

Designed to unravel complex chemical structures

Thermo Scientific Orbitrap IQ-X
Tribrid mass spectrometer



The future of small-molecule analysis is here

Designed for small-molecule analysis, the Thermo Scientific™ Orbitrap IQ-X™ Tribrid™ mass spectrometer redefines small molecule identification and characterization of unknown compounds. The trusted Tribrid architecture provides the richest MSⁿ data by leveraging the best quadrupole, linear ion trap and Thermo Scientific™ Orbitrap™ mass analyzers combined with intelligent data acquisition. Ease-of-use hardware improvements for automatic, hands-free calibration along with a fit-for-purpose software interface allow you to overcome the traditional bottlenecks in small molecule structure elucidation workflows.



The Orbitrap IQ-X Tribrid instrument seamlessly integrates with our industry-leading solutions—including Thermo Scientific™ Vanquish™ Duo UHPLC Systems, Thermo Scientific™ FAIMS Pro Duo interface, and Thermo Scientific™ Compound Discoverer™ software—for a complete workflow for small molecule structural characterization.

- **Increase certainty**

Real-Time Library Search increases confidence in unknown metabolite annotation and structure assignment of lipid isomers through search-driven, real-time spectral matching against local mzCloud™ or Thermo Scientific™ mzVault™ spectral libraries. Using decision-based triggering of MSⁿ or alternate fragmentation scans, you can tailor the analysis based on what information is needed and what is already known about the analytes in question.

- **Acquire rich, meaningful data**

Expanded Thermo Scientific™ AcquireX™ intelligent data acquisition workflows increase sample profiling efficiency and depth of analysis by automating inclusion/exclusion list creation for MSⁿ. The MSⁿ mass range has also been extended down to *m/z* 40 to capture low-mass fragments and differentiate challenging isomers.

- **Expand experimental possibilities**

The Orbitrap IQ-X Tribrid mass spectrometer provides experimental versatility for structural determination with collision-induced dissociation (CID), high-energy collision dissociation (HCD), and optional Thermo Scientific™ Ultraviolet Photodissociation (UVPD). Collision energies (CE) can be optimized in real time by making use of assisted CE determination. Optionally available are the Thermo Scientific™ 1 Million (1M) Resolution option to resolve isobaric components and fine isotopes, and the FAIMS Pro Duo interface for orthogonal selectivity based upon differential ion mobility.

- **Spend more time on reviewing results, less on instrument setup**

The Auto-Ready ion source standardizes calibration for consistent instrument performance with automated, remote calibration. Pre-built methods and optimized templates enable you to analyze complex samples effortlessly. Method templates define data acquisition for a variety of small molecules using combinations of high-resolution accurate-mass (HRAM) and ion trap mass analyzers with MSⁿ fragmentation using CID, HCD, or optional UVPD. The instrument increases sample throughput with fast polarity switching to acquire positive and negative mode data in a single run.



Drug metabolism and metabolomics



DNA/RNA-based drugs



Environmental and food safety



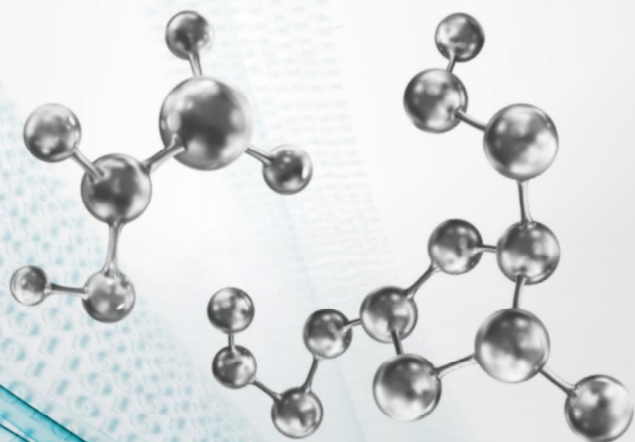
Extractables and leachables



Lipidomics

Next-generation Tribrid mass spectrometer for small molecules

Designed with new capabilities, the Orbitrap IQ-X Tribrid mass spectrometer is the cutting edge of small molecule analysis. Proven and trusted Tribrid architecture combines quadrupole, ion trap, and HRAM Orbitrap mass analyzer technologies for acquisition of the richest MSⁿ data for every sample. All fragmentation techniques—CID, HCD, and optional UVPD—are available at any stage of MSⁿ, with subsequent mass analysis in either the ion trap or ultra-high-resolution Orbitrap mass analyzer.



