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Micromass Quattro Premier LC/MS/MS

High Performance LC/MS/MS to meet your demanding quantification needs

Specialized quantitative applications, including ADME screening, bioanalysis, clinical analysis, as well as food safety and environmental monitoring, require high sensitivity, high performance LC/MS/MS instrumentation. Compliance with stringent regulatory guidelines may also be necessary with these applications.

Now you can achieve high performance and low detection limits in a compact, easy-to-use system that includes the Waters Micromass Quattro Premier Tandem Quadrupole Mass Spectrometer, featuring T-Wave (traveling wave collision cell) technology. To ensure high quality, secure data- from method development to high throughput quantitative analyses- MassLynx 4.0 software and its dedicated application managers make your operating system easier than ever before.

Powerful Technology Platform- Quattro Premier Mass Spectrometer

The Micromass Quattro Premier provides a powerful platform for MS analyses, upon which total system solutions may be designed to maximize performance for your application.

- Zspray- premium API interface for sensitivity and robustness
 - Compact size- uses only 18.9" (48 cm) of linear bench space
 - Sensitivity- Enhanced ion optics using T-Wave technology for high efficiency ion transmission
 - Fast analysis- T-wave collision cell for optimum performance at fast acquisition rates
 - Dynamic range- up to 5 orders of magnitude for accurate determination across a wide concentration range
 - DDA- Data Directed Analysis for intelligent, automated MS to MS/MS switching within a single analytical run
 - Integrated syringe pump- under Masslynx control
 - Gas flow control- software regulation of source and collision gases
- Options
- IonSABRE APCI Probe- high performance APCI probe for enhanced sensitivity at high flow rates
 - APPI/APCI dual ionization source- Atmospheric pressure photo and chemical ionization in a single

analysis for the comprehensive analysis of nonpolar compounds

- ESCi Multi-Mode Ionization Source- APCI and ESI in the same analysis for increased ionization

coverage for a wide range of compound classes

- MUX-technology- 4 way electrospray ionization interface for high throughput parallel analyses

Why LC/MS/MS?

LC/MS/MS is the industry standard for dedicated quantitative analysis, with the tandem quadrupole mass

spectrometer being the primary instrument for accurate, sensitive determination of compounds.

The flexibility of the tandem quadrupole configuration provides several distinct modes of analysis, enabling

compound identification, structural elucidation, determination of characteristic compound classes and highly

selective quantification.

- MS Scan
- Selected Ion Recording (SIR)
- Product ion scan
- Constant neutral loss scan
- Precursor ion scan
- Multiple Reaction Monitoring (MRM)

Quattro Premier Performance Specifications

Electrospray Positive Ion

The measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 609 to m/z 195 on injection of 5 pg of reserpine is $\geq 500:1$. This is based on a 5- μL injection of a 1 pg/ μL reserpine solution in 70:30 acetonitrile/water (no additives) at a flow rate of 200 $\mu\text{L}/\text{min}$ in MRM mode, 0.5 second dwell, span 0 Da.

The resolution of the precursor and product ions is <1 Da peak width at half-height.

Electrospray Negative Ion

The measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 503 to m/z 179 on injection of 25 pg of raffinose is $\geq 50:1$. This is based on a 5- μL injection of a 5 pg/ μL raffinose solution in 70:30 acetonitrile/water (no additives) at a flow rate of 200 $\mu\text{L}/\text{min}$ in MRM mode, 0.5 second dwell, span 0 Da.

The resolution of the precursor and product ions is <1 Da peak width at half-height.

MS Resolution

The resolution is demonstrated using a 1 $\mu\text{g}/\mu\text{L}$ solution of PPG 2000 in 50:50 acetonitrile/water containing 1-mM ammonium acetate. The peaks at m/z 2009.5 and 2010.5 should be resolved with a valley between them of no more than 15% of the height of the 2010.5 peak. It is recommended that fifteen 1-second scans are summed and the resulting spectrum smoothed (two passes, 0.5 Da SG).

