

Thermo Scientific Q Exactive GC Orbitrap GC-MS/MS System

Higher Quality Data, Most Comprehensive Analysis

- Resolving power of up to 100,000 (FWHM) at m/z 272
- Routine sub ppm mass accuracy
- < 6 fg OFN Instrument Detection Limit
- EI/CI Thermo Scientific™ ExtractaBrite™ ion source removable under vacuum through vacuum interlock
- Vent-free column exchange with source plug
- Advanced Quadrupole Technology (AQT) for superior precursor isolation
- High sensitivity MS/MS experiments with Higher-Energy Collisional Dissociation (HCD) cell



The Thermo Scientific™ Q Exactive™ GC hybrid quadrupole Orbitrap mass spectrometer provides an unmatched combination of sensitivity, mass-accuracy and resolving power, helping answer today's most challenging analytical questions. With best-in-class performance characteristics for both quantitative and discovery workflows, the Q Exactive GC system allows the

most comprehensive characterization of complex samples. The full MS scanning sensitivity combined with the selectivity achieved at resolutions of 50,000 and higher provides detection limits comparable to the best GC-triple quadrupoles while operating in an untargeted full MS scan mode. The included chemical ionization source provides soft ionization for pseudo-molecular ion generation, and the analytical quadrupole and HCD cell allow for structural characterization experiments through MS/MS fragmentation. This world-class performance and comprehensive toolkit comes in a user-friendly bench-top design, with standard ease-of-use features including vent-free source and column exchange. Step into the next chapter of GC-MS technology with the first commercial Orbitrap-based GC-MS: the Q Exactive GC Orbitrap GC-MS/MS system.



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Hardware Specification

Ion Source

- Thermo Scientific™ ExtractaBrite™ Electron Ionization (EI) source
- Ion source includes ion volume, repeller, source lenses, RF lens and dual filaments in all ionization modes, programmable from 50 °C to 350 °C
- Chemical Ionization (CI) source for acquisition with Positive Ion Chemical Ionization (PCI) and Negative Ion Chemical Ionization (NICI)
- Remove entire ion source or change to CI source in under 2 minutes without venting
- Vent-free column exchange with new, patented source plug
- Combination EI/PCI/NICI ion volume can be used without need for source interchange

MS Ion Optics

- Advanced prefiltering and axial field bent flatapole ion guide reduces noise by preventing neutrals from entering the quadrupole

Quadrupole Mass Filter

- Advanced Quadrupole Technology (AQT) featuring a segmented Thermo Scientific™ HyperQuad™ mass filter provides increased ion transmission and superior isolation window shape
- Variable precursor ion 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

Orbitrap Mass Analyzer

- Nitrogen-filled C-Trap
- Highly efficient ion transfer to Orbitrap mass analyzer
- Straight multipole collision cell for HCD
- Low-noise image current preamplifier
- 16-bit signal digitalization

Data Acquisition

- Ultrafast real-time data acquisition and instrument control system
- Fully automated tune and calibration via instrument control software
- Automatic gain control

EI Full MS Installation Specifications

- 1 μ L of 100 fg/ μ L octafluoronaphthalene (OFN) will produce a minimum signal-to-noise of 10,000:1 at a minimum resolution of 50,000 (FWHM) and a mass error of less than 1 part per million (ppm) while scanning from m/z 50 to m/z 300.
- The area precision of eight sequential injections of 1 μ L, 10 fg/ μ L OFN will result in an instrument detection limit (IDL) of 6 fg or less (OFN) derived at the 99% confidence level.*

**Demonstrated at installation with purchase of Thermo Scientific™ TriPlus™ RSH Autosampler and Q Exactive GC system IQ/OQ. Otherwise, a signal-to-noise of greater than 1000:1 will be demonstrated on a single 1 μ L injection of a 10 fg/ μ L OFN standard.*

PCI Full MS Installation Specifications

- 1 μ L of 10 pg/ μ L benzophenone (BZP) will produce a minimum signal-to-noise of 150:1 while scanning from m/z 80 to m/z 230.

