

Supporting Information

Heterogenous huntingtin N-terminal monomeric and multimeric structures destabilized by covalent modification of heteroatomic residues

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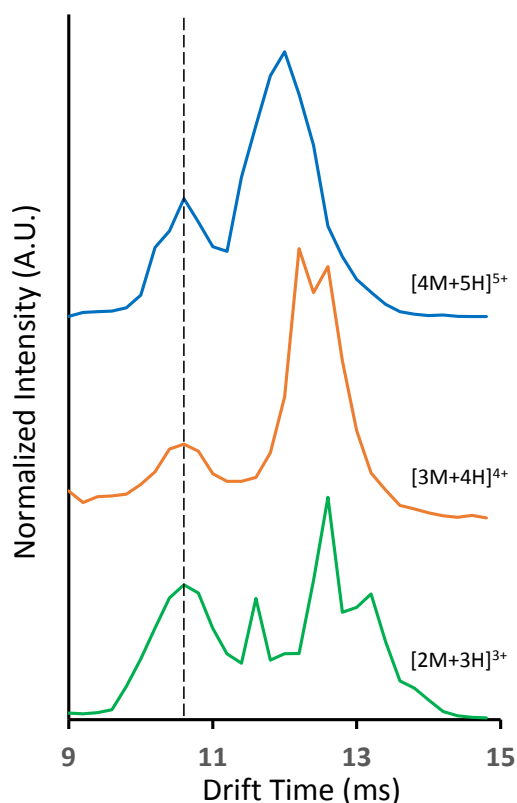


Figure S1 – Extracted t_D distributions for dimer (green), trimer (orange), and tetramer (cyan) ions. The dotted box shows the feature at 10.6 ms for all ions, suggesting that this feature arises from dissociation of a higher-order complex(es) after the drift separation has occurred.

