

The next-generation Orbitrap Exploris 120 mass spectrometer

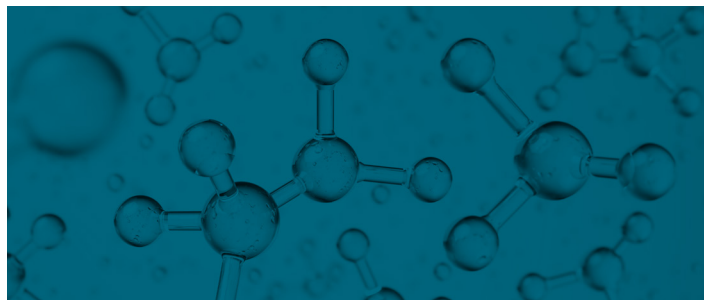
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Thermo Fisher Scientific has developed a next-generation quadrupole-Orbitrap™ hybrid mass spectrometer (Figure 1) designed to provide the productivity, operational simplicity and ruggedness needed to accelerate your qualitative and quantitative analyses from method development to everyday testing through consistent and accurate data using proven Orbitrap technology. This benchtop system continues the expansion of our next-generation Thermo Scientific™ Orbitrap Exploris™ series product portfolio, taking advantage of a multitude of key ion-optical and instrument design solutions (Figure 2) to extend the capabilities beyond that of the previous Thermo Scientific™ Q Exactive™ series of instruments.

The highly optimized design permits a significantly smaller physical footprint with inclusion of high-performance components and many new functionalities that significantly advance performance for many critical application areas. Some of these include:

- Uncover and quantify more analytes with a fast-scanning (up to 22 Hz scan rate, depending on resolution setting) High-Field Orbitrap mass analyzer with 120,000 maximum resolution (FWHM) at m/z 200
- Analyze more with an extended mass range from m/z 40 up to m/z 3,000



- Fast polarity switching with one full experimental cycle acquired at >1.4 Hz. The cycle consists of acquiring one full scan MS in positive and negative polarities at a resolution setting of 60,000
- Ion Routing Multipole used for ion routing and to perform higher-energy collisional dissociation (HCD) fragmentation
- Increase your confidence using the Thermo Scientific™ EASY-IC™ which provides automated introduction of an internal calibrant to consistently achieve high mass accuracy (<1 ppm mass measurement error for at least 5 days)
- Reduce time spent on instrument method set up using the Thermo Scientific™ Orbitrap Exploris Instrument Control Software that is consistent across the Thermo Scientific™ Tribid™ MS and Thermo Scientific™ TSQ™ triple quadrupole MS platforms. The Tune and Method Editor ecosystem also delivers intuitive method programming with ready-to-go templates for the most popular experiments
- Choose from a wider selection of scan modes including Full scan, MS² (DDA with Top4 @ 14 Hz), tMS², tSIM, AIF, DIA and MSX
- Improved robustness and system quality with modified instrument architecture and rugged component design

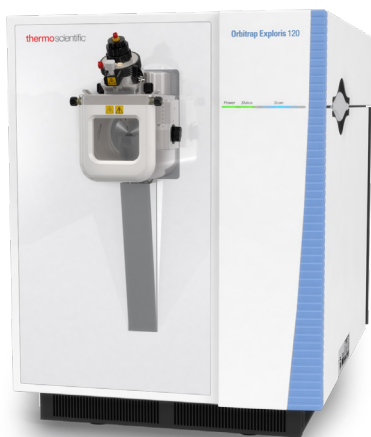


Figure 1. The next generation Thermo Scientific™ Orbitrap Exploris™ 120 instrument, a quadrupole-Orbitrap benchtop mass spectrometer.

