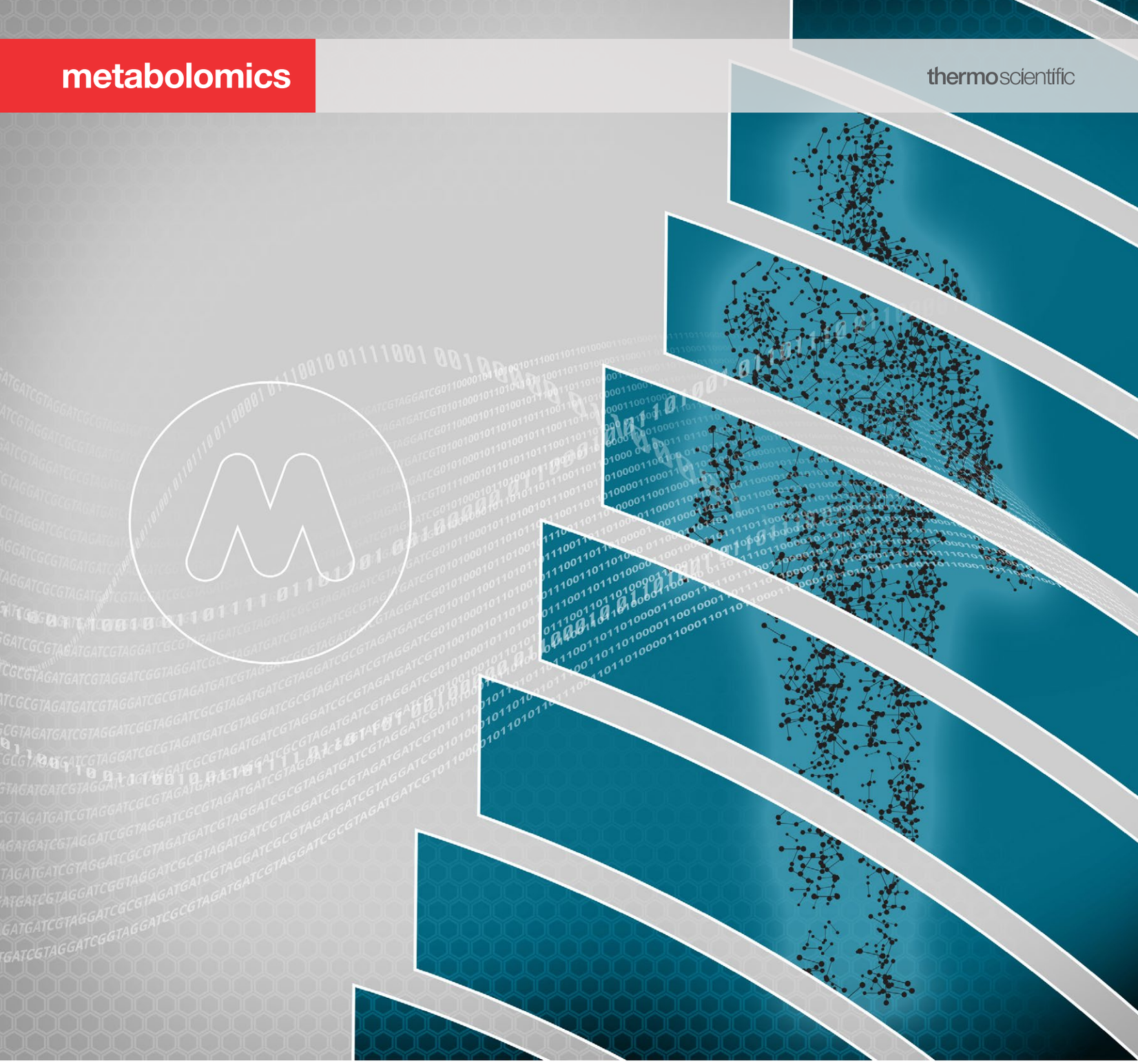
metabolomics

thermoscientific



GO BEYOND

to realities unexplored

Comprehensive workflows, integrated solutions

ThermoFisher SCIENTIFIC

Metabolomics—the total package

We're committed to helping researchers and scientists in academia and industry harness the power of metabolomics to gain in-depth biological insight, facilitate biomarker discovery, and advance scientific research.

By collaborating with key opinion leaders and others within the scientific community, we've developed leading solutions in the areas of separation, detection, and software. And we'll continue to pursue advancements to delve deeper into the metabolome, so you can go beyond the edge of what we ever thought possible.

Moving metabolomics forward requires an all-in commitment. That's why we've invested heavily in developing new metabolomics software that lives up to the high standards set by our leading instrumentation. Now you can have the total package needed to perform increasingly complex analysis, and easily translate your metabolomics data into valuable discoveries for your next step.

A multitude of discoveries

With its close link to phenotype, metabolomics is an ideal approach in areas of human health such as disease research, mechanisms of drug metabolism, drug safety studies and in the advance of precision medicine.

Metabolomics approaches have also found wide applicability to other research areas such as the food and beverage industry, biofuels, and biochemicals.

We collaborate with leading metabolomics researchers across industries to deliver results for diverse applications

Human health
Metabolomics reveals metabolic signatures of disease in areas such as cancer, diabetes, and cardiovascular disease leading to insights for translational research and targeted diagnostics that advance precision medicine.

Plant science
Metabolomics can help researchers understand the factors contributing to plant traits that influence yield, stress tolerance, seed quality, disease resistance, and mode of action of pesticides, knowledge of which will help to optimize crop development and production.

Food science
Through metabolomics, food scientists can rapidly obtain valuable information about the biochemical composition of foods. This helps in the derivation of components for food flavors and shelf life, leading to better control over food quality, among other factors.

Nutrition and diet
Using metabolomics, the biochemical profile of food components and its interaction with the biochemical networks of living organisms can be studied to provide information regarding the potential role of nutrition in health. This can help guide diet-based disease treatments and prevention.

Drug development
Metabolic profiling has the potential to identify markers arising from drug-induced toxicity—leading to improvements in public safety and optimizing drug development.

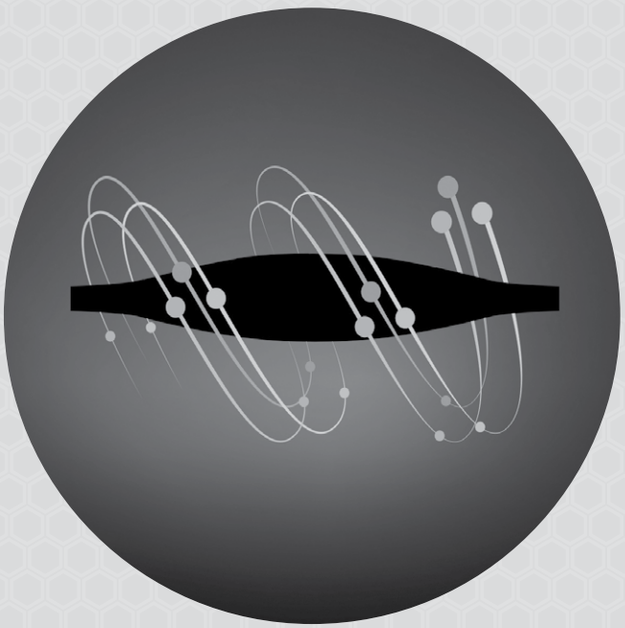
Environmental science
Environmental metabolomics is an emerging approach to characterizing the effects of disease and toxic chemicals on sentinel species to understand their possible impact on humans. It is also a useful tool for carrying out chemical risk assessment of pharmaceuticals, pesticides, and other chemicals, and maintaining healthy livestock and fish.

Biofuels and bioengineering
Metabolomics can help researchers identify microbial strains and engineer novel metabolic routes for biomass production and conversion. This could potentially increase production of biofuels needed to meet future energy demands.

The core of successful metabolomics—powered by Orbitrap mass spectrometry

The success of metabolomics research lies with proven Thermo Scientific™ Orbitrap™ mass analyzer technology. Workflows that include Orbitrap mass spectrometers have been widely adopted for life science applications such as proteomics and in the last few years, this technology is becoming established for metabolomics and lipidomics.

Orbitrap mass spectrometers represent the leading mass spectrometry (MS) technology for analyzing samples that are complex both in the sheer number of analytes present and the type of sample matrix, such as plasma, tissue, urine and others. Additionally, with a breadth of chromatographic separations and integrated data analysis tools, Orbitrap MS-based workflows enable researchers to successfully analyze physiochemically diverse samples in metabolites—making us the leader in metabolomics, delivering solutions to keep you at the forefront of science.



Diverse instrument portfolio to support metabolomics analysis

Harnessing the power of chromatographic separation

Since endogenous metabolites are diverse in their physicochemical properties and abundance, a truly comprehensive metabolomics study will require multiple separation techniques.

This complexity demands sophisticated methods of separation and detection—high-resolution separation that is designed for high-resolution detection by Orbitrap mass spectrometers.

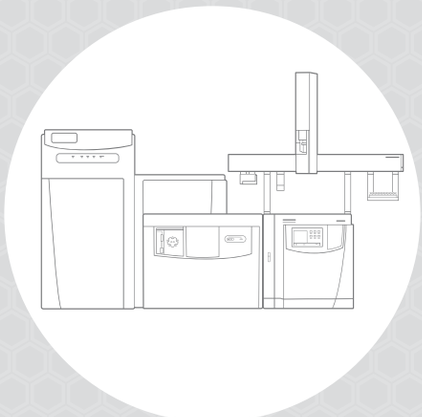
The integration of each of the chromatographic separation methods (liquid, gas, and ion) with the high-resolution detection system (Orbitrap mass spectrometer) enables broader, deeper, and faster analysis of complex and diverse metabolites—offering a robust system that is more effective than the sum of its parts.

Seamless integration with Orbitrap mass spectrometers

Thermo Scientific™ products deliver comprehensive breadth in separation of analytes with gas, liquid, and ion chromatography systems. When combined with the leading Orbitrap mass spectrometer, our technologies enable broader and deeper analysis into the metabolome.

With high robustness and technical reproducibility, these solutions provide novel yet stringent results for high-impact discoveries.

LC-MS: Thermo Scientific™ Vanquish™ Duo UHPLC system with Thermo Scientific™ Orbitrap ID-X™ Tribrid™ mass spectrometer.

