# [INSTRUMENT SPECIFICATIONS]

THE SCIENCE OF WHAT'S POSSIBLE.

# Waters Xevo TQ MS

The Waters<sup>®</sup> Xevo<sup>™</sup> TQ Mass Spectrometer is an advanced, bench top, tandem quadrupole mass spectrometer designed for ultra high performance LC/MS/MS applications. Unlike conventional tandem quadrupole mass spectrometers, the Xevo TQ MS utilizes unique T-Wave<sup>™1</sup> and ScanWave<sup>™</sup> enabled collision cell technology to provide a highly flexible analytical tool capable of supporting both quantitative and qualitative studies on a single MS platform. The Xevo TQ MS is a robust platform for quantitative LC/MS/MS, featuring high speed MRM (Multiple Reaction Monitoring), with enhanced full scan spectral acquisition modes providing additional qualitative LC/MS/MS capabilities.

The system incorporates IntelliStart<sup>™</sup> 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	<ul> <li>High performance ZSpray<sup>™</sup> dual-orthogonal API sources:</li> <li>1) Multi mode source – ESI/APCI/ESCi<sup>®</sup> (standard) NB – Dedicated APCI requires an additional probe (optional)</li> <li>2) Dual mode APPI/APCI source (optional)</li> <li>3) Nano-flow ESI source (optional)</li> <li>4) Atmospheric pressure solids analysis probe - ASAP (optional)</li> <li>5) Atmospheric pressure gas chromatography ion source - APGC (optional)</li> </ul>
	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 customer serviceable elements Plug and play probes De-clustering cone gas Software control of gas flows and heating elements
lon source transfer optics	High efficiency hexapole ion guide
Mass analyzer	Two high resolution 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 up to $4 \times 10^6$
Vacuum system	Two air-cooled vacuum turbomolecular pumps evacuating the source and analyzer; One rotary backing pump
Dimensions	Width:61.0 cm (24.0 in.)Height:70.7 cm (27.8 in.)Depth:90.4 cm (35.6 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 The following MassLynx Quantification Work-flow Tools are also included as standard
IntelliStart Technology	System parameter checking and alerts Integrated sample/calibrant delivery system + programmable divert valve Automated mass calibration Automated sample tuning Automated SIR and MRM method development LC/MS System Check – automated on-column performance test
Quantification methods database	Quanpedia™ – a data base for storing and sharing user defined LC/MRM acquisition methods and associated processing methods for the targeted quantification of named compounds is provided as standard; database entries (greater than 1000 compounds) for a number of applications are also provided as a standard
Auto-Dwell feature for MRM 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 is acquired. The Auto-Dwell feature can dynamically optimize MRM cycle times to accommodate retention time windows that either partially or completely 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.
MRM 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. This ensures 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 enh	anced)
Precursor ion scan	
Constant neutral loss	
Selected ion recording (SIR)	
Multiple reaction monitoring (M	RM)
Survey scan modes Full scan MS triggered product i	on scan
Precursor ion scan triggered pro	duct ion scan
Constant neutral loss triggered	product ion scan
Quan Qual mode MRM triggered ScanWave enhan	ced product ion spectral acquisition
Mass range 2 to 2048 m/z	
Scan speed Up to 10,000 Da/s	
Examples of achievable acquisit	on rates:
10 scans per second (m/z 100 t	o 1000)
20 scans per second (m/z 50 to	500)
Mass stability Mass drift is less than 0.1 amu o	ver a 24 hour period
Linearity of response The linearity of response relativ	e to sample concentration, for a specified compound, is five orders
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Polarity switching time	20 ms to switch between positive and negative ion modes
MS to MS/MS switching time	5 ms
ESCi mode switching time	20 ms to switch between ESI and APCI
MRM acquisition rate	Minimum dwell time of 1 ms per MRM channel
Inter-channel cross talk	The inter-channel cross talk between two MRM transitions, acquired using an MRM dwell time of 10 ms and an inter-channel delay time of 10 ms, will be less than 0.02%
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 1024 MRM channels when operating in GLP/secure mode (32 functions, 32 channels per function)
Mass resolution	Automatically adjusted (IntelliStart) to desired resolution; (0.40 Da, 0.75 Da or 1.00 Da FWHM)
MRM sensitivity (ESI+)	A 50 fg on-column injection of reserpine will give a chromatographic signal-to-noise greater than 500:1 (Gradient separation, LC mobile phase flow rate of 0.8 mL/min, MRM transition <i>m/z</i> 609 > 195)
MRM sensitivity (ESI-)	A1 pg on-column injection of chloramphenicol will give a chromatographic signal-to-noise greater than 1,000:1 (Gradient separation, LC mobile phase flow rate of 0.8 mL/min, MRM transition <i>m/z</i> 321 > 152)
MRM sensitivity (APCI+)	A 10 pg on-column injection of of 17- $\alpha$ -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 <i>m/z</i> 331 > 109)

It should be noted that the above are not standard installation specifications. All Xevo TQ MS instruments will be installed and tested in accordance with standard performance tests as detailed in Waters document (715001885, Xevo TQ MS Installation Checklist). 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 productand specification information.

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, W02007125354, W02007052025, W0200804710, W02006129106).





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