

MALDI MS in-source decay of glycans using a glutathione-capped iron oxide nanoparticle matrix

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Support information

Contents

Experimental

Figure S-1. UV- vis absorption spectra of iron oxide nanoparticle dispersion at various particle size, shape, and capping molecules.

Figure S-2. ESI MS mass spectrum of maltoheptaose tricosaacetate.

Figure S-3. Expansion of MALDI/TOF ISD mass spectra of maltoheptaose acquired using iron oxide nanoparticle matrices with various capping molecules.

Experimental: Nanoparticle synthesis and characterization and mass spectrometry experiments followed same procedures as in text. Extra capping molecules utilized for supplemental figures include: Tween 80, Polyacrylic acid, polyethylenimine, and dopamine.

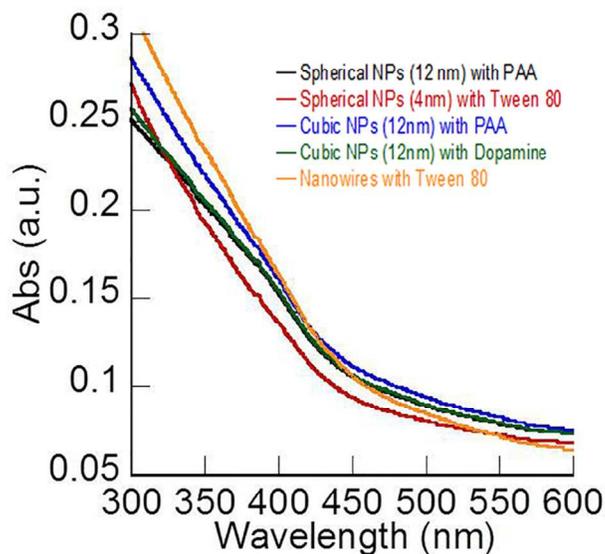


Figure S-1. UV- vis absorption spectra of iron oxide nanoparticle dispersion at various particle size, shape, and capping molecules. PAA, polyacrylic acid. The spectra demonstrate that iron oxide absorption is relatively insensitive to the changes in particle size (4 nm versus 12 nm), shape (cubic, spherical, and nanowire), and capping molecules (PAA, dopamine, and Tween 80). Spherical NPs (4 nm) are only capped with Tween 80 and PAA capping was unsuccessful at this size.

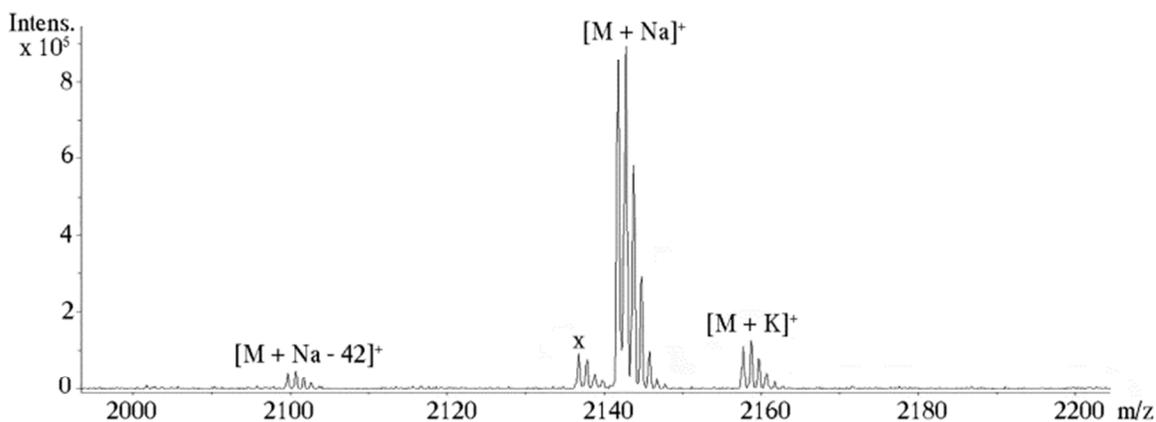


Figure S-2. ESI MS mass spectrum of maltoheptaose tricosacetate. The ESI MS spectrum shows the presence of precursor ions $[M + Na]^+$ and $[M + K]^+$. The 42 (CH_2CO) loss peak is less than 5% intensity of the $[M + Na]^+$ precursor ion. x marks a contamination peak.

