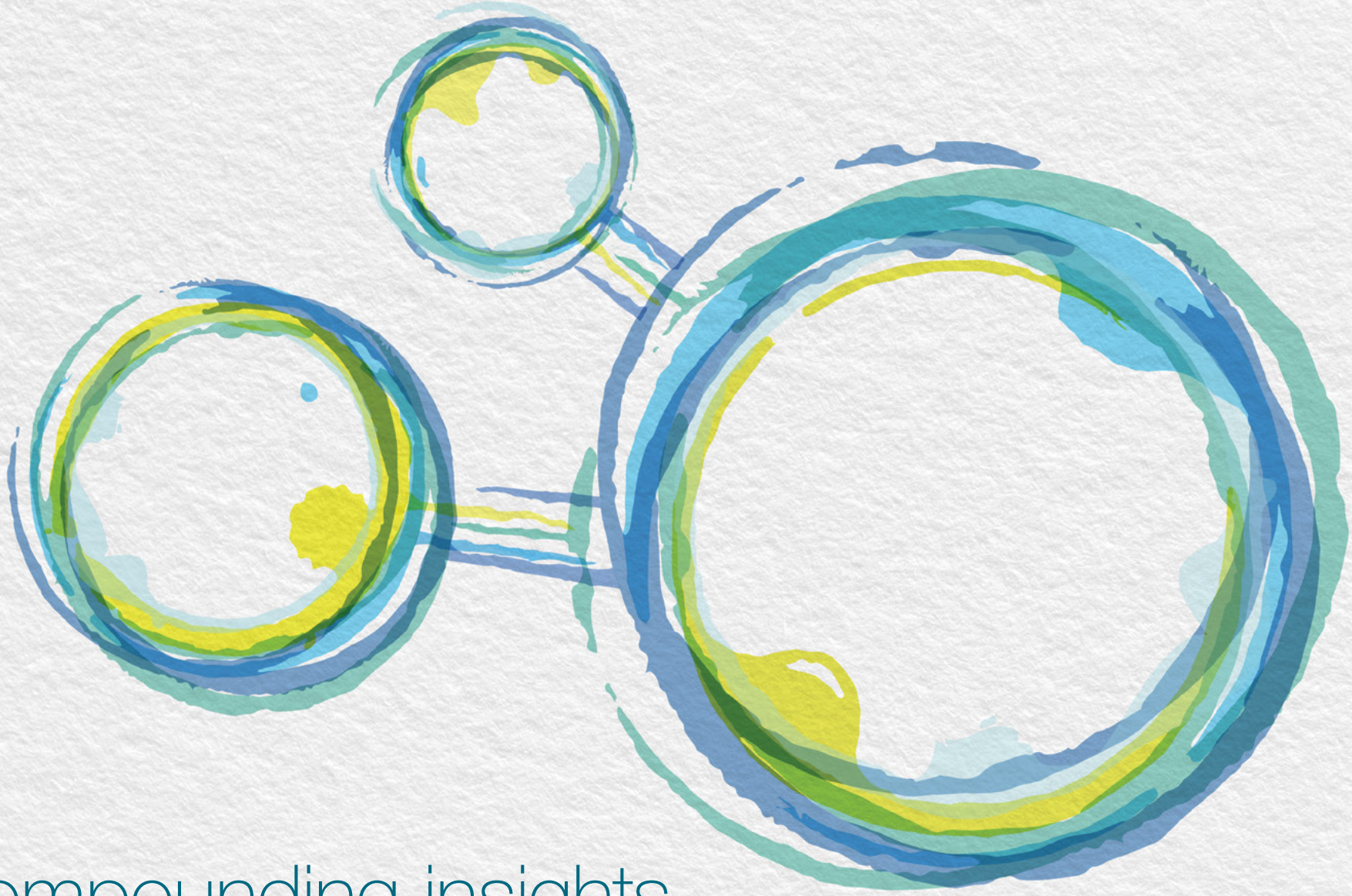


Compounding insights

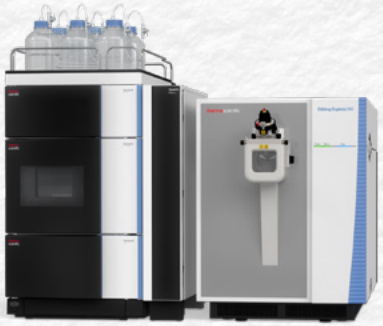
Thermo Scientific Compound Discoverer Software