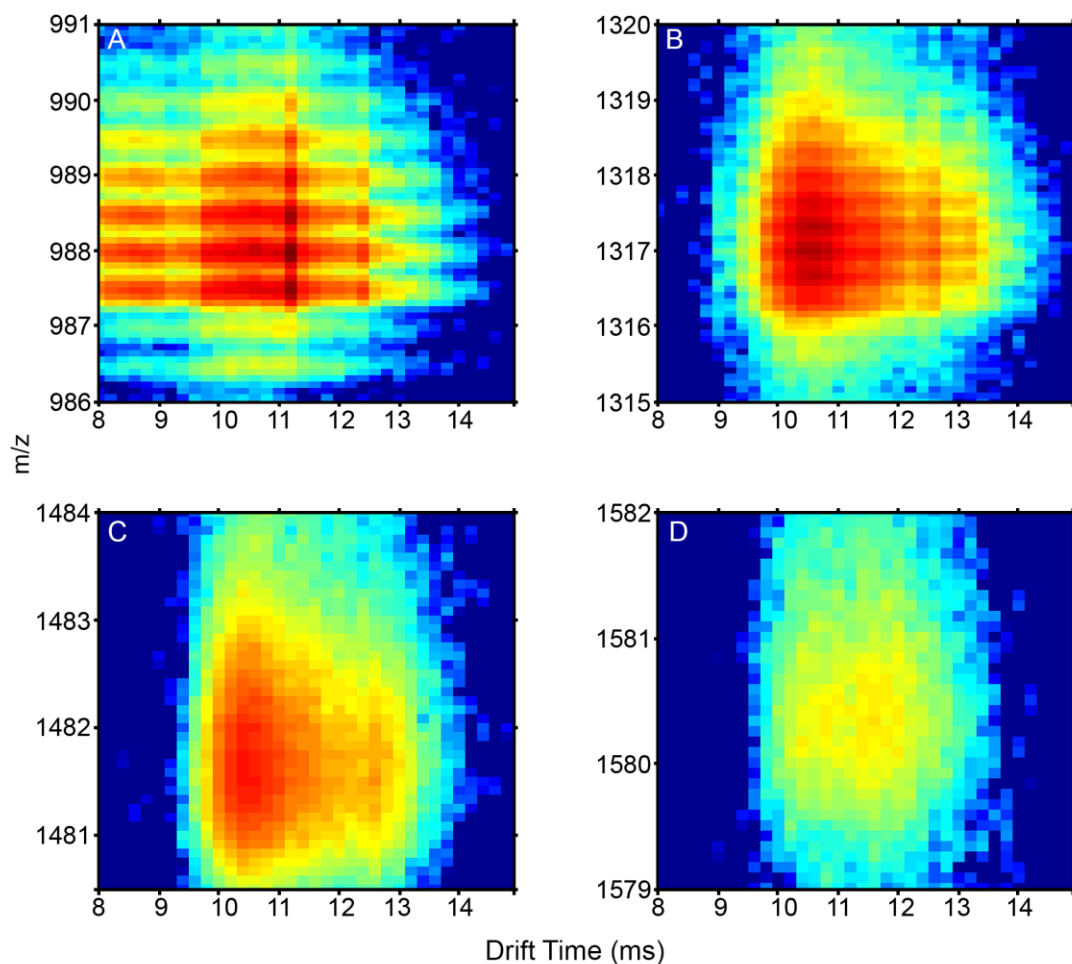


Figure S2 – 2D IMS-MS distributions of monomer (A), dimer (B), trimer (C), and tetramer (D) collected with the drift tube exit lens turned to 120 V. Note the large increase in the features at 10.6 ms through all species, compared to Figure 2 in the main manuscript. This increase is a direct result of higher order multimer ($n > 4$) dissociation at the rear of the drift tube.

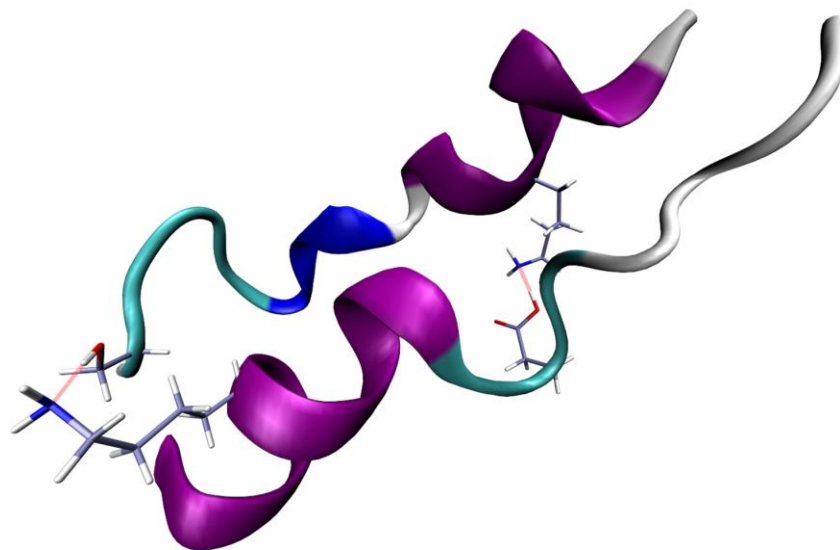


Figure S3 – Hypothetical elongated Nt17 homodimer showing Lys6 interactions. Red lines indicate H-bonds between Lys6 and Ser16, and Lys6 and Glu12.

