

Orbitrap IQ-X Tribrid mass spectrometer

Designed to unravel complex chemical structures

The Thermo Scientific™ Orbitrap IQ-X™ Tribrid™ mass spectrometer redefines small molecule identification and characterization by leveraging the proven and trusted Tribrid architecture with intelligent MSⁿ acquisition using Real-Time Library Search to improve annotation and structural characterization of unknown analytes. This instrument delivers unrivaled performance and ease-of-use with an integrated autocalibration source that simplifies maintenance combined with a fit-for-purpose software interface to overcome the traditional bottlenecks in small molecule structural identification and characterization.



Orbitrap IQ-X Tribrid mass spectrometer features and benefits

- A combination of the best of quadrupole, linear ion trap and Thermo Scientific™ Orbitrap™ mass analyzer technologies for acquisition of the richest MSⁿ data
- Automated, remote, and hands-free calibration with the Auto-Ready ion source, allowing the user to spend more time obtaining results and less time on instrument setup
- Real-Time Library Search provides higher confidence for small molecule analysis using real-time spectral matching for decision-based triggering of MSⁿ acquisition events
- Expanded Thermo Scientific™ AcquireX workflow capabilities produce easy, intelligent acquisitions to discover more compounds with unique fragmentation patterns, enhancing your results
- Expectational mass accuracy to <1 ppm with Thermo Scientific™ EASY-IC™ ion source
- Flexible fragmentation techniques for structural determination of lipids, metabolites, and other small molecules utilizing Collision induced association (CID), Higher-energy collisional dissociation (HCD) and optional Ultraviolet Photodissociation (UVPD)
- Improved unknown analysis with ultra-high 500,000 resolution at m/z 200, and fine isotope detection with optional Thermo Scientific™ 1,000,000 (1M) resolution at m/z 200
- Thermo Scientific™ OptaMax™ NG ion source for enhanced usability and robustness with a redesigned HESI sprayer and built-in APCI assembly
- Expansive collection of application specific, small molecule one-click method templates for metabolomics, lipidomics, metabolite ID, impurities, extractables and leachables, and more

Proven Tribrid architecture

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

Hardware specifications

OptaMax NG ion source

- Outstanding performance with improved sprayer alignment and stability
- Interchangeable HESI/APCI probe
- Enhanced exhaust port efficiently removes solvent vapor, improving uptime and reducing chemical noise

Thermo Scientific™ Auto-Ready ion source

- Integrated source with dedicated emitter and ion transfer tube simplifies maintenance and calibration
- Trigger on-demand or scheduled system checks and calibrations from anywhere without disruption to your LC-MS configuration
- Calibration and maintenance results are controlled and reported directly in the instrument control software interface
- internal Thermo Scientific™ Pierce™ FlexMix™ Calibration solution consumable lasts ≥ 3 months with regular use

Electrodynamic Ion Funnel

- Efficiently captures ions as they enter the mass spectrometer
- Automatic tuning results in gentle transmission curves and reduces ion losses, increasing sensitivity

Thermo Scientific™ EASY-IC™ ion source

- Generates internal calibrant ions for real-time mass calibration of spectra in positive and negative modes
- Provides < 1 ppm RMS drift over 24 hours, measured with FlexMix Calibration solution

Advanced Active Ion Beam Guide

- Advanced Active Ion Beam Guide with an axial field and low pass filtering reduces noise by preventing neutrals and high-velocity clusters from entering the quadrupole mass filter

Quadrupole mass filter

- 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
- Enables high efficiency HCD fragmentation

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
- Optional resolving power of 1M at m/z 200 provides improved performance at high resolutions

Dual-pressure linear ion trap

- Dual-dynode detector with high linear dynamic range for improved quantification
- MS^n precursor isolation from m/z 50 to 2,000
- Low-pressure cell for improved scan speed, resolving power, and mass accuracy
- High efficiency, CID favors first generation fragment ions

Vacuum system

- Split-flow turbomolecular pump controlling vacuum in three regions
- Stainless steel high-vacuum analyzer chamber
- Advanced Vacuum Technology reducing the pressure in the ultra-high vacuum region to $< 2 \times 10^{-10}$ enhancing transmission of the ions to the Orbitrap mass analyzer

Optional hardware

Thermo Scientific™ UVPD ion source

- UVPD includes a Class 1, 213 nm laser system with 2.5 kHz repetition rate, delivering $> 1.2 \mu J$ per pulse

Thermo Scientific™ 1M resolution

- Compact size, located entirely within the footprint of the instrument, 1M resolution enables mass measurements at ultra-high resolution of 1,000,000 FWHM at m/z 200

