Waters Xevo TQ-S

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 required 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)

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 in 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

CE and NTRL

System Software Specifications

Software

Systems supported on MassLynx^{tm} version 4.1 or later; Open Lynx^{tm} and TargetLynx^{tm} 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.

Performance Specifications

Acquisition Modes

Full scan MS
Product ion scan (ScanWave enhanced)
Precurser 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 procut ion spectra.
Constant neutral scan data acts as an automatic trigger for the collection of ScanWave-enhanced product in 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 quantitave 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 transition, 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 300:1 (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-a-hydroxyprogesterone will give a chromatographic signal-to-noise greater than 100:1 (LC mobile phase flow rate of 0.8 mL/min, MRM transition m/z 331 > 109).

MRM Signal-to-noise definition

Signal is defined as the height of the chromatographic peak of interest and noise is defined as the RMS of a continuous section of the mass chromatogram.

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, WO2007022025, Wo2006129106, WO200804710).
4. StepWave (Patent WO2009/037483 A2).