

Orbitrap ID-X Tribrid mass spectrometer

Transforming small molecule identification and structure elucidation

Keywords

[Orbitrap ID-X mass spectrometer](#),
AcquireX, small molecule identification,
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The Thermo Scientific™ Orbitrap ID-X™ Tribrid™ mass spectrometer redefines small molecule identification and characterization by leveraging the proven and trusted Tribrid architecture with new automated data acquisition and processing routines. The new instrument, with its fit-for-purpose user interface, is designed to overcome the traditional bottlenecks in small molecule structural identification and characterization.

Novel Orbitrap ID-X MS features

- Thermo Scientific™ OptaMax™ NG ion source for enhanced usability and robustness with a redesigned HESI sprayer and built-in APCI assembly
- Streamlined calibration routines with improved Thermo Scientific™ Orbitrap™ mass analyzer calibration for ions with $m/z < 200$
- User interface and default parameters optimized for small molecule analysis
- Assisted CE provides real-time collision energy optimization
- AcquireX data acquisition mode for all-inclusive, automated sample profiling that enables MS^n analysis to be truly compatible with an LC-timescale
- Expansive collection of application specific small molecule methods for metabolomics, lipidomics, metabolites, impurity, extractables and leachables, which are organized as easy-to-use, one-click method templates
- MS^n Library Builder method enables the collection of high-quality, fragment ion-rich MS^n spectra for the creation of local library

Proven Tribrid architecture

- Tribrid architecture combines a quadrupole mass filter, a dual-cell linear ion trap, and the [Orbitrap mass analyzer](#) for fast, selective, and sensitive MSⁿ analyses
- High-field Orbitrap mass analyzer for ultra-high resolution and the fastest acquisition rates
- Dual fragmentation techniques—CID and HCD—are available at any stage of MSⁿ, with subsequent mass analysis in either the ion trap or Orbitrap mass analyzers

Hardware specifications

OptaMax NG ion source

- Outstanding performance without adjustments
- Improved sprayer alignment and stability
- Inter-changeable HESI/APCI probe
- Enhanced exhaust port efficiently removes solvent vapor, improving uptime and reducing chemical noise

Ion optics

S-Lens

- Progressively spaced stacked-ring ion guide (S-Lens) captures and efficiently focuses ions into a tight beam while minimizing in-source dissociation

Active beam guide

- Reduces noise by preventing neutrals and high-velocity clusters from entering the quadrupole mass filter
- Axial field along the length of the rods improves ion transfer robustness

Quadrupole mass filter

- MS/MS precursor ion selection with high efficiency transmission from m/z 50 to 2,000
- Highly specific precursor isolation window widths down to 0.4 amu

Ion-routing multipole

- Provides efficient ion trapping and ion transfer to the Orbitrap and linear ion trap mass analyzers
- Performs higher-energy collisional dissociation (HCD) to obtain fragment ion spectra with multiple generations of product ions, similar to the triple quadrupole fragmentation process

Orbitrap mass analyzer

- High-field Orbitrap mass analyzer with resolving power up to 500,000 FWHM at m/z 200 and isotopic fidelity up to 240,000 FWHM

Dual-pressure linear ion trap

- Dual-dynode detector with high linear dynamic range for improved quantitation
- MSⁿ precursor isolation from m/z 50 to 2,000
- Low-pressure cell for improved scan speed, resolving power, and mass accuracy
- High efficiency, collision induced dissociation (CID) favors first generation fragment ions

Vacuum system

- Split-flow turbomolecular pump regulates vacuum in multiple regions
- Precise and accurate low mTorr pressure control in the ion-routing multipole
- Differentially pumped to $<2 \times 10^{-4}$ Torr in the ion trap chamber
- Differentially pumped to $<2 \times 10^{-10}$ Torr in Orbitrap mass analyzer

Optional Thermo Scientific™ EASY-IC™ ion source

- Generates internal calibrant ions for real-time mass calibration of every Orbitrap mass analyzer spectrum

Performance characteristics

Mass range

- m/z 50–2,000

Orbitrap mass analyzer resolution

- 7,500–500,000 (FWHM) at m/z 200

Scan rate (under defined conditions)

