

# 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 MS<sup>n</sup> 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 MS<sup>n</sup> 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 MS<sup>n</sup> 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 MS<sup>n</sup> 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 MS<sup>n</sup>, 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  $\geq 3$  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  $\mu\text{L}$  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

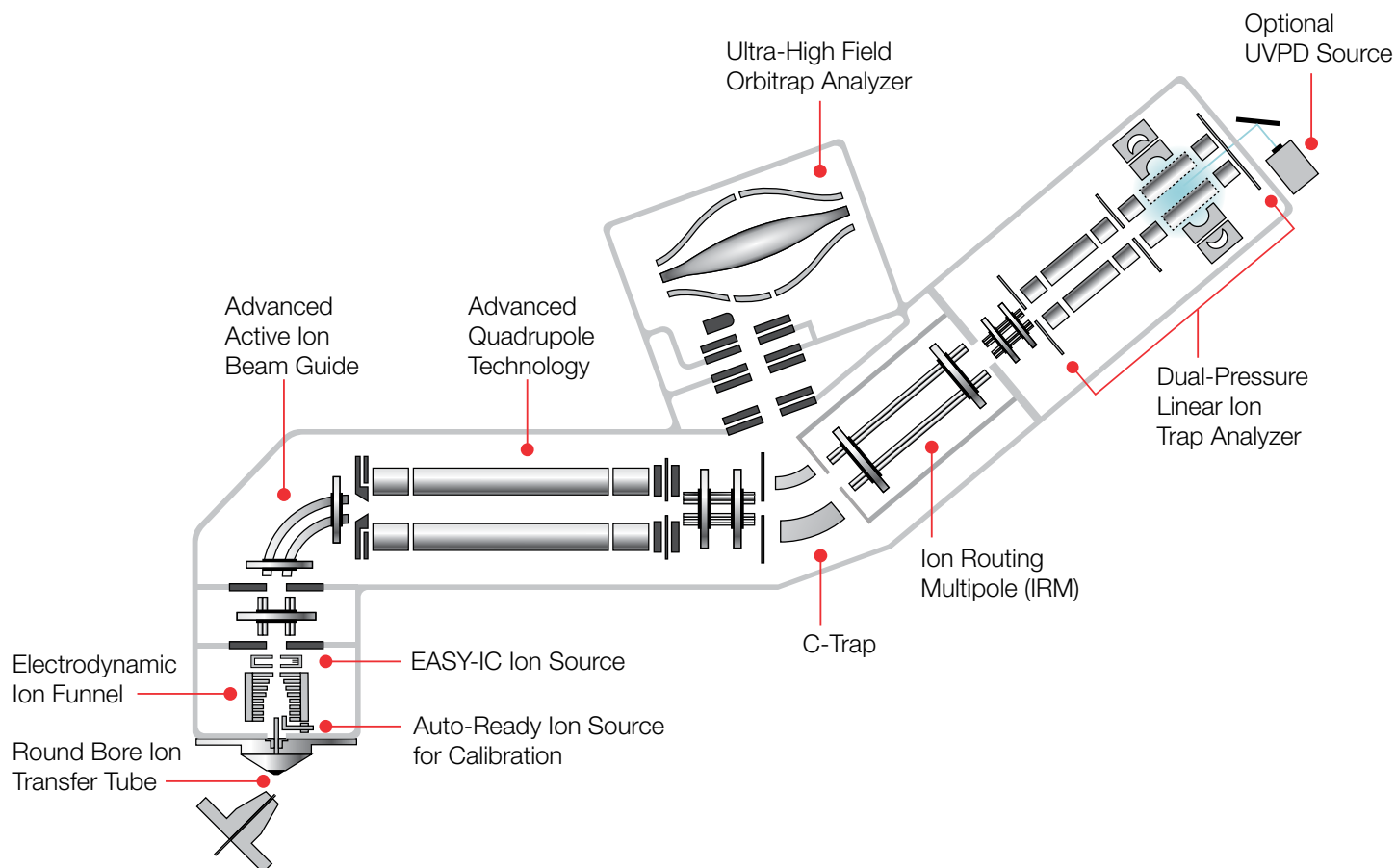
- Up to 10 precursors per acquisition using the quadrupole mass filter for targeted  $MS^2$  and Selected Ion Monitoring (SIM)

### 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 MS<sup>n</sup> 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 MS<sup>n</sup> 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
- MS<sup>n</sup> Library Builder method acquires high-quality, fragmentation-rich MS<sup>n</sup> 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 MS<sup>n</sup> acquisition events. Real-Time Library Search enables library directed MS<sup>n</sup> 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 MS<sup>n</sup> analysis of oligo nucleotides and for the MS<sup>n</sup> 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 MS<sup>n</sup> 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 MS<sup>2</sup> acquisition mode allows rapid profiling of complex samples
- Data dependent MS<sup>3</sup> and higher order fragmentation methods allow in-depth characterization of precursors to aid unknown small molecule structure elucidation
- MS<sup>n</sup>, for n = 1 through 10
- Advanced scan filters allow highly specific and customizable MS<sup>n</sup> 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 MS<sup>n</sup> Quality Trigger triggers complementary ITMS<sup>n</sup> acquisitions if the corresponding FTMS<sup>n</sup> 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](https://thermofisher.com/OrbitrapIQ-X)