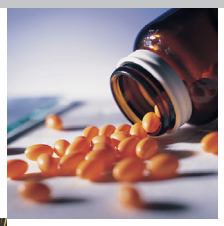
Product Specifications

**The Thermo Scientific TSQ Quantum XLS defines a new standard of excellence in GC-MS/MS structure selective detection for multi-component target compound quantitation in food safety, environmental, forensic, toxicological, pharmaceutical, clinical research, and petrochemical laboratories.**

# Thermo Scientific TSQ Quantum XLS

## The Next Evolution in GC-MS/MS Systems



- **Highest sensitivity in class by DuraBrite™ IRIS source technology**
- **Highest selectivity for complex matrix samples with enhanced mass resolution *(H-SRM)***
- **Analyze a virtually unlimited number of target compounds in one GC run, with two transitions each**
- **EZ-method setup from Excel® tables with timed-SRM at compound retention times**
- **Simultaneous quantitation and confirmation with QED-MS/MS**
- **Exchangeable ion volumes – no need to vent the vacuum**
- **PPINICI™ Pulsed Positive Ion Negative Ion Chemical Ionization for sample screening**
- **Convertible between GC/MS and LC/MS**

With the Thermo Scientific TSQ Quantum XLS we continue the successful and well-known TSQ™ triple quadrupole mass spectrometer series, combined with the power, performance and flexibility of the Thermo Scientific TRACE GC Ultra gas chromatograph.

The TSQ Quantum XLS delivers unsurpassed performance with superior robustness and confidence, especially for complex matrix samples with the new DuraBrite IRIS ion source technology. With best-in-class hyperbolic quadrupoles with highest ion transmission and innovative detection, the TSQ Quantum XLS is the most selective and sensitive GC-triple quadrupole mass spectrometer available today, while providing reliable results 24 × 7 in high-throughput working environments. 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 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 especially designed for demanding pesticides and drug analysis
- Standard EI, 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 µA
- 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

- Patented high precision Thermo Scientific HyperQuad mass analyzers Q1 and Q3 provide superior and unique combination of higher mass resolution and increased sensitivity
- Highly selective Selected Reaction Monitoring (H-SRM) with increased mass resolution at 0.4 Da peak width (FWHM)
- Highly selective Selected Ion Monitoring (H-SIM) mode
- Mass resolution adjustable from 0.4 Da to 5.0 Da peak width (FWHM) (Q1)
- 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 H-SRM operation
- Fast MRM scan speed of more than 300 SRM/s
- 90° high-efficiency noise-cutting collision cell
- Crosstalk free CID operation
- CID gas pressure programmable through the software
- Collision gases argon (specified) or nitrogen
- Mass range of *m/z* 10–3000
- 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

- Patented off-axis ion detection system
- Fast switching (< 25 ms) post-acceleration conversion dynode with ±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
- Highly Selective Reaction Monitoring (H-SRM) for optimal selectivity
- Selected Ion Monitoring (SIM) in Q1 or Q3
- Highly selective Selected Ion Monitoring (H-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

### TRACE GC Ultra™ Gas Chromatograph

See the TRACE GC Ultra product specification for additional specifications 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 – 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 $N_2$, -30 °C with $CO_2$ 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
- Purge and Trap, thermal desorption and pyrolysis sampling system optional available

### Direct Probe System Options

- Quick, simple method for sample introduction directly into the ion source
- Direct Inlet Probe (DIP) for using aluminum crucibles, max. temp. 350 °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

### LC-MS Options

- Convertible to LC-MS mode by replacing EI/CI source with an optional dedicated LC-MS source
- Interchangeable H-ESI and APCI ionization probes
- Thermo Scientific Ion Max API source
- Enhanced sensitivity and ruggedness
- Sweep gas reduces chemical noise
- Optimal 60-degree spray angle for best sensitivity and ruggedness
- 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
- Automated valve for making manual loop injections or diverting LC flow stream to waste
- Automated infusion with syringe pump
- Automated loop injection from syringe pump for analyte optimization

** Sold under license from Supelco®*

### 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
- 19-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/MS Specifications

All specification measurement are performed using a Thermo Scientific TRACE TG-SQC fused silica capillary column, 15 m × 0.25 mm ID × 0.25 µm film.

