Heparin Hexasaccharide MS Standard 6

40 nmol Lot: 0011305 Store at –20°C Exp: 5/15

Description: The Heparin Hexasaccharide MS Standard 6 is a MS standard of defined sequence and structure. This highly purified hexasaccharide with six 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 GAGs. Glycosaminoglycans (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_{3}O_{49}S_{6}

Exact Mass: 1,533.05

Mass-to-Charge Ratios: [M-1H]+ 1532.04; [M-2H]2- 765.52; [M-3H]3- 510.01; [M-4H]4- 382.25

Absorbance Extinction Coefficient: 3800 L· mol⁻¹· cm⁻¹

Denotes either glucuronic acid or iduronic acid.
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%.

MS Analysis of Heparin Hexasaccharide MS Standard 6: The hexasaccharide MS Standard 6 was diluted to 100 pmol/µl in a solution of Methanol:Water (30:70; v:v). The 100 pmol/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 382.74; the theoretical value after hydrogen-shift rearrangement is 382.75.