

The Thermo Scientific TSQ Quantum XLS Ultra triple quadrupole mass spectrometer is the highest performing GC-MS/MS instrument with unsurpassed matrix selectivity, analytical performance, and lab productivity – the new “Gold Standard” from Thermo Fisher Scientific, the technology leader in GC-MS/MS.

## Thermo Scientific TSQ Quantum XLS Ultra

The “Gold Standard” in GC-MS/MS



- Highest sensitivity in class with DuraBrite™ IRIS source technology
- HyperQuad™ technology with high mass resolving quadrupoles for unsurpassed matrix selectivity with best in class sensitivity
- Ultra high selectivity for complex matrix samples with enhanced mass resolution (*U-SRM*)
- Analyze a virtually unlimited number of target compounds in one GC run, with two transitions each
- Simultaneous quantitation and confirmation with QED-MS/MS
- Exchangeable ion volumes – no need to vent the MS for preventive maintenance
- PPINICI™ Pulsed Positive Ion Negative Ion Chemical Ionization for sample screening

The Thermo Scientific TSQ Quantum XLS Ultra GC-MS/MS is based on the successful TSQ Quantum XLS system by using HyperQuad technology for highly increased analyte selectivity by increased mass resolution.

The TSQ Quantum XLS Ultra™ GC-MS/MS addresses the requirements of the most demanding analytical tasks in clinical, forensic, toxicology, pharmaceutical, and metabolomics, and especially in routine food safety and environmental analysis for increased target compound selectivity in real life samples.

Increase lab productivity and save precious sample prep time. More compounds can be screened in one run. The TSQ Quantum XLS Ultra GC-MS/MS is specially suited for multi component trace analysis in on run, and is already prepared for Fast-GC applications on 10 to 15 m column lengths.

HyperQuad technology used in the TSQ Quantum XLS Ultra GC-MS/MS delivers superior sensitivity with exceptional precision at the lowest concentration levels. Get to lowest LOQs – at low fg levels for TCDD with LODs <1 ppb in common challenging biological matrices such as food and feed, urine, blood, plant tissues.

State-of-the-art electronics and comprehensive diagnostics are hallmarks of our instruments. Data processing is masterfully facilitated by the unique workflow oriented Thermo Scientific QuanLab Forms processing software, providing compliant reporting with international standards.

Providing industry-leading features and performance, the TSQ Quantum XLS Ultra GC-MS/MS defines the new standard of excellence in GC-MS/MS analysis.



## Hardware Features

### DuraBrite IRIS Source Technology

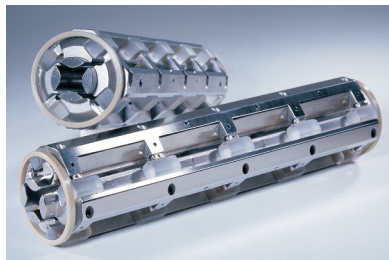
- DuraBrite IRIS source with pre-filter allows detection of low level analytes in complex matrix samples and provides unparalleled uptime along with superior sensitivity
- Exchange ion volumes for extended uptime, or switch from EI to PCI/NCI in only minutes without breaking system vacuum
- Highly inert ion source specially designed for demanding pesticides and drug analysis
- Standard EI, optional CI operation
- Dedicated closed EI, CI, or combined EI/CI ion volumes, maximizing performance in EI, positive ion CI, and negative ion CI
- Computer-controlled CI reagent gas flow control for high quantitative accuracy and day-to-day calibration stability
- No tools required for routine source maintenance
- Unique electron lens isolates filament from contaminants of the source
- Uniquely increased filament lifetime, and improve ionization efficiency for maximum sensitivity
- Electron beam collimating magnets further increase ionization efficiency
- Electron energy adjustable between 0 and 140 eV
- Emission current up to 1000  $\mu\text{A}$
- Independently controlled ion source heating adjustable from 125–350 °C for stable operation and superior chromatographic integrity
- GC transferline interface temperature up to 350 °C

### Inlet/Vacuum Interlock

- Interlock for ion volume exchange with exchange tool is standard
- Allows quick and easy exchange of ion volumes for routine source maintenance without breaking vacuum
- Offers for fast switching from EI to CI, from GC to solid probe analysis without removing the GC transfer line

