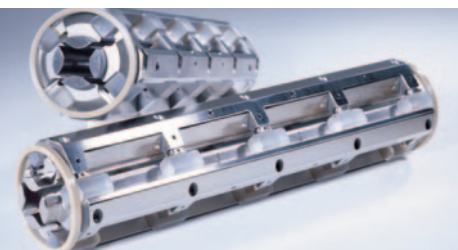


The Thermo Scientific TSQ Quantum Ultra triple quadrupole mass spectrometer defines a standard of excellence for your quantitative analysis needs.

Thermo Scientific TSQ Quantum Ultra/ Ultra AM/ Ultra EMR



- **Ultimate productivity for bioanalytical analysis**
- **Universal Thermo Scientific Ion Max source with Heated Electrospray Ionization (HESI-II)**
- **Unmatched sensitivity and specificity with H-SRM**
- **Supports 21 CFR Part 11 compliance through Thermo Scientific LCQUAN software**
- **3000 amu mass range with Thermo Scientific TSQ Quantum Ultra EMR**

The TSQ Quantum Ultra family's innovative technology provides wide linear dynamic range and low sensitivity limits, defining a high standard of excellence in mass spectral quantitation. It features the revolutionary Ion Max™ source with interchangeable

HESI-II, ESI and APCI probes, a titanium skimmer with hard-edged skimming and larger aperture for increased robustness and sensitivity, and a redesigned ion transfer tube lens with wider aperture for enhanced ion focusing and ion transmission. The Ion Max source also allows full probe adjustment in the x, y, and z directions. The probe position can be optimized for maximum robustness and sensitivity with any given combination of flow rate, solvent, and ionization mode. Its new, ultra high temperature, self-cleaning APCI probe, with ceramic heater, virtually eliminates carryover. All of this comes with the benefits of constant neutral loss scanning, parent scanning, high-resolution precursor ion selectivity, Selected Reaction Monitoring (SRM) and Highly Selective Reaction Monitoring (H-SRM).

The TSQ Quantum Ultra EMR™ offers higher resolution, higher resolution precursor selection, and an Extended Mass Range of up to 3000 daltons. This extended mass range capability allows high-resolution analysis of a whole new class of biopolymers including peptides, polysaccharides, intact proteins, and oligonucleotides. It combines the benefits of the TSQ Quantum Ultra, including constant neutral loss scanning, parent scanning, high-resolution precursor ion selectivity, SRM and H-SRM to deliver a complete solution for the proteomics and large molecule research community.

The Thermo Scientific TSQ Quantum Ultra AM has the additional capability of routine accurate mass measurements on the chromatographic timescale. Its meticulously engineered analyzer control circuitry takes full advantage of the high-resolution Thermo Scientific HyperQuad quadrupole mass analyzers, enabling accurate mass measurement capabilities that are easier to use and have a greater dynamic range than those of instruments based on quadrupole/time-of-flight technology.

Hardware Features

Ion Max API Source

- Enhanced sensitivity and ruggedness
- Sweep gas reduces chemical noise
- Optimal 60-degree spray angle for best sensitivity and ruggedness
- Interchangeable HESI-II, ESI, and APCI ionization probes

- APPI/APCI combination probe
- Removable ion transfer tube provides vent-free maintenance
- High temperature, self-cleaning APCI heater employing state-of-the-art ceramic heater technology
- X, Y, and Z probe positioning adjustments for all ionization probes
- Automatic source recognition for ease of use and simplified data logging
- Dual square profile quadrupole ion guides for the highest ion transmission

Triple Stage Quadrupole

- Dual HyperQuad™ precision hyperbolic quadrupole mass analyzers for ultra performance
- Large 6-mm field radius provides high transmission and superior peak shape
- 90-degree square profile quadrupole ion guide with noise-reducing geometry
- Software control and automated optimization of collision energy and gas pressure
- Fully automated system calibration, tuning, and compound optimization

Vacuum System

- Four-stage differentially pumped vacuum manifold
- Advanced triple inlet turbomolecular pump integrated with vacuum manifold
- Dual rotary vacuum pump configuration

