

Xevo TQ-XS

Xevo® TQ-XS is an advanced benchtop tandem quadrupole mass spectrometer which expands the scope of ultimate sensitivity analysis. It features StepWave XS™ ion transfer optics delivering enhanced sensitivity, robustness, and reliability; passively removing gas load and undesirable neutral contaminants while actively transferring ions into the mass analyzer.

Sensitivity benefits are more accessible as the Xevo TQ-XS also features a tool-free probe design which allows users much easier maintenance, optimization and improved reproducibility between operators. Method transfer onto the Xevo TQ-XS is made simple by the Xtended Dynamic Range (XDR™) detector which allows six orders of linear dynamic range. Wider compound coverage without changing ionization technique is delivered by the revolutionary UniSpray™ source option.

In addition to these benefits, users can combine quantitative MRM with qualitative MS data acquisition through RADAR™ and confirm low levels of compounds using ScanWave™ enhanced Product Ion Confirmation scanning. The MassLynx® software supporting this instrument ensures that automated system optimization, status monitoring, results review, and reporting is a smooth process using IntelliStart™ and TargetLynx XS.™



SYSTEM HARDWARE SPECIFICATIONS

API sources and ionization modes	High performance ZSpray™ dual-orthogonal API sources: 1) Multi-mode source - tool free ESI/APCI/ESCI® (standard) NB – Dedicated APCI requires an additional probe (optional) 2) UniSpray ion source (optional) 3) Tool-free APCI probe (optional) 4) Dual mode APPI/APCI source (optional) 5) NanoFlow™ ESI source (optional) 6) ASAP (optional) 7) APGC ion source (optional) 8) ionKey™ source (optional) Optimized gas flow dynamics for efficient ESI desolvation (supporting LC flow rates up to 2 mL/min) Tool-free source exchange Vacuum isolation valve Tool-free access to user serviceable elements Plug-and-play probes De-clustering cone gas Software control of gas flows and heating elements
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UniSpray ion source option	UniSpray is a novel ionization technique designed to broaden the scope of compounds which can be analyzed in a single run, including those which typically optimize in ESI, APCI or APPI. Enhanced ionization efficiency and desolvation allow the potential to combine several methodologies into one, or simply enable the operator to keep the same source for multiple methods, requiring less time performing set-up and routine maintenance, and more time delivering results.
Ion source transfer optics	StepWave XS ion transfer optics (US patent - US9035241) delivering class leading UPLC®-MS/MS sensitivity. The unique off-axis design and segmented quadrupole second stage dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyzer at the same time as actively eliminating undesirable neutral contaminants.
Mass analyzer	Two high-resolution, high-stability quadrupole analyzers (MS1/MS2), plus pre-filters to maximize resolution and transmission while preventing contamination of the main analyzers.
Collision cell	T-Wave™ enabled for optimal MS/MS performance at high data acquisition rates; ScanWave enabled for enhanced MS/MS spectral performance (product ion scanning); Software programmable gas control.
Detector	Low-noise, off-axis, long-life photomultiplier XDR detector.
Vacuum system	Three air-cooled turbomolecular vacuum pumps One vacuum backing pump
Dimensions	Width: 61.0 cm (24.0 in.) Height: 70.7 cm (27.8 in.) Depth: 99.5 cm (39.0 in.)
Regulatory approvals	CE and NRTL

SYSTEM SOFTWARE SPECIFICATIONS

Software	Systems supported on MassLynx version 4.2 or later; OpenLynx™ and TargetLynx XS Application Managers are included as standard.
IntelliStart Technology	System parameter checks and alerts Integrated sample/calibrant delivery system + programmable divert valve Automated mass calibration Automated sample tuning Automated SIR and MRM method development UPLC-MS/MS System Check – automated on-column performance test
Automated MRM scheduling (acquisition rate assignment)	Dwell time, inter-channel delay time and inter-scan delay time for individual channels in a Multiple MRM experiment can be automatically assigned (using the Auto-Dwell feature) to ensure that the optimal number of MRM data points per chromatographic peak are acquired. The Auto-Dwell feature dynamically optimizes MRM cycle times to accommodate retention time windows that overlap. This greatly simplifies MRM method creation, irrespective of the number of compounds in a single assay, while at the same time ensuring the very best quantitative performance for every experiment.