Mass Measurement Accuracy

The mass measurement accuracy is measured from the mean of five repeat analyses of the

[M+NH₄]⁺ peak at m/z 1004.622 from 1 µg/µL PEG 1000 in 50:50 acetonitrile/water containing 2 mM ammonium acetate. The mean measured mass will be 1004.622 +0.05 Da. The standard deviation of the mean will be <0.05 Da.

A mass calibration will be performed using the [M+H]⁺ peaks from a separate analysis over the mass range m/z 700 to 1300 and the resolution on the [M+H]⁺ peak at m/z 1031.62 must be between 0.3 and 0.4 Da wide at half height after smoothing.

APCI Positive Ion

Measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 331.2 to m/z 109.1 on injection of 50 pg of 17- α -hydroxyprogesterone will be $\geq 70:1$, using a 5 µl injection of a 10 pg/µl 17- α -hydroxyprogesterone solution in 70:30 acetonitrile/water (no additives) at a flow rate of 1 mL/min in MRM mode, 0.2 second dwell, span 0 Da.

The resolution of the precursor and product ions will be <1 Da peak width at half height

Quattro Premier Overview

The Quattro Premier™ is a high-performance tandem quadrupole mass spectrometer designed for routine LC/MS/MS operation

The Quattro Premier may be coupled to either of two types of inlet:

- An HPLC system, to provide molecular weight information from an LC run or perform target analysis and quantification.
- A syringe pump, for analysis of precious, low-concentration compounds

The sample is ionized at atmospheric pressure in the source. The ions enter the vacuum system through a sampling cone, then pass through the source travelling-wave (T-Wave™) ion guide into the first quadrupole, where they are filtered according to their mass-to-charge ratio (m/z). The mass-separated ions pass into the T-Wave collision cell where they either undergo collision-induced decomposition (CID) or pass to the second quadrupole. Any fragment ions are then mass-analyzed by the second quadrupole. The transmitted ions are detected by a conversion dynode, phosphor, and photomultiplier detection system. The output signal is then amplified, digitized, and passed to the control system.

Sample Inlet

An HPLC system or infusion pump delivers sample to a ZSpray™ Ionization Source. The ionization technique (see [Section F.1](#)) is selected by installing the appropriate probe. An ESI (electrospray ionization) probe is supplied as standard. An APCI (atmospheric pressure chemical ionization) is available as an option. Recognition pins on the probe identify the ionization method to the system. The source can also be operated as an ESCi™ multi-mode ionization source to combine ESI and APCI operation in a single run (see [Chapter 4](#)). In this case the ESI probe is used together with an APCI corona discharge pin, which is supplied as standard.

Vacuum System

An external backing pump and internal turbomolecular pumps generate vacuum in the instrument. The backing pump may be a rotary pump or, optionally, an oil-free scroll pump.

The control system monitors the turbomolecular pump speeds and continuously monitors

the vacuum using an integral Pirani gauge. The Pirani gauge stops instrument operation if a vacuum loss is detected.

A vacuum isolation valve allows routine source maintenance to be performed without breaking the vacuum.

MassLynx Control System

The Quattro Premier is controlled by the PC-based MassLynx™ software. MassLynx also controls the HPLC system, autosampler, and divert/injector valve, if applicable. A second PC, embedded in the Quattro Premier, processes the acquired data. Communication between the MassLynx PC and the embedded PC is via a network link.

Analog inputs allow data acquisition from conventional LC detectors like an ultraviolet (UV) detector or evaporative light scattering detector (ELSD). Data from selected UV photo diode array detectors (for example, the Waters 996 PDA detector) can also be acquired.

The MassLynx software allows the following processes:

- Configuring the Quattro Premier.
- Creating inlet and MS methods that define operating parameters for a run.
- Tuning and calibrating the Quattro Premier.
- Running samples.
- Monitoring the run.
- Acquiring data.



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