Waters
THE SCIENCE OF WHAT'S POSSIBLE.™

SYNAPT G2-S High Definition MS (HDMS) System

High performance, versatility, and workflow efficiency of your MS system all play a crucial role in your ability to successfully reach your scientific and business goals – and that's what drives the evolution of Waters® SYNAPT® technology.

SYNAPT G2-S combines revolutionary StepWave™ ion optics with proven Quantitative Tof (QuanTof™) and High Definition MS™ technologies to provide the highest levels of sensitivity, selectivity, and speed. With Waters' leading MS Informatics, SYNAPT G2-S will help you efficiently extract the maximum information from your most challenging samples – in less time – so you can be first to discover, first to publish, first to succeed.

SYNAPT G2-S HDMS is a high resolution exact mass MS/MS platform designed to get you to the right result, faster – no matter how challenging your application is. When you want to reach beyond the boundaries of conventional mass spectrometry, SYNAPT G2-S High Definition Mass Spectrometry™ (HDMS™) provides a new dimension to your discovery capability by combining high efficiency ion mobility based measurements and separations with high performance tandem mass spectrometry. By enabling you to differentiate samples by size, shape, and charge – as well as mass – this unique capability allows you to make discoveries that simply aren't possible any other way.

PERFORMANCE SPECIFICATIONS

The SYNAPT G2-S HDMS System can operate in two modes:	(a) TOF mode (b) Mobility-TOF mode
TOF Mass Resolution in Positive Ion	(a) Sensitivity Mode 10,000 FWHM measured on the $(M + 6H)^{6+}$ isotope cluster from bovine insulin (*m/z* 956) (b) Resolution Mode 20,000 FWHM measured on the $(M + 6H)^{6+}$ isotope cluster from bovine insulin (*m/z* 956) (c) High Resolution Mode 40,000 FWHM measured on the $(M + 6H)^{6+}$ isotope cluster from bovine insulin (*m/z* 956)

TOF Mass Resolution in Negative Ion	(a) Sensitivity Mode 10,000 FWHM measured on the $(M - 4H)^{4-}$ isotope cluster from bovine insulin (*m/z* 1431) (b) Resolution Mode 20,000 FWHM measured on the $(M - 4H)^{4-}$ isotope cluster from bovine insulin (*m/z* 1431) (c) High Resolution Mode 40,000 FWHM measured on the $(M - 4H)^{4-}$ isotope cluster from bovine insulin (*m/z* 1431)
Positive Ion MS Sensitivity	a) Sensitivity Mode The peak at *m/z* 556 from a solution of 50 pg/µL leucine enkephalin in 50/50 acetonitrile/water + 0.1% formic acid, infused at a flow rate of 5 µL/min, will have an intensity of greater than 41,600 ions per second. The instrument will be tuned to 10,000 resolution (as demonstrated on bovine insulin) and the mass range will be set to a maximum of 1200 *m/z*. (b) Resolution Mode The peak at *m/z* 556 from a solution of 50 pg/µL leucine enkephalin in 50/50 acetonitrile/water + 0.1% formic acid, infused at a flow rate of 5 µL/min, will have an intensity of greater than 20,800 ions per second. The instrument will be tuned to 20,000 resolution (as demonstrated on bovine insulin) and the mass range will be set to a maximum of 1200 *m/z*. (c) Enhanced Duty Cycle (EDC) Mode The peak at *m/z* 556 from a solution of 10 pg/µL leucine enkephalin in 50/50 acetonitrile/water + 0.1% formic acid, infused at a flow rate of 5 µL/min, will have an intensity of greater than 24,800 ions per second. The instrument will be tuned to 20,000 resolution (as demonstrated on bovine insulin), with sensitivity set to a maximum at 556 *m/z*.
Negative Ion MS Sensitivity	(a) Sensitivity Mode The peak at *m/z* 503 from a solution of 500 pg/µL raffinose in 70/30 acetonitrile/water (no additives), infused at a flow rate of 5 µL/min, will have an intensity of greater than 44,800 ions per second. The instrument will be tuned to 10,000 resolution (as demonstrated on bovine insulin), and the mass range will be set to a maximum of 1200 *m/z*. (b) Resolution Mode The peak at *m/z* 503 from a solution of 500 pg/µL raffinose in 70/30 acetonitrile/water (no additives), infused at a flow rate of 5 µL/min, will have an intensity of greater than 22,400 ions per second. The instrument will be tuned to 20,000 resolution (as demonstrated on bovine insulin), and the mass range will be set to a maximum of 1200 *m/z*.
Positive Ion MS/MS Sensitivity	(a) Sensitivity Mode Using a [Glu[1]] -Fibrinopeptide B solution of 100 fmol/µL, at a flow rate of 5 µL/min and with the instrument tuned for 10,000 resolution (as demonstrated on bovine insulin), the intensity of the most intense y" sequence ion from the MS/MS spectrum of the doubly charged precursor ion (785.8 *m/z*) will be greater than 3,200 ions per second. The instrument mass range will be set to a maximum of 2000 *m/z*.