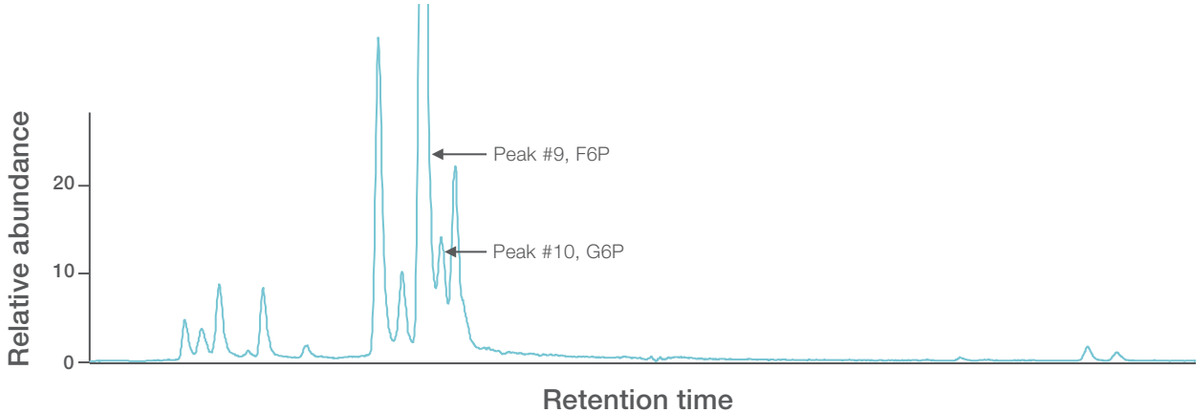


GC-MS: Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system with proven Thermo Scientific™ TRACE™ 1300 Series GC injectors.

IC-MS: Thermo Scientific™ Dionex™ ICS-5000+ Capillary HPIC™ system with Thermo Scientific™ Q Exactive™ HF hybrid quadrupole-Orbitrap™ mass spectrometer.

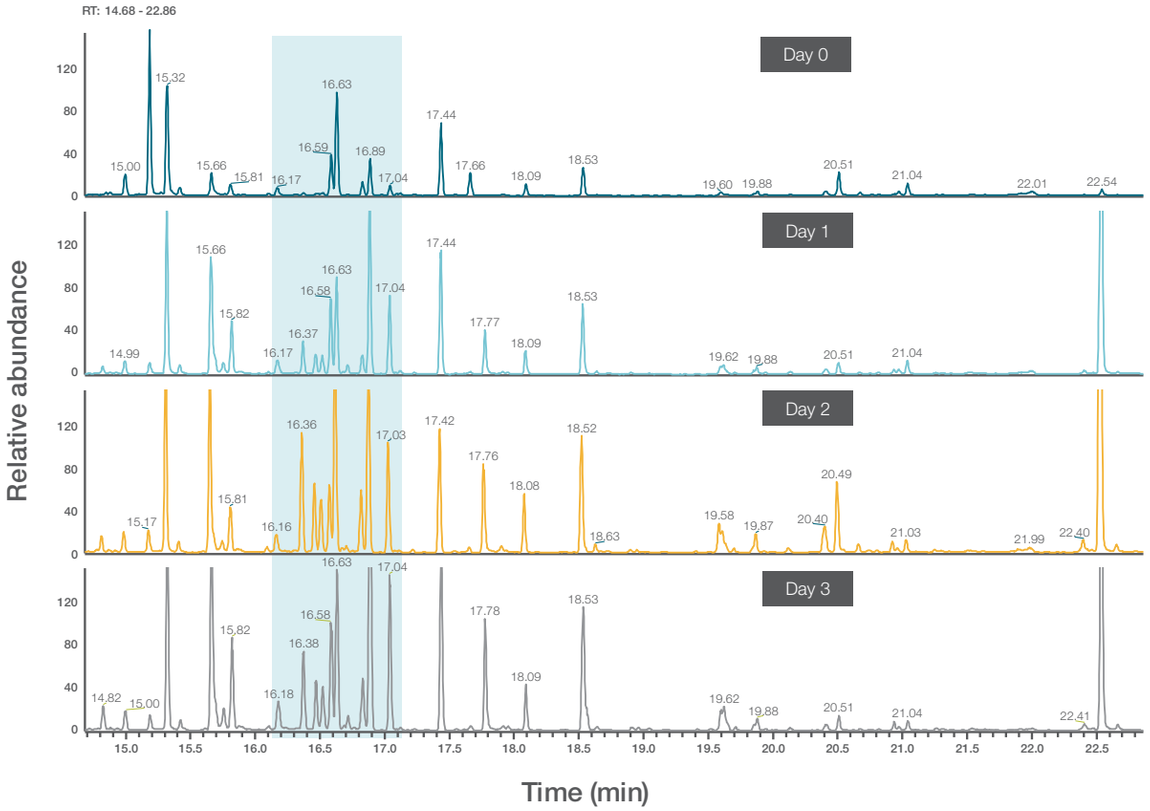
Comprehensive coverage of the metabolome

Enabled by orthogonal separations and deep coverage with Orbitrap mass spectrometry



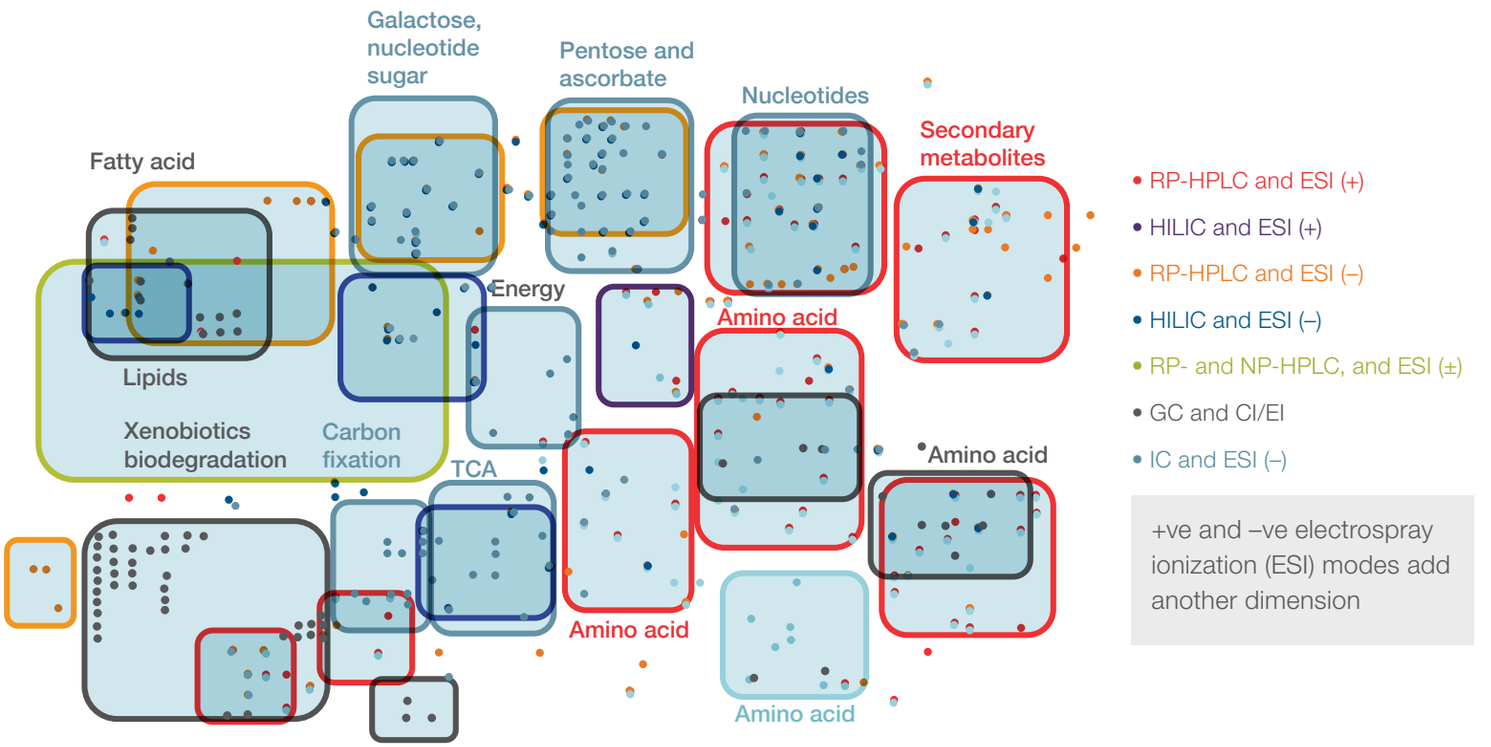
Separation of 11 monophosphate isomers of sugar by IC-MS.

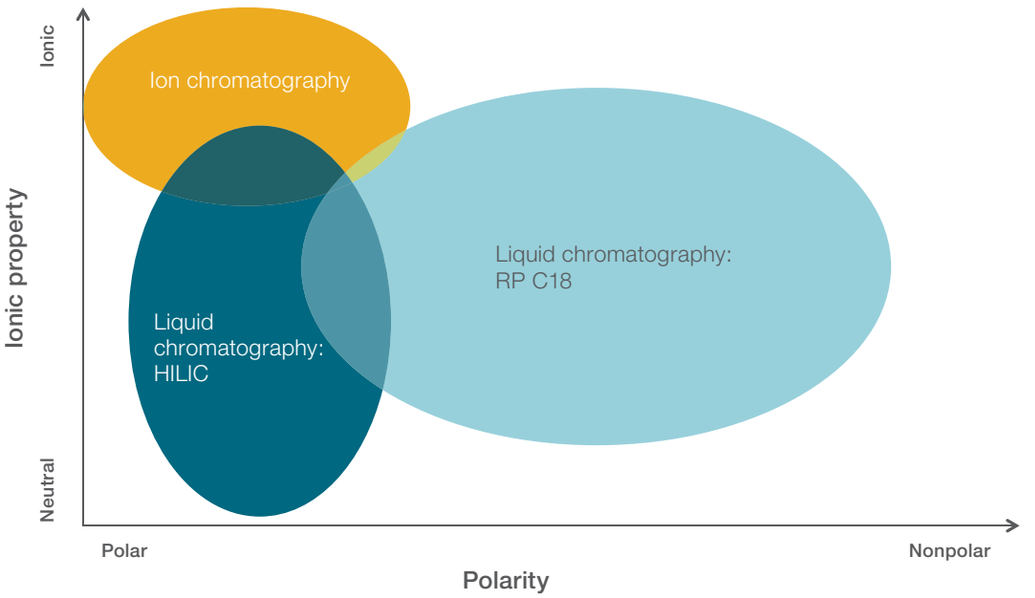
IC: Ion chromatography (IC)-MS is best suited for charged or very polar metabolites such as sugar phosphates and amino acids that are difficult to analyze by LC-MS. IC has high resolving power, and many isomers can be separated prior to mass spectrometry using this technique.



Quantitation of components in rat muscle homogenate by GC. Rat muscle tissues were decayed for 0–3 days (top to bottom). The peaks in the highlighted region indicate the change in intensity over time.