ThermoFisher SCIENTIFIC

Integrated, complete, toolset solves small-molecule analysis challenges

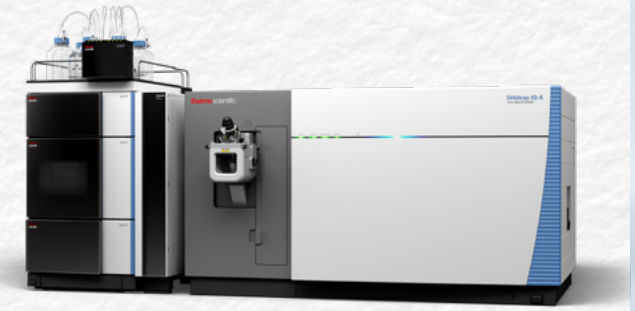
Thermo Scientific™ Orbitrap™ mass spectrometers produce information-rich data. The challenge for small-molecule analysis is to efficiently extract high-confidence understanding from this comprehensive data, without need for an expert user.

Thermo Scientific™ Compound Discoverer™ software solves this challenge. With a comprehensive, integrated set of libraries, databases, statistical analysis and visualization tools linked in customizable workflows, the software streamlines unknown identification, determination of real differences between samples, and elucidation of biological pathways.



Thermo Scientific™
Orbitrap Exploris™ 240 mass spectrometer

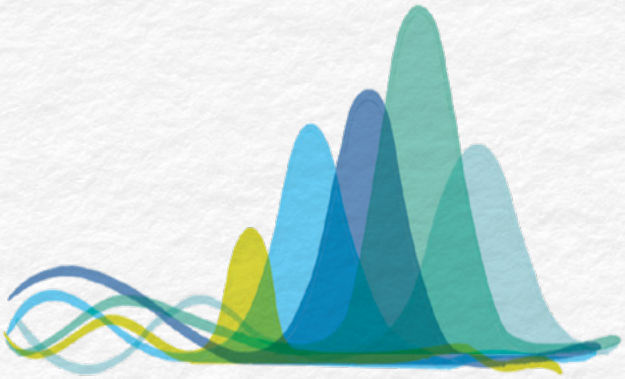
Thermo Scientific™
Orbitrap Exploris™ GC 240 mass spectrometer

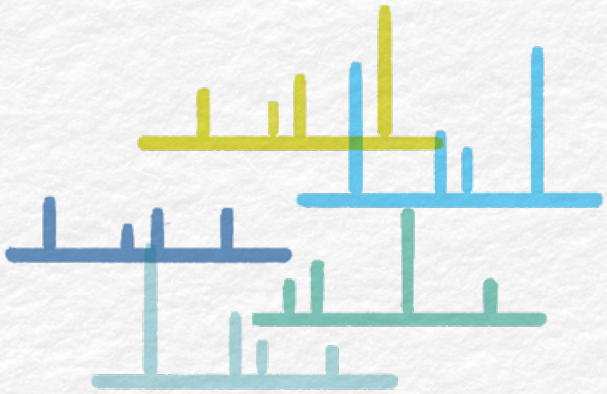


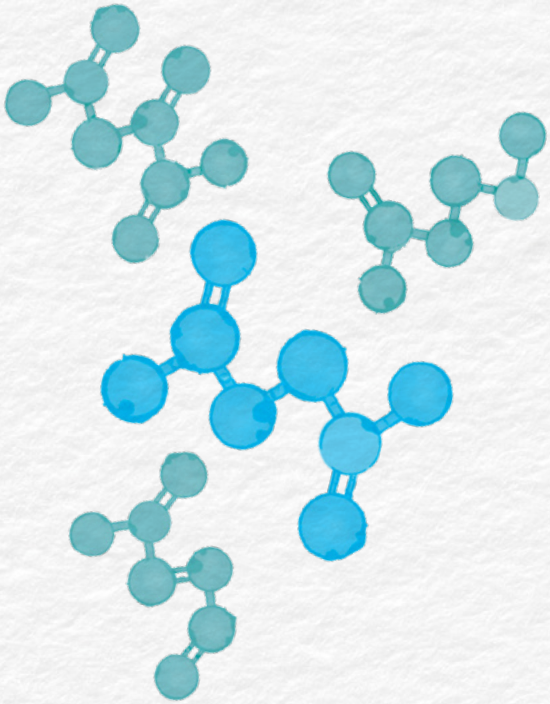
Thermo Scientific™
Orbitrap IQ-X™ Tribrid™ mass spectrometer

Reveal the highest confidence data using Compound Discoverer software on liquid chromatography (LC), gas chromatography (GC), and mass spectrometry (MS) instrumentation