	(b) Resolution Mode Using a [Glu[1]] -Fibrinopeptide B solution of 100 fmol/µL, at a flow rate of 5µL/min and with the instrument tuned for 20,000 resolution (as demonstrated on bovine insulin), the intensity of the most intense y" sequence ion from the MS/MS spectrum of the doubly charged precursor ion (785.8 *m/z*) will be greater than 1,600 ions per second. The instrument mass range will be set to a maximum of 2000 *m/z*.
Negative Ion MS/MS Sensitivity	(a) Sensitivity Mode Using a solution of 500 pg/µL raffinose in 70/30 acetonitrile/water, at a flow rate of 5 µL/min and with the instrument tuned for 10,000 resolution (as demonstrated on bovine insulin), the intensity of the fragment ion at 179.1 *m/z* in the MS/MS spectrum of the precursor ion at 503.2 *m/z* will be greater than 3,200 ions per second. The instrument mass range will be set to a maximum of 1200 *m/z*. (b) Resolution Mode Using a solution of 500 pg/µL raffinose in 70/30 acetonitrile/water, at a flow rate of 5 µL/min and with the instrument tuned for 20,000 resolution (as demonstrated on bovine insulin), the intensity of the fragment ion at 179.1 *m/z* in the MS/MS spectrum of the precursor ion at 503.2 *m/z* will be greater than 1,600 ions per second. The instrument mass range will be set to 1200 *m/z*.
Mass Scale Calibration Accuracy	The mass measurement accuracy of the instrument in High Resolution mode, using internal lock masses, is such that the RMS error between the measured and the accepted masses of peaks which have sufficient intensity, and are free from interference from other masses, will be less than 1 ppm over the range 150 to 900 *m/z*.
Mass Measurement Accuracy	The mass measurement accuracy of the instrument, in High Resolution mode, will be better than 1 ppm RMS, based on 10 consecutive repeat measurements of the $[M + Na]^+$ ion of raffinose (*m/z* 527.1588), using the $[M + H]^+$ ions of leucine enkephalin (*m/z* 556.2771) and 4-acetamidophenol (*m/z* 152.0712) as the LockSpray lockmasses. Analyte and lockmass peaks must have sufficient intensity and be free of interference from other masses.
Mass Range	The TOF mass range is 20 to 100,000 *m/z* in Resolution mode, and 20 to 32,000 *m/z* in High Resolution mode. The *m/z* transmission range for a quadrupole in non-resolving mode is 20 to 16,000 *m/z* for a 4000 *m/z* quadrupole, and 20 to 32,000 *m/z* for an 8000 *m/z* quadrupole.
Acquisition Rate	Mass spectra can be acquired up to a rate of 30 scans per second (mode dependent).
Dynamic Range	The dynamic range in High Resolution mode, defined as the range of peak intensities that will give better than 3 ppm accurate mass RMS for 10 sec of data without pDRE (programmable Dynamic Range Enhancement), is at least 4 orders of magnitude, when measured on the *m/z* 556.2771 peak from leucine enkephalin.
High Mass Precursor Selection	Applicable to instruments with 8000 *m/z* and 32,000 *m/z* quadrupoles only. The low energy MS/MS spectrum of *m/z* 5569.1 from a solution of 2 µg/µL sodium iodide in 50/50 isopropanol/water will contain only *m/z* 5569.1 and its fragments. The intensity of the largest fragment ion will be less than 5% of the intensity of the precursor ion. MS/MS data will be acquired over the mass range 100 – 8000 *m/z*, with collision energy of 10 eV.