Enhanced capabilities

Real-Time Library Search uses Real-Time MS² spectral matching against local mzCloud or mzVault spectral libraries for decision-based triggering. This leads to higher confidence metabolite annotation, and improved characterization of unknowns.

Segmented quadrupole delivers higher transmission at narrower isolation widths, down to 0.4 *m/z*, improving selectivity for co-eluting compounds.

New AcquireX acquisition workflows increase coverage and throughput with the flexibility to submit several experiments from a single sequence, and with new algorithms for improved background exclusion and component detection.

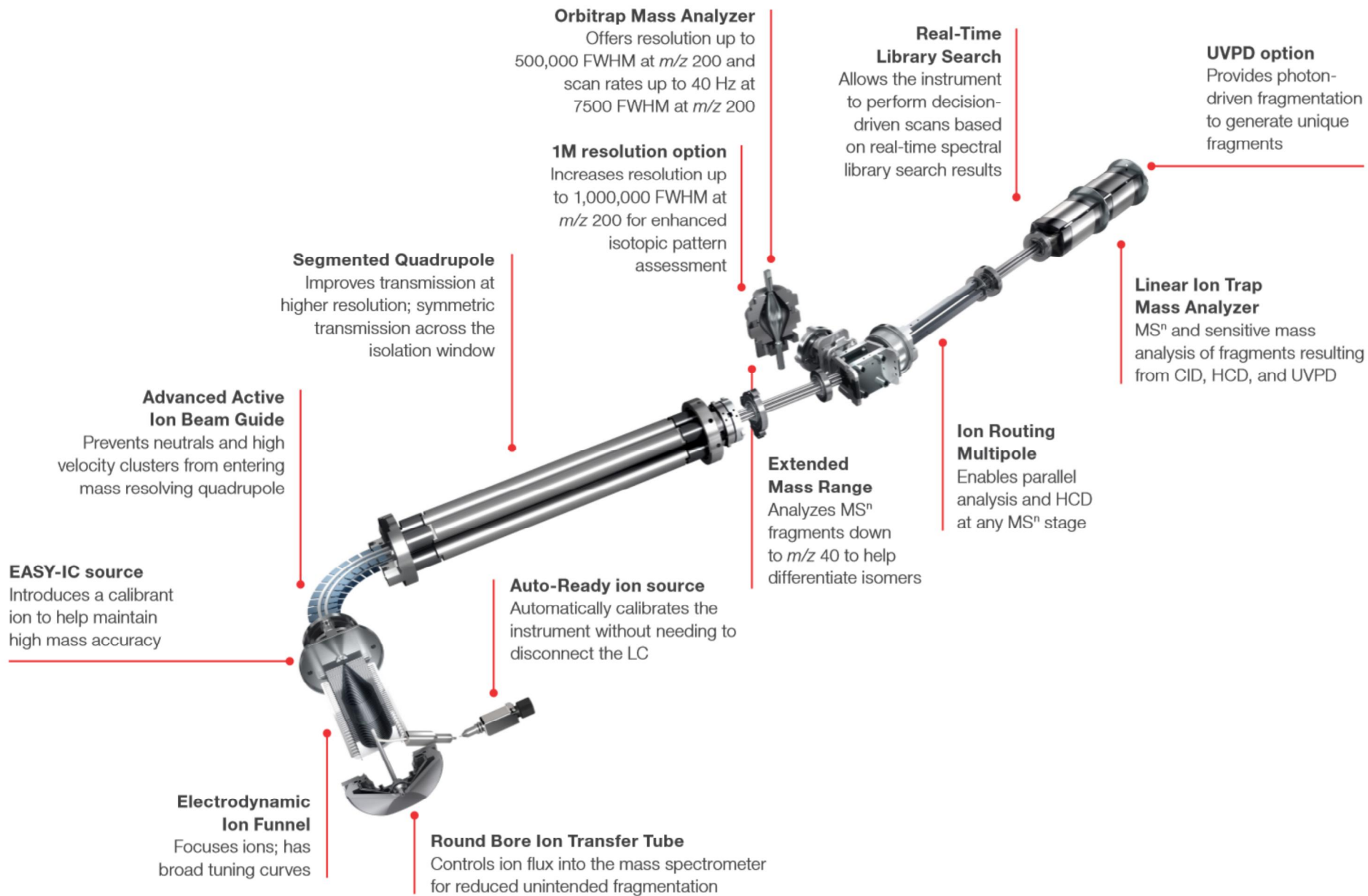
Auto-Ready ion source provides scheduled, or on demand, remote system checks and calibrations, without disruption to your LC-MS system.