- Orbitrap mass analyzer MSⁿ up to 30 Hz
- Ion trap MSⁿ up to 40 Hz

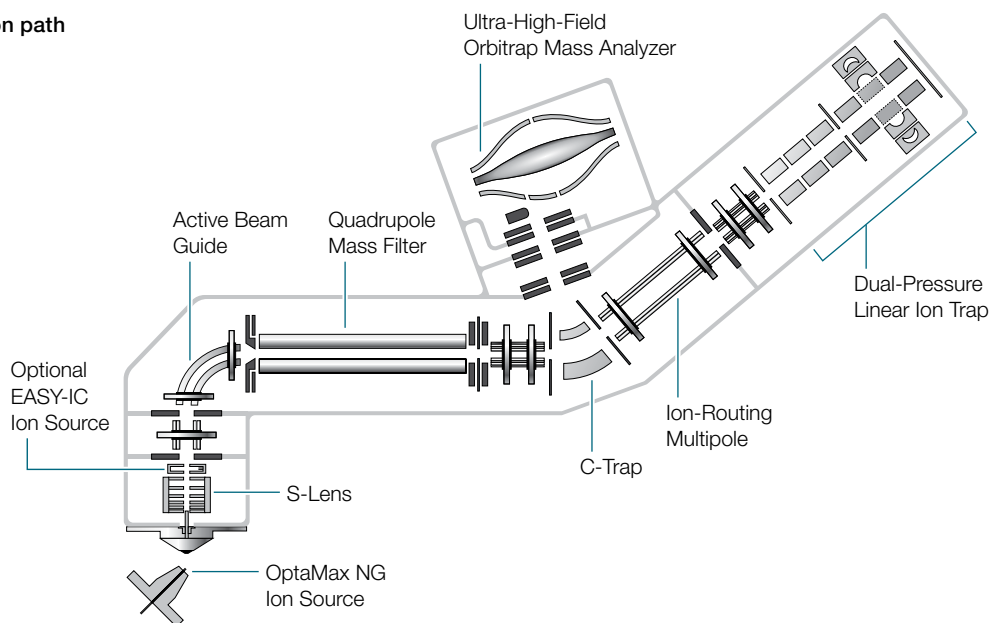
Mass accuracy (under defined conditions)

- <3 ppm RMS using external calibration
- <1 ppm RMS using internal calibration

MS/MS electrospray ionization (ESI) ion trap sensitivity

- 2 μL of a 50 fg/ μL solution of reserpine (100 fg total) injected at a flow of 500 $\mu\text{L}/\text{min}$ will produce a minimum signal-to-noise ratio of 100:1 for the transition of the isolated protonated molecular ions at m/z 609 to the largest two product ions, m/z 397 and m/z 448, when the mass spectrometer is operated at unit resolution in the full-scan MS/MS mode, m/z 165–615. The test requires the HESI probe.

Orbitrap ID-X MS ion path



Dynamic range

- >5,000 within a single scan

MS scan power

- MSⁿ, for n = 1 through 10

Multiplexing using ion-routing multipole

- Up to 10 precursors per scan using the quadrupole mass filter for targeted MS² and Selected Ion Monitoring (SIM)

Polarity switching

- One full cycle in 1.1 sec (one full scan in positive mode and one full scan in negative mode at a resolution setting of 30,000)

Analog inputs

- One analog input (0–1 V)
- One analog input (0–10 V)

Software features

Data system

- [Thermo Scientific™ Xcalibur™ software](#) for data processing and automated data acquisition
- Tune software for instrument control, system calibration, diagnostics, and manual data acquisition
- Method Editor software with comprehensive small molecule application-specific templates and a drag-and-drop user interface to facilitate method development

Operation modes

- *Background Exclusion* AcquireX workflow utilizes an exclusion reference to automatically generate an exclusion list that directs the MS away from fragmenting background ions in favor of sample specific compounds

- *Exclusion and Component Inclusion* AcquireX workflow utilizes the exclusion and inclusion references to automatically generate the corresponding exclusion and inclusion lists allowing the triggering of MSⁿ scans on unique precursor ions of interest that are only present in the sample