### Installation Specifications

***Electron Ionization SRM***

Hot splitless injection of 1 µL of a 100 fg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a minimum S/N ratio of **> 2500:1** for the transition of *m/z* 271.99 to the product ion of *m/z* 240.99 when operated in selected reaction monitoring mode (SRM) at five scans per second, using mass resolution of 0.7 Da FWHM.

***Positive Chemical Ionization SRM***

Hot splitless injection of 1 µL of a 100 fg/µL standard of benzophenone (BZP) in n-heptane will produce a minimum S/N ratio of **> 150:1** for the transition of the protonated molecular ion at *m/z* 183.08 to the fragment ion at *m/z* 105.03 when operated in selected reaction monitoring mode (SRM) at five scans per second with mass resolution set to 0.7 Da FWHM and methane as reagent gas.

### Typical Specifications

***Selectivity Specification***
***Electron Ionization H-SRM in Matrix***

Hot splitless injection of 1 µL of a 100 fg/µL standard of octafluoronaphthalene (OFN) with 1% diesel oil in iso-octane will produce a minimum S/N ratio of **> 500:1** for the transition of *m/z* 271.99 to the product ion of *m/z* 240.99 when operated in the highly selective reaction monitoring mode (H-SRM) at five scans per second, using the higher mass resolution set to 0.4 Da FWHM.

***Quantitative Precision Specification***

10 sequential injections of 100 fg OFN will produce an area precision of < 8% RSD at 0.7 Da mass resolution (FWHM).

***Electron Ionization H-SRM***

Hot splitless injection of 1 µL of a 100 fg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a minimum S/N ratio of **> 2500:1** for the transition of *m/z* 271.99 to the product ion of *m/z* 240.99 when operated in the highly selective reaction monitoring mode (H-SRM) at five scans per second, using the higher mass resolution set to 0.4 Da FWHM.

***Electron Ionization Full Scan***

Hot splitless injection of 1 µL of a 1 pg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a S/N ratio of **> 400:1** for *m/z* 271.99 when scanning from 200–300 Da at five scans per second.

***Electron Ionization SIM***

Hot splitless injection of 1 µL of a 25 fg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a S/N ratio of **> 50:1** for *m/z* 271.99 when operated in selected ion monitoring mode (SIM) at five scans per second, with mass resolution set to 0.7 Da FWHM.

***Electron Ionization H-SIM***

Hot splitless injection of 1 µL of a 25 fg/µL standard of octafluoronaphthalene (OFN) in iso-octane will produce a S/N ratio of **> 50:1** for *m/z* 271.99 when operated in the highly selective ion monitoring mode (H-SIM) at five scans per second, using the higher mass resolution set to 0.4 Da FWHM.

***Positive Chemical Ionization H-SRM***

Hot splitless injection of 1 µL of a 100 fg/µL standard of benzophenone (BZP) in n-heptane will produce a minimum S/N ratio of **> 150:1** for the transition of the protonated molecular ion at *m/z* 183.08 to the product ion at *m/z* 105.03 when operated in the highly selective reaction monitoring mode (H-SRM) at five scans per second with the higher mass resolution set to 0.4 Da FWHM, and methane as reagent gas.

***Positive Chemical Ionization Full Scan***

Hot splitless injection of 1 µL of a 10 pg/µL standard of benzophenone in n-heptane will produce a S/N ratio of **> 25:1** for the protonated molecular ion at *m/z* 183.08 when scanning from 80 – 230 Da at two scans per second with mass resolution set to 0.7 Da FWHM, and methane as reagent gas.