GC: Samples that are volatile and amenable to chemical derivatization are well suited for gas chromatography (GC)-MS. GC offers high resolving power for separation of isomers. Plant secondary metabolites are well suited to analysis using this technique.





LC: Liquid chromatography (LC)-MS offers the broadest coverage of metabolites through the ability to use different column chemistries, such as reversed-phase high-performance liquid chromatography (RP-HPLC) for nonpolar to moderately polar metabolites, and hydrophobic interaction liquid chromatography (HILIC) for ionic and polar compounds not retained by RP. Ultra high-performance LC (UHPLC) systems and columns are available for high-resolution separations.

Leading-edge metabolomics

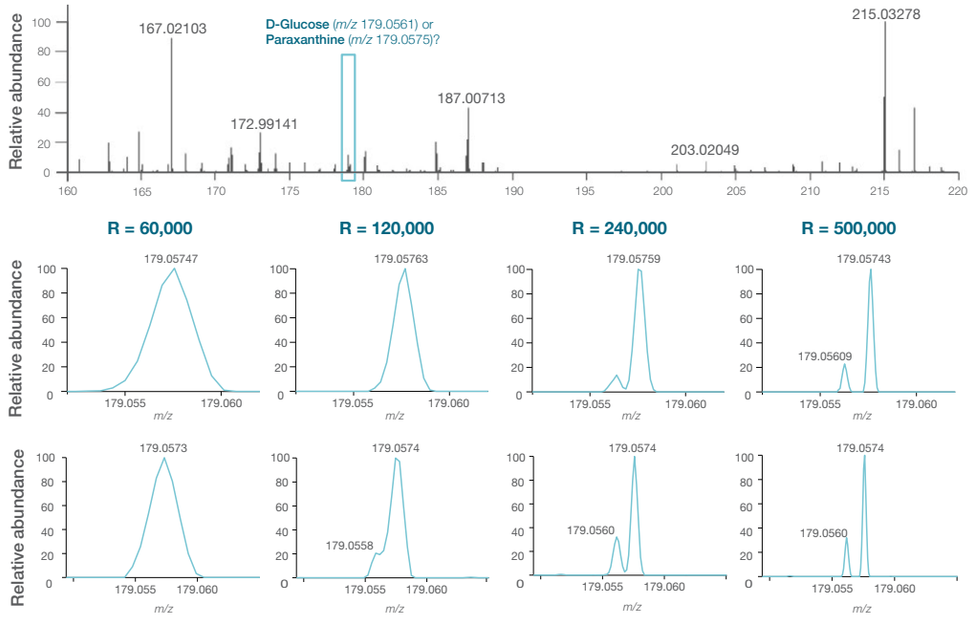
Powered by Orbitrap mass spectrometry

When combined with advanced separation techniques, industry-leading Orbitrap mass spectrometers provide high-resolution accurate mass (HRAM) measurements and sensitivity required for metabolomics.

This powerful technology delivers high-throughput and quantitative capabilities, expanding the scope of our understanding of metabolites involved in cell metabolism and biological pathways, and in putative biomarker discovery.

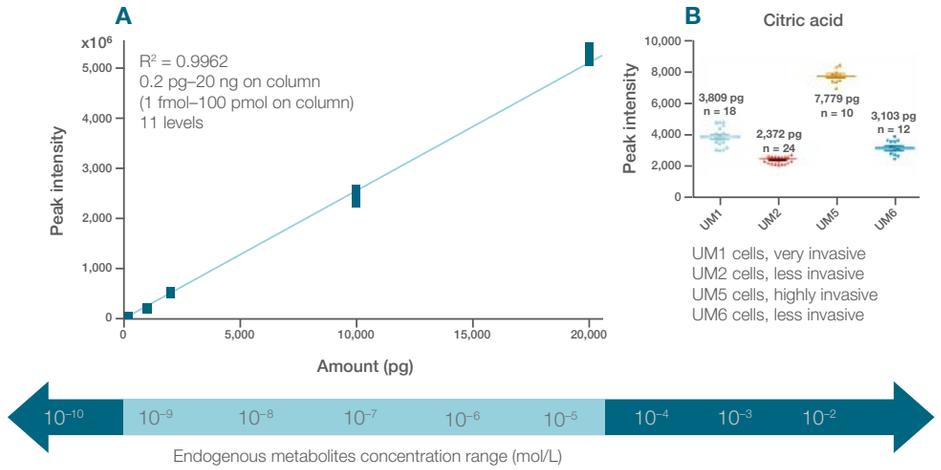
Key attributes of HRAM Orbitrap MS for successful metabolomics

HRAM: With up to 500K resolution, Orbitrap mass analyzers enable more confident identification and quantitation due to high specificity, allowing accurate mass assignments, especially for metabolites of similar mass, and isotope-labeling studies.



The very high resolving power of Orbitrap mass analyzers resolves isobaric metabolites from a complex mixture in (A) plasma extract and (B) a standard mix of D-glucose and paraxanthine at concentrations of 50 mM and 0.1 mM, respectively.

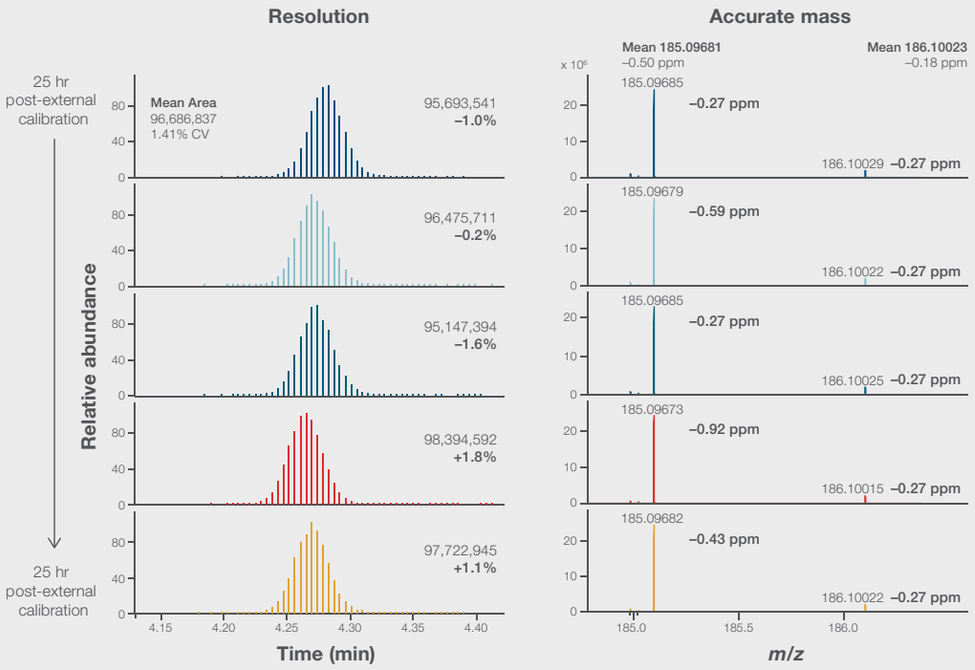
Sensitivity: Metabolomics is and always has been a quantitative science. There are orders-of-magnitude differences between concentrations of different endogenous metabolites that must be detected for a comprehensive and meaningful view of their biological states. Orbitrap mass analyzer technology enables quantitation down to low-femtomole concentrations, with up to five orders of linear dynamic range with tight coefficients of variation (CV).



Sensitivity of Orbitrap mass analyzer: (A) Quantitation of citric acid was achieved at low-femtomole sensitivity using full scan MS. (B) Shows the amount of endogenous citric acid obtained from each plate containing ~3 × 106 cells.

Technical reproducibility

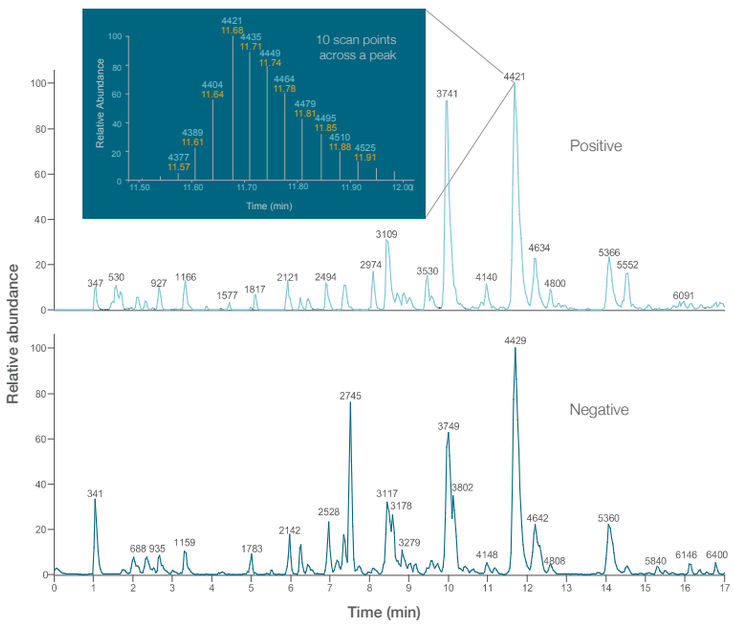
Due to its sensitivity and selectivity, Orbitrap mass spectrometer-based techniques have become the method of choice for metabolomics research. To find meaningful answers within the large number of datasets typically found with metabolomics studies, the mass spectrometer must provide accurate and reproducible data from run to run, without the need for internal calibration.



Full scan MS R = 70,000; Peak width = 3.6 s, mean 14.5 scans; D3-hippuronic acid, theoretical *m/z* = 185.0969.

Fast polarity switching

A combination of separation techniques (GC, IC, and LC (RP or HILIC)) can help achieve a more comprehensive view of the metabolome. Additionally, more coverage can be obtained using both positive and negative ionization modes on the mass spectrometer. Polarity switching on an Orbitrap mass spectrometer can be achieved in a single run, enabling a more productive analysis.

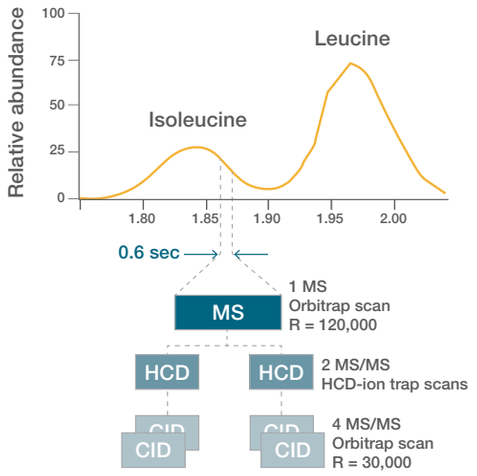


Base peak chromatograms of positive and negative ion modes of bovine heart lipid extract (1 µg on column) in a single run.

