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Waters Xevo TQ-S

Xevo® TQ-S is an advanced benchtop tandem quadrupole mass spectrometer, designed to meet the needs of your most demanding quantitative LC/MS/MS applications. Xevo TQ-S features revolutionary off-axis StepWave™ ion transfer optics that 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.

Xevo TQ-S also features ScanWave™ collision cell technology to provide the very best high-speed MRM , an enhanced product ion spectral acquisition capability and a valuable, information-rich acquisition mode known as RADAR™ The system incorporates IntelliStart™ Technology, for automated system optimization and status monitoring, ensuring that the highest quality data is routinely available to all levels of operator.

SYSTEM HARDWARE SPECIFICATIONS

API sources and ionization modes	High performance ZSpray™ dual-orthogonal API sources: 1) Multi-mode source – ESI/APCI/ESCi® (standard) NB – Dedicated APCI requires an additional probe (optional) 2) APCI IonSABRE II probe (optional) 3) Dual mode APPI/APCI source (optional) 4) nanoFlow ESI source (optional) 5) ASAP (optional) 6) APGC ion source (optional) 7) TRIZAIC™ ion 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
Ion source transfer optics	StepWave ion transfer optics (Waters patent pending) delivering class leading UPLC/MS/MS sensitivity. The unique off-axis design dramatically increases the efficiency of ion transfer from the ion source to the quadrupole MS analyser 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 detector; Digital dynamic range of 4×10^6

Vacuum system	Three air-cooled turbomolecular vacuum pumps; Two vacuum backing pumps
Dimensions	Width: 61.0 cm (24.0 in.) Height: 70.7 cm (27.8 in.) Depth: 99.5 cm (39.0 in.)
Regulatory approvals	IVD, CE, and NRTL

SYSTEM SOFTWARE SPECIFICATIONS

Software	Systems supported on MassLynx™ version 4.1 or later; OpenLynx™ and TargetLynx™ 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 quantita tive 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

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)
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 10,000 Da/s Examples of achievable acquisition rates: 10 scans per second (m/z 50 to 1000) 20 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-S site preparation guide)
Linearity of response	The linearity of response relative to sample concentration, for a specified compound, is five orders of magnitude from the limit of detection
Polarity switching time	20 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 250 MRM data points per second; Minimum dwell time of 1 ms per MRM channel; Minimum inter-channel delay of 3 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 3 ms, is less than 0.01%
Number of MRM channels	Up to 16,384 MRM channels (512 functions, 32 channels per function) can be monitored in a single acquisition; up to 8,000 MRM channels when operating in GLP/secure mode (250 functions, 32 channels per function)
Mass resolution	Automatically adjusted (IntelliStart) to desired resolution; The valley between the m/z 2034.63 and m/z 2035.63 peaks is < 12% of the average height of the two peaks
MRM sensitivity (ESI+)	A 50 fg on-column injection of reserpine will give a chromatographic signal-to-noise greater than 3,000:1 (Gradient separation, LC mobile phase flow rate of 0.8 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 3,000:1 (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 of 17-α-hydroxyprogesterone will give a chromatographic signal-to-noise greater than 100:1 (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-S instruments will be installed and tested in accordance with standard performance tests as detailed in Waters document (715002460, Xevo TQ-S 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 (Patent WO 2009/037483 A2).

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