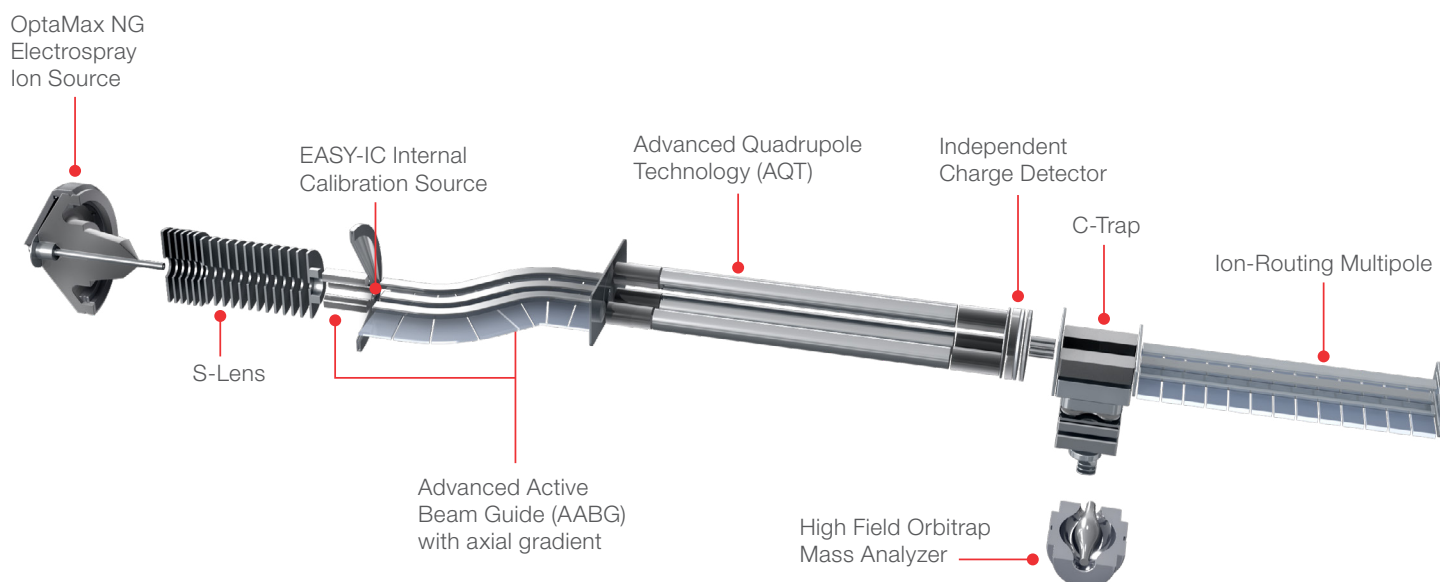


Figure 2. Schematic of the instrument with key items highlighted.

Description of instrumental features and key prove points

Ion source housing and source selection

The next generation Thermo Scientific™ OptaMax™ source housing is compatible with the H-ESI II (Heated Electrospray Ionization) and Thermo Scientific™ EasySpray™ sources used with Thermo Scientific™ Orbitrap Fusion™ Lumos™ Tribid™ MS and Thermo Scientific™ TSQ Altis™, Thermo Scientific™ Quantis™, and Thermo Scientific™ Fortis™ triple quadrupole mass spectrometers. ESI, APCI, APPI and other probes can be used with the H-ESI II source, accommodating many ionization methods to broaden your analytical capabilities.

Ion source interface

Robustness and sensitivity inlet, coupled to a round bore ion transfer tube that is removable without breaking vacuum and progressively spaced stacked-ring ion guide (S-lens) with a resolving injection filter, delivers high transmission and focusing of ions. This inlet design has a proven track record for delivering exceptional performance on the Thermo Scientific™ Q Exactive™ HF mass spectrometers.

Internal calibration

All applications benefit from the highest possible mass measurement accuracy. The Orbitrap Exploris 120 MS routinely achieves sub-3ppm accuracy for most applications over a wide dynamic concentration range. With the standard EASY-IC (Internal Calibration) system, sub-ppm accuracies are achieved with automated introduction of an internal reference mass during sample analysis (Figure 3), improving analytical confidence for every scan during an analysis for up to 5 consecutive days.

