# Heparin Hexasaccharide MS Standard 7

1-800-632-7799
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P0739S 001140616061

# P0739S

**40 nmol** **Lot: 0011406**

**Store at –20°C** **Exp: 6/16**

**Description:** The Heparin Hexasaccharide MS Standard 7 is a MS standard of defined sequence and structure. This highly purified hexasaccharide with seven sulfates is prepared from a digest of porcine mucosal heparin using *Bacteroides* Heparinase I.

Among the modern ionization techniques for the analysis of biomolecules, Electrospray Ionization (ESI) has proven the most effective for the mass spectrometry (MS) analysis of sulfated carbohydrates, called Glycosaminoglycans (GAGs). GAGs are acidic molecules with numerous sulfate groups and are easily ionized and produce abundant negative ions. Sulfates are the most labile functional groups and are more fragile than peptides and less acidic glycans. Due to sulfate lability, GAGs can be difficult to analyze by ESI mass spectrometry without using finely tuned ESI parameters. Optimization of the ESI tuning parameters will result in little or no in-source fragmentation of sulfated GAGs.

Highly sulfated heparin hexasaccharides with defined structure can be used to optimize the ESI tuning parameters in various mass spectrometers. Extent and position of sulfation can lead to varying degrees of lability for every oligosaccharide. The lability of the sulfate groups increases as the size of the heparin oligosaccharide increases. Successful tuning parameters are more easily achieved using a highly sulfated hexasaccharide standard as compared to a disaccharide standard.

**Source:** Prepared from a digest of porcine mucosal heparin using *Bacteroides* Heparinase I

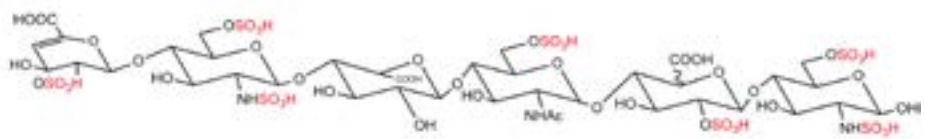
Supplied as: dried powder

**Formula:** $C_{38}H_{59}N_3O_{52}S_7$

**Exact Mass:** 1,613.01

**Mass-to-Charge Ratios:** $[M-1H]^{1-}$1612.00; $[M-2H]^{2-}$ 805.50; $[M-3H]^{3-}$ 536.66; $[M-4H]^{4-}$ 402.24

**Absorbance Extinction Coefficient:** 3800 L· $mol^{-1}$· $cm^{-1}$



ΔUA2S - GlcNS6S - IdoA - GlcNAc6S - UA2S - GlcNS6S

Denotes either glucuronic acid or iduronic acid.

***Heparin Hexasaccharide MS Standard 7.***

## Suggested Usage Parameters

**Ion Trap MS:** Thermo Scientific Velos LTQ mass spectrometer equipped with a heated electrospray standard source (HESI-II probe) run in the negative ion mode. Optimized settings were determined by direct injection of 100 pmol/µl and a 5 µl/min flow rate. Recommended ESI source settings: spray voltage 3.5 kV; capillary temperature 250°C; sheath gas 11 psi, Aux gas and Sweep gas Flow rates 0, S-lens RF level% 14. Recommended Ion Optics settings: Multiple 00 offset 2.5 V, Lens 0 voltage 6.5 V, Multiple 0 offset 7.0 V, Lens 1 voltage 16 V, Multiple 1 offset 6.5 V, Multiple RF Amplitude 600, Front lens 7.75 V.b

**Time of Flight MS:** Agilent 6210 Time of Flight mass spectrometer equipped with a chip-cube nanospray interface in the negative ion mode. Optimized ESI source settings were determined by fast injection analysis (FIA; 8 µl/injection of 100 pmol/µl). Recommended ESI source settings: spray voltage 1.9 kV; capillary temperature 320°C; drying gas 4 L/min, skimmer 50 V, Octipole1 RF-Vpp 300 V and fragmentor voltage 100 V.