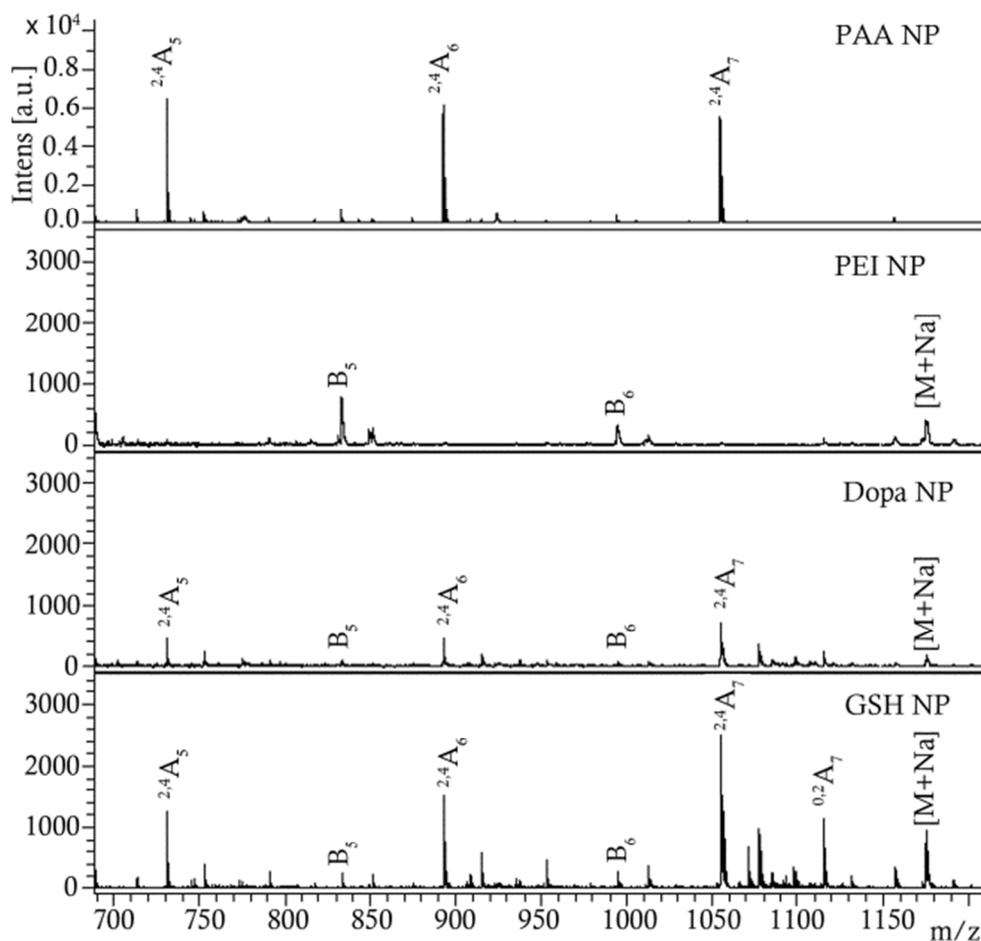


Figure S-3. Expansion of MALDI/TOF ISD mass spectra of maltoheptaose acquired using iron oxide nanoparticle matrices with various capping molecules. PAA, polyacrylic acid; PEI, polyethylenimine; Dopa, dopamine; GSH, glutathione. To prevent aggregation of the nanoparticles, NaOH (20 mM) is added to PAA, Dopa, and GSH capped nanoparticles, while 0.1 mM HCl is added to PEI capped nanoparticles. The absence of cross-ring fragmentation in PEI spectrum may be related to less abundant Na^+ ions. In PAA spectrum, $^{2,4}A_n$ cross-ring fragmentation dominates. Dopa spectrum is very similar to GSH spectrum but less intense. GSH is chosen as the best capping molecule for it provides a variety of fragmentation species at comparable intensity.