***Positive Chemical Ionization SIM***

Hot splitless injection of 1 µL of a 1 pg/µL standard of benzophenone in n-heptane will produce a S/N ratio of **> 50:1** for the protonated molecular ion at *m/z* 183.08 at five scans per second with mass resolution set to 0.7 Da FWHM, and methane as reagent gas.

***Negative Chemical Ionization Full Scan***

Hot splitless injection of 1 µL of a 1 pg/µL standard of OFN in iso-octane will produce a S/N ratio of **> 2500:1** for *m/z* 271.99 when scanning from 200–300 Da at five scans per second with mass resolution set to 0.7 Da FWHM, and methane as the reagent gas.

***Negative Chemical Ionization SIM***

Hot splitless injection of 1 µL of a 25 fg/µL standard of OFN in iso-octane will produce a S/N ratio of **> 200:1** for *m/z* 271.99 when operated in selected ion monitoring mode (SIM) at five scans per second, with mass resolution set to 0.7 Da FWHM, and methane as reagent gas.

## LC/MS Specifications

***Electrospray (H-ESI)***

A 5 µL loop injection of a 2 pg/µL (3.250 fmol/µL) reserpine solution at a flow rate of 400 µL/min 50/50 IPA/water will produce a S/N ratio of **> 100:1** for the transition of the protonated molecular ion at *m/z* 609.30 to the fragment ion at *m/z* 195.10 when operated in selected reaction monitoring mode (SRM) with mass resolution set to 0.7 Da FWHM.

***Atmospheric Pressure Chemical Ionization (APCI) and Atmospheric Pressure Photoionization (APPI)***

A 5 µL loop injection of a 2 pg/µL (3.250 fmol/µL) reserpine solution at a flow rate of 1 mL/min 50/50 IPA/water will produce a S/N ratio of **> 100:1** for the transition of the protonated molecular ion at *m/z* 609.3 to the fragment ion at *m/z* 195.1 when operated in selected reaction monitoring mode (SRM) with mass resolution set to 0.7 Da FWHM.

## System Dimensions/Weights

Complete GC-MS system requires 2.5 m of workbench space. Optional LC will require additional workbench space.

### TSQ Quantum XLS

*(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 x 17 in)
Weight: 5 kg (11 lbs)

### Laser Printer

20 × 41 × 46 cm (8 × 16 × 18 in)
Weight: 7 kg (15 lbs)

## Installation Requirements

### Power

***TSQ Quantum XLS 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

***Optional Liquid Chromatograph*****

- 120 V AC at 10 amps or 230 V AC at 5 amps, single phase, with earth ground
- Stable voltage, free of spikes

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

### 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%
- One high-purity (99% pure) nitrogen gas supply for the API source (optional). Required pressure is 690 ± 140 kPa (100 ± 20 psi). Maximum consumption of nitrogen gas is 20 L/min (56 SCFH). (Optional, for LC/MS)

### 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

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

**www.thermoscientific.com**



**Africa-Other** +27 11 570 1840
**Australia** +61 2 8844 9500
**Austria** +43 1 333 50 34 0
**Belgium** +32 53 73 42 41
**Canada** +1 800 530 8447
**China** +86 10 8419 3588
**Denmark** +45 70 23 62 60
**Europe-Other** +43 1 333 50 34 0
**Finland/Norway/Sweden** +46 8 556 468 00
**France** +33 1 60 92 48 00
**Germany** +49 6103 408 1014
**India** +91 22 6742 9434
**Italy** +39 02 950 591
**Japan** +81 45 453 9100
**Latin America** +1 608 276 5659
**Middle East** +43 1 333 50 34 0
**Netherlands** +31 76 579 55 55
**South Africa** +27 11 570 1840
**Spain** +34 914 845 965
**Switzerland** +41 61 716 77 00
**UK** +44 1442 233555
**USA** +1 800 532 4752

*Thermo Fisher Scientific, San Jose, CA USA is ISO Certified.*
PS10296_E 04/10M

Thermo SCIENTIFIC