- *Deep Scan* AcquireX workflow provides the ultimate depth and coverage for complex samples by combining the efficiency of the inclusion and exclusion list-based MSⁿ triggering with automated re-injections, where each re-injection is informed by the preceding LC-MS analysis through dynamic updating of the exclusion and inclusion lists

- MSⁿ Library Builder method acquires high-quality, fragmentation-rich MSⁿ product ion spectra utilizing Assisted CE for improved signal to noise for the HCD and CID product ions

- Data dependent MS² acquisition mode allows rapid profiling of complex samples

- Data dependent MS³ and higher order fragmentation methods allow in-depth characterization of precursors to aid unknown small molecule structure elucidation

Exclusive technologies

- AcquireX allows automated re-interrogation of the sample aided by automatically updated inclusion and exclusion lists
- Assisted CE mode utilizes hidden ion trap scans to assess the optimal collision energy in real-time, automatically generating precursor ion specific breakdown curves to select the collision energy needed to sufficiently deplete a given precursor ion. This mode is ideally suited for the MSⁿ Library Builder method.

- Complete experimental flexibility where precursor fragmentation can take place in the ion-routing multipole (HCD) or in the ion trap (CID) with fragment detection in the linear ion trap or Orbitrap mass analyzers at any stage of MSⁿ analysis
- Normalized Collision Energy for both CID and HCD fragmentation techniques ensures reproducible data from day to day and instrument to instrument
- Dynamic Scan Management allows for intelligent, real-time scheduling, parallelization, and prioritization of scan events. It also enables selection, sorting, and routing of precursors to different fragmentation modes and analyzers based on user-selected parameters, including precursor *m/z* and/or intensity.

Advanced data-dependent experiments

- AcquireX automated acquisition workflows allow comprehensive sample interrogation by incorporating automated sample re-injection logic aided by automatically generated and updated inter-run inclusion and exclusion lists
- Advanced scan filters allow highly specific and customizable MSⁿ data acquisition. For example:
 - ‘Targeted Mass Difference’ filter selects only precursors that have peaks with a specified mass difference
 - ‘Targeted Isotope Ratio’ filter selects only precursors that have peaks with the defined intensity ratio and mass difference
 - ‘Targeted Loss Inclusion’ filter selects only precursors that have the defined targeted mass loss
 - ‘Targeted Mass Trigger’ triggers a scan only if the system detects a product ion from the user defined list
 - A new ‘MSⁿ Quality Trigger’ triggers complementary ITMSⁿ scans if the corresponding FTMSⁿ scan S/N drops below a user-definable threshold
- Isolation window offset allows for custom centering of the isolation window when working with broad isotopic distributions or with compounds that have unique isotopic distributions due to chemical labeling

Optional application-specific software

- [Thermo Scientific™ Compound Discoverer™ software](#)—an integrated solution for small-molecule identification
- [Thermo Scientific™ Mass Frontier™ software](#)—predictive fragmentation software for spectral interpretation, local library generation and classification to identify unknowns

Installation requirements

Power

- Instrument: 230 Vac ± 10% single phase, 15 Amp, 50/60 Hz, with earth ground
- Data system: 120 or 230 V single phase, 50/60 Hz, with earth ground

Gas

- Ultra-high-purity helium (99.999%) with less than 1 ppm each of water, oxygen, and total hydrocarbons
- High-purity nitrogen (99.5% pure, flow rate 15 L/min) gas supply for the ion source
- Ultra-high-purity nitrogen (UHP, 99.999%) with less than one ppm each of water and oxygen for the ion-routing multipole and IC

Size

- 1270 × 767 × 703 mm (w, d, h); The system comes mounted on a 1320 × 788 × 726 mm (w, d, h) table, similar to a standard lab bench

Weight

- 318 kg with table but without data system, vacuum rough pump, and optional items

Environment

- System averages 2,800 W (10,000 Btu/hr) output
- Operating environment must be 16–26 °C and relative humidity must be 50–80% with no condensation
- Optimum operating temperature is 18–21 °C

Find out more at thermofisher.com/OrbitrapID-X

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