Detection System

- Off-axis continuous dynode electron multiplier with extended dynamic range
- ±15 kV post-acceleration conversion dynode

- Integrated electron multiplier eliminates field emission and microphonic noise
- Digital electronic noise reduction

Integrated Divert Valve

- Fully automated data system control enables switching the solvent front, gradient end point, or any portion of the HPLC run to waste
- Automatic system optimization by loop injections
- User-definable default state of the valve, either “to waste-load” or “to source-inject”

Integrated Syringe Pump

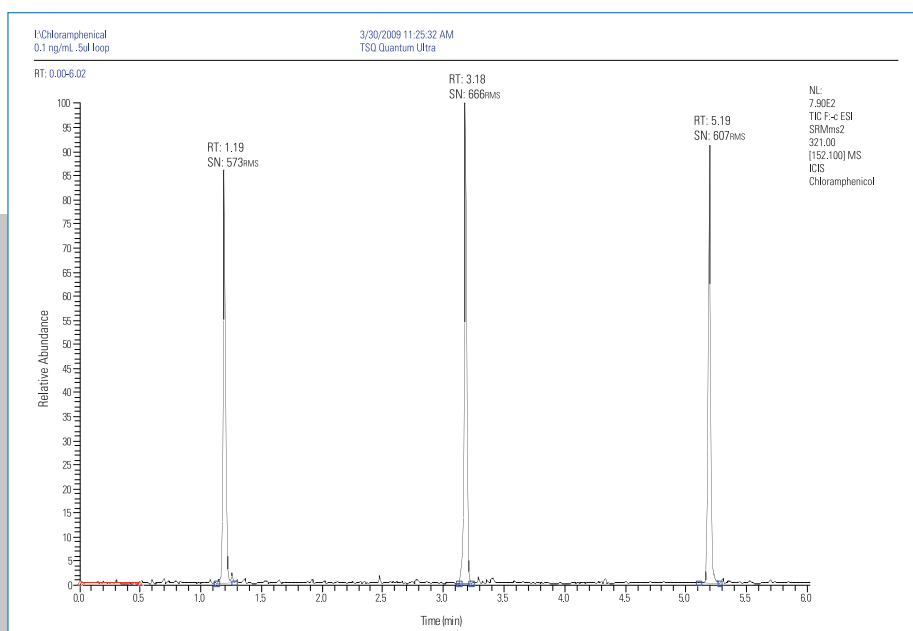
- Automated infusion and loop injections under full data system control

Source Options

- ESI probe compatible with liquid flow rates of 1 µL/min to 1 mL/min, without splitting
- APPI/APCI combination probe compatible with liquid flow rates of 50 µL/min to 2 mL/min, without splitting
- APCI probe compatible with liquid flow rates of 50 µL/min to 2 mL/min, without splitting
- Metal needle option for ESI with configurations for low-flow or high-flow analysis
- NanoSpray source supports both static and dynamic nanospray experiments, compatible with liquid flow rates of 50 nL/min* to 50 µL/min
- HESI-II source compatible with liquid flow rates of 1 µL/min to 2 mL/min, without splitting

*Lower limit depends on gauge of needle used.

Typical TSQ Quantum Ultra sensitivity for 0.5 pg chloramphenicol injected on a Thermo Scientific Hypersil GOLD aQ 20 X 2.1 mm 1.9 µm particle packed column at a flow rate of 500 µL/min 30:70 water/methanol. Operating in negative ion mode monitoring the transition 321.0→152.1. Three consecutive injections on the column are visible and showing excellent s/n of better than 570.



System Control

- Powerful embedded computer system with Motorola PowerPC® processor
- Integrated Serial Peripheral Interconnect (SPI) bus for reliable electronic communications between system modules
- Dedicated SHARC™ digital signal processor (DSP) for dedicated instrument control
- Fast 100BASE-T Ethernet port for PC-to-instrument communications

Data Acquisition

- Real-time, high-speed, digital signal processing with dedicated SHARC digital signal processor (DSP)
- High-speed analog-to-digital converter (ADC) with 195 kHz sampling rate
- Adjustable scan speeds to 5000 Da/sec
- High-resolution centroiding