MS^n capabilities for the structural elucidation of metabolites

Multiple-stage mass spectrometry (MS^n) offers a solution for *de novo* identification and structural elucidation. MS^n is usually achieved using ion traps and Thermo Scientific™ Tribrid™ mass spectrometers such as the Orbitrap ID-X Tribrid mass spectrometer.

This is an advanced technique, requiring high-resolution, accurate-mass (HRAM), and speed on an HPLC time scale, with a variety of dissociation modes such as high-energy collisional dissociation (HCD) and collision-induced dissociation (CID).



MS^n improves the ability to confidently identify isomeric metabolites and elucidate structures of unknowns.

Numerous metabolites, unlimited possibilities

Solutions designed to meet your metabolomics goals

Several approaches to metabolomics research are available depending on your goals. The untargeted discovery approach can be used to identify putative biomarkers, understand metabolism on a system-wide scale, and detect unknown metabolites in routine applications. Targeted approaches are best suited to a focused study of a subset of known compounds, to verify and/or validate results from the discovery or hypothesis-driven phase, or for the routine detection and quantitation of compounds.

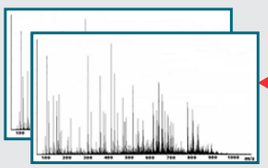
We provide a range of solutions and workflows that are specifically designed to meet your needs.

1 Chromatographic separations

- GC
- LC: HILIC
- LC: RP-HILIC (C-18)
- IC

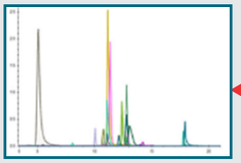
2 Mass spectrometry

Untargeted metabolomics
What is the global metabolite profile of a sample?



HRAM detection by Orbitrap mass spectrometry

Discovery phase



HRAM detection by Orbitrap mass spectrometry

Targeted metabolomics
What are the levels of specific metabolites in a sample?

Selected reaction monitoring (SRM) by triple quadrupole mass spectrometry

From discovery or hypothesis driven

3 Data analysis

Profiling
Statistical analysis
Identification
Pathway analysis

Profiling
Quantitation
Statistical analysis

Quantitation
Statistical analysis
Reporting

Go beyond traditional untargeted metabolomics

Explore all relevant compounds present in your complex samples

- Annotate and identify biomarkers
- Understand cellular metabolism
- Identify trends between samples and populations
- Overcome the technical limitations associated with studying the most challenging samples

Both our separation technologies and HRAM Orbitrap mass spectrometers are proven to be highly reproducible, sensitive, and capable of measuring a wide range of metabolites, from very hydrophilic to hydrophobic, for comprehensive coverage.

With specially designed metabolomics software, you can examine the rich HRAM Orbitrap mass analyzer data more efficiently and convert these large data sets into meaningful insights.

Ultimate tool for small molecule characterization and structure elucidation

Acquisition and interpretation of mass spectra to characterize and identify unknowns is a formidable task in untargeted metabolomics. Sample complexities, background interferences, compound structural diversity, and lack of robust data processing tools can make it difficult to set up analytical methods and interpret data. Overcoming these bottlenecks requires advances in both data acquisition and computational tools.

Equipped with the novel, automated Thermo Scientific™ AcquireX intelligent data acquisition workflow that includes various characterization capabilities using intelligent MS^n and a multitude of mass spectral data-processing tools, the Orbitrap ID-X Tribrid mass spectrometer can help you extract meaningful data faster and with higher confidence.

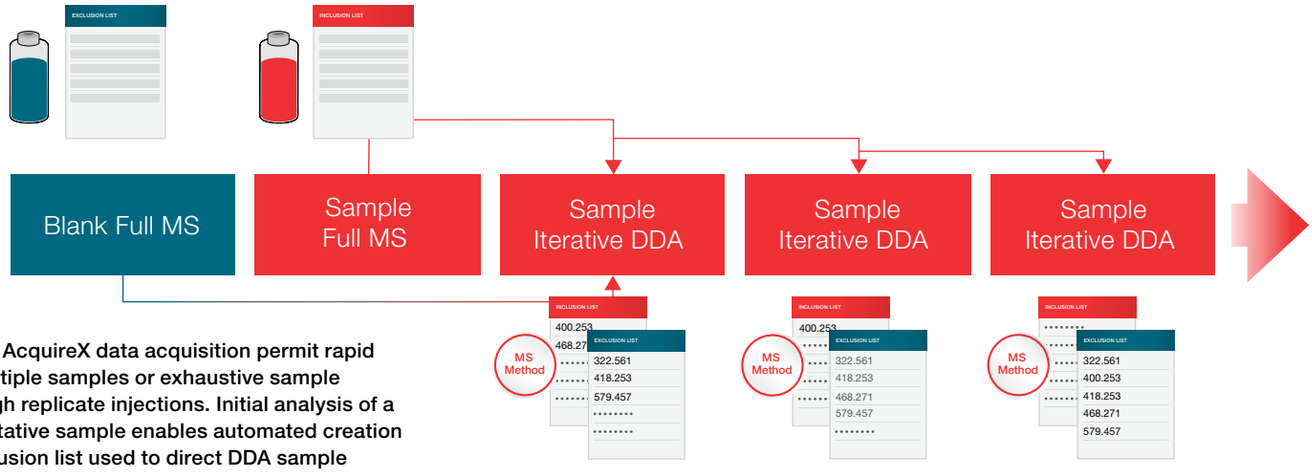
Orbitrap ID-X Tribrid mass spectrometer

Increased coverage and confidence in unknown identification

More meaningful data, not just more data

Fragmentation spectra provides more spectral information to increase the confidence of unknown annotation. AcquireX intelligent acquisition generates more fragmentation spectra for sample relevant compounds, avoids unrelated background ions, and removes redundancies by using fully automated iterative inclusion and exclusion lists. Available on the latest generation Orbitrap Tribrid MS systems, AcquireX takes advantage of knowledge to drive acquisition where the blank sample generates a list of ions to exclude for subsequent fragmentation and a matrix sample generates a list of true sample components to prioritize for data dependent MS^2 and MS^n acquisition.

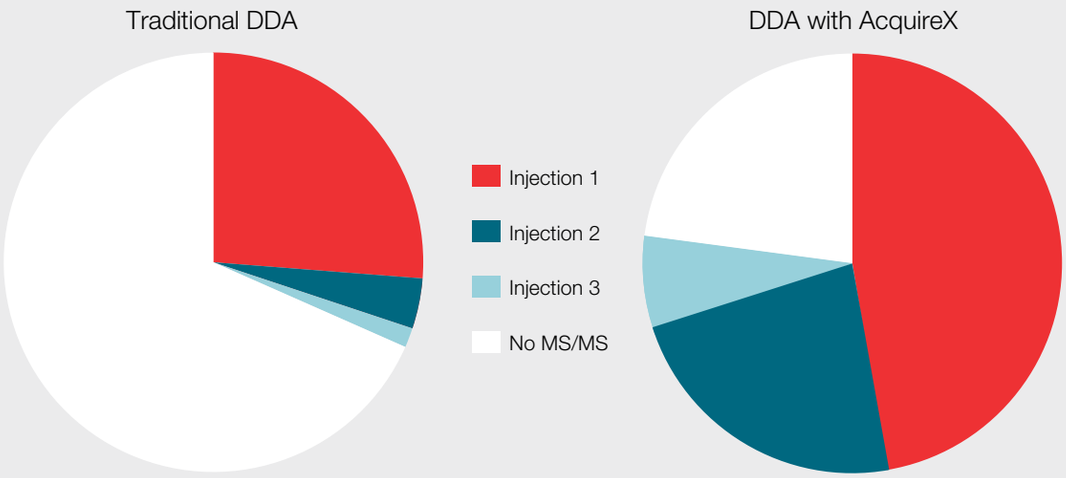
AcquireX data acquisition



The three modes of AcquireX data acquisition permit rapid profiling across multiple samples or exhaustive sample interrogation through replicate injections. Initial analysis of a blank and representative sample enables automated creation of an inclusion/exclusion list used to direct DDA sample analysis. Each replicate injection increases the number of compounds sampled with distinguishable fragmentation spectra for sample and study characterization.

Higher Efficiency

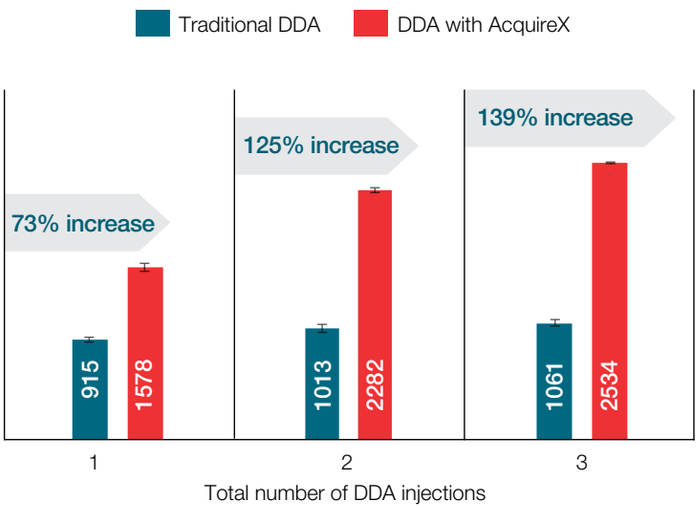
Number of compounds with fragmentation spectra



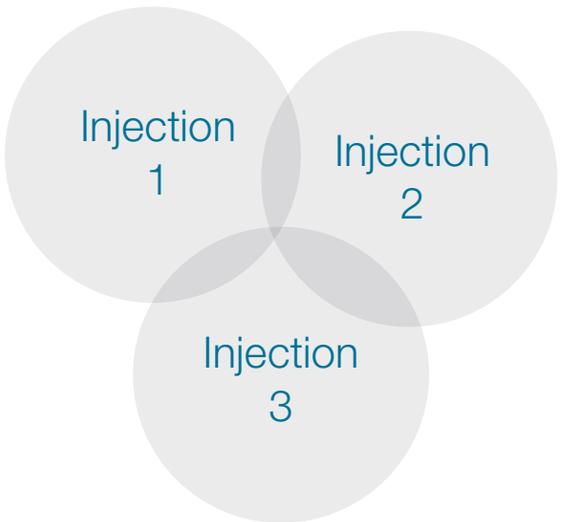
The Orbitrap ID-X Tribrid mass spectrometer improves precursor sampling by automatically updating the inclusion/exclusion lists following each replicate. The data-informed AcquireX approach utilizes sequential injections to interrogate more unique sample components through MS^n acquisition. AcquireX more than doubled the number of unique compounds with fragmentation spectra in human plasma (NIST SRM1950) in comparison to traditional DDA, resulting in a greater metabolome coverage.

