Supporting Information

Enhanced Top-Down Protein Characterization with Electron Capture Dissociation and Cyclic Ion Mobility Spectrometry

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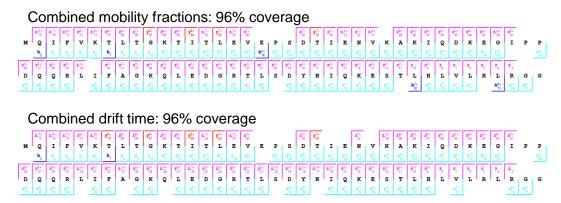


Figure S1. Product ion maps for pre-IMS ECD of 10+ ubiquitin produced by the combined results of four mobility fraction (top), or a single mass spectrum produced by combing the entire drift time range.

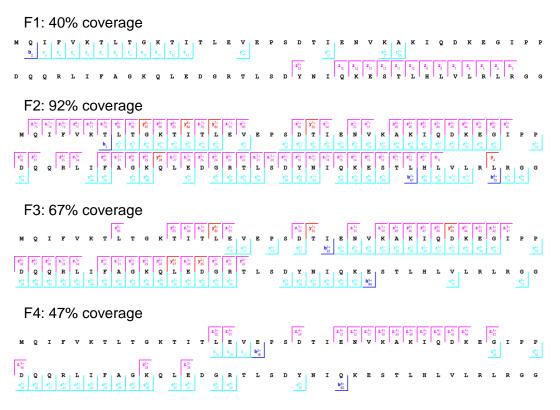


Figure S2. Product ion maps for each mobility fraction from pre-IMS ECD of 10+ ubiquitin.

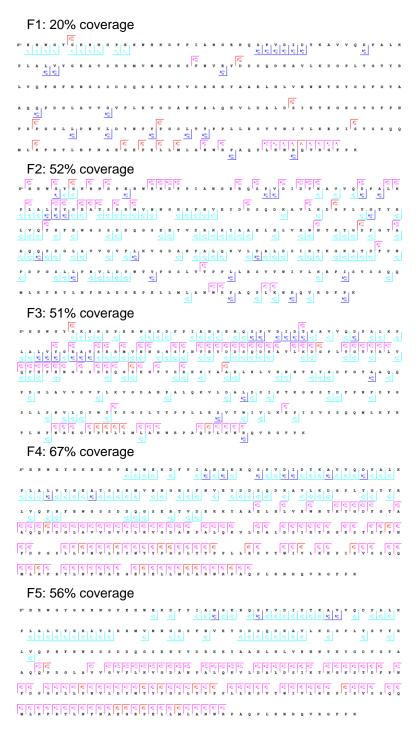


Figure S3. Product ion maps for the five mobility fractions produced by pre-IMS ECD of 35+ bovine carbonic anhydrase II.

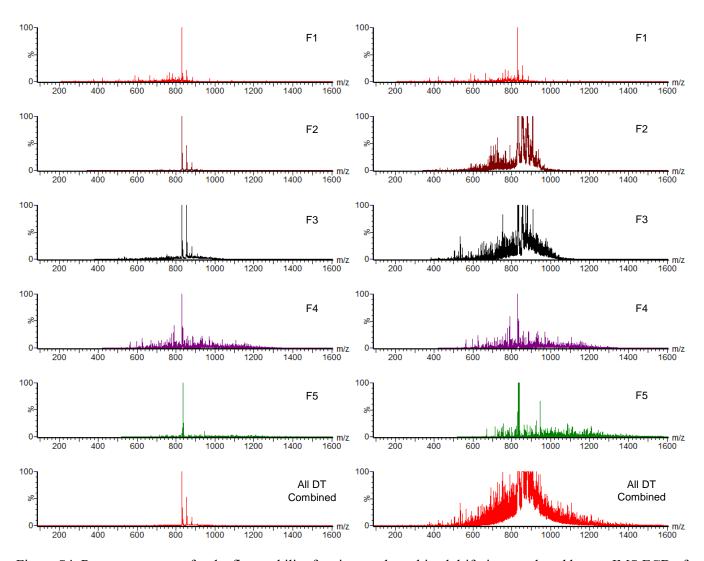


Figure S4. Raw mass spectra for the five mobility fractions and combined drift time produced by pre-IMS ECD of 35+ bovine carbonic anhydrase. Spectra in the right column are zoomed in to an intensity of 4.8E3.

