



Figure S1: MSⁿ of N-acetyl glucosamine and glucuronamide. A, MS² spectrum of N-acetyl glucosamine showing losses of one, two and three water molecules. The boxed product ion (m/z 168.065) was targeted for MS⁴ analysis. B, MS⁴ spectrum of m/z 168 (222.0900@cid30.00 204.0800@cid30.00 168.0600@cid30.00). C, MS² spectrum of glucuronamide showing losses of one, two and three water molecules. The boxed product ion (m/z 140.034) was targeted for MS³ analysis. D, MS³ spectrum of m/z 140 (194.0600@cid50.00 140.0340@cid25.00). The proposed structure and fragmentation of the dehydrated parent ions are shown. Both spectra were acquired by direct infusion into the Orbitrap Lumos instrument.