Supplementary Data

for

Platform Dependencies in Bottom-up Hydrogen/Deuterium Exchange Mass Spectrometry

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Supplementary Data

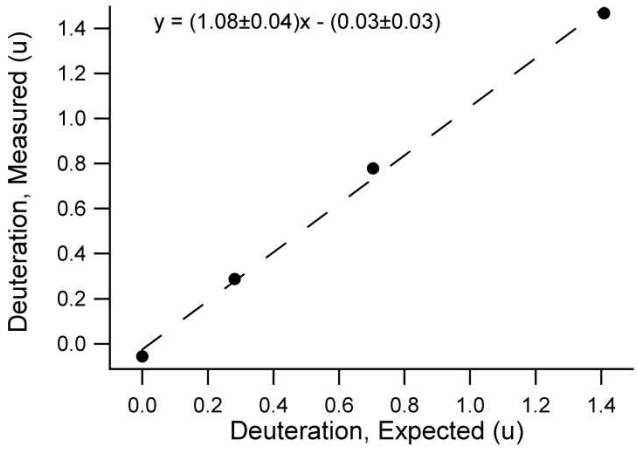

Figure S1. Deuteration measurement for AEGFSAI (1+) on the 5600 TripleTOF as a function of expected deuteration value. Deuteration was achieved by incubation and equilibration of the peptide in 0, 2, 5 and 10% D_2O (with 30% acetonitrile and 0.1% formic acid). This solution was directly sprayed into the instrument. In this way, issues of back-exchange could be avoided and the expected deuteration level readily calculated. Note that the deuteration is more extensive that would be expected for conventional HDX-MS experiments, as the labile hydrogens on the side chains and peptide termini are also exchanged.

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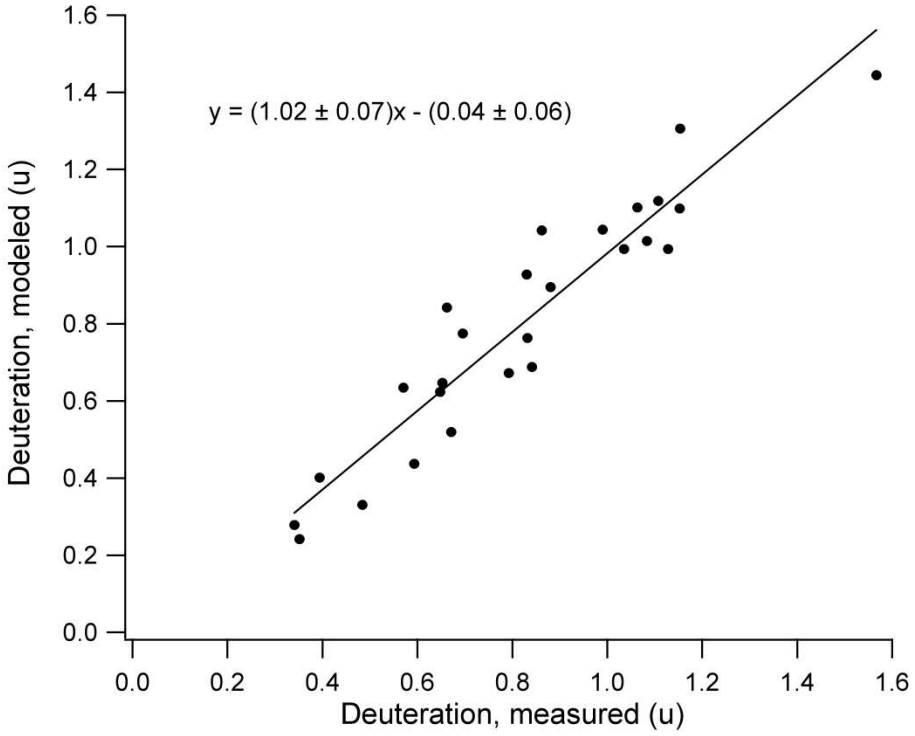

Figure S3. Comparison between the modeled deuteration (accounting for interference) and the measured deuteration. Modeling was based upon transients sampled for 770 msec to represent the 60k resolution data, and built from the doubly-charged peptide set. In this exercise, the simulations incorporated the full isotopic composition for each peptide (i.e., contributions from minor isotopes such as 15N, 17O, 18O and native 2H) and the deuteration levels from the TOF data were taken to be the true values.

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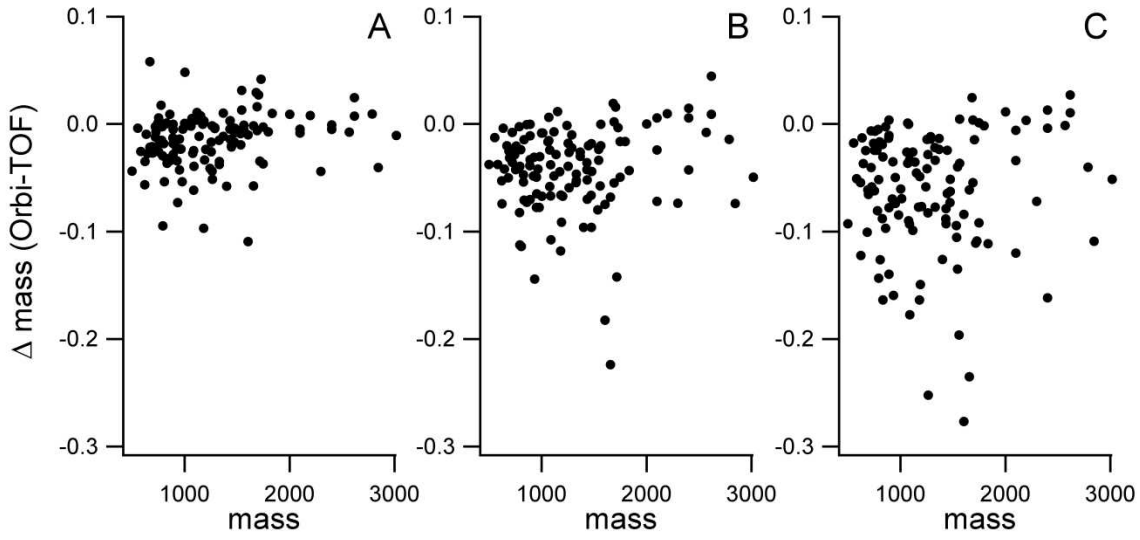

Figure S3. Effect of Orbitrap resolution on centroid mass measurements for undeuterated peptides, where Δmass represents the difference between the Orbitrap data and the 5600 TOF data for a set of common peptides from the PNK digest. (A) The 30k resolution Orbitrap setting, (B) the 60k resolution Orbitrap setting, and (C) the 100k resolution Orbitrap setting. All masses in unified atomic mass units (u).