Sample to structure—pathways to insight







Know more unknowns

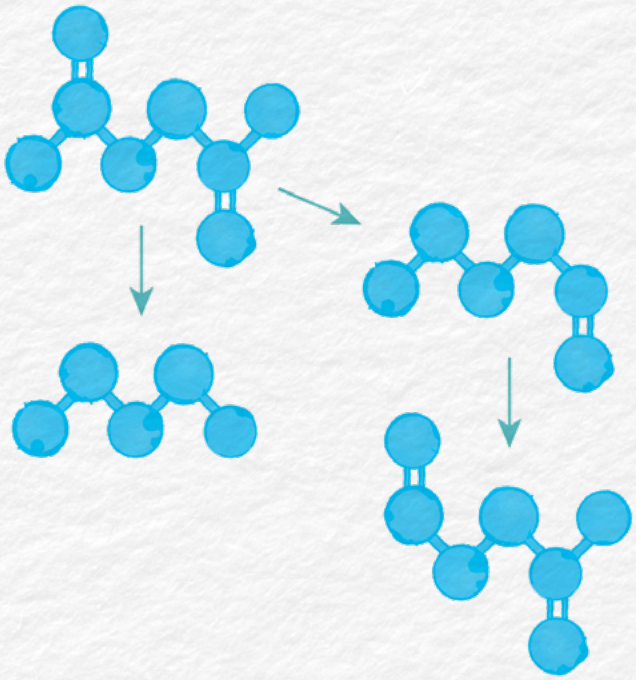
- Identify compounds using MS/MS libraries
- Determine elemental composition using high-resolution full MS isotopes and MS/MS data
- Search online chemical databases
- Gain confidence in ID with automated MS^n tree search against mzCloud

Go from spectra to structure

- Perform spectral library and similarity searches to identify compounds
- Search chemical databases for putative candidates
- Annotate spectra with predicted fragmentation, automatically
- Increase certainty using multi-factorial Peak Quality Factors to reveal, identify, and quantify with confidence

Find real differences

- Perform statistics and differential analysis using t-tests, ANOVA, PCA, PLS-DA, volcano plots, box-and-whisker plots, and more
- View trend charts to visualize peak areas, average peak area per group or fractional label incorporation over time
- Review heatmaps of peak areas, CV values, adjusted p-values, and more



Understand biological pathways

- Perform stable isotope labeling (“metabolic flux”) experiments
- View pathways using Thermo Scientific™ Metabolika™, KEGG, and BioCyc databases
- Map detected compounds, statistical data and fractional label incorporation to pathways

Supports a breadth of applications

Impurities and degradants

Identification of impurities and degradation products in drugs and foods is a critical aspect of product safety testing. Compound Discoverer software tools and customizable approaches enable confident detection of related components in complex samples.

Environmental and food safety

Food and environmental fate studies, and the analysis of contaminants in soil and water, often require identification of unknown compounds. Compound Discoverer software is ideally applicable to the analysis of metabolic fate and unknown compound identification of food and environmental degradants and contaminants.

Metabolite identification

The detection of related components in biological samples and the subsequent determination of their structures are key aspects of research. Compound Discoverer software allows you to find, identify and flexibly report metabolites of interest.

Forensic toxicology

Targeted screening applications only find what is targeted. Compound Discoverer software enables forensic toxicologists to find unknown metabolites of drugs of abuse and structurally related designer drugs. This information can then be transferred back to screening methods to help you keep up with an ever-expanding array of new drugs and their metabolites.