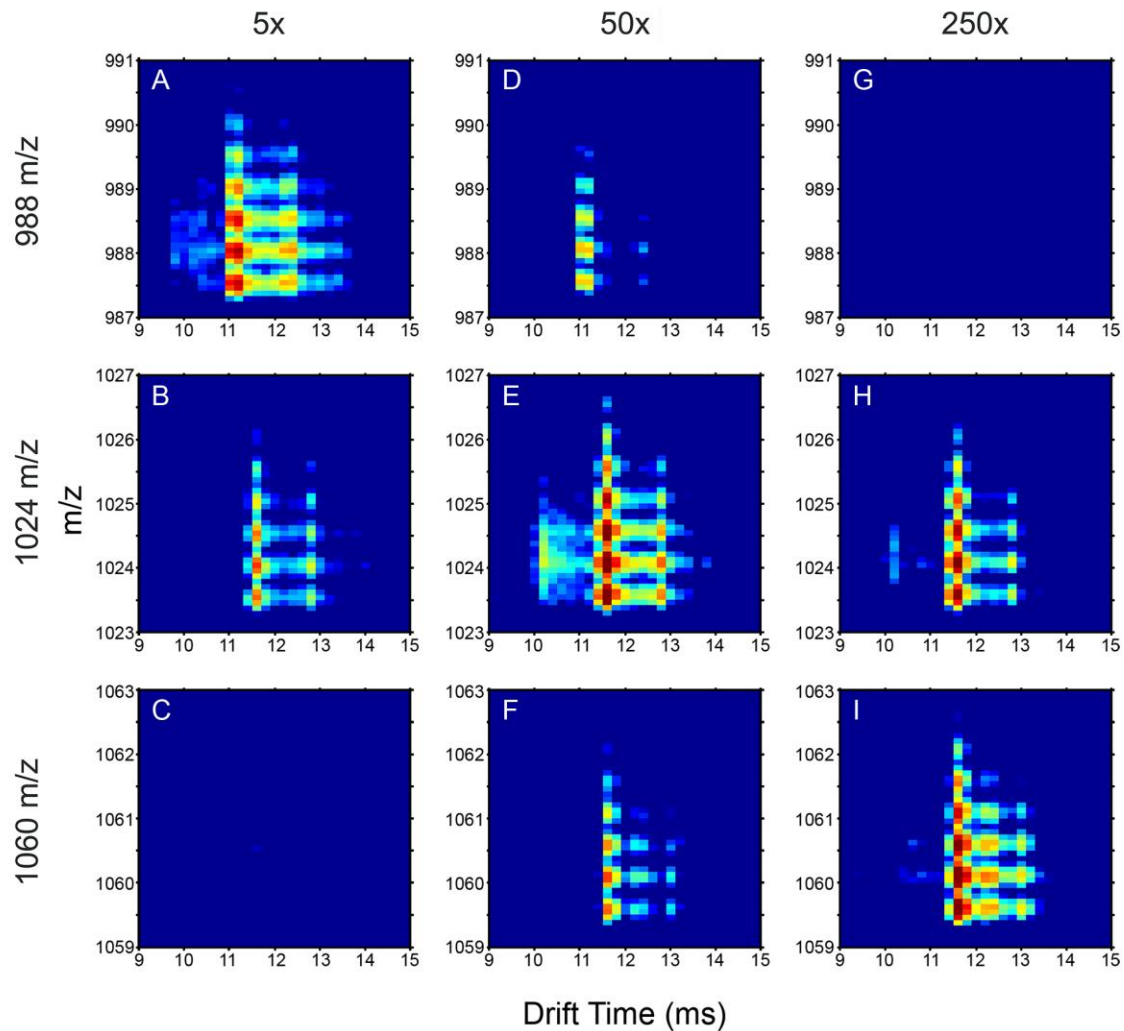


Figure S4 – 2D IMS-MS distribution showing expanded regions of unlabeled, singly-, and doubly-modified Nt17 at the 5x, 50x, and 250x DEPC concentrations. Note the appearance of the intermediate doubly-modified species (1060 m/z, 50x and 250x).