Expanded experimental options

UVPD produces fragment ions indicative of double bond locations and other unique structurally diagnostic information for analysis of various compound classes, including lipids and glucuronides.

1M provides higher resolution and fine isotope information to help determine elemental composition of the analytes.

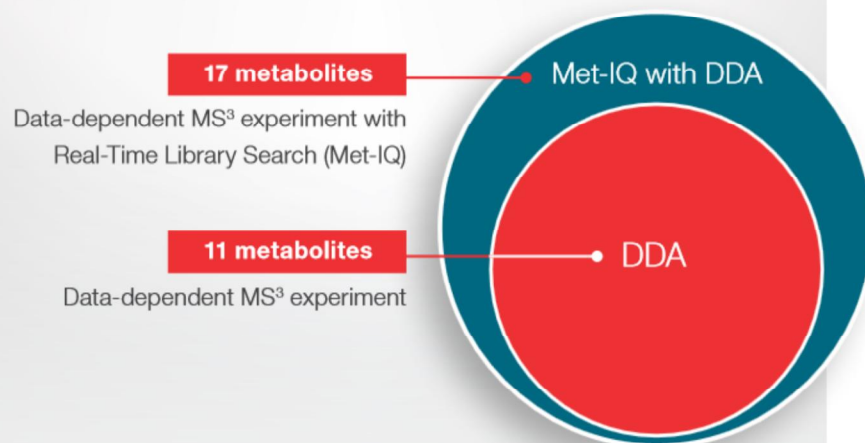
FAIMS Pro Duo interface is a differential ion mobility device that increases selectivity and reduces interferences, for improved detection with expanded lower limits of quantitation (LOQ).



Improved structural characterization with Real-Time Library Search

Acquisition and interpretation of mass spectra to characterize small-molecule unknowns can be a formidable task. Sample complexity, background interferences, compound structural diversity, and the shortage of robust data processing tools can make it difficult to set up analytical experiments and interpret data.

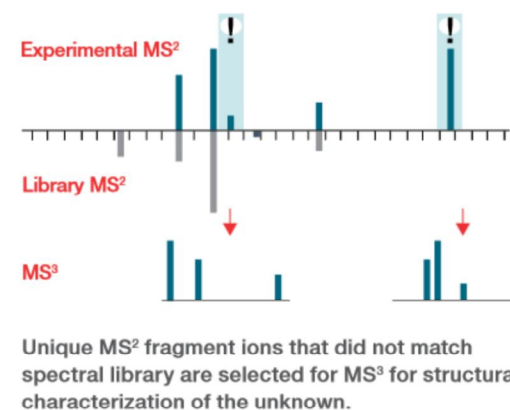
The Orbitrap IQ-X Tribrid mass spectrometer overcomes these challenges with advanced data acquisition and processing tools that are accessed in a single powerful instrument control software, harmonized across all next-generation Thermo Scientific™ mass spectrometers.



Real-Time Library Search guides data acquisition and analysis

Using an offline version of mzCloud or a custom-built spectral library, Real-Time Library Search evaluates MS² spectra in real time to trigger additional scan events based on the search results.

- Unknowns can preferentially trigger MSⁿ or alternate fragmentation events on fragments that did not match spectral library, to obtain more structural information.
- Additional scans can be triggered on possible isomers to aid in differentiation.
- Compounds with a library match can be blocked from triggering additional scans to instead collect data on other unknowns.



Find more metabolites with less effort using Met-IQ

The Met-IQ data acquisition strategy uses Real-Time Library Search to find spectral similarities with library compounds. When an MS² spectrum is similar to a library spectrum, such as a drug-metabolite compared to the original drug, additional information is collected. This has multiple benefits:

- Only compounds with matching fragments are selected for additional scans, it also identifies them as potential targets during the data processing step.
- Limiting additional data collection to only structurally related compounds means the instrument spends more time collecting MS² spectra for a more in-depth analysis.
- Analyzing metabolized amprenavir six additional potential drug metabolites were found in a single run using Met-IQ acquisition compared to a traditional data dependent acquisition (DDA).

Sample provided by Dr. Shuguang Ma, Genentech, South San Francisco, CA
For research purposes only.