Metabolomics

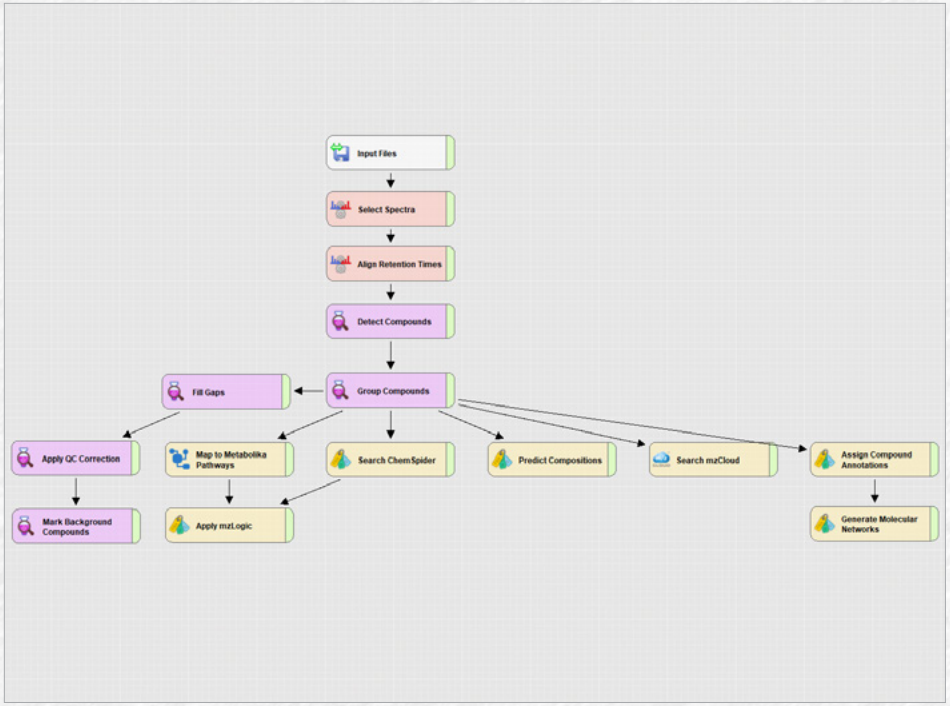
By integrating the tools necessary to determine components of interest in large complex metabolomics datasets, Compound Discoverer software offers a solution for quickly finding and identifying important statistical differences between sample sets. Compound Discoverer software also provides easy visualization of fractional label incorporation over time on metabolic pathways, eliminating the tedious manual steps used to examine the production and consumption of metabolites during qualitative flux analyses.

Speed, simplicity, and flexibility match your requirements

Easily customizable workflows

Compound Discoverer software empowers data processing with its customizable workflows. Drag and drop workflow nodes from an extensive list of processing tools into workflow trees that specify your desired data flows. Save your workflow as a template or pick from many pre-made templates to simplify setup.

Get up and running quickly with the Study and Analysis Wizard. Add your data, define your study and sample groups, pick a workflow template and start processing. You can also save time by partially re-running a workflow if needed.



Compound Discoverer workflows reduce the processing clicks needed to transform mass spectral data into results.

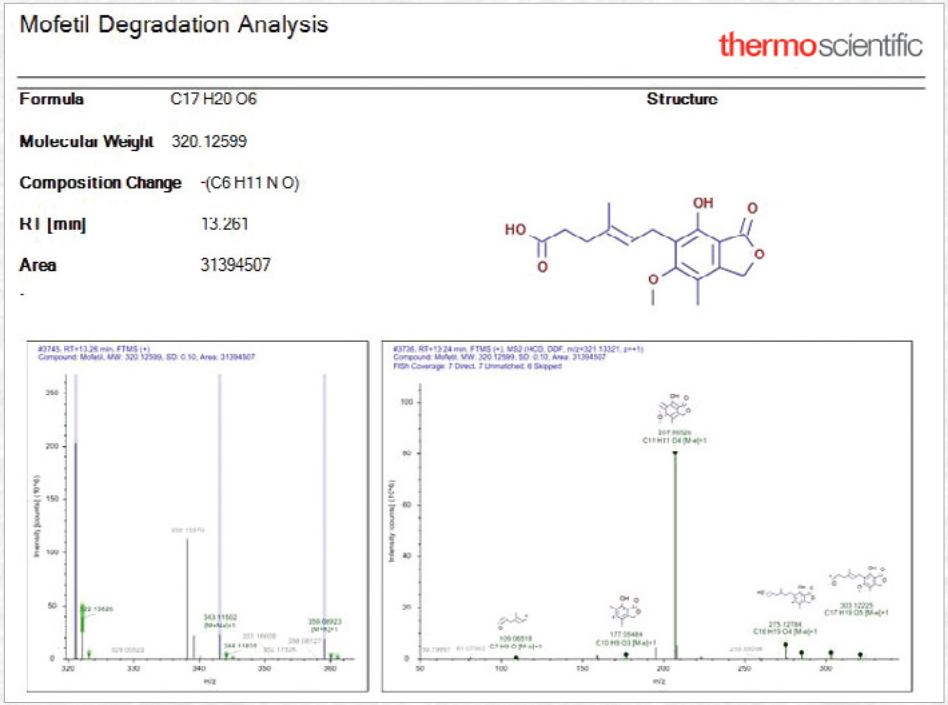
Interactively linked results

Compound Discoverer software makes it easy to visualize results in a meaningful way. Customizable data visualization allows you to review only the data you choose. Configurable layouts let you quickly change between views. Multiple monitor support ensures that you can view more data at once.