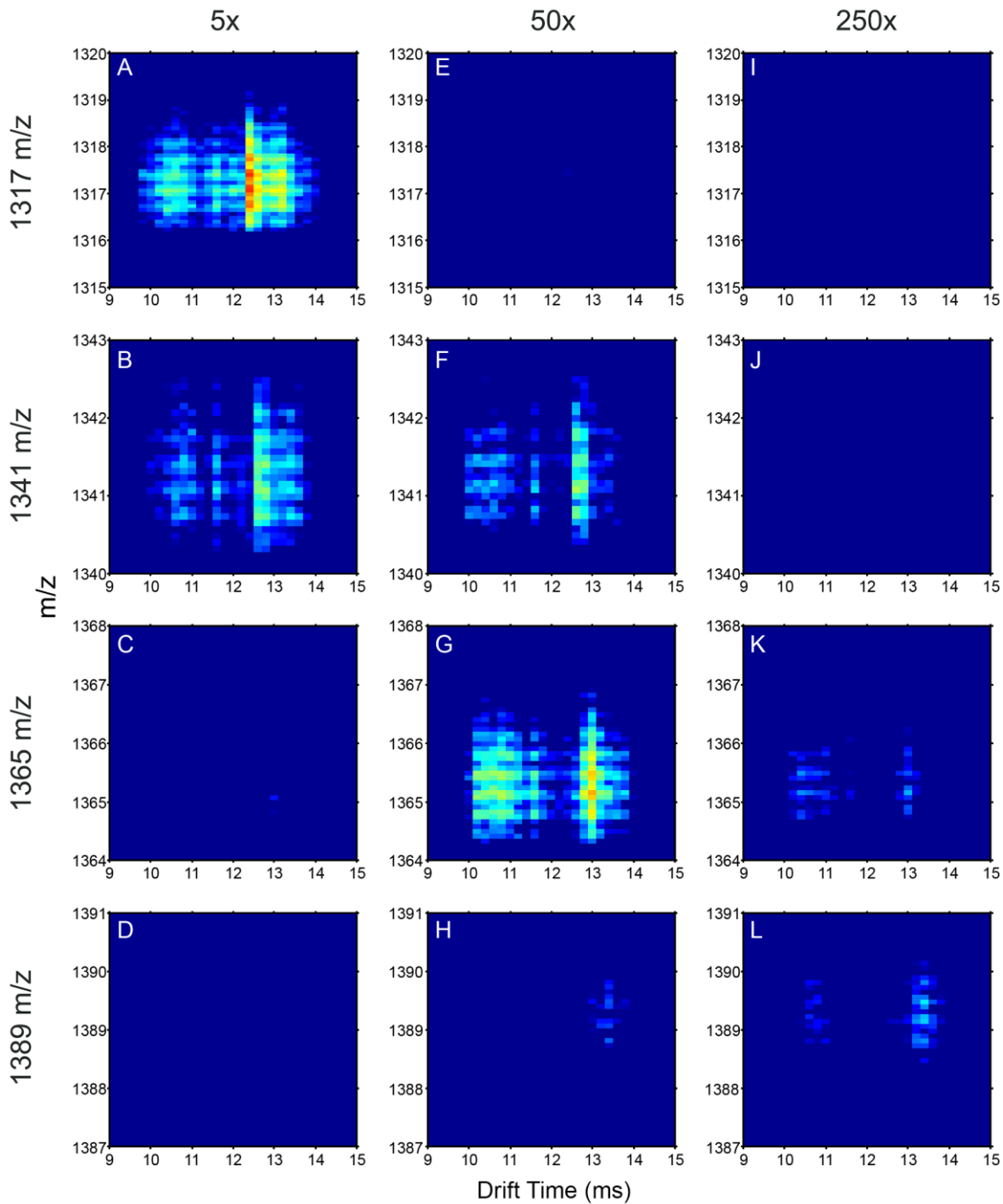


Figure S5 – 2D IMS-MS distributions of modified dimer species. The overall abundance of multimer decreases as a function of label concentration.

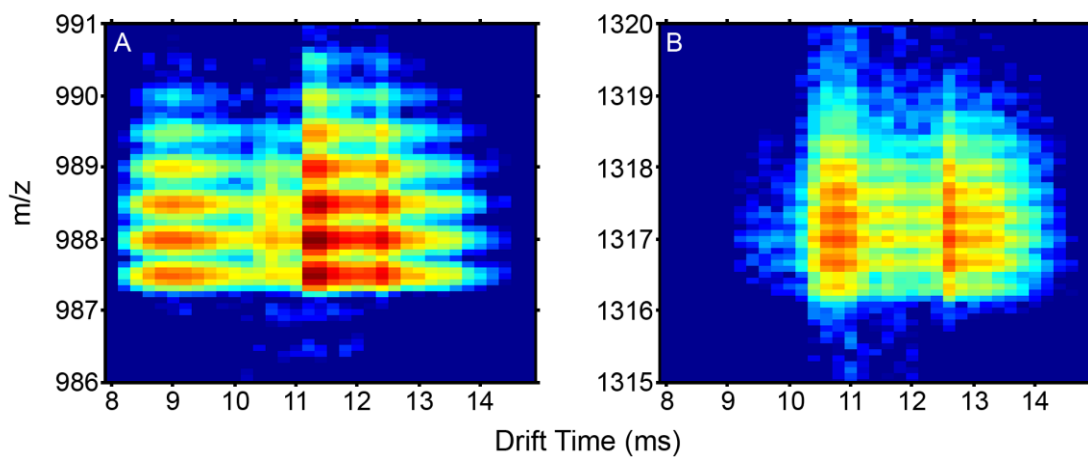


Figure S6 – 2D IMS-MS distributions of Nt17 monomer (A) and dimer (B) with 1% ACN. No additional conformers are apparent in the monomer distribution that would correspond to the doubly modified conformer at 12.2 ms shown in Figure 4 and Figure S3. Additionally, no significant reduction in dimer abundance is observed.