Automated MRM scheduling (acquisition window assignment)	Multiple MRM experiments can be scheduled (manually or automatically using the Quanpedia™ database) using retention time windows to optimize the cycle time for each MRM channel monitored. If required, MRM retention time windows can overlap partially or completely, ensuring that MRM data acquisition rates will be optimal for the quantification of all analytes in a given assay.
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PERFORMANCE SPECIFICATIONS

Acquisition modes	Full scan MS Product ion scan (ScanWave enhanced) Precursor ion scan Constant neutral loss scan Selected ion recording (SIR) Multiple reaction monitoring (MRM) Simultaneous Full scan and MRM (RADAR)
Survey scan modes	Full scan MS data acts as an automatic trigger for the collection of ScanWave-enhanced product ion spectra Precursor ion scan data acts as an automatic trigger for the collection of ScanWave-enhanced product ion spectra Constant neutral scan data acts as an automatic trigger for the collection of ScanWave-enhanced product ion spectra
Product ion confirmation (PIC) mode	MRM data acts as an automatic trigger for the collection of ScanWave-enhanced product ion spectra.
RADAR	An information rich acquisition approach that allows you to collect highly specific quantitative data for target compounds while providing the ability to visualize all other components.
Mass range	2 to 2048 m/z
Scan speed	Up to 20,000 Da/s Examples of achievable acquisition rates: 20 scans per second (m/z 50 to 1000) 40 scans per second (m/z 50 to 500)
Mass stability	Mass assignment will be within +/- 0.05 Da over a 24 hour period (the instrument must be operated in conformance with the laboratory environmental guidelines given in the Xevo TQ-XS site preparation guide).
Linearity of response	The linearity of response relative to sample concentration, for a specified compound, is six orders of magnitude from the limit of detection.
Polarity switching time	15 ms to switch between positive and negative ion modes
MS to MS/MS switching time	3 ms
ESCI mode switching time	20 ms to switch between ESI and APCI
MRM acquisition rate	Maximum acquisition rate of 500 MRM data points per second; Minimum dwell time of 1 ms per MRM channel; Minimum inter-channel delay of 1 ms

Inter-channel cross talk	The inter-channel cross talk between two MRM transitions, acquired using an MRM dwell time of 1 ms and an inter-channel delay time of 1 ms, is less than 0.01%.
Number of MRM channels	Up to 32,768 MRM channels (1,024 functions, 32 channels per function) can be monitored in a single acquisition; up to 1,024 MRM channels when operating in GLP/secure mode (32 functions, 32 channels per function).
Mass resolution	Automatically adjusted (IntelliStart) to desired resolution; (0.50 Da, 0.75 Da or 1.00 Da FWHM)
MRM sensitivity (ESI+)	A 1 pg on-column injection of reserpine will give a chromatographic signal-to-noise greater than 500,000:1, using raw unsmoothed data (Gradient separation, LC mobile phase flow rate of 0.4 mL/min, MRM transition m/z 609 > 195)
MRM sensitivity (ESI-)	A 1 pg on-column injection of chloramphenicol will give a chromatographic signal-to-noise greater than 500,000:1, using raw unsmoothed data (Gradient separation, LC mobile phase flow rate of 0.8 mL/min, MRM transition m/z 321 > 152)
MRM sensitivity (APCI+)	A 1 pg on-column injection of 17- α -hydroxyprogesterone will give a chromatographic signal-to-noise greater than 300:1, using raw unsmoothed data (Gradient separation, LC mobile phase flow rate of 0.8 mL/min, MRM transition m/z 331 > 109)

It should be noted that the above are not standard installation specifications. All Xevo TQ-XS instruments will be installed and tested in accordance with standard commissioning tests as detailed in Waters document (Xevo TQ-XS Installation Checklist). Performance specifications given in this document and installation test criteria are routinely reviewed to ensure quality is maintained and are therefore subject to change without notice. See Site Preparation Guide and Product Release Notes for additional product and specification information.

Related Patents:

1. The traveling wave device described here is similar to that described by Kirchner in US Patent 5,206,506; 1993.
2. ZSpray (US Patent 5,756,994).
3. ScanWave (Patents US7405401, WO2007125354, WO2007052025, WO200804710, WO2006129106).
4. StepWave (US Patent 9,035,241).

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