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CERTIFICATE OF ANALYSIS

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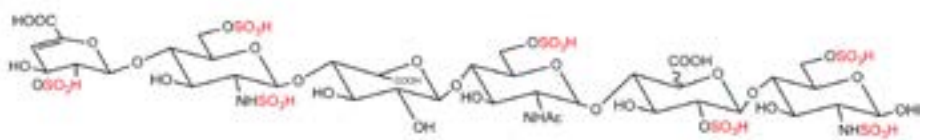

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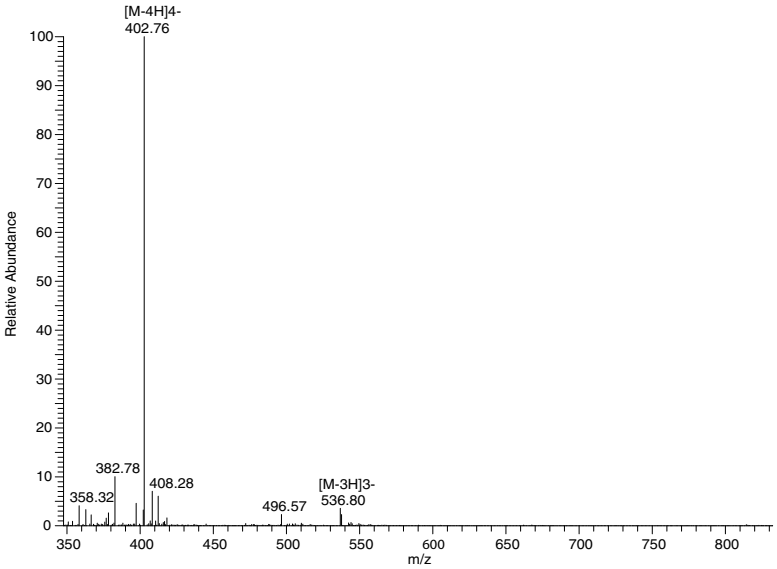
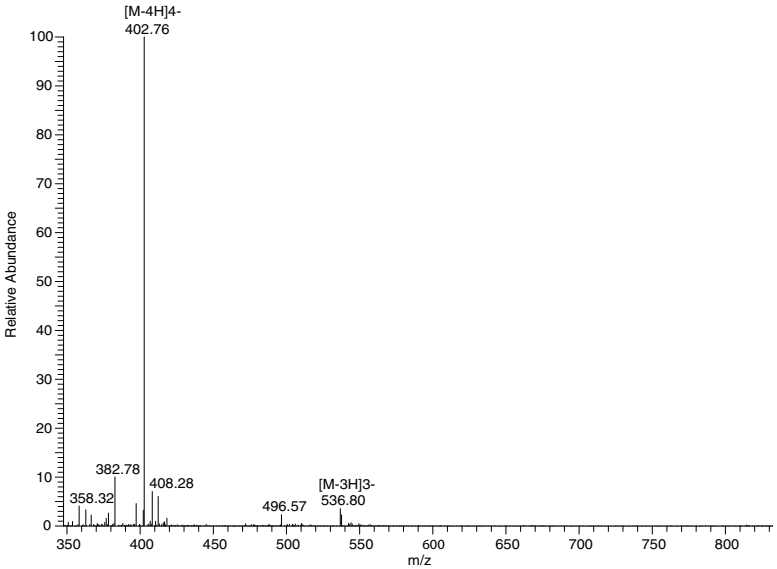



***MS Analysis of Heparin Hexasaccharide MS Standard 7:*** *The hexasaccharide MS Standard 7 was diluted to 100 pmol/µl in a solution of Methanol:Water (30:70;v:v). The 100pmol/µl solution was analyzed by direct injection with a flow rate of 5 µl/min on an Velos LTQ Ion Trap mass spectrometer equipped with a heated electrospray standard source (HESI-II probe) using the suggested usage parameters. Note: High charge states can lead to hydrogen-shift rearrangement resulting in loss of the double bond with the addition of two hydrogens. In this case, the [M-4H]4- ion has an observed value of 402.73; the theoretical value after hydrogen-shift rearrangement is 402.74.*



**Single Quadrupole MS:** An Agilent 1200 series HPLC connected on-line with an Agilent 6120A Quadrupole mass spectrometer equipped with a standard electrospray source in the negative ion mode. Optimized ESI source settings were determined by fast injection analysis (FIA; 25 µl/injection of 100 pmol/µl). Recommended ESI source settings: spray voltage 2 kV; capillary temperature 295°C; nebulizer gas 35 psi and fragmentor voltage 50 V.

**Quality Assurance:** Composite hexasaccharide mass signal-to-noise ratio is greater than or equal to 95%.

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