Application-specific methods are one click away

The intuitive method editor features a drag-and-drop user-friendly interface with predefined, optimized method templates.

- Run advanced experiments effortlessly with method templates for a large range of applications.
- Edit parameters in easily accessible panels, featuring recommended defaults for each experiment.

AcquireX workflows

Real-Time Library Search

Go from data to actionable results with a suite of software tools

m/z™ mzCloud™ mass spectral library
A database with over 19,000 compounds to help annotate a wide variety of unknowns

Thermo Scientific™ mzVault™ spectral library
Curates custom libraries from known standards



Thermo Scientific™ mzLogic Algorithm
Compares spectra against an extensive library of fragmentation data to get the highest confidence candidates for unknowns

Thermo Scientific™ Mass Frontier™ spectral interpretation software
Helps analyze a compound's fragments and structure

Thermo Scientific™ Xcalibur™ software
Provides a centralized platform for instrument control and a wide variety of data processing tools

Thermo Scientific™ AcquireX™ intelligent data acquisition software
Allows automatic generation of inclusion/exclusion lists and iterative sample interrogation

Thermo Scientific™ Compound Discoverer™ software
Identifies unknowns and performs statistical analysis

Thermo Scientific™ Almanac™ application
Provides remote access to instrument health and alerts to any issues

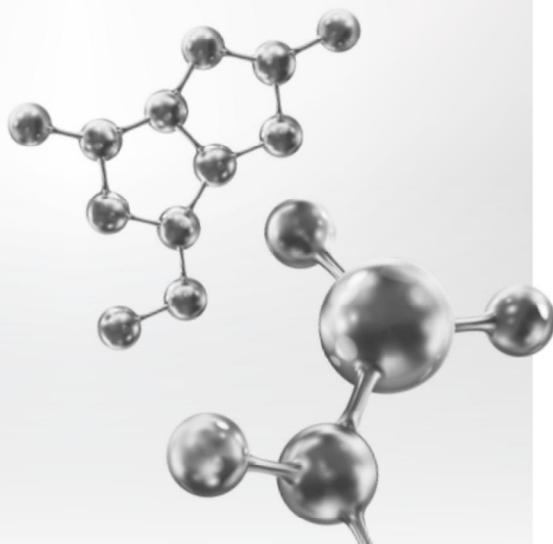
Thermo Scientific™ LipidSearch™ software
Enables rapid high confidence analysis of lipids

Thermo Scientific™ TraceFinder™ software
Provides high speed quantitative processing of large data sets

Thermo Scientific™ FreeStyle™ software
Allows for rapid and straightforward examination of chromatograms and mass spectra

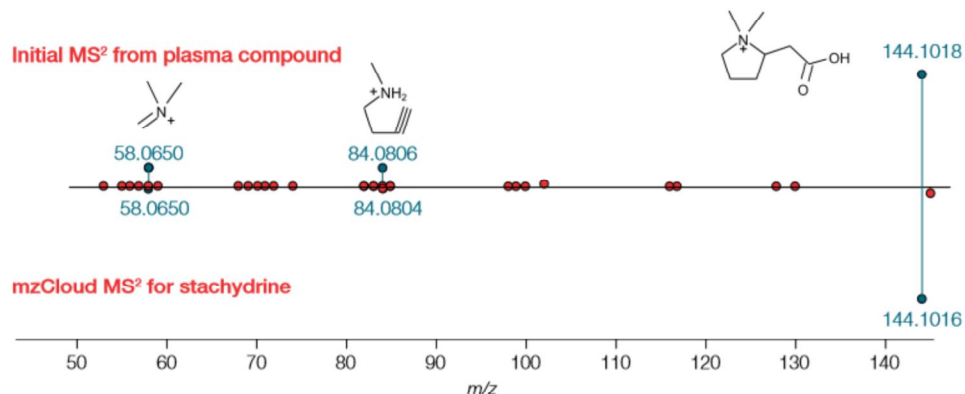
Metabolomics like never before

The Orbitrap Tribrid IQ-X mass spectrometer offers a streamlined approach to routinely achieve comprehensive metabolome coverage with confident compound annotation through comparison against spectral libraries or by *de novo* structural elucidation of unknown metabolites. The power of the Orbitrap mass analyzer combined with AcquireX data acquisition workflows and Real-Time Library Search of MSⁿ spectra redefines possibilities for small molecule research. Optional UVPD generates unique fragments for unparalleled lipid structure characterization.