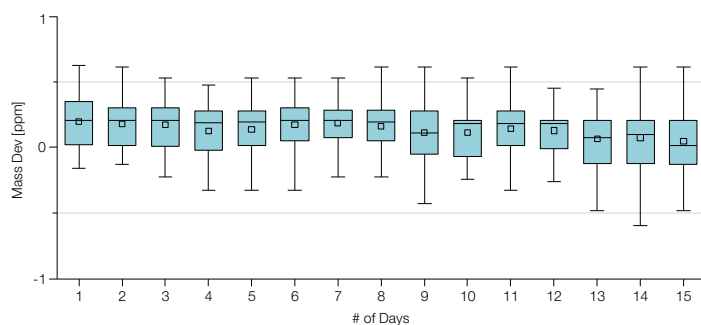


Figure 3. The Easy-IC internal calibrant consistently achieves high mass accuracy of less than <1 ppm for at least 5 days. Veterinary drug with continuous polarity switching for mass range 160–900 were used for these measurements.

Quadrupole mass filter

The quadrupole mass filter enables precursor ion selection before the C-Trap, using hyperbolic quadrupole rods. The mass resolving quadrupole has a segmented design with RF-only segments at the entrance and exit of the device. The combination of high-quality hyperbolic quadrupole rods with RF application allows for very high ion transmission at narrow isolation widths—providing excellent selectivity with minimal loss of sensitivity.

The resolution of the mass filter can be as high as 0.4 Da for ions < m/z 400, supporting highly specific precursor selection while maintaining excellent transmission. The instrument can be operated using the following isolation widths at variable scan ranges when using the quadrupole:

- 0.4 Da and full mass range (m/z 40–400)
- 0.7 Da and full mass range (m/z 400–700)
- 1.0 Da and full mass range (m/z 700–1000)
- 1.5 Da and full mass range (m/z 1000–1500)
- 2.0 Da and full mass range (m/z 1500–2000)

Ion-routing multipole (IRM)

In common with the Orbitrap Tribid platform, the next generation quadrupole-Orbitrap mass spectrometer includes an IRM, which accumulates and distributes ions within the system. Ions can be retained and fragmented using Higher Energy Collisional Dissociation (HCD) or sent to the C-trap for introduction to the Orbitrap mass analyzer. HCD spectra can be generated by user-defined absolute CE (collision energy) or NCE (normalized collision energy), as with other Thermo Scientific mass spectrometers, facilitating easy method development and cross-platform parameter transfer.

High-field Orbitrap mass analyzer

The next generation quadrupole-Orbitrap instrument features a high-field Orbitrap mass analyzer. The combination of the physical size of the Orbitrap central electrode with the ultra-high vacuum obtained inside the Orbitrap analyzer enables a mass resolving power of 120,000. This Table 1 summarizes the relationship between transient length/scan rate and achievable resolving power (measured at m/z 200).

Table 1. Mass resolution versus transient length and scan rate in the new quadrupole-Orbitrap hybrid mass spectrometer.

Resolution at m/z 200	Transient length (ms)	Scan rate (Hz)
15,000	32	22
30,000	64	12
60,000	128	7
120,000	256	3

The ability to choose different combinations of resolution, transient length, and scan rate allows for acquisition of highest quality data across a wide variety of applications, all available with experimental method templates meaning you can acquire the highest quality data with ease.

Serviceability

The improvements on the next-generation hybrid-Orbitrap mass spectrometer were designed to allow for minimal downtime when the instrument is being serviced. The simplified ion source from the Orbitrap Tribrid series allows for quicker capillary replacement and source cleaning. If the internal quadrupole requires cleaning, access is obtained by simply lifting the lid to the ion optics following system vent. The quadrupole can be easily removed from the ion rail for cleaning and there is no need to disassemble any electrical connections manually. Once the instrument is ready to restore vacuum, an automatic breakout of the Orbitrap manifold is performed to minimize downtime. Finally, a single 6 stage turbo molecular pump (TMP) has been employed to keep the system under vacuum, keeping the mechanics to optimum requirements.

