Thermo Scientific Q Exactive

Benchtop Quadrupole-Orbitrap Mass Spectrometer

Identify, quantify and confirm with unmatched confidence using the Q Exactive mass spectrometer.

- Resolving power up to 140,000
- Maximum scan speed 12 Hz
- Intra-scan dynamic range > 5000:1
- · Quadrupole mass filter
- · Spectral multiplexing for enhanced duty cycle
- · S-Lens ion source for enhanced sensitivity





The Q Exactive benchtop LC-MS/MS combines high-performance quadrupole precursor selection with high-resolution, accurate-mass (HR/AM) Orbitrap detection to deliver high performance and tremendous versatility.

With a fast scan speed and multiplexing capabilities, the Q Exactive mass spectrometer is an outstanding detector for fast chromatography separation techniques. The superior quality of Q Exactive MS/MS data enables identification and quantitation of more compounds with greater confidence.

The Q Exactive LC-MS/MS system not only offers broad screening capabilities but also excels at targeted quantitation experiments, making it a versatile addition to any laboratory. Fast, alternating positive-negative scan modes allow for the most comprehensive approaches, saving time during screening experiments. The benchtop system is ideally suited for drug metabolism, proteomics, environmental analysis, food safety and clinical research applications.



Thermo Scientific Q Exactive MS system.

Hardware Specifications

Thermo Scientific Ion Max API Source

- Enhanced sensitivity and ruggedness
- Sweep Gas reduces chemical noise
- 60° interchangeable ion probe orientation
- Removable metal ion transfer capillary provides vent-free maintenance

Ion Source

- H-ESI II probe with Dual Desolvation Zone technology equipped as standard
- A progressively spaced stacked ring ion guide (S-lens)
- The S-lens is a radio frequency (RF) device that captures and efficiently focuses the ions in a tight beam
- Large variable spacing between electrodes allows for better pumping efficiency and improves ruggedness

Transfer Ion Optics

- Advanced ion guides for high sensitivity and ruggedness
- High stability and ion transmission efficiency

Quadrupole Mass Filter

- Thermo Scientific HyperQuad mass filter provides superior and unique combination of resolution and sensitivity
- Variable precursor isolation width selection from 0.4 Da to full mass range

Vacuum System

- Differentially pumped vacuum system with final vacuum $< 1 \times 10^{-9}$ mbar
- Two split-flow turbomolecular pumps and one rotary vane pump
- · Seven vacuum regions

Orbitrap Mass Analyzer

- · Gas (nitrogen) filled C-Trap
- Highly efficient ion transfer to Orbitrap analyzer
- Straight multipole collision cell for HCD
- Orbitrap analyzer with 5 kV central electrode voltage
- · Low-noise image current pre-amplifier
- 16-bit signal digitalization

Data Acquisition

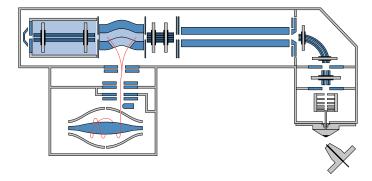
- Ultra fast real-time data acquisition and instrument control system
- Fully automated calibration via instrument control software
- Automated gain control

Performance Characteristics	
Resolving power	Up to 140,000 @ m/z 200
Mass range	50 to 6,000 <i>m/z</i>
Scan rate*	Up to 12 Hz at resolution setting of 17,500 @ m/z 200
Mass accuracy *	Internal: < 1 ppm RMS External: < 3 ppm RMS
Sensitivity	Full MS: 500 fg Buspirone on column S/N 100:1 SIM: 50 fg Buspirone on column S/N 100:1
Dynamic range	> 5000:1
Polarity switching	One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 35,000)
Multiplexity	up to 10 precursors/scan
Analog inputs	One (1) analog input (0 – 1 V) One (1) analog (0 – 10 V)

^{*} Under defined conditions

Options

- Nanospray source supports static packed tip and dynamic nanospray experiments, compatible with liquid flow rates of 50 nL/ min to 2 µL/min
- NanoSpray Flex Ion source single set-up for all online nanoflow applications
- ESI probe compatible with liquid flow rates of < 1 µL/min to 1 mL/min without splitting
- APCI source compatible with liquid flow rates of 50 μL/min to 2 mL/min without splitting
- APCI/APPI source compatible with liquid flow rates of 50 µL/min to 2 mL/min without splitting
- Metal needle kits for high and low flow analyses



Schematic Schematic of the Thermo Scientific Q Exactive Benchtop LC-MS/MS.