Intelligent solutions to metabolomics problems

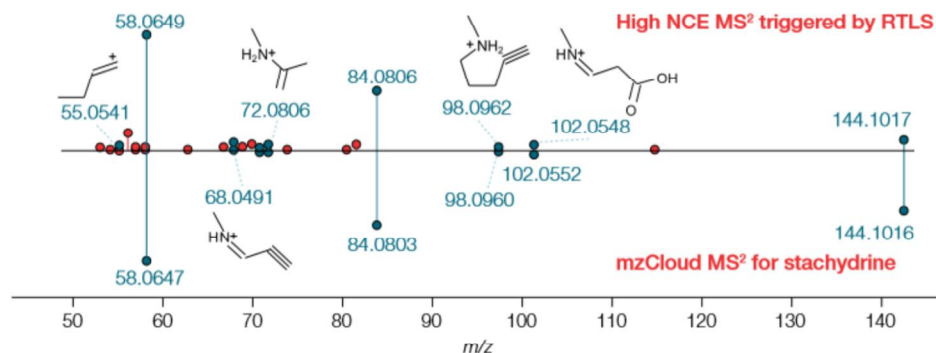
Getting comprehensive data in metabolomics is challenging. There are complex matrices and an extensive number of unknowns to be investigated. Using Real-Time Library Search, data can be collected intelligently to ensure not only comprehensive coverage, but also that the most useful structural information is being collected the first time.



Mirror plot of stachydrine and unknown compound triggered for MSⁿ.

Real-Time Library Search for added confidence

Static parameters do not always yield sufficient information, compounds can be under-fragmented or missing a critical fragment for confident annotation. Using Real-Time Library Search, the instrument interrogates the library in real time and collects additional data on poorly annotated compounds. For example, stachydrine yields few structural peaks using standard settings (see above). Triggering a higher normalized collision energy (NCE) scan guided by Real-Time Library Search results acquires the information needed for confident annotation.



Mirror plot of stachydrine and unknown compound triggered for additional MSⁿ scans.

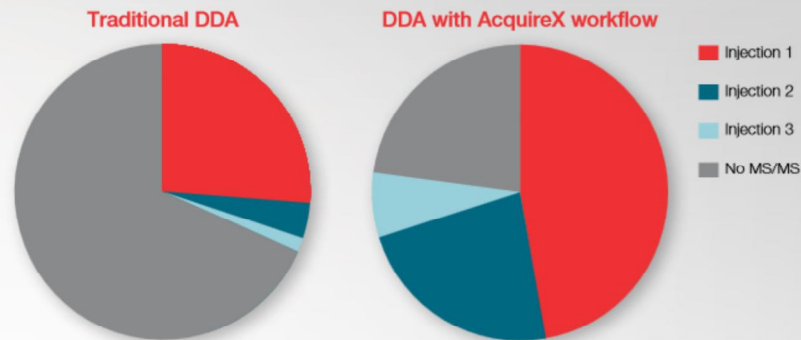
Results obtained in collaboration with Dr. Gary Patti, Washington University in St. Louis, MO.
For research purposes only.

Comprehensive sample coverage with AcquireX data acquisition

AcquireX data acquisition automates generation of inclusion and exclusion lists between runs to target new compounds in subsequent runs and increase the depth of coverage. The number of unique compounds with fragmentation spectra in human plasma (NIST SRM1950) obtained using AcquireX workflows are more than doubled compared to traditional DDA.

Sequence Design							
AcquireX Template Injections							
#	Name	Type	Group	Instrument Method	Vial	Inj Vol (µl)	Comment
1	Blank_01	Blank	1	MS1	1	10.00 µl	group 1
2	ExclusionRef_01	Exclusion	1	MS1	2	10.00 µl	
3	Sample_01	Inclusion	1	MS1	3	10.00 µl	
4	Sample_02	Inclusion	1	MS1	4	10.00 µl	group 2
5	ID_01	Id	1	MSn incl_excl	5	10.00 µl	
6	ID_02	Id	1	MSn incl_excl	5	10.00 µl	
7	ID_03	Id	1	MSn incl_excl	5	10.00 µl	group 2
8	Wash	Unknown	1	MS1	20	10.00 µl	
9	ExclusionRef_01	Exclusion	2	MS1	5	10.00 µl	
10	ExclusionRef_02	Exclusion	2	MS1	6	10.00 µl	group 2
11	Sample_01	Inclusion	2	MS1	7	10.00 µl	
12	Sample_02	Inclusion	2	MS1	8	10.00 µl	
13	Sample_03	Inclusion	2	MS1	9	10.00 µl	group 2
14	ID_01	Id	2	MSn incl_excl	10	10.00 µl	