"Confident metabolite identification remains a challenging step in the untargeted metabolomics workflow where the data acquired are applied to derive the structure of all metabolites detected. Progress has been made to putatively annotate metabolites using MS or MS/MS data using established UHPLC/MS assays through the use of metabolomics database and mass spectral library searching workflows. The Orbitrap ID-X Tribrid MS delivers complementary information with multiple dissociation techniques and robust MS^n data required to deduce structural information and increase confidence in metabolite annotation. With built-in intelligent data acquisition, AcquireX, we now collect more informative data, and not just more data, we can maximize metabolome coverage and increase confidence in the identification on unknowns applying intelligent-DDA approaches."

—Warwick Dunn, PhD, Professor in Analytical and Clinical Metabolomics, Phenome Centre Birmingham, School of Biosciences and Institute of Metabolism and Systems Research, University of Birmingham, UK



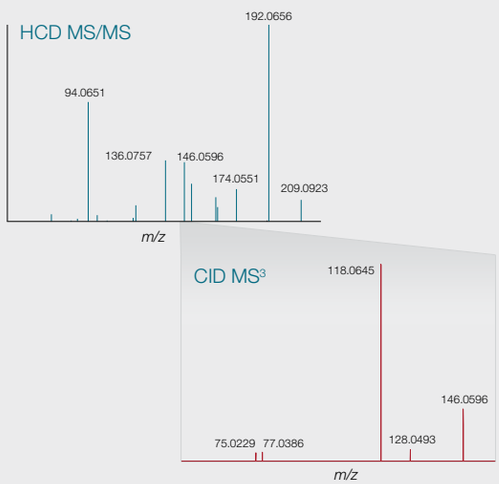
Detect up to 140% more unique unknown compounds that are truly experimentally related, even at low abundance as shown in this example of three replicate injections of the NIST SRM 1950 plasma extract sample.



The AcquireX Intelligent data acquisition approach samples more compounds with distinguishable product ion spectra. With each iteration and subsequent injection, the same compounds chosen to be fragmented are eliminated, minimizing redundancy.

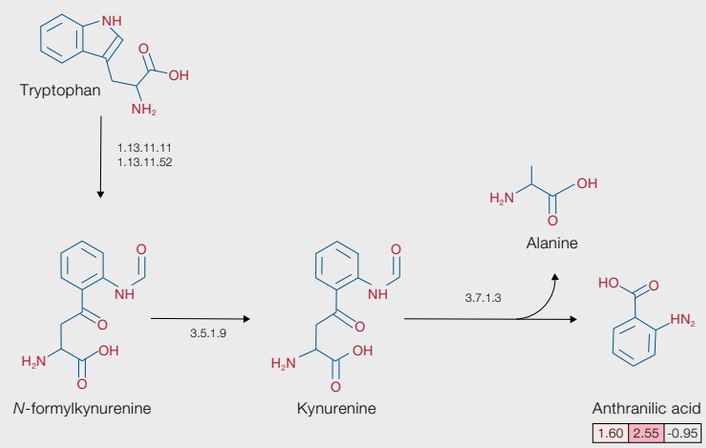
Higher Quality

Complimentary MS^n fragmentation of kynurenine metabolite



The Orbitrap ID-X Tribrid mass spectrometer offers MS^n fragmentation and the flexibility of complementary HCD and CID techniques to increase the probability of generating information-rich product-ion spectra across more compound classes. In this example, fragmentation of the metabolite kynurenine illustrates the complementarity of HCD and CID.

Metabolite intermediate kynurenine identified in a Crohn's disease study



Annotation of more high-quality spectra leads to improved metabolome coverage, comprehensive pathway annotation, and functional interpretation of results. Confident annotations of metabolites in the tryptophan degradation pathway enabled detection of changes in the levels of anthranilic acid in a comparison among healthy donors and donors with Crohn's disease.

Targeted metabolomics

Validation of identified metabolites using a quantitative approach

Rapid large-scale targeted profiling

- Target selected metabolites and compounds from either untargeted discovery or hypothesis-driven data
- Apply high-throughput and sensitive techniques
- Target and verify putative biomarkers or compounds indicative of quality, origin, and toxicity before developing routine assays

Large-scale metabolomics quantitation using HRAM Orbitrap MS-based workflows enables you to rapidly evaluate and screen known metabolites. As untargeted analyses are performed, the same system can also be used for targeted profiling with the same high selectivity, post-acquisition flexibility, and retrospective data analysis of compounds by MS/MS.

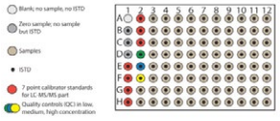
Fast, robust routine quantitation

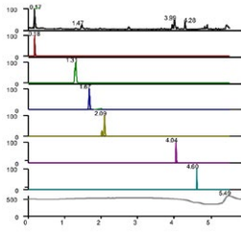
- Target known, well-characterized metabolites and compounds
- Apply high-throughput and sensitive techniques
- Customize reports

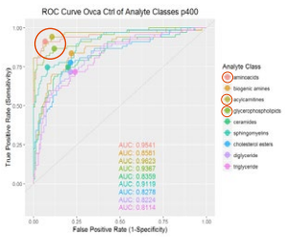
For targeted lists of known, well-characterized metabolites and compounds, Thermo Scientific™ TSQ™ triple quadrupole mass spectrometers offer sensitive, fast, and robust quantitation of metabolites.

Standardized and quantitative HRAM LC-MS metabolomics workflow

Targeted metabolomics offers researchers the possibility to quantify selected metabolites. The Absolute*IDQ*® p400 HR kit is the first standardized solution for broad metabolic and lipid profiling developed and verified for use with Orbitrap mass spectrometers**, covering key metabolites relevant to pathophysiological processes and disease specific markers. This workflow delivers quantification of hundreds of metabolites with high throughput and the reproducibility needed for rigorous and confident results.







Sample labeling and preparation

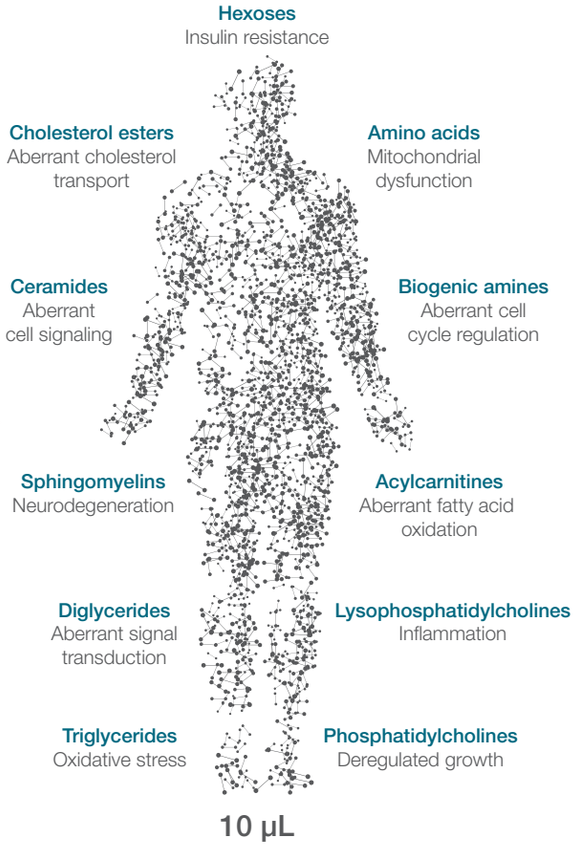
Biocrates Absolute*IDQ*® p400 HR kit verified for Thermo Scientific™ Q Exactive™ MS

LC-MS/MS and FIA MS/MS analysis

Thermo Scientific™ Q Exactive™ MS family

Quantification and kit validation analysis

Biocrates Met*IDQ*™ software

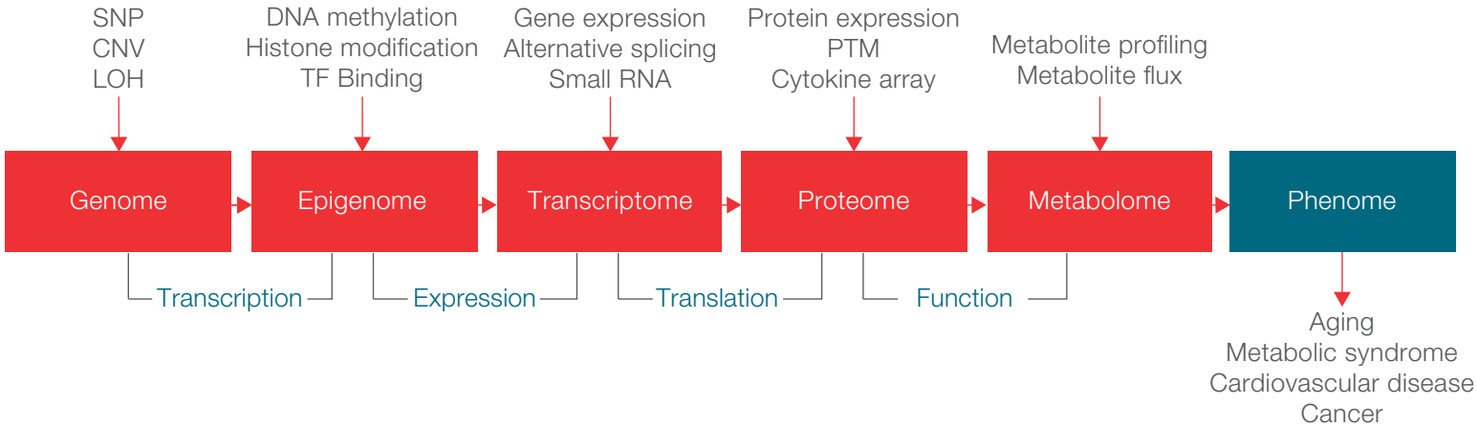


** Thermo Scientific Q Exactive series MS (excluding Thermo Scientific™ Q Exactive HF-X hybrid quadrupole-Orbitrap™ mass spectrometer)

Tools for translational research

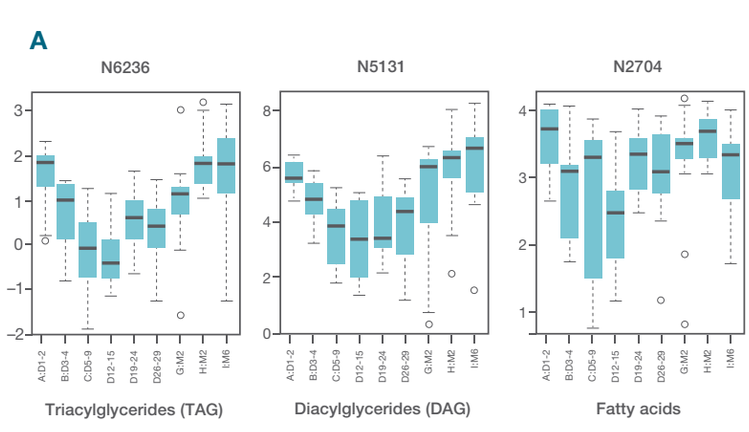
Large-scale metabolic phenotyping

As metabolism is closely associated with the dynamics of the human phenotype, metabolic phenotyping (phenome studies) can be applied to large-scale analysis of thousands of samples per study to identify a single metabolite signature that relates to disease onset and progression, or response to treatment. Several research initiatives are underway worldwide using this approach.