Confidently uncover more analytes

The Orbitrap Exploris 120 mass spectrometer significantly improves data accuracy by discriminating ions of interest and interfering ions which differ by even a small mass increment down to the low mass-to-charge (m/z) range. Orbitrap High Resolution Accurate Mass Spectrometry (HRAM) technology greatly reduces the likelihood of false positives or negatives in complex samples.

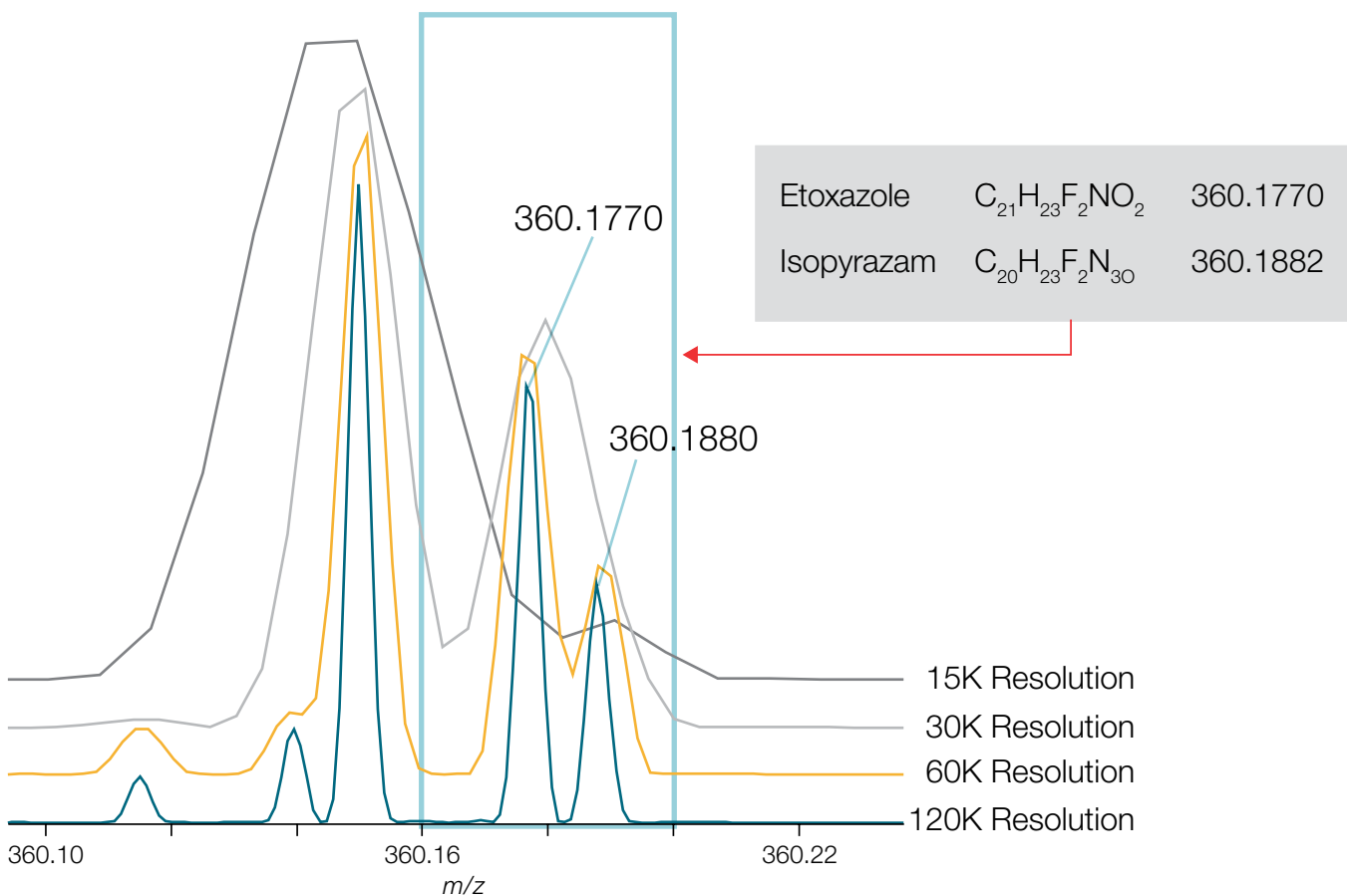


Figure 4. Full-scan mass spectrum of Etozazole and Isopyrazam, at a resolution (R) setting up to 120,000 (FWHM) at m/z 200, demonstrates outstanding resolving power.

