Fragmentation of Integral Membrane Proteins in the Gas Phase

Owen S. Skinner, Adam D. Catherman, Bryan P. Early, Paul M. Thomas, Philip D. Compton, and Neil L. Kelleher

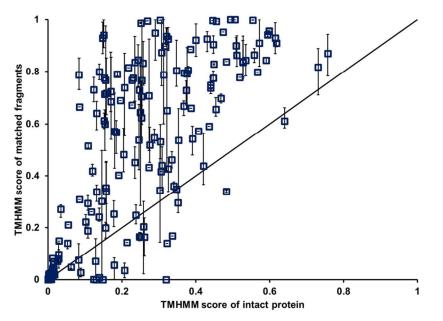


Figure S1. Experimental variability of the average TMHMM scores of matched fragment ions for proteins identified in one or more of the CAD runs. Open boxes indicate the average TMHMM score over the three runs, with error bars stretching from the minimum to the maximum average TMHMM score observed.

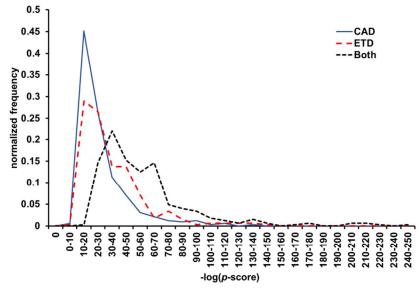


Figure S2. The distribution of the $-\log(p\text{-score})$ for the proteins included in the study after searching and scoring with fragments from CAD, ETD, and both methods in tandem. Each increasing integer on the x-axis is an order-of-magnitude increase in database search specificity.

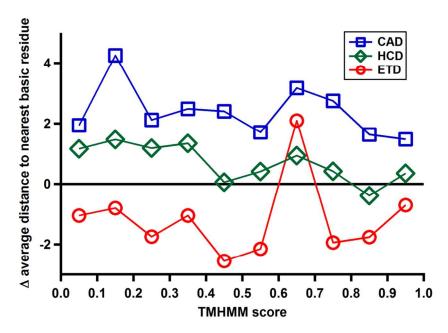


Figure S3. A plot showing the difference in distance between random fragmentation and observed products from CAD, HCD, and ETD. Fragment ions are binned by TMHMM scores that differ by increments of 0.1; each symbol represents the average value of the bin for the type of fragmentation method indicated in the figure key in the upper right.

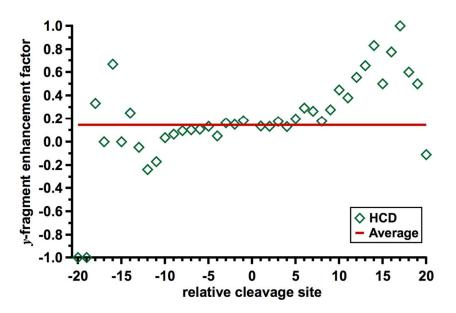


Figure S4. The *y*-fragment enhancement factor of HCD products as a function of distance from the nearest Asp (D), Ala (A), or Phe (F) residue.