> "Compound Discoverer software is a powerful, versatile, and easy-to-use solution for MS-based isotopic labeling studies. Implementation of the software has drastically reduced our lead time and improved the impact of our research."
>
> Juan Moises Sanchez,
> — Associate Scientist,
> Bioanalytical Chemistry, Intrexo

Share results with tailored reporting

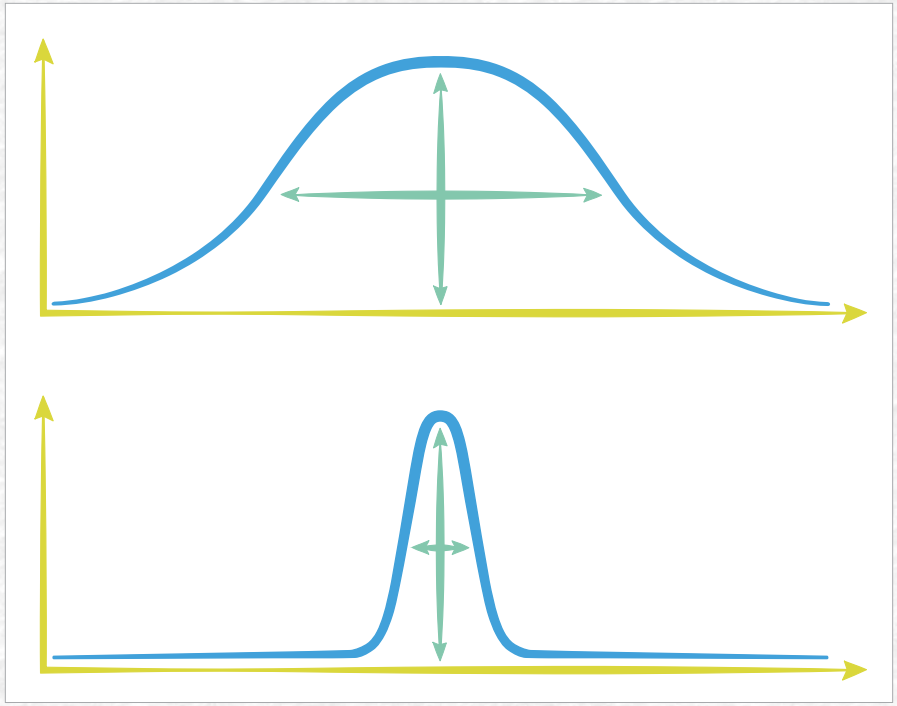
Powerful data-processing tools quickly create valuable results, but these results and supporting information must also be shared. Compound Discoverer software provides customizable reporting so results can be easily transferred to others that need them. Multiple output formats also allow you to transfer data to informatics software.



Tailored reporting helps you make real use of results.

Reveal higher quality chromatographic peaks

Peak Quality Factors provide a dedicated scoring mechanism to identify high-quality chromatographic peaks, by measuring certain properties such as jaggedness or symmetry, which describe the overall peak quality. The aggregated Peak Quality Factor score can then be used to filter out low-quality peaks, resulting in higher quality data.



Compound Discoverer software measures and reports peak quality.

Know more unknowns

Unknown identification is one of the toughest challenges in many small-molecule analyses. By integrating multiple tools for gathering identification information, Compound Discoverer software enables you to identify more of your unknowns.

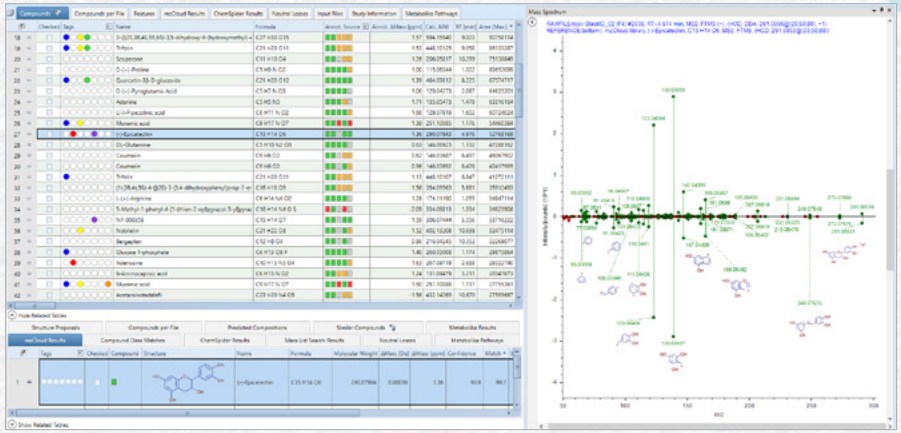
Automatically identify components

Identify automatically more unknowns faster—with online mzCloud spectral libraries or localized Thermo Scientific™ mzVault™ spectral libraries:

- Search mzCloud spectral libraries to gain even more information to use for unknown identification
- Export spectra of interest to save in mzVault libraries directly from Compound Discoverer software