Software Features

Data System

- High performance PC with Intel® Pentium® microprocessor
- · High resolution LCD color monitor
- Microsoft Windows® 7 operating system
- · Microsoft Office software package
- Thermo Scientific Xcalibur processing and instrument control software
- · New workflow based method editor

Operation Modes

- Full MS with high resolution accurate mass detection
- Selected Ion Monitoring (SIM) with high resolution accurate mass detection
- Parallel reaction monitoring (PRM) for improved screening and quantitative confidence
- Data-Idependent Acquisition (DIA) for unbiased identification and quantitative analysis
- MS/MS of isolated ions with high resolution accurate mass detection
- All Ion Fragmentation (AIF) in the HCD collision cell with high resolution accurate mass detection

- In-source fragmentation of all ions in the source region
- Positive/negative ion switching on chromatographic timescale
- Data Dependent on-the-fly decision making
- Timed SIM for scheduled data acquisition of the targets of interest

Exclusive Technologies

- Unique, patented* Thermo Scientific Automatic Gain Control (AGC) ensures that the Orbitrap is always filled with the optimum number of ions for all scans
- High performance HCD collision cell for highest performance MS/MS fragmentation
- Collision energy profiling using different collision energies for HCD fragmentation
- · Advanced signal processing
- Interleaved operation
- Multiplex-MS for simultaneous detection of up to 10 precursor ions in the Orbitrap mass analyzer



The Thermo Scientific Q Exactive™ mass spectrometer with the Thermo Scientific Ultimate 3000 RSLC.

Specifications

Installation Requirements

Power

 $2 \times 230 \text{ Vac} \pm 10\%$ single phase, 15 Ampere, 50/60 Hz, with earth ground for the instrument 120 or 230 Vac single phase with earth ground for the data system

Gas

Nitrogen

High purity nitrogen gas supply (99% pure at 800 ± 30 kPa (8.0 ± 0.3 bar, 116 ± 4 psi))

Environment

System averages 2,500 W (~9,000 Btu/h) output when considering air conditioning needs Operating environment must be 15 - 26 °C (59 - 78 °F) and relative humidity must be 40–70% with no condensation

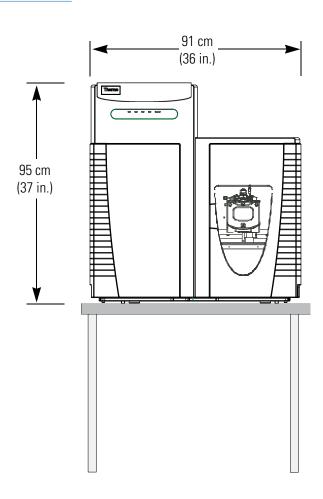
Weight

Q Exactive mass spectrometer: 182 kg (401 pounds) without forevacuum pump Forevacuum pump: 62 kg (136 pounds)

Dimensions

Q Exactive mass spectrometer: $(h \times d \times w)$

 $95 \times 83 \times 91$ cm $(37 \times 33 \times 36 \text{ inches})$



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Africa +43 1 333 50 34 0
Australia +61 3 9757 4300
Austria +43 810 282 206
Belgium +32 53 73 42 41
Canada +1 800 530 8447
China 800 810 5118 (free call domestic)
400 650 5118

Denmark +45 70 23 62 60 Europe-Other +43 1 333 50 34 0 Finland +358 9 3291 0200 France +33 1 60 92 48 00 Germany +49 6103 408 1014 India +91 22 6742 9494 Italy +39 02 950 591 Japan +81 45 453 9100 Korea +82 2 3420 8600 Latin America +1 561 688 8700 Middle East +43 1 333 50 34 0 Netherlands +31 76 579 55 55 New Zealand +64 9 980 6700 Norway +46 8 556 468 00 Russia/CIS +43 1 333 50 34 0 Singapore +65 6289 1190 Spain +34 914 845 965 Sweden +46 8 556 468 00 Switzerland +41 61 716 77 00 UK +44 1442 233555 USA +1 800 532 4752