Software Features

Scan Functions

- Highly sensitive full-scan MS in Q1 or Q3
- Selected Ion Monitoring (SIM) in Q1 or Q3
- Selected Reaction Monitoring (SRM) for the most demanding bioanalytical assays
- Product Ion Scanning
- Precursor Ion Scanning
- Neutral Loss Scanning
- H-SRM
- Reverse Energy Ramp MS/MS spectra (RER) gives information rich MS/MS spectra for solid compound identification

Advanced Experiments with Data-Dependent Acquisition Mode

- Available from all scan functions
- Thermo Scientific Dynamic Exclusion allows acquisition of MSⁿ spectra from lower intensity ion species
- Polarity switching capabilities
- AutoSIM
- Quantitation-Enhanced Data-Dependent MS/MS (QED-MS/MS) for simultaneous compound confirmation and quantitation

Accurate Mass Calibration

- Internal lock mass for best performance
- External lock mass for interference-free measurement
- Post-acquisition processing

Data System

- Thermo Scientific Xcalibur processing and instrument control software
- Data system control of all instrument parameters
- Superior comprehensive instrument diagnostics
- Automated optimization of all instrument parameters including gas pressures and collision energy within an experiment
- Direct control of multiple vendor LC systems and autosampler configurations through Xcalibur™ data system software
- High performance PC with Intel® Pentium® microprocessor and Microsoft® Windows® operating system
- 19-inch viewable ultra-sharp, flat screen display monitor

Optional Thermo Scientific Application-Specific Software

- LCQUAN™ quantitation software supports 21 CFR Part 11 compliance
- Mass Frontier™ – spectral interpretation and classification software for the identification of unknowns
- MetWorks™ – automated metabolite identification, component detection and predicted fragmentation in one intuitive workplace
- QuickQuan™ – high-throughput, automated quantitation software for early drug discovery
- QuickCalc™ software powered by Gubbs Inc. GMSU – quantitation and reporting solution for high-throughput ADME laboratories

- Watson LIMS™ – highly specialized protocol-driven Laboratory Information Management System designed to support DMPK/Bioanalytical studies in drug development
- Galileo LIMS™ – fully integrated system for *in vitro* ADME experiments in a single client-server application
- TraceFinder™ – simplifies method development and routine analysis in food safety and environmental laboratories