Determine elemental composition—including fine isotopes, using HRAM MS, MS/MS, and MS^n data

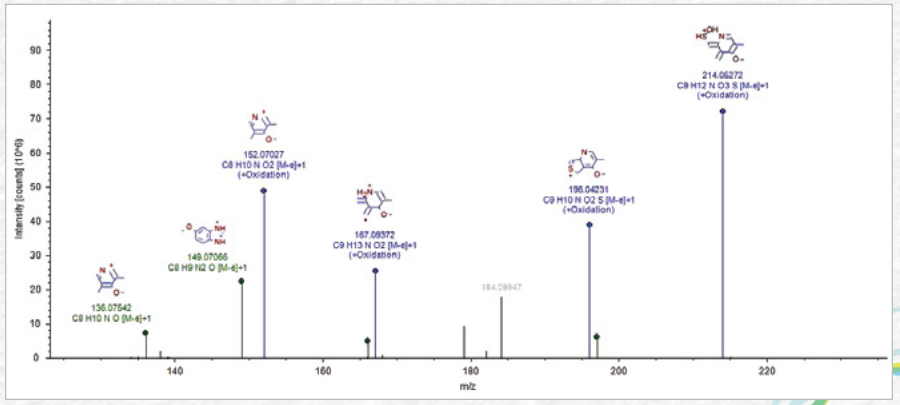
Access further annotations—use information to search multiple chemical databases for annotation



Automatically identify unknown compounds using the mzCloud spectral library, without leaving Compound Discoverer software.

Elucidate structures

Compound Discoverer software simplifies determination of compound structure by predicting and displaying fragments onto spectra using the built in HighChem Fragmentation Library of reference fragmentation mechanisms. This feature allows annotation of either expected compounds such metabolites, impurities, or breakdown products, and of putative structures supplied by chemical databases or the user.



Structurally annotated peaks provide more certainty in results and allow visualization of modified portions of expected compounds.

Rank order putative results

Database searches alone only produce putative candidates for identification. With the new mzLogic algorithm, you can use the extensive fragmentation spectral information in mzCloud to rank order putative database results. Combining mzCloud similarity searching with structure similarity matching provides improved candidate ranking.

Comprehensive mzCloud advanced mass spectral library

mzCloud is the world's most extensively curated mass spectral fragmentation library. Beyond generating matches for identification, integrated batch searching of mzCloud can also produce similarity matches. Searching makes use of stepped collision energy scans to automatically model results using the library's multiple energy levels of reference fragmentation data.

mzCloud

- Extensively-curated online library
- Includes compounds relevant to all applications
- Highly-curated, highest-quality data
- Multiple energy levels represented
- Supports both research and targeted screening workflows

Turn data into knowledge

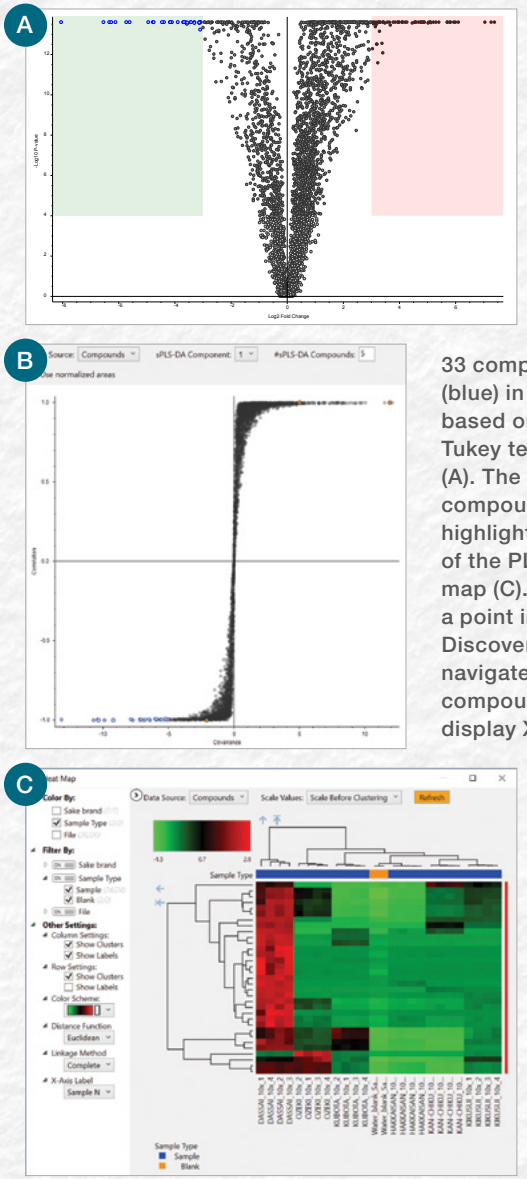
Compound Discover software supplies a suite of tools—KEGG and BioCyc, and Metabolika biological pathway databases, advanced statistics, hypothesis testing, and flexible visualization of complex data—that take you far beyond compound detection, enabling you to understand complex systems. These tools build on the certainty provided by the identification and structural elucidation capabilities of Compound Discoverer software, because confidence in pathway analysis is dependent on the confidence in underlying identifications.