Thermo Scientific™ FAIMS Pro™ Duo interface

- Performs online gas-phase separation based on differential ion mobility for orthogonal separation and selectivity
- Optimized performance for 100 nL/min to 1 mL/min flow rates

Performance characteristics

Mass range

- Full MS mass range: 50–2,000 m/z
- MS^n mass range (detection only): 40–2,000 m/z

Orbitrap mass analyzer resolution

- 7,500–500,000 (FWHM) at m/z 200
- 1M option: up to 1,000,000 (FWHM) at m/z 200

Acquisition rate (under defined conditions)

- Orbitrap mass analyzer MS^n up to 40 Hz
- Ion trap MS^n up to 45 Hz

Mass accuracy (under defined conditions)

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

MS^2 electrospray ionization (ESI) ion trap sensitivity

2 μL of a 50 $\text{fg}/\mu\text{L}$ solution of reserpine (100 femtograms total) injected at a flow of 500 $\mu\text{L}/\text{min}$ will produce a minimum signal-to-noise (S/N) 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^2 mode, m/z 165–615. The test requires HESI III probe.

Dynamic range

- >5,000 within a single MS acquisition

Multiplexing using the ion-routing multipole

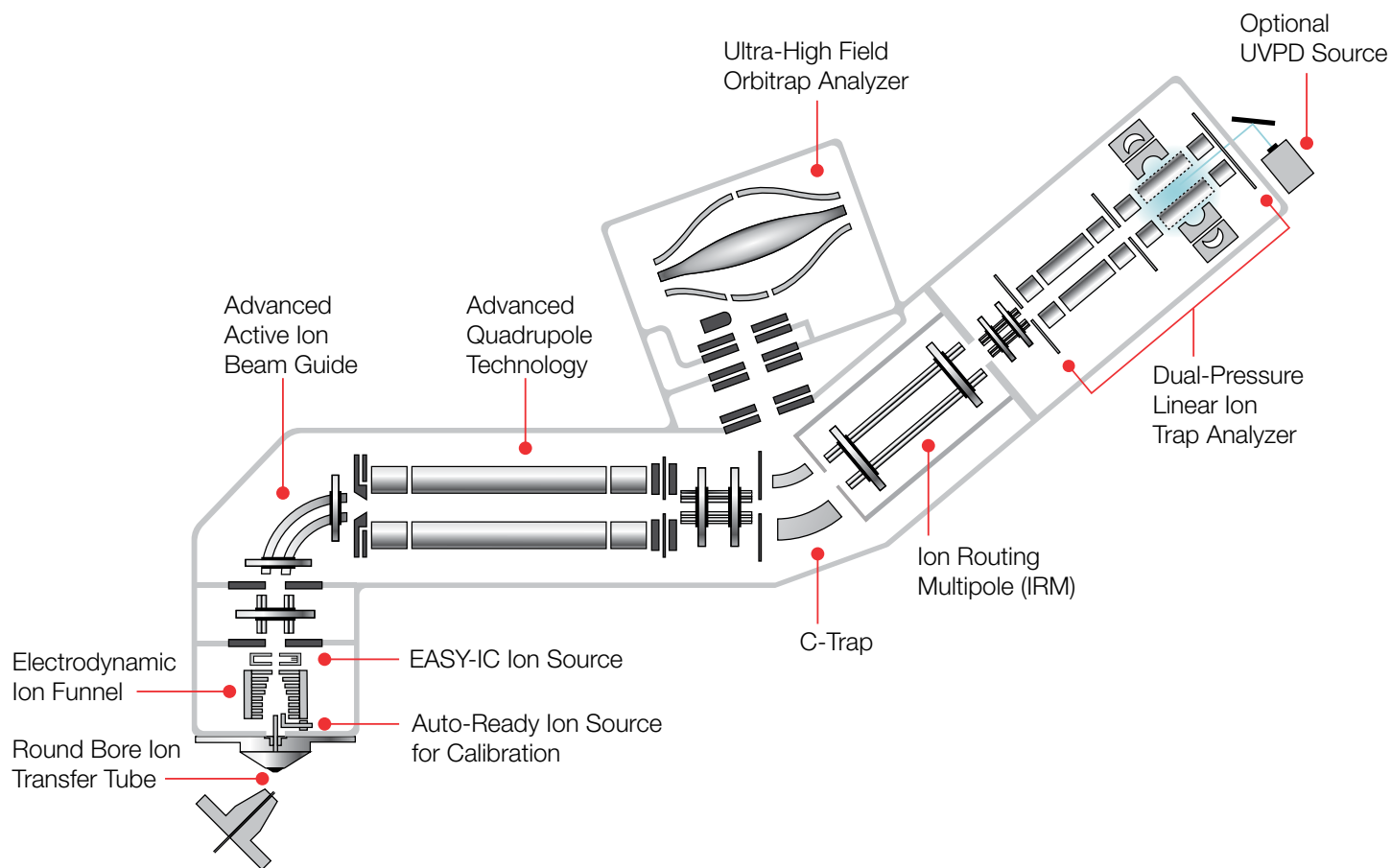
- Up to 10 precursors per acquisition using the quadrupole mass filter for targeted MS^2 and Selected Ion Monitoring (SIM)