Number of compounds with fragmentation spectra



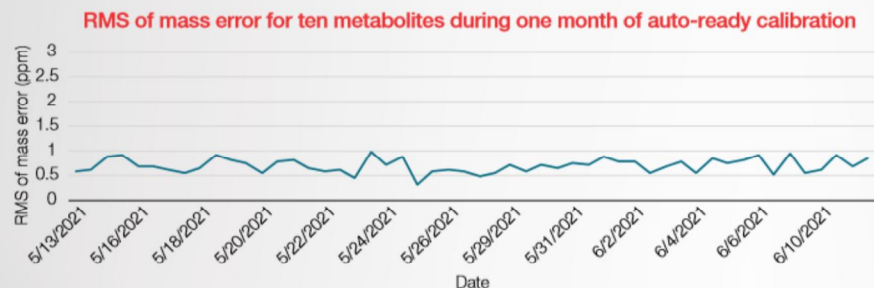
Additional advanced Deep Scan workflow

A comprehensive user interface allows you to queue multiple experiments in one sequence....

.....and generate a combined inclusion/exclusion list from multiple samples to account for variable conditions, reducing the risk of missing low level compounds.

Auto-Ready ion source for effortless calibration

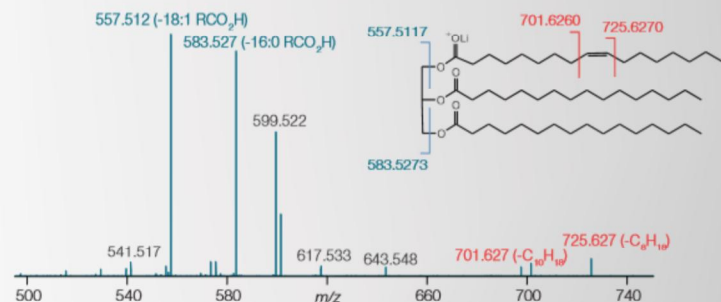
The Auto-Ready ion source simplifies calibration by integrating a dedicated pump, emitter, ion transfer tube, and container of Thermo Scientific™ Pierce™ FlexMix™ Calibration Solution inside the instrument. The mass spectrometer will calibrate itself regularly during scheduled off hours without interrupting data acquisition. During a months worth of experiments, ten metabolites showed a root mean square (RMS) of less than 1 ppm using the Auto-Ready ion source for scheduled mass and system calibrations, and EASY-IC ion source to maintain mass accuracy between calibrations.



A breakthrough in lipid structural elucidation

Using soft fragmentation techniques such as CID or HCD, it is impossible to locate double bonds in the acyl chain of lipid molecules. Optional UVPD produces structurally diagnostic information including ions indicative of double bond locations and site-specific glucuronidation.

UVPD hardware is enclosed inside the mass spectrometer with MSⁿ fragments generated in the linear ion trap. Both the ion trap and Orbitrap mass analyzers detect these fragments to provide unambiguous characterization of various lipid classes.



HRAM UVPD MS² spectrum of [M+Li]⁺ precursor ions of TG 16:0/16:0/18:1, with two fragment ions diagnostic of the double bond location (data obtained on Thermo Scientific™ Orbitrap™ Fusion Lumos™ mass spectrometer).

Characterize and quantify small-molecule structures with greater confidence

Combined with powerful spectral library and data processing software the Orbitrap IQ-X Tribrid mass spectrometer provides the ultimate solution for accuracy efficiency and overall productivity of drug impurity and metabolite identification extractable and leachable analysis and other related applications

Optional UVPD allows generation of unique fragments complementary to CID and HCD to obtain detailed structural information for high-confidence identification of unknown compounds. Optional rM adds enhanced resolution and fine isotope detection to improve determination of elemental composition and enhance stable isotope labeling experiments. Optional FAIMS Pro Duo interface increases selectivity and provides orthogonal gas-phase fractionation using differential ion mobility