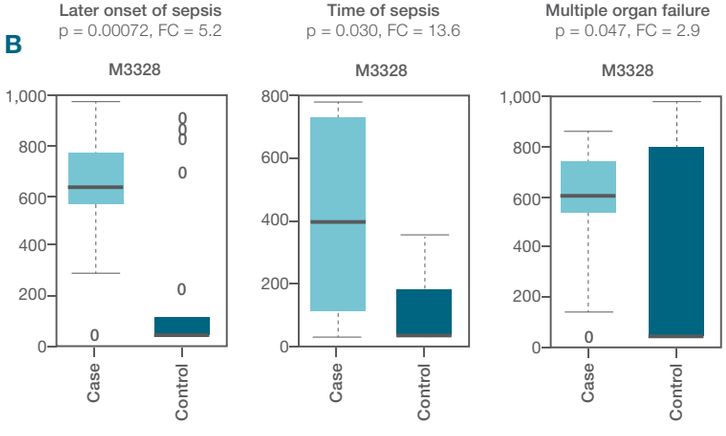


Due to their proven sensitivity, dynamic range, broad coverage, and high throughput, Orbitrap mass spectrometers are ideally suited to both small-scale metabolomics and large-scale metabolic phenotyping.

The Phenome Centre Birmingham, UK, employs multiple Orbitrap LC-MS mass spectrometers with the aim to complete more than 15,000 assays per year to study human metabolism and its role in health and disease. One such study applied a nontargeted discovery–based metabolomics approach to investigate metabolic changes that relate to phenotypic changes, following burn trauma in an adult population. The study showed expected (e.g., fatty acid and carbohydrate metabolism) and unexpected (e.g., tryptophan metabolism) metabolic changes longitudinally, which may allow the development of improved nutritional support following trauma (A in figure). The study also identified putative prognostic markers of outcome, such as M3328 (e.g., later sepsis onset), which, following validation and replication, may be used to provide stratification and personalized treatment path (B in figure).



Hypermetabolism is observed across many different metabolic classes in an adult sample population following burn trauma.



A single metabolite shows promise as a biomarker for stratification, as it shows statistically significant changes before sepsis and during sepsis, and is also predictive of multiple organ failure.

PHENOME CENTRE BIRMINGHAM

UNIVERSITY OF BIRMINGHAM

Data courtesy of the Phenome Centre Birmingham, UK.

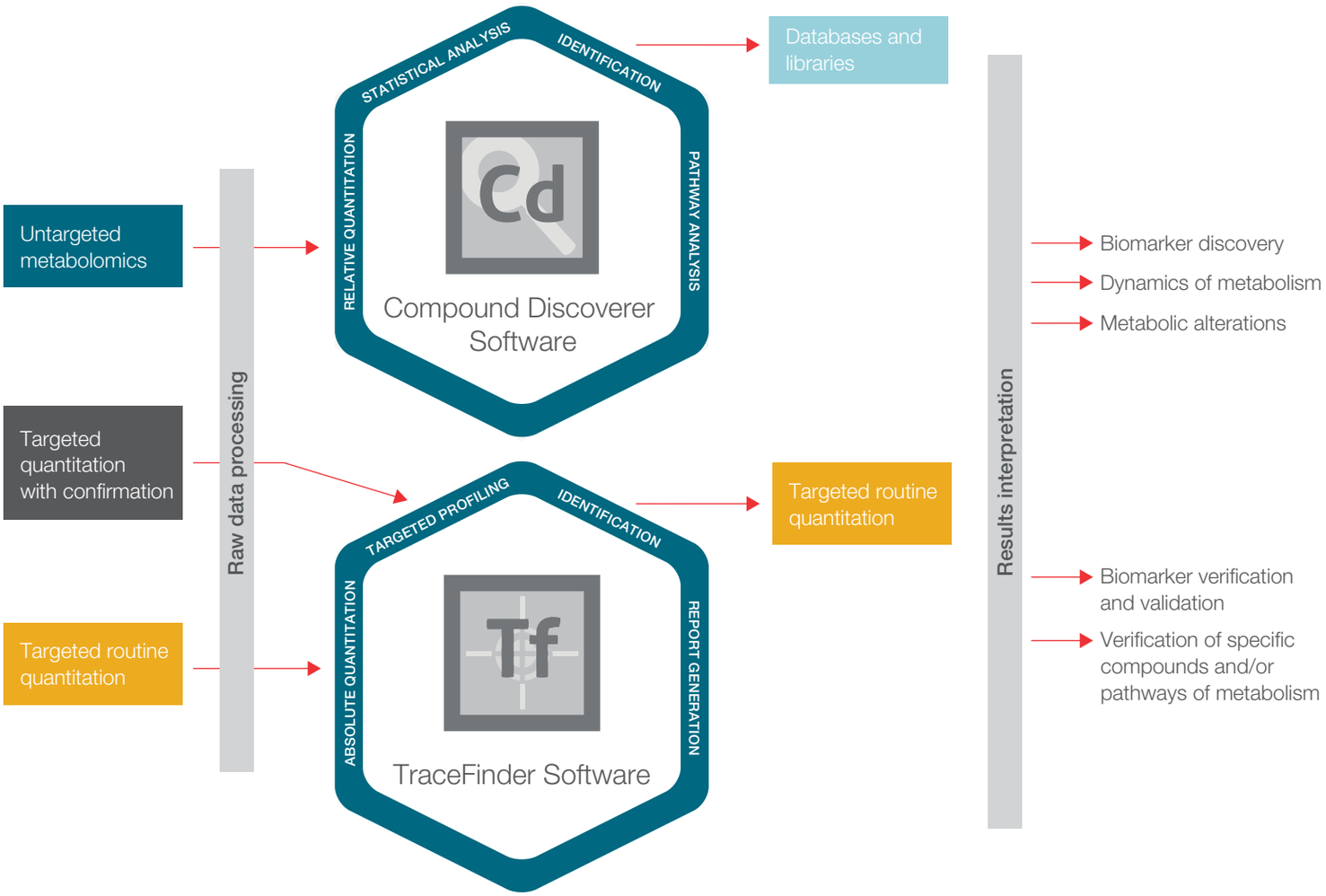
Streamlined data analysis solutions

Delivering the total package

We have invested heavily in developing new metabolomics software that lives up to the high standards set by our leading instrumentation—promising the same standards of quality, usability, and performance.

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 architecture. Get simplified analysis of large-scale data.



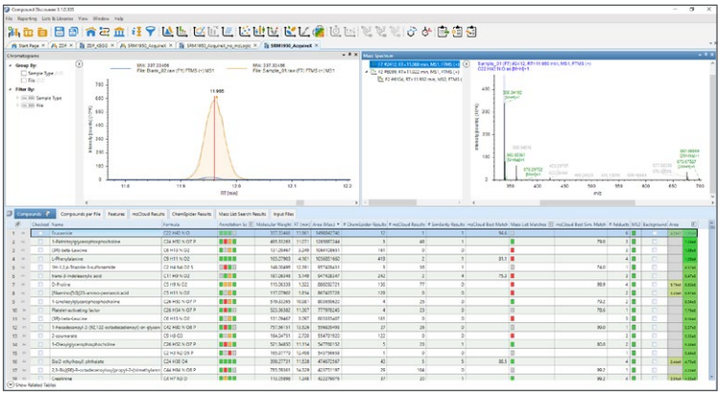
User-friendly software experience

Compound Discoverer software

Create actionable insights by streamlining data analysis and processing that provides unknown feature detection, data reduction to reduce false positives, statistical analysis, annotation tools to build confidence, and pathway mapping for metabolite associations. Thermo Scientific™ Compound Discoverer™ software easily transforms complex, unknown mass spectra into confident elucidation of compounds, enabling biological interpretation of the metabolome and confidence in pathway analysis.

Intuitive-user experience

The Data Results View is intuitively laid out creating an effortless experience. Chromatographic and mass spectral information are displayed side-by-side for corresponding compounds selected in the results table. Additional compound details, such as database and library search results, are easily accessible through the Related Tables feature. Icons to filter, graph, and plot are conveniently arranged at the top of the window, allowing you to smoothly transition between data outputs with minimal mouse clicks.

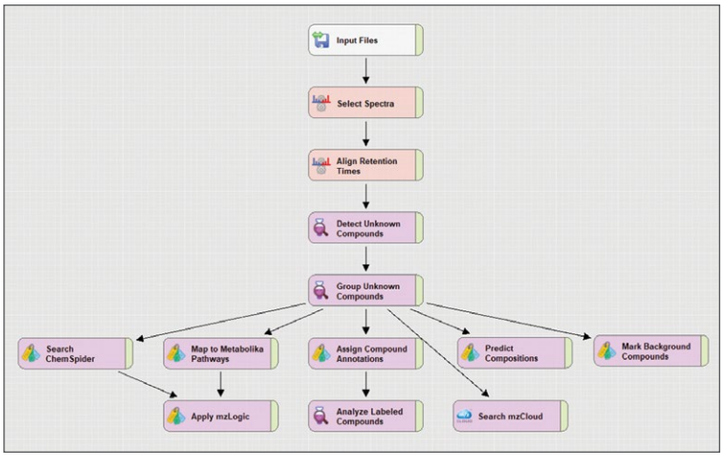


Results layout is arranged to easily review data.