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

- Channel 1 analog input (0–10 V),
- Channel 2 analog input (0–2 V)



Orbitrap IQ-X Tribrid mass spectrometer schematic

Software features

Thermo Scientific™ Xcalibur™ software

- Xcalibur software is the control software for the next-generation Thermo Scientific mass spectrometer portfolio
- Accelerates familiarization and reduces training requirements

Orbitrap IQ-X Tribrid MS instrument control software

- 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 intuitive method development

AcquireX workflows

- AcquireX data acquisition workflows provide comprehensive small molecule sample profiling on an LC timescale using automated, logic-based sample re-injection with inter-run inclusion and exclusion lists
- Background Exclusion AcquireX workflow utilizes an exclusion reference, such as a matrix blank, to automatically generate an exclusion list that directs the MS away from interrogating background ions in favor of sample specific compounds
- Exclusion and Component Inclusion AcquireX workflow utilizes a reference sample to automatically generate the corresponding exclusion and inclusion lists allowing the triggering of MSⁿ acquisitions on unique precursor ions that are only present in the sample of interest
- Deep Scan AcquireX workflow provides 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 updates of the exclusion and inclusion lists
- Advanced Deep Scan AcquireX workflow provides higher confidence for small-molecule analysis expanding the Deep Scan workflow with increased flexibility to submit several experiments from a single sequence including; copy/fill-down, export/import sequence, and insert blank/wash
- MSⁿ Library Builder method acquires high-quality, fragmentation-rich MSⁿ product ion spectra utilizing Assisted CE for improved S/N for the HCD and CID product ions

Enhanced technologies

- Real-Time Library Search provides higher confidence small molecule analysis with real-time spectral matching against a local, customizable mzVault library for decision-based triggering of MSⁿ acquisition events. Real-Time Library Search enables library directed MSⁿ data acquisition to increase confidence in metabolite annotation, including structurally related compounds and improve structured assignment of isomeric species, unknown characterization, and addition applications.
- Assisted CE mode utilizes ion trap acquisitions to assess the optimal collision energy in real-time, automatically generating precursor ion specific breakdown curves to select the collision energy required to sufficiently deplete a given precursor. This mode is ideally suited for MSⁿ analysis of oligo nucleotides and for the MSⁿ Library Builder method and additional applications.
- Complete experimental flexibility where precursor fragmentation can take place in the ion-routing multipole (HCD) or in the ion trap (CID or UVPD) with fragment detection in the linear ion trap or Orbitrap mass analyzer 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 acquisition 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.
- Improved Advanced Precursor Determination (APD) enhances detection and monoisotopic mass assignment for halogenated compounds, leading to fewer redundancies in acquisition

Data acquisitions methods

- 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
- MSⁿ, for n = 1 through 10
- 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 an acquisition only if the system detects a product from the user defined list
 - A MSⁿ Quality Trigger triggers complementary ITMSⁿ acquisitions if the corresponding FTMSⁿ acquisition 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
- A Mild Trapping mode can be optionally applied for particularly labile compounds as a global setting that amends the entire analysis

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 and local library generation for unknown compound identification

- Thermo Scientific™ LipidSearch™ software—processes LC-MS data to provide accurate lipid identification, which automatically integrates complex data into reports and dramatically reduces data analysis time

Installation requirements

Power

- 230 Vac ± 10% single phase, 15 Amp, 50/60 Hz, with earth ground for the instrument
- 120 or 230 Vac single phase with earth ground for the data system

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 API source and the ion routing multipole

Dimensions (w, d, h)

1270 × 767 × 703 mm (50 × 30.2 × 27.7 in)

Weight

318 kg (700 lbs) without data system, vacuum rough pumps and optional items

Environment

- System averages 2,800 W (10,000 Btu/hr) output when considering air conditioning needs
- Operating environment must be 16–26 °C (59–78 °F) and relative humidity must be 50–80% with no condensation
- Optimum operating temperature is 18–21 °C (65–70 °F)

Data system

- High-performance PC with Intel® microprocessor
- High-resolution LED color monitor
- Microsoft® Windows® 10 operating system

 Learn more at thermofisher.com/OrbitrapIQ-X