## Triple Quadrupole Mass Analyzer

- High precision Thermo Scientific HyperQuad mass analyzers Q1 and Q3 provide superior and unique combination of higher mass resolution and increased sensitivity



Thermo Scientific HyperQuad rods

- Mass stability  $\pm 0.1$  Da over >24 hours
- Ultra high selective Selected Reaction Monitoring (U-SRM) with increased mass resolution down to 0.1 Da peak width (FWHM)
- Ultra high selective Selected Ion Monitoring (U-SIM) mode
- Mass resolution adjustable from 0.1 Da to 5.0 Da peak width (FWHM) (Q1 and Q3)
- Variable peak width selection in all scan modes
- MRM Multi-compound detection with up to 3,000 SRM transitions in one analytical GC run
- Minimum dwell time 1 ms for SRM and U-SRM operation
- Fast MRM scan speed of more than 300 SRM/s
- 90° high-efficiency noise-cutting collision cell
- Collision energy range 0–200 eV
- Crosstalk free CID operation
- CID gas pressure programmable through the software
- Collision gases argon (specified) or nitrogen
- Mass range up to  $m/z$  1500
- Full mass scan rate of 5,000 Da/s

### Vacuum System

- Unique close-coupled triple inlet turbo molecular pumping 270 L/s
- Two stages of pumping provide optimal vacuum throughout GC-MS/MS analyzer
- Single mechanical pump 30 L/min, floor standing

## Detection System

- Off-axis ion detection system
- Fast switching (<25 ms) post-acceleration conversion dynode with  $\pm 10$  kV applied voltage
- Off-axis continuous dynode electron multiplier with increased dynamic range >10 E6 (electronic)
- System integrated electron multiplier eliminates field emission and microphonic noise
- Centroid or profile data acquisition modes
- PPINICI mode to acquire positive ion CI and negative ion CI spectra in alternating scans

## Scan Modes

- Highly sensitive full-scan MS in Q1 or Q3
- Selected Reaction Monitoring (SRM) for demanding quantitative assays
- Ultra high Selective Reaction Monitoring (U-SRM) for optimal selectivity
- Selected Ion Monitoring (SIM) in Q1 or Q3
- Ultra high selective Selected Ion Monitoring (U-SIM) mode
- Product Ion Scan
- Precursor Ion Scan
- Neutral Loss Scan

## Advanced Data-Dependent Experiments

- Available from all scan functions
- Dynamic Exclusion™ allows acquisition of MS/MS 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
- Reverse Energy Ramp MS/MS spectra (RER) gives information-rich MS/MS spectra from a range of collision energies for solid compound identification e.g. using spectral library comparison

## Thermo Scientific TRACE GC Ultra Gas Chromatograph

See the TRACE GC Ultra™ multi-channel GC product specification for additional details for the gas chromatograph.

- Multi-level temperature program with seven ramps and eight levels settable from 0.1–120 °C/min
- Eight independent, heated zones for individual control of injectors and detectors plus auxiliary zones

- Digital Carrier Gas Controller (DCC) including gas saver
- Optimized Geometry Split/splitless injector (SSL), temperature range 50 °C to 400 °C in 1 °C increments. Standard with large volume splitless capability for injection volumes up to 50 µL using concurrent solvent recondensation (CSR).
- Maximum oven temperature 450 °C
- Superior oven cool-down for increased sample productivity, from 450 °C to 50 °C in 250 seconds

### GC Options

- Broad range of GC options for maximum versatility
- B.E.S.T. PTV cold injection system for split/splitless, large volume and automated on-column injections (optional, heating rate: up to 14.5 °C/sec (870 °C/min). Programmability: 3 ramps/4 plateaus. Air-cooled down to few degrees above ambient temperature. Sub-ambient: -50 °C with liquid N<sub>2</sub>, -30 °C with CO<sub>2</sub> options.
- Matrix backflush of pre-column for routine matrix sample analysis
- AI/AS 3000 Series II autosampler ideal for routine liquid sample injections
- TriPlus autosampler for liquid, headspace and solid phase microextraction (SPME\*) sampling capabilities