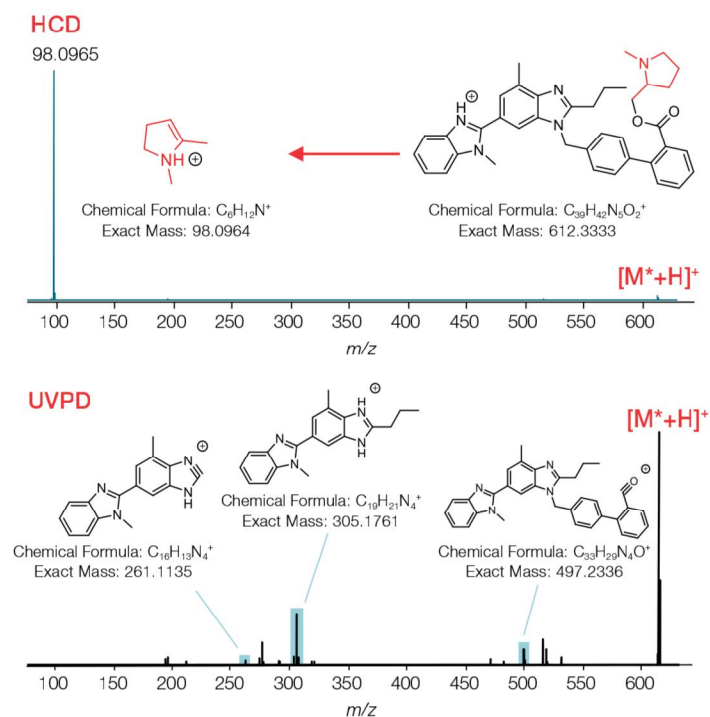


UVPD source shown as positioned inside the mass spectrometer.



Alternate fragmentation with UVPD

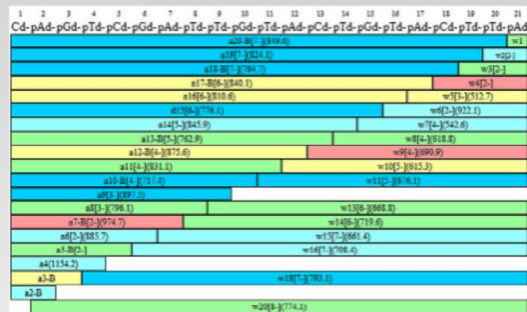
Certain compounds break apart to yield fragments with minimal structural information using HCD and CID. Adding the UVPD option provides an alternate mode of fragmentation to help elucidate complex structures. For example, derivatized telmisartan yields only a non-informative fragment using HCD (top panel shown below). Using UVPD, multiple structurally significant fragments are generated and the structure can be characterized (bottom panel).



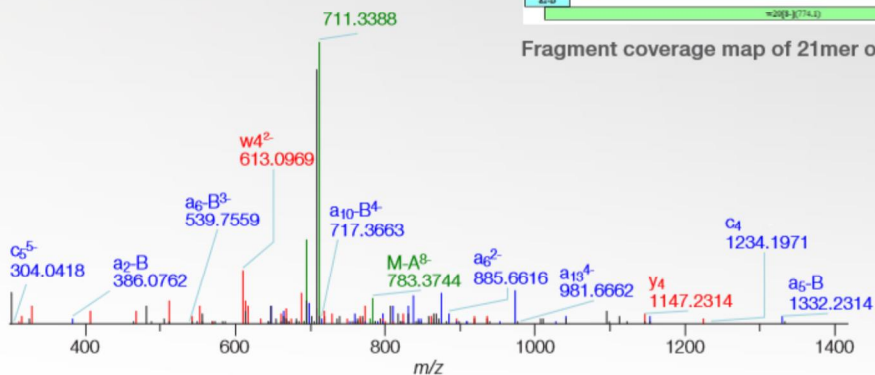
MS² spectra of derivatized telmisartan using HCD (top) and UVPD (bottom) fragmentations.

Comprehensive oligomer analysis

Nucleic acid oligomers are an emerging compound class that have shown promise as biopharmaceuticals. Using assisted CE, the Orbitrap IQ-X Tribrid mass spectrometer can determine an optimal CE for fragmentation to help achieve complete sequence coverage. Additionally, UVPD results in efficient fragmentation regardless of the charge state of the oligomer, reducing the need for lengthy method optimization.