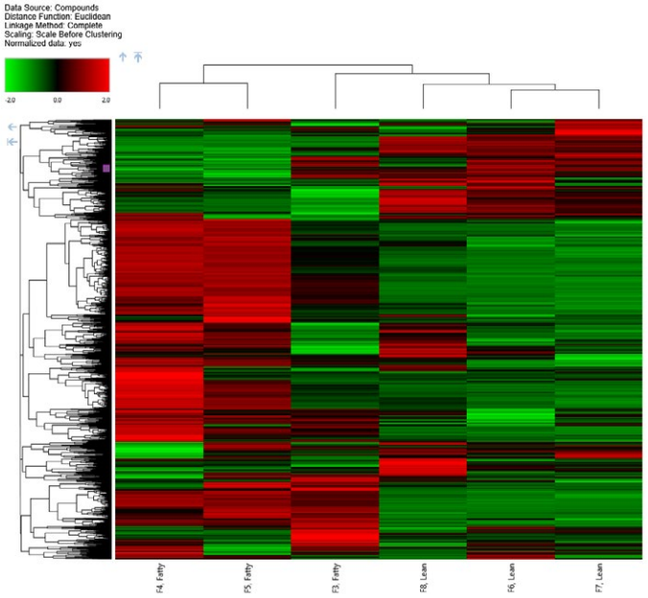
Easily customized workflows

Compound Discoverer software provides unlimited flexibility, making it easy to design a workflow that matches your metabolomics goals.

Unique to Compound Discover software, customized workflows are easy to build by dragging and dropping workflow nodes—data processing algorithms—into workflow trees that specify desired data flows. Workflow trees make it easy to visualize and modify workflows.



Workflow trees make it easy to create, review, and change your data processing workflows.



Reveals real differences

Compound Discoverer software makes it easy to visualize results in a meaningful way to quickly find real statistical differences—the differences that matter—between sample sets.

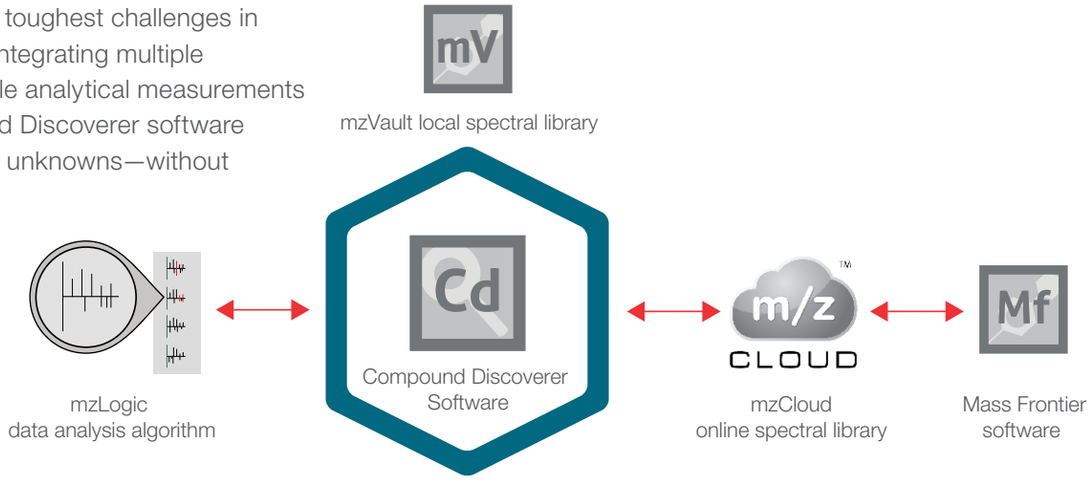
Customizable data visualization allows you to review only the data you choose. Configurable layouts let you quickly change between views. Multiple monitor support ensures that you can view more data once.

Hierarchical clustering enables sample grouping by similar datapoints for visualization and data mining.

Know your unknowns

Powerful unknown identification capabilities

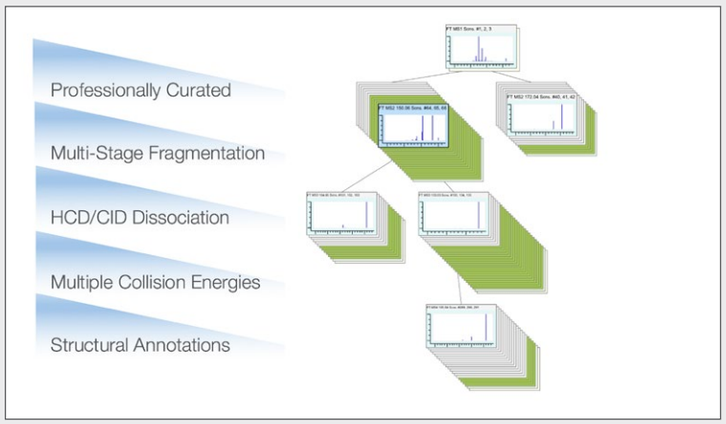
Unknown identification is one of the toughest challenges in many small-molecule analyses. By integrating multiple annotation tools that support multiple analytical measurements from mass spectral data, Compound Discoverer software enables you to identify more of your unknowns—without leaving the software application.



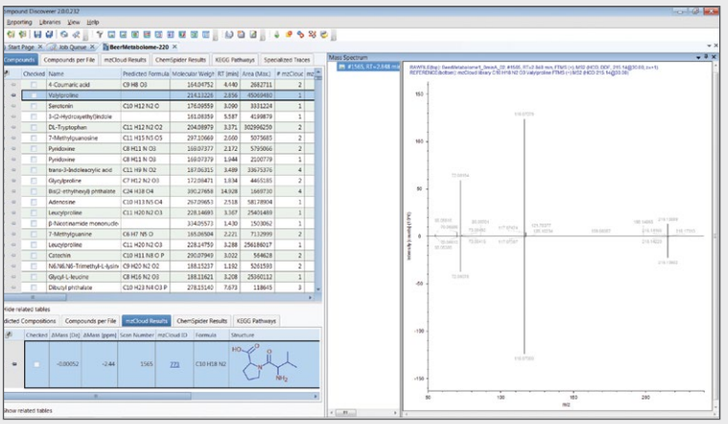
Comprehensive advanced mass spectral library

mzCloud is the industry's most extensively curated mass spectral fragmentation library. Automatically identify more unknowns faster against both the online Thermo Scientific™ mzCloud and in-house Thermo Scientific™ mzVault™ spectral libraries.

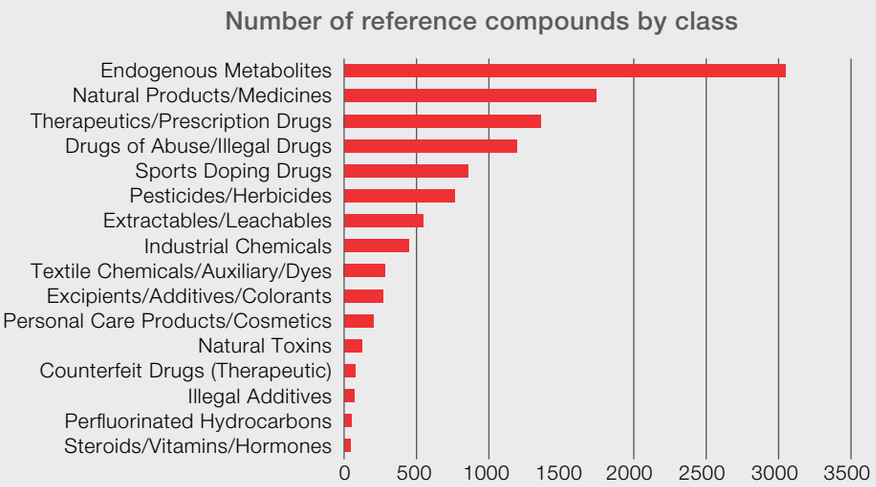
Beyond generating matches for identification, integrated batch searching of the mzCloud library can also produce similarity matches. Searching makes use of stepped collision energy scans to automatically model results using the library's multiple energy levels of reference fragmentation data.



Spectral trees consisting of MS^2 and MS^n fragmentation spectra are created for each compound using a range of collision energies. All spectra include structural annotation to accelerate structure elucidation.



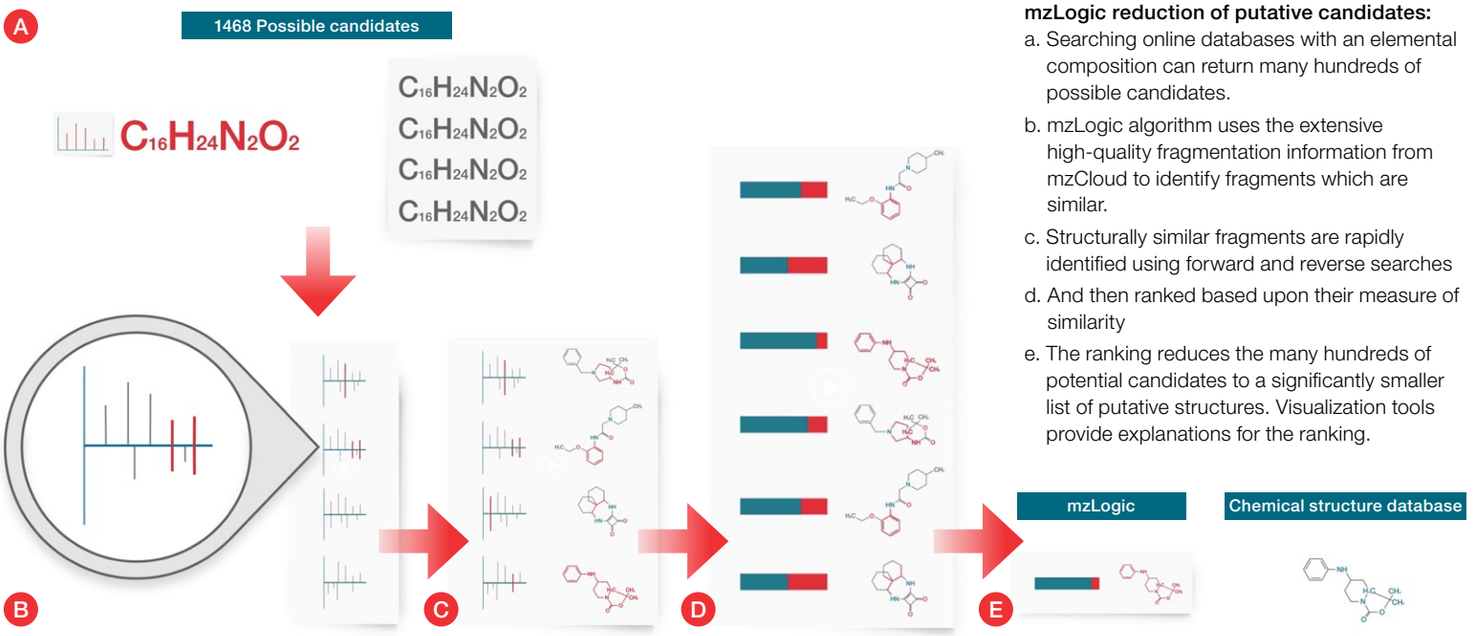
Mirror plot showing precursor and product ion matching of raw data against the library.