System Specifications

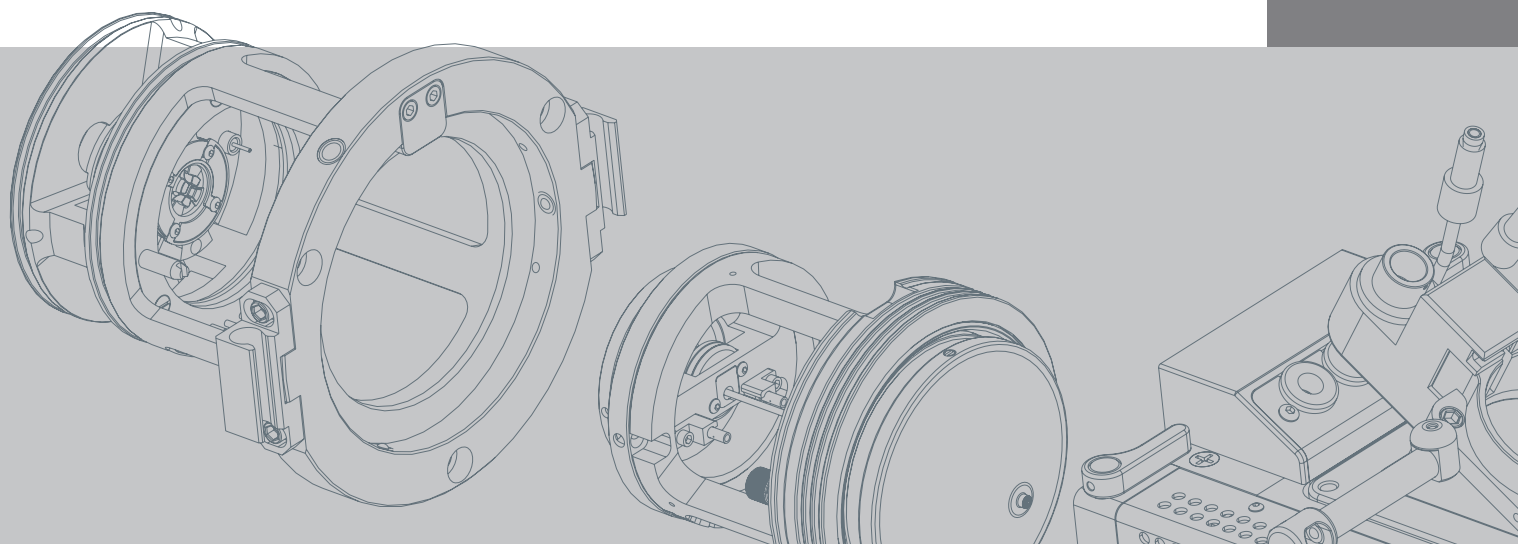
Sensitivity

Heated Electrospray (HESI) at Unit Resolution

A 5 µL injection of a 100 fg/µL (0.3250 fmol/µL) reserpine solution on a Hypersil GOLD aQ 20 X 2.1 mm 1.9 µm particle packed column at a flow rate of 500 µL/min 30:70:0.1 water/Acetonitrile/Formic acid will produce a minimum signal-to-noise ratio of 150:1 for the transition of the protonated molecule at m/z 609.3 to the fragment ion at m/z 195.1 when operated in selected reaction monitoring mode (SRM) with Q1 and Q3 resolution set to 0.7 Da FWHM.

Heated Electrospray (HESI) at High Resolution

A 5 µL injection of a 100 fg/µL (0.3250 fmol/µL) reserpine solution on a Hypersil GOLD aQ 20 X 2.1 mm 1.9 µm particle packed column at a flow rate of 500 µL/min 30:70:0.1 water/Acetonitrile/Formic acid will produce a minimum signal-to-noise ratio of 150:1 for the transition of the protonated molecule at m/z 609.3 to the fragment ion at m/z 195.1 when operated in selected reaction monitoring mode (SRM) with Q1 resolution set to 0.2 Da FWHM and Q3 resolution set to 0.7 Da FWHM.



Atmospheric Pressure Chemical Ionization (APCI) and Atmospheric Pressure Photoionization (APPI) at Unit Resolution

A 5 μL injection of a 100 $\text{fg}/\mu\text{L}$ (0.3250 $\text{fmol}/\mu\text{L}$) reserpine solution on a Hypersil GOLD aQ 20 X 2.1 mm 1.9 μm particle packed column at a flow rate of 500 $\mu\text{L}/\text{min}$ 30:70:0.1 water/Acetonitrile/Formic acid will produce a minimum signal-to-noise ratio of 150:1 for the transition of the protonated molecule at m/z 609.3 to the fragment ion at m/z 195.1 when operated in selected reaction monitoring mode (SRM) with Q1 and Q3 resolution set to 0.7 Da FWHM.

APCI and APPI at High Resolution

A 5 μL injection of a 100 $\text{fg}/\mu\text{L}$ (0.3250 $\text{fmol}/\mu\text{L}$) reserpine solution on a Hypersil GOLD aQ 20 X 2.1 mm 1.9 μm particle packed column at a flow rate of 500 $\mu\text{L}/\text{min}$ 30:70:0.1 water/Acetonitrile/Formic acid will produce a minimum signal-to-noise ratio of 150:1 for the transition of the protonated molecule at m/z 609.3 to the fragment ion at m/z 195.1 when operated in selected reaction monitoring mode (SRM) with Q1 resolution set to 0.2 Da FWHM and Q3 resolution set to 0.7 Da FWHM.

Mass Accuracy—TSQ Quantum Ultra AM

Infusion of a mixture of polyethylene glycols (PEGs) of average molecular weights 200, 400, 600, and 1000 at 50 $\text{pmoles}/\mu\text{L}$ produces 27 ammoniated PEG ions from 124 to 1268 Da. Accurate mass data is generated on each of the 25 ions from 168 to 1224 Da using the neighboring peaks as internal lock masses. The mass of each ion is determined from the average of up to 100 scans and the error between the expected mass and the measured mass is expressed in mmu and ppm . The root mean square (RMS) average is computed from the errors of the 25 individual ions. The RMS error will be less than or equal to 5 ppm .