MALDI PERFORMANCE SPECIFICATIONS

Mass Resolution in Positive Ion	(a) Resolution Mode 16,000 measured on the (M + H)+ isotope cluster from insulin B chain (*m/z* 3494.6) (b) High Resolution Mode 32,000 measured on the (M + H)+ isotope cluster from insulin B chain (*m/z* 3494.6)
Mass Resolution in Negative Ion	(a) Resolution Mode 16,000 measured on the (M - H)- isotope cluster from insulin B chain (*m/z* 3492.6) (b) High Resolution Mode 32,000 measured on the (M - H)- isotope cluster from insulin B chain (*m/z* 3492.6)
Positive Ion MS Sensitivity	Measured in Sensitivity Mode The peak at *m/z* 1570.6774 from 10 fmol of [Glu[1]] -Fibrinopeptide B will have an intensity of greater than 30,000 counts acquired from an entire line through a sample well. The instrument *m/z* range will be set to 2000. When this combined acquisition is smoothed (5 window, 1 number Savitzy Golay) and background subtracted the signal-to-noise ratio will be greater than 90:1 when compared to a region of the *m/z* scale between 1768 and 1818.
Negative Ion MS Sensitivity	Measured in Sensitivity Mode The peak at *m/z* 1568.6618 from 100 fmol of [Glu[1]]-Fibrinopeptide B will have an intensity of greater than 30,000 counts acquired from an entire line through a sample well. The instrument *m/z* range will be set to 2000. When this combined acquisition is smoothed (5 window, 1 number Savitzy Golay) and background subtracted the signal-to-noise ratio will be greater than 90:1 when compared to a region of the *m/z* scale between 1768 and 1818.
Positive Ion MS/MS Sensitivity	Measured in Sensitivity Mode The peak at *m/z* 1056.4750 (y9) from 10 fmol of [Glu[1]] -Fibrinopeptide B will have an intensity of greater than 1000 counts for an entire line through a sample well. The instrument *m/z* range will be set to 2000 (Precursor+50) and the collision energy and instrument conditions set such that the intensity of this peak will be greater than 40% of the intensity of the precursor peak. When this combined acquisition is smoothed (5 window, 1 number Savitzy Golay) and background subtracted the signal-to-noise ratio should be greater than 60:1 for the *m/z* 1056.4750 peak when compared to a region of the *m/z* scale between 1450 and 1490.
Mass Measurement	Measured in Sensitivity Mode, Positive Ion The mass measurement accuracy will be better than 1 ppm RMS, measured from a mixture of PEG oligomers between *m/z* 700 – 2500; using an internal reference peak and an instrument calibration that covers the same mass range.

MOBILITY-TOF MODE PERFORMANCE SPECIFICATIONS

The Triwave™ cell is the enabling technology of the SYNAPT G2-S HDMS System. It is comprised of three main components:

(a) TRAP T-Wave
Ensures high-efficiency by trapping ions prior to ion mobility separation;
the trap can also operate as a collision cell.

(b) IMS T-Wave
Provides reproducible separation of ions based on their mobility.

(c) TRANSFER T-Wave
Transfers separated ions to the oa-TOF for mass analysis;
the TRANSFER T-Wave can also operate as a collision cell.

Mobility Functionality	Separation of ions based on their mobility (size, shape, and charge) Time Aligned Parallel (TAP) fragmentation High Duty Cycle (HDC) for extended detection limits over a wide *m/z* range Drift Time measurements: Record drift times between 33 µs and 90 ms
Ion Mobility Resolution	Infusion of a mixture of the inverse peptides ser-asp-gly-arg-gly and gly-arg-gly-asp-ser will yield doubly-charged molecular ions at *m/z* 246.1. The mobility separation of the *m/z* 246.1 ion species in Nitrogen will give two distinct arrival time peaks from which a mobility resolution (Ω/ΔΩ) of >36 will be demonstrated using collision cross section (Ω) values of 222.7 and 211.7 A2 for the ser-asp-gly-arg-gly and gly-arg-gly-asp-ser peptides respectively. (Values taken from: C Wu, WF Siems, J Klasmeier and HH Hill, Anal. Chem., 72 (2000) 391.)
Control of Mobility Separation	Control of Triwave height and velocity with linear ramps or user defined programs Ability to use different gases for mobility separation Automated control of mobility conditions for routine operation Comprehensive manual control of mobility and Triwave operation for research use

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Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com