High confidence quantitation results with improved scan rate

The Orbitrap Exploris 120 MS instrument triggers even more precursor ions for MS/MS with an improved scan rate of up to 22 Hz so you can generate quantitation results rapidly and confidently.

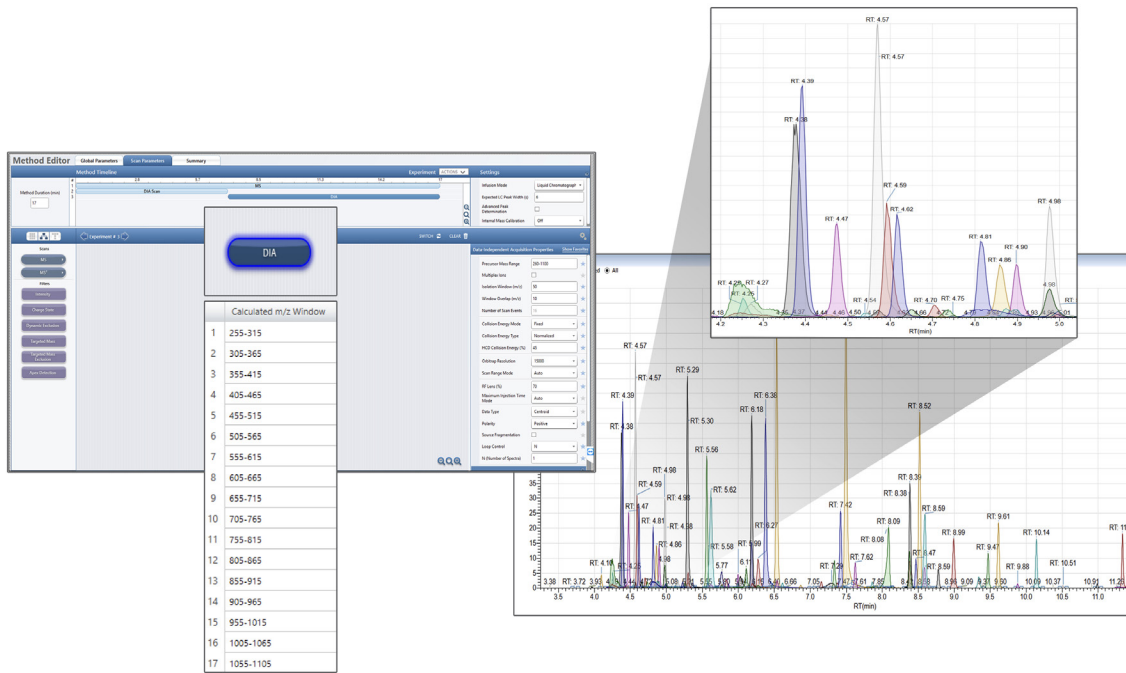


Figure 5. Quantitation of all compounds in bovine muscle matrix is easily achieved by excellent scan speed even when multiple precursor ion m/z isolation windows are selected in a DIA experiment.

Analyze samples twice as fast with rapid polarity switching

The Orbitrap Exploris 120 MS instrument enables positive and negative mode switching with a single cycle rate of approximately 1.4 Hz. Compared to other high-resolution MS instruments, the mass resolution and mass stability do not need to recover after polarity switching, saving you time.