Performance Characteristics

Resolving Power:	100,000 @ m/z 272
Mass Range:	50 to 3,000 m/z
Scan Rate:*	Up to 18 Hz at resolution setting of 12,500 @ m/z 272
Mass Accuracy:**	Internal: <1 ppm RMS External: <3 ppm RMS
Quantitative Dynamic Range*:	>10 ⁶
In-Spectrum Dynamic Range:	>5000:1
Multiplexity:	Up to 10 precursors/scan

* Under defined conditions

** Under conditions defined in 1 μ L, 100 fg/ μ L octafluoronaphthalene EI Full MS installation specification

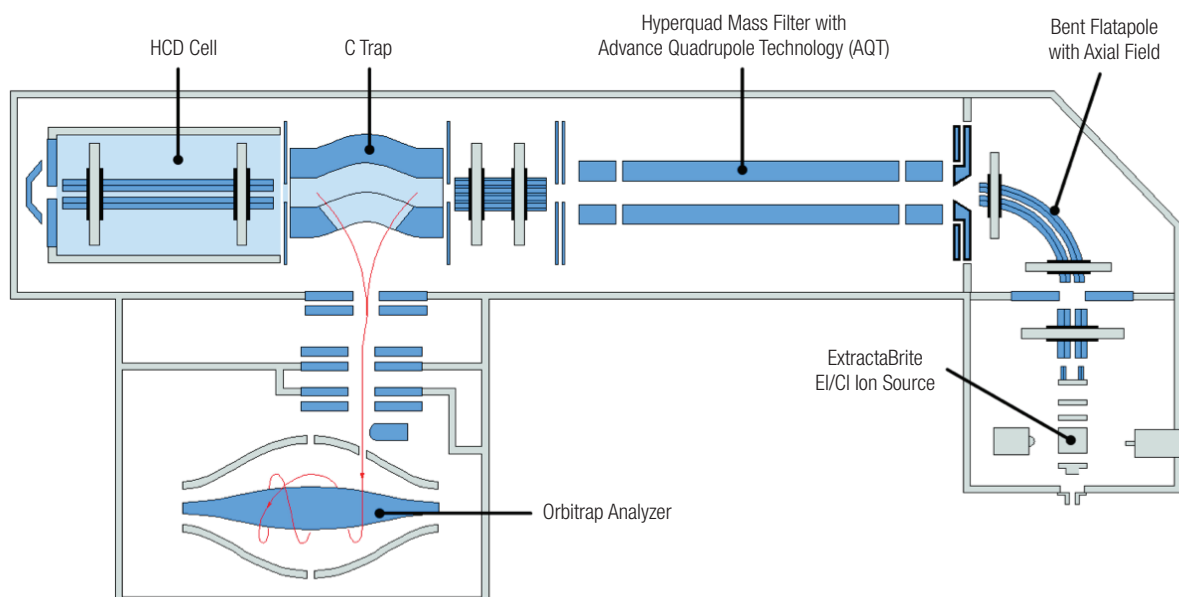


Figure 1. Q Exactive GC system schematic design.

Software Features

Data System

- High-performance PC with Intel® microprocessor
- High-resolution LCD color monitor
- Microsoft Windows 7® operating system
- Microsoft Office® software package
- Thermo Scientific™ Xcalibur™ instrument control and data processing software
- Workflow-based method editor
- Thermo Scientific™ TraceFinder™ software for quantitation, targeted screening, and high resolution spectral deconvolution with accurate mass library search
- NIST spectral library included

Gas Chromatograph

Thermo Scientific™ TRACE™ 1310 GC: Complete icon-driven touch screen user interface for direct local instrument control

GC mainframe included with system.

Injectors, detectors, autosampler and other options sold separately.

- User-installable injector or detector assembly can be installed in less than 2 minutes
- 0.001–1000 kPa digitally controlled carrier gas with gas saver and septum purge
- Split/Splitless (S/SL) injector with optional large volume kit for injections up to 50 µL
- Multi-mode programmed temperature vaporization (PTV) injector including on-column capabilities and large volume injection up to 250 µL
- Integrated backflush optional for both S/SL and PTV
- 1000 kPa digitally controlled carrier gas with gas saver and septum purge
- Detector fast data acquisition rate: up to 300 Hz

Oven Temperature

- Operating temperature range: ambient + 3 °C to 450 °C
- Operating temperature range with liquid N₂ Cryo: -100 °C to 450 °C
- Operating temperature range with CO₂ Cryo: -50 °C to 450 °C



Figure 2. Q Exactive GC mass spectrometer with TriPlus RSH autosampler.