\* Sold under license from Supelco®

### Direct Probe System Options

- Quick, simple method for sample introduction directly into the ion source
- Direct Inlet Probe (DIP) for using glass crucibles, max. temp. 450 °C
- Direct Exposure Probe (DEP/DCI) analysis of highly polar, thermally labile, or suspended solid compounds using fast heating filament with max. temp. ca. 1600 °C
- Powerful screening techniques that are compatible with all modes of ionization and mass analysis
- Switch to solid probe analysis in minutes with GC interface undisturbed

### System Control

- Embedded computer with Motorola PowerPC processor
- Integrated Serial Peripheral Interconnect (SPI) bus
- I/O coprocessor with nonvolatile memory
- AD SHARC digital signal processor (DSP) for dedicated instrument control
- 100BASE-T Ethernet port for instrument data system communications

### Data Acquisition

- Real-time, high-speed, digital signal processing with dedicated AD SHARC DSP
- Digital sampling rate up to 195,000 samples per second
- High mass resolution centroid calculation

### Instrument Diagnostics

- Graphical diagnostics for all power supplies, electronic circuits and pumping system
- Remote access allows Thermo Fisher Scientific engineers to troubleshoot via modem
- Electronic logbook of diagnostic results

### Data System

- Thermo Scientific Xcalibur processing and instrument control software
- QuanLab™ Forms software for routine data analysis and reporting
- Autotune
- Auto mass calibration
- Data system control of GC, MS and autosamplers
- Superior comprehensive instrument diagnostics
- Automated optimization of all instrument parameters including gas pressures and collision energy within an experiment
- High performance PC with Intel® Core™ 2 Duo and Microsoft® Windows® operating system
- 21-inch viewable ultra sharp flat-screen display monitor

### Optional Application Specific Software and Mass Spectrum Libraries

- Thermo Scientific ToxLab and EnviroLab forms are dedicated for toxicology and environmental applications
- Thermo Scientific LCQUAN quantitation software supports 21 CFR Part 11 compliance
- Thermo Scientific MetWorks automated metabolite identification using spectral trees
- Mass Frontier™ spectral interpretation and classification software to identify unknowns
- Thermo Scientific Pesticide library
- NIST library, including collection of MS/MS spectra
- Wiley Registry of Mass Spectral Data, Full Version
- Wiley Registry of Mass Spectral Data with NIST, Full Version
- Wiley Mass Spectra of Pesticides
- Wiley Mass Spectra of Designer Drugs

- Wiley Mass Spectra of Androgens, Estrogens, and other Steroids
- Wiley Mass Spectra of Flavors and Fragrances
- Wiley Maurer-Weber-Pfleger mass spectral library, including printed version

### Performance Specifications

GC triple stage mass spectrometers are most frequently applied to trace quantitative analysis in complex matrix. This means that the ability of the system to select against matrix (reduce chemical noise) is a critical performance factor to be taken into consideration. This can be demonstrated with a signal-to-noise ratio (S/N). In addition, a S/N ratio also provides a guarantee against instrument contamination on installation. Finally, low level precision and instrument detection limits (IDL) provide the complete picture.

### Installation Checkout Specifications

#### Single Reaction Monitoring (SRM) Performance in Solvent Standard

##### EI SRM (U-SRM)

An injection of **100 fg OFN** in solvent will produce an RMS **S/N of ≥12000:1** using the 271.99 > 240.99 *m/z* transition. Quadrupole 1 and quadrupole 3 are set to transmit at 0.2 Da FWHM and 0.7 Da FWHM respectively (U-SRM). Scan rate is ≥five scans per second.

##### PCI SRM

An injection of **100 fg BZP(d<sub>10</sub>)** in solvent will produce an RMS **S/N of ≥300:1** using the 193.14 ≥ 110.07 *m/z* transition. Quadrupole 1 and quadrupole 3 are set to transmit at 0.7 Da FWHM and 0.7 Da FWHM respectively. Scan rate is ≥five scans per second. Methane is used as reagent gas.

### Reference Specifications

#### Instrumental Detection Limit Performance in Solvent Standard<sup>1</sup>

##### EI SRM IDL<sup>2</sup>

**≤6 fg OFN.** Determined from ten injections of a 20 fg/µL **in solvent** using statistical methods (99% confidence). Precision is specified at ≤11% at this low concentration.