Unknown analysis means you may not know what you are looking for. The mzCloud mass spectral library contains small molecules representing broad chemical diversity ranging from endogenous metabolites to exogenous chemicals. New entries are continuously added, keeping the library up-to-date.

Identify unknowns more efficiently

What happens when you don't get a match from your library search or you have hundreds of potential structure matches and confirming potential structural matches still remains a challenge? The mzLogic algorithm compares mzCloud library similarity matches against database hits, looking for maximum common substructure. It then ranks putative hits based on structure overlap, leveraging real fragmentation information to rank structure candidates for true unknowns, increasing efficiency and confidence in small-molecule unknown identification.



mzLogic reduction of putative candidates:

a. Searching online databases with an elemental composition can return many hundreds of possible candidates.

b. mzLogic algorithm uses the extensive high-quality fragmentation information from mzCloud to identify fragments which are similar.

c. Structurally similar fragments are rapidly identified using forward and reverse searches

d. And then ranked based upon their measure of similarity

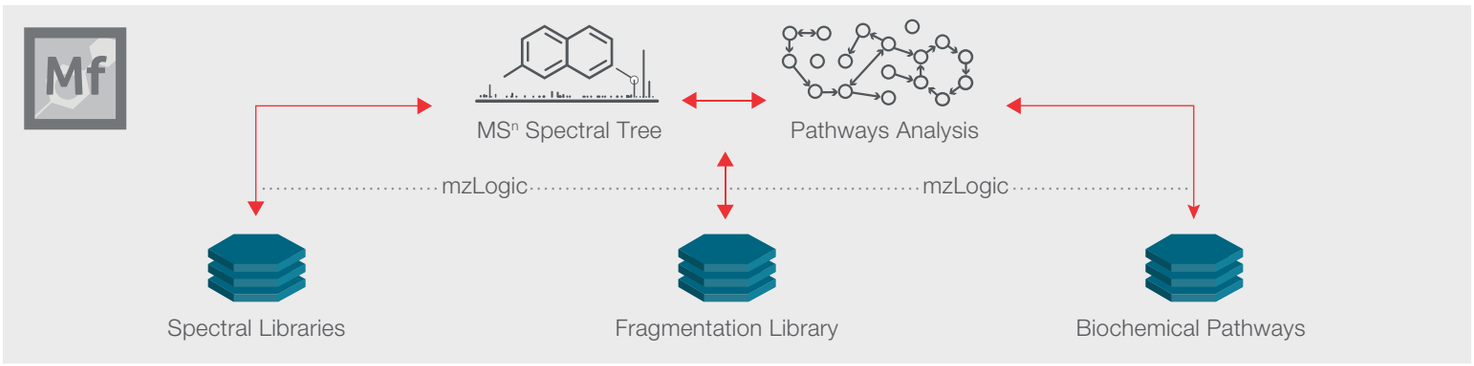
e. The ranking reduces the many hundreds of potential candidates to a significantly smaller list of putative structures. Visualization tools provide explanations for the ranking.

Absolute confidence for proposed structures

Interpretation and characterization of mass-spectral data can be an enormous challenge due to extreme compound structural diversity and complex samples. Thermo Scientific™ Mass Frontier™ software solves this challenge through powerful algorithms and fully-curated knowledge databases of spectral and fragmentation data, as well as the ability to confidently interrogate your fragmentation data through the use of fragmentation assignments which use more than 99% of all published fragmentation mechanisms.

This approach adds greater certainty to putative structure identification through the deep fragmentation and characterization information provided by the high-quality data and extensive spectral trees in the mzCloud library.

The new curator module automates spectral tree curation, fragment annotation and mass recalibration for your proprietary compounds to build a high quality curated local MS^n library.



Mass Frontier software structure elucidation platform.

Accurate lipid identification and profiling

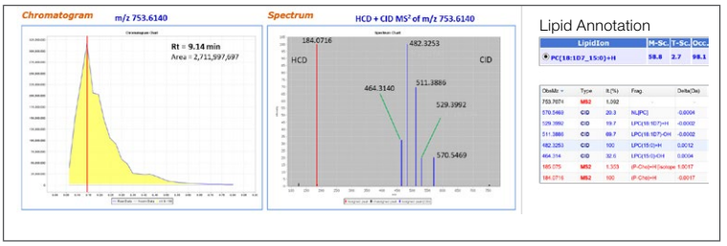
LipidSearch software

Lipidomics is a rapidly growing field of study that is crucial for understanding the underlying mechanisms for disease progression. Accurate identification and relative quantitation of lipids from biological samples requires sophisticated software with a comprehensive database. Thermo Scientific™ LipidSearch™ software delivers an easy-to-use, automated workflow that enables lipid identification and integration of the entire dataset into concise reports showing statistical differences between sample groups.

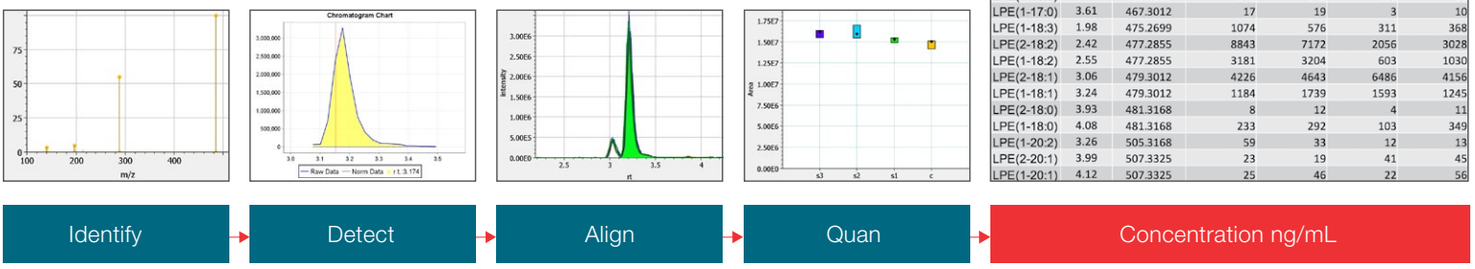
Confident annotation and identification

The software includes unique peak detection algorithms that are customized for LC-data dependent MS/MS, including the ability to combine information from Orbitrap Tribrid mass spectrometer CID/HCD fragmentations and MS^2 and MS^3 spectra.

These algorithms were introduced to reduce false positives, improve quantitation using labeled internal standards, and automate searching of MS^n data obtained by both HCD and fragmentation methods.



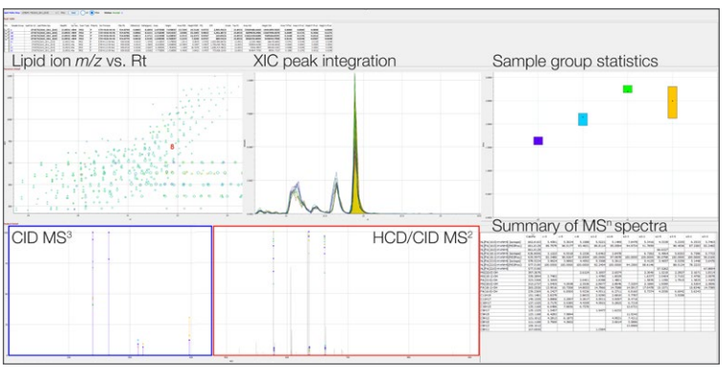
LipidSearch software combines data from both HCD and CID MS^2 searches to improve confidence in lipid annotation.



LPE	Rt min	[M+H]⁺ m/z	Conc C	Conc S1	Conc S2	Conc S3
LPE(1-16:1)	2.21	451.2699	131	267	354	452
LPE(1-16:0)	3.07	453.2855	242	642	158	710
LPE(1-17:0)	3.61	467.3012	17	19	3	10
LPE(1-18:3)	1.98	475.2699	1074	576	311	368
LPE(2-18:2)	2.42	477.2855	8843	7172	2056	3028
LPE(1-18:2)	2.55	477.2855	3181	3204	603	1030
LPE(2-18:1)	3.06	479.3012	4226	4643	6486	4156
LPE(1-18:1)	3.24	479.3012	1184	1739	1593	1245
LPE(2-18:0)	3.93	481.3168	8	12	4	11
LPE(1-18:0)	4.08	481.3168	233	292	103	349
LPE(1-20:2)	3.26	505.3168	59	33	12	13
LPE(2-20:1)	3.99	507.3325	23	19	41	45
LPE(1-20:1)	4.12	507.3325	25	46	22	56

LipidSearch software workflow.

The alignment algorithm merges positive and negative ion annotations at the same retention time into a single report and summarizes the MS^n spectral annotations. The relative amounts of the annotated lipid are displayed along with the statistical differences between the sample groups.



Alignment results view showing HCD/CID MS^2 and CID MS^3 data for triglyceride (16:0_18:1_22:0).

Comprehensive database coverage

Annotation of lipids via untargeted lipidomics requires a sophisticated software with an extended lipid database. The LipidSearch software database includes defined structures and more than 92 sub-classes and 1.4 million species.

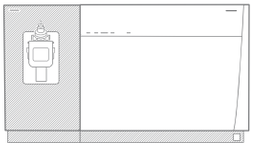
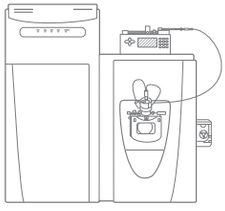
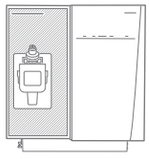
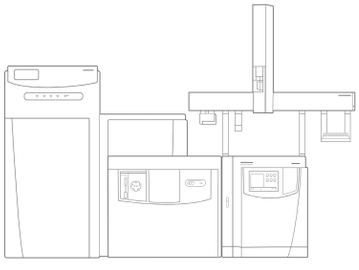
Fragmentation patterns are calculated and improved using expert knowledge based on experimental results. Lipid adduct ions and MS^n fingerprints are also included. Data are stored in XML files that are easily customized.

Comprehensive portfolio

Our complete Thermo Scientific instrument and software lineup

One resource

Thermo Fisher Scientific™ is a partner in the life sciences, providing innovative metabolomics solutions to address the challenges of biological research. We enable end-to-end workflows with column chemistries, comprehensive separation systems, mass spectrometry and integrated software.

Instrument lineup	Software lineup
 Orbitrap ID-X Tribrid mass spectrometer	Compound Discoverer software
 Q Exactive HF mass spectrometer	mzCloud mass spectral library
 Thermo Scientific™ TSQ Altis™ triple quadrupole mass spectrometer	mzVault spectral library
 Vanquish Duo UHPLC system	LipidSearch software
 Dionex ICS-5000+ Capillary HPIC system	Mass Frontier software
 Q Exactive GC Orbitrap mass spectrometer	TraceFinder software

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