Performance Specifications

Mass Range

- 10–1500 Da (TSQ Quantum Ultra/Ultra AM)
- 10–3000 Da (TSQ Quantum Ultra EMR)

Resolution

- 7500 (FWHM) at m/z 508 of polytyrosine
- Resolution is continuously adjustable to better than 0.1 Da peak width (FWHM) across the entire mass range.

Mass Stability

TSQ Quantum Ultra/Ultra EMR

- Mass assignment will be within ± 0.050 Da over a 24 hour period. The laboratory room temperature must be maintained between 15–27 $^{\circ}\text{C}$ (59–81 $^{\circ}\text{F}$). The optimum temperature of operation is between 18–21 $^{\circ}\text{C}$ (65–70 $^{\circ}\text{F}$). The room temperature may not change by more than 5 $^{\circ}\text{C}$ (9 $^{\circ}\text{F}$) during this period.

TSQ Quantum Ultra AM

- Mass assignment will be within ± 0.025 Da over a 24 hour period. The laboratory room temperature must be maintained between 15–27 $^{\circ}\text{C}$ (59–81 $^{\circ}\text{F}$). The optimum temperature of operation is between 18–21 $^{\circ}\text{C}$ (65–70 $^{\circ}\text{F}$). The rate of change in temperature may not exceed 2 $^{\circ}\text{C}$ per hour (3.6 $^{\circ}\text{F}/\text{hr}$) and not by more than 5 $^{\circ}\text{C}$ (9 $^{\circ}\text{F}$) during this period.

Installation Requirements

Power

- One 230 Vac $\pm 10\%$, 50/60 Hz at 16 A minimum
- Four 120 Vac $+6\text{--}10\%$, 50/60 Hz at 20 A or four 230 V $\pm 10\%$ AC, 50/60 Hz at 13 A
- Earth ground hardwired to main panel
- Free from voltage variations above or below the recommended operating range

Gas

- Collision gas: 99.995% pure Argon
- Collision gas supply pressure: 135 ± 70 kPa (20 ± 10 psig)
- Sheath/aux/sweep gas: 99% pure Nitrogen
- Sheath/aux/sweep gas supply pressure: 690 ± 140 kPa (100 ± 20 psig)
- Maximum sheath gas consumption: ~ 20 L/min.

Environment

- Functional temperature range: 15 $^{\circ}\text{C}$ to 27 $^{\circ}\text{C}$ (59 $^{\circ}\text{F}$ to 81 $^{\circ}\text{F}$)
- Optimal temperature range: 18 $^{\circ}\text{C}$ to 21 $^{\circ}\text{C}$ (65 $^{\circ}\text{F}$ to 70 $^{\circ}\text{F}$)
- TSQ Quantum Ultra heat output: 2,300 W (8,000 Btu/h)
- Particulate matter: < 3,500,000 particles per cubic meter of air (< 100,000 particles of > 5 μm diameter per cubic foot of air)
- Relative humidity: 20% to 80%, without condensation
- Floors must be free of vibration.

Dimensions

- TSQ Quantum Ultra family: 61 cm \times 56 cm \times 79 cm (h \times w \times d)
- Liquid chromatograph*: 61 cm \times 76 cm \times 61 cm (h \times w \times d)
- Minitower computer: 48 cm \times 18 cm \times 43 cm (h \times w \times d)
- Monitor: 41 cm \times 41 cm \times 43 cm (h \times w \times d)
- Forepumps (each): 30 cm \times 20 cm \times 64 cm (h \times w \times d)
- Laser printer: 20 cm \times 41 cm \times 46 cm (h \times w \times d)

Weight

- TSQ Quantum Ultra: 118 kg
- Liquid chromatograph*: 45 kg
- Minitower computer: 14 kg
- Monitor: 5 kg
- Forepumps (each): 34 kg
- Laser printer: 7 kg

*Values are for the Thermo Scientific Surveyor LC system. Other LC systems will vary.

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