#### Single Reaction Monitoring (SRM) Performance in Complex Matrix<sup>1</sup>

##### Matrix EI U-SRM

An injection of **100 fg OFN in 1% Diesel solution** will produce an RMS **S/N of ≥2000:1** using the 271.99 > 240.99 *m/z* transition. Quadrupole 1 and quadrupole 3 are set to transmit at 0.2 Da FWHM and 0.7 Da FWHM respectively. Scan rate is ≥five scans per second.

## Other Performance Specifications<sup>1</sup>

Specification	S/N Value	Compound/inj. amount	Signal (Da)	Q1 FWHM (Da)	Q3 FWHM (Da)
EI Full Scan	≥500:1	1 pg OFN	271.99 (200-300 Da Scan)	0.7	0.7
EI SIM	≥50:1	25 fg OFN	271.99	0.7	0.7
EI U-SIM	≥50:1	25 fg OFN	271.99	0.2	0.7
PCI U-SRM	≥150:1	100 fg BZP (d <sub>10</sub> )	193.14 > 110.07	0.2	0.7
PCI SIM	≥50:1	1 pg BZP (d <sub>10</sub> )	193.14	0.7	0.7
PCI Full Scan	≥50:1	10 pg BZP (d <sub>10</sub> )	193.14	0.7	0.7
NCI SIM	≥300:1	10 fg OFN	271.99	0.7	0.7
NCI Full Scan	≥4000:1	1 pg OFN	271.99 (200-300 Da Scan)	0.7	0.7

### System Dimensions/Weights

Complete GC-MS system requires 2.5 m of workbench space.

#### TSQ Quantum XLS Ultra

(height × width × depth)  
69 × 56 × 79 cm (27 × 22 × 31 in)  
Weight: 118 kg (260 lbs)

#### TRACE GC Ultra

44 × 61 × 65 cm (17 × 24 × 26 in)  
Weight: 55 kg (121 lbs)

#### Forepump (Floor Standing)

30 × 20 × 64 cm (12 × 8 × 25 in)  
Weight: 34 kg (75 lbs)

#### Minitower Computer

48 × 18 × 43 cm (19 × 7 × 17 in)  
Weight: 14 kg (31 lbs)

#### Monitor

41 × 41 × 43 cm (16 × 16 × 17 in)  
Weight: 5 kg (11 lbs)

### Installation Requirements

#### Power

##### TSQ Quantum XLS Ultra System

- One 230 V AC ± 10% at 30 amps, 50/60 Hz, single phase, with earth ground, dedicated to the instrument

##### Data System

- 120 V AC at 10 amps or 230 V AC at 5 amps, single phase, with earth ground

#### Gas Supply

- Collision gas: 99.995% pure Argon
- Helium: purity 99.999% with less than one ppm each of water, oxygen, and total Hydrocarbons
- Collision gas pressure: 135 ± 70 kPa (20 ± 10 psig)
- CI reagent gases: methane, isobutane, ammonia or carbon dioxide with purity 99.99% (PPINICI for CI operation only)

#### Environment

- System averages 4,420 W (15,380 Btu/h) output when considering air conditioning needs. Operating environment must be 15–27 °C (59–81 °F) and relative humidity must be 40–80% with no condensation.
- Optimum operating temperature is 18–21 °C (65–70 °F)

- Functional temperature range: 15–27 °C (59–81 °F)
- Optimal temperature range: 18–21 °C (65–70 °F)
- Particulate matter: <100,000 particles of >5 µm diameter per cubic foot of air (<3,500,000 particles per cubic meter of air)
- Relative humidity: 20–80%, without condensation
- Floors must be free of vibration

### References

- Reference specifications are given as typical instrument performance and not confirmed upon installation.
- Instrument detection limit (IDL) is statistically based (99% confidence) using an on-column concentration close to the IDL. This allows for the best view of performance near to the detection limit. Ion statistics, injection and chromatographic performances causes peak area precision to increase as the detection limit of the instrument is approached. It is difficult to extrapolate an IDL from precision measurements made at higher concentrations.

**See further installation details in the separate pre-installation requirement document.**

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