Oven Performance

- Number of ramps/plateaus: 32/33
- Maximum heating rate: 125 °C/min
- Oven cool-down (22 °C ambient): 450 °C to 50 °C in <4 min

GC Analytical Performance

- Retention time repeatability: <0.0008 min
- Peak area repeatability: <0.5 % RSD
- Pressure set points minimum increments: 0.01 kPa–0.001 psi in all ranges

Operation Modes

- Full MS with high-resolution accurate-mass detection
- Selected Ion Monitoring (SIM) with high-resolution accurate-mass detection
- Timed SIM for scheduled data acquisition of targets of interest
- Parallel Reaction Monitoring (PRM) for fast, sensitive MS/MS experiments
- Positive/negative ion switching on chromatographic timescale
- On-the-fly data-dependent decision making

Exclusive Technologies

- Automatic Gain Control (AGC) ensures that the Orbitrap mass analyzer 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
- Spectrum multiplexing for simultaneous detection of up to 10 precursor ions in the Orbitrap mass analyzer

Installation Requirements

Power

- 2 × 230 VAC ± 10% single phase, 15 A, 50/60 Hz, with earth ground for the instrument
- 120 or 230 VAC single phase with earth ground for the data system

Gas

Helium

- High-purity helium gas supply (99.999% pure)
- Regulator output pressure adjustable from 300 to 1000 kPa (3 to 10 bar, 45 to 145 psi)

Methane (required for CI installation)

- High-purity methane gas supply (99.999% ultra high purity)
- Regulator output pressure adjustable from 35 to 240 kPa (0.3 to 2.4 bar, 5 to 35 psi)

Nitrogen

- High-purity nitrogen gas supply (99.999% ultra high purity)
- Regulator output pressure at 800 ± 30 kPa (8.0 ± 0.3 bar, 116 ± 4 psi)

Environment

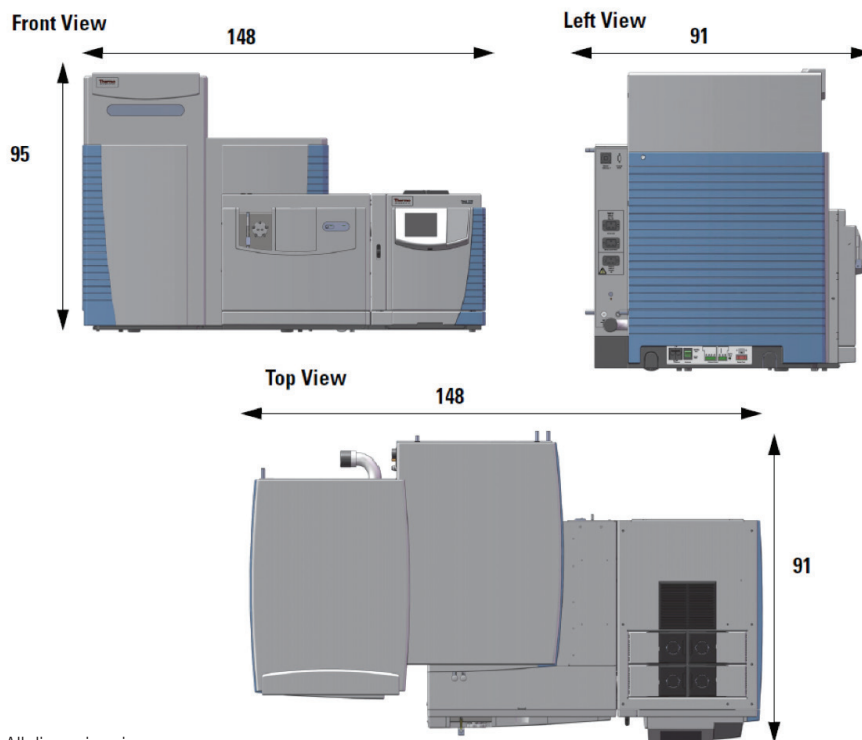
- Air conditioning load for a typical Q Exactive GC system (with data system, GC, and autosampler) approximately 4.6 kW (16,000 BTU/h)
- Operating environment must be constant temperature between 15–26 °C (59–78 °F) and relative humidity must be 40–70% with no condensation

Weight

- Q Exactive GC mass spectrometer: 254 kg (560 pounds) with Q Exactive MS, TRACE 1310 GC and TriPlus RSH Autosampler without forevacuum pump
- Forevacuum pump: 24 kg (52 pounds)

Dimensions

- Q Exactive GC Orbitrap GC-MS/MS system: (h × d × w) 95 × 91 × 148 cm (37 × 36 × 58 inches)



www.thermoscientific.com/QExactiveGC

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