Find and visualize real differences

Whether you are performing metabolomics research or looking for emerging environmental contaminants, the powerful Compound Discoverer software toolset enables you to quickly find real statistical differences—the differences that matter—between sample sets. Quickly view trends in components across a study, or identify the key components of interest between multiple sample groups using interactively linked displays. Move quickly from high-level PCA visualizations to individual components with one click.

Capabilities

- Interactive differential analysis; PCA; ANOVA; volcano, box-whisker, and trend line plots; PLS-DA; and t-tests
- Visualization of fractional label incorporation for multiple samples (isotopologue plot) and for trends over time (trendline chart)
- Heat map-like tables are included for normalized and original peak areas, ratios, two-fold log change, CV values, p and adjusted p-values
- Pathway mapping and visualization using Metabolika, KEGG, and BioCyc
- Interactive heatmaps with hierarchical clustering
- Powerful and flexible result table filtering, along with automatic background removal



33 compounds were selected (blue) in the Volcano plot based on p-value (ANOVA, Tukey test) and fold change (A). The same set of compounds is automatically highlighted in the S-plot (B) of the PLS-DA and the heat map (C). When clicking on a point in a plot, Compound Discoverer software will navigate to the corresponding compound in the table and display XIC and spectrum.

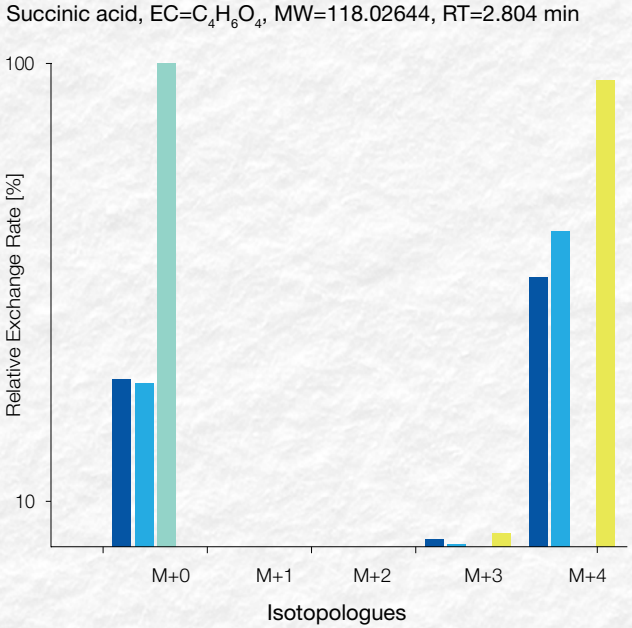
Streamline stable isotope labeling flux analysis

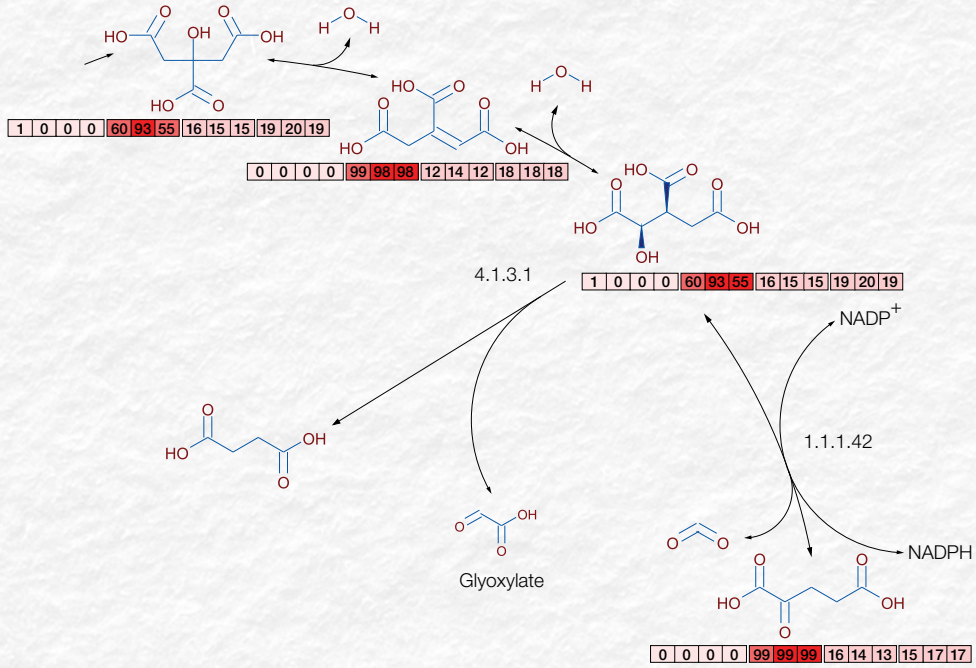
Stable isotope labeling experiments (qualitative flux analysis) are fundamental to understanding metabolic pathways and fluxes. Compound Discoverer software makes full use of HR Orbitrap mass spectrometer data to offer advanced, streamlined untargeted workflows for stable isotope labeling. Using an unlabeled reference sample, Compound Discoverer software automatically detects all compounds, determines their elemental composition, and identifies their labeled counterparts in labeled samples. Any isotopic label can be used and the label is the only user-entered parameter required for automatic isotopologues detection.