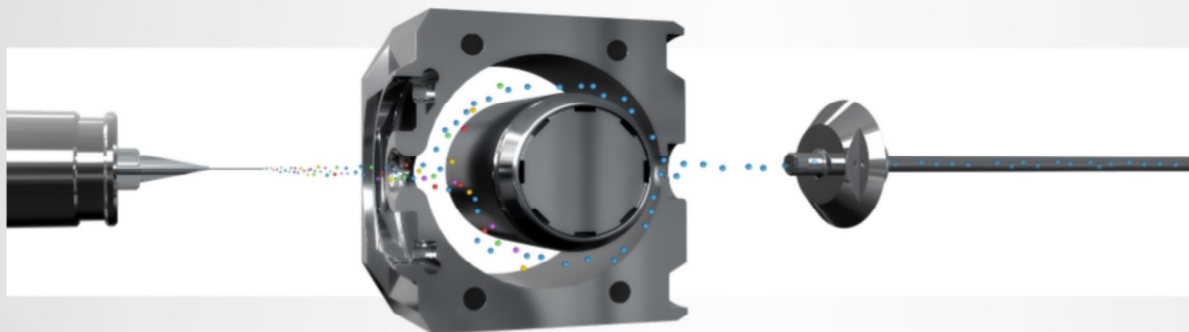
Fragment coverage map of 21mer oligonucleotide.



Assisted CE HCD MS² spectra of 21mer oligonucleotide.

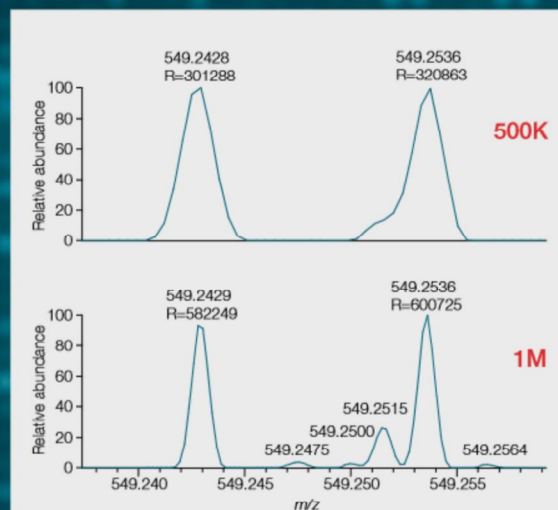
Increased sensitivity with FAIMS Pro Duo interface

The Orbitrap IQ-X Tribrid mass spectrometer is compatible with the FAIMS Pro Duo interface option to increase the limit of quantitation for select compounds. For example, monensin analyzed in muscle meat matrix, the limit of quantitation was improved by an order of magnitude when the experiment was performed using the FAIMS Pro Duo interface, shown below.

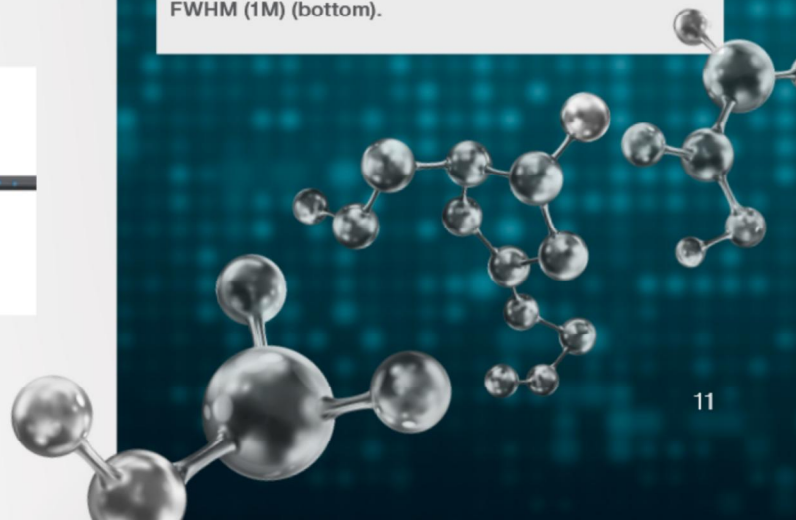


1M resolution for fine isotope structure

Sometimes a compound can have a fine isotope structure that cannot be resolved using high resolution settings. Using optional 1M, even the most complicated isotopic fine patterns can be resolved, providing unambiguous determination of the elemental composition. For example, the compound shown in the top spectrum could belong to $C_{28}H_{35}NO_7S$ and $C_{30}H_{32}N_3O_4P$. Using 1M, the identity is clearly determined as $C_{28}H_{35}NO_7S$.



SIM scan of extractable and leachable compound collected at 500,000 FWHM (top) and 1,000,000 FWHM (1M) (bottom).



ALM

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