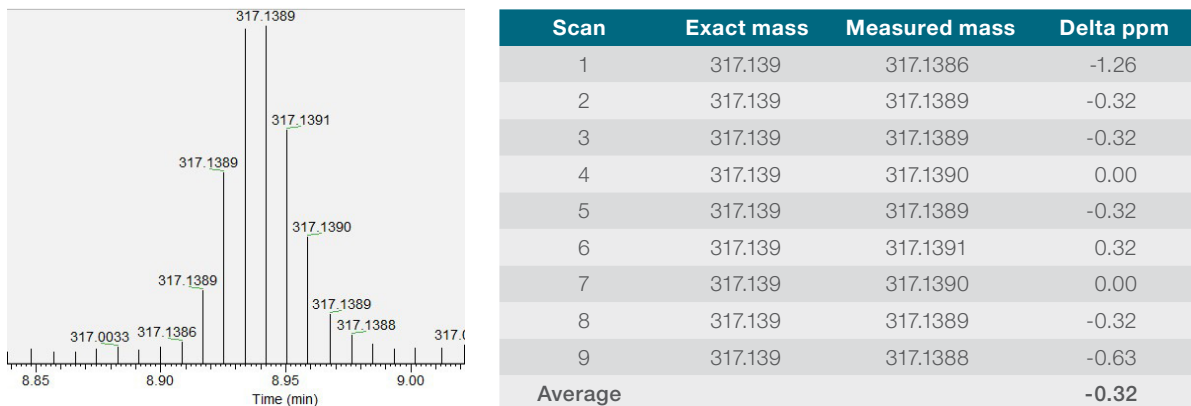


Figure 6. Full scan MS acquired data for 90 ng/g Zearalenone in corn feed demonstrates preservation of mass accuracy stability during polarity switching.

Conclusions

In addition to generating accurate high resolution mass spectrometry results with the proven Orbitrap HRAM technology, productivity has been redefined for small molecule researchers. This includes improvements to increase the ease-of-use of the instrument control software, with application modes and pre-built method templates that are fully customizable. Designed for robust performance and operational simplicity, the new instrument ensures your laboratory will run seamlessly. Instrument downtime has been minimized with the ability to perform a single calibration for the entire mass range and improved serviceability to minimize downtime.

Features	Benefits	Technology
High Resolution	High selectivity to resolve analytes from matrix interferences down to a few mDa	120,000 (FWHM) at m/z 200
Sub-ppm Mass Accuracy	Increased confidence in molecular formula	EASY-IC Internal Calibrant source
Speed	Fast scan rates for improving small molecule identification and quantitation	Up to 22 Hz at resolution setting 15,000 (FWHM) at m/z 200
Easy-to-set up method	Pre-built method templates that are fully customizable using a drag-n-drop flexible user interface	Orbitrap Exploris Instrument Control Software
Acquisition modes including: DDA, DIA, PRM, and AIF	Multiple novel methods that improve screening and quantitation for target verification	Segmented Quadrupole, Independent charge detector, AGC

Size, weight and site requirements

- Size: 763 × 534 × 703 mm (30 × 21 × 28 inches) (length × width × height)
- Weight: 120 kg (264 pounds) without data system, vacuum rough pumps and optional items.
- Power: 208–240 V AC ±10% single phase, 10 A, 50/60 Hz for MS instrument alone. 200–240 V AC single phase with earth ground for the data system, external syringe pump and divert valves.
- Source Gas: Nitrogen, 99% or better (high purity), max. 45 L/min, pressure 0.6 ±0.05 MPa.
- HCD Gas: Nitrogen, 99.999% or better (ultra-high purity), max. 0.04 L/min, pressure 0.6 ±0.05 MPa.

Operating environment

- Laboratory temperature: 18–27 °C
- Maximum temperature fluctuation: 1 °C/10 min
- Humidity: 20–80%, non-condensing and noncorrosive atmosphere
- Maximum altitude: 3,000 m above sea level

Roughing pumps

- Source vacuum pump: SOGEVAC SV 65 BI

Complete system (including data system)

- Noise emission: Below 70 dB(A)
- Heat generation: 3,440 W

Find out more at thermofisher.com/OrbitrapExploris120