Compound Discoverer software reports the fractional label incorporation (exchange rate) after natural abundance correction for each compound. The exchange rate and other statistical data can be overlaid onto pathways using Metabolika, which is integrated with Compound Discoverer software.

Exchange Rate [%]

0	1	2	3	4
0	0	0	3	97
0	0	0	3	97
0	0	0	4	96
30	0	0	1	69
32	0	0	0	68
34	0	0	2	65
38	0	0	2	60
39	0	0	2	59
41	0	0	0	59
100	0	0	0	0
100	0	0	0	0
100	0	0	0	0
100	0	0	0	0
100	0	0	0	0
100	0	0	0	0





Compound Discover software supports untargeted stable isotope labeling workflows with visualizations of fractional label incorporation. Left-to-right: Details for fractional label incorporation (exchange rate) for isotopologues of succinic acid ($C_4H_6O_4$) across 15 samples; isotopologue plot showing exchange rates for isotopologues of succinic acid measured for 4 samples; Metabolika pathways showing a detail of the TCA cycle with data overlay of the overall exchange rates measured across 4 sample groups with multiple replicates.

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The complete package for small-molecule unknown data processing

Compound Discoverer software provides customers with a complete software platform for small-molecule research with unprecedent unknown identification in a customizable/ease of use single platform enabling sample to structure information.

Compound Discoverer software addresses small molecule identification needs and workflows including untargeted metabolomics, drug metabolism, impurity, E&L, environmental, food & beverage, and forensic research.

Try before you buy: Compound Discoverer software

Whether you are a new user or upgrading, try the latest version of Compound Discoverer software to experience the only software that fully utilizes data generated by HRAM Thermo Scientific Orbitrap mass spectrometers at thermofisher.com/compounddiscovererfreetrial.

mzVault updates

Compound Discoverer software ships with the latest revision of the mzVault spectral library. Approximately every 6 months, Thermo Fisher Scientific provides an updated local mzCloud library as an mzVault database file, which you can access at thermo.flexnetoperations.com.

mzCloud advanced mass spectral database

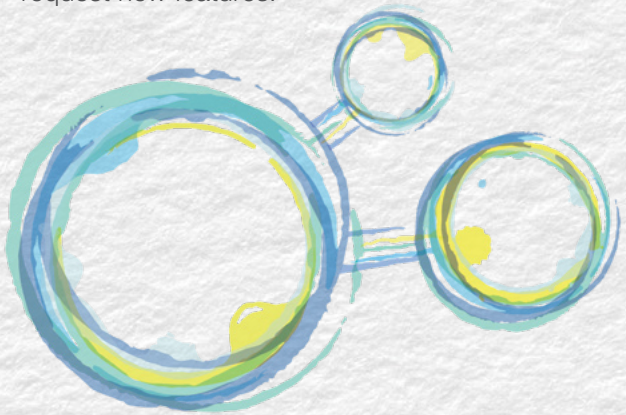
www.mzcloud.org

Orbitrap LC-MS and GC-MS systems

We offer a wide portfolio of Orbitrap-based mass spectrometer systems, including systems combined with ion traps and quadrupole mass filters, to address all your analysis needs at thermofisher.com/orbitrap.

For more information

Join the mycompounddiscoverer.com community today to stay up to date on new features, upcoming events, request help, access tutorials, and to request new features.



Find out more at **thermofisher.com/compounddiscoverer**

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