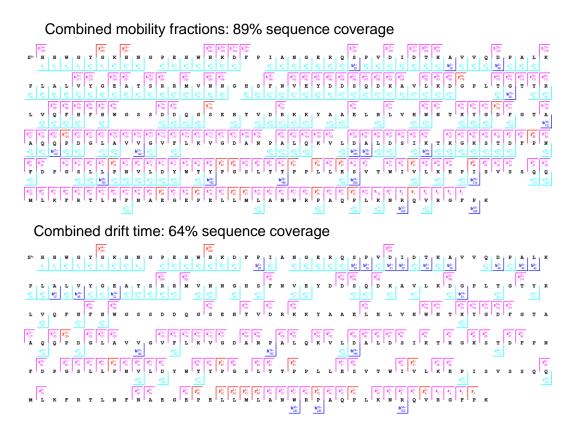


Figure S5. Product ion maps for pre-IMS ECD of 35+ bovine carbonic anhydrase II produced by the combined results of five mobility fraction (top) or a single mass spectrum produced by combing the entire drift time range.

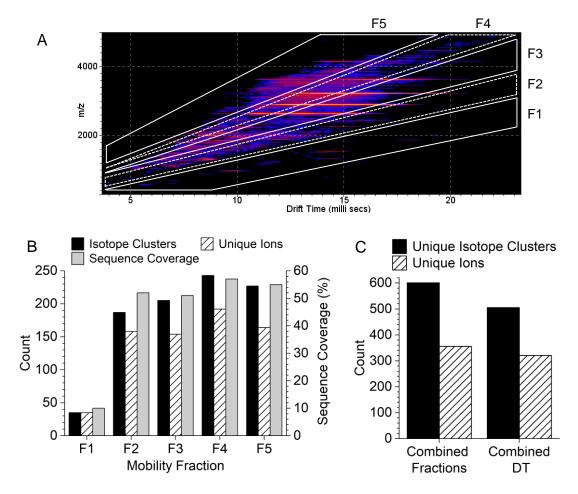


Figure S6. The 2D mobiligram (m/z vs. drift time) for pre-cIMS ECD of the 11+ charge state of bovine carbonic anhydrase II (A) with outlined mobility fractions. The number of annotated isotope clusters/unique ions and sequence coverage for in each mobility fraction (B). Comparison of the number of unique isotope clusters and unique ions observed from a single mass spectrum from all drift times combined and the combined results of the four mobility fractions (C).

F1: 11% sequence coverage
L V Q F H F H W G S S D D Q G S E H T V D R K X Y A A E L H L V H W M T K Y G D F G T A
AQQPDGLAVVGVFLKVGDANPALQKVLDALDSIKTKGKSTDFFN
F D P O S L L P N V L D V N T Y P O S L T T P P L E S V T N I V L K E P I S V S S Q Q N L K F R T L N F N A E O E P E L L N L A N N R P A Q F L K N N Q V N Q P P K
N L K P R T L N P N A E G E P E L L N L A N N R P A Q P L K N R Q V R G P P K
F2: 52% sequence coverage
C COCCCC SCOC COC SOCIOCIOS COC
C C C C C C C C C C C C C C C C C C C
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F3: 51% sequence coverage
P 1 1 V 0 E T S R R V V N 0 S F N V E D S 0 D K A V L X D 0 F T T T X C C C C C C C C C
LVOTET PO SSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSSS
C CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
F4: 57% sequence coverage Fig. 8 of 0 x 1 x 0 x 1 x 0 x 1 x 0 x 1 x 0 x 0 x
P, L, A, L, V, Y, G, E, A, T, S, R, R, N, V, N, N, G, H, S, F, N, V, E, Y, D, D, S, Q, D, K, A, V, L, K, D, G, P, L, T, G, T, Y, R
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CC C CCC CCC CCC CCC CCC CCC CCC CCCC CCCC
C CC CC CCCC CCC CCC CCC CCC CCC CCC C
F5: 55% sequence coverage
Figure Coverage
FLACCECECE E VECCEC CCCCCC CCCCCCCCCCCCCCC
S SINCE SELECTED SELE
C C C C C C C C C C C C C C C C C C C
H 1 K 7 R 7 1 N 7 H A 8 0 E 7 E 1 1 N 1 A H W R P A 0 P 1 K H R 0 V R 0 F P K

Figure S7. Product ion maps for the five mobility fractions produced by pre-IMS ECD of 11+ bovine carbonic anhydrase II.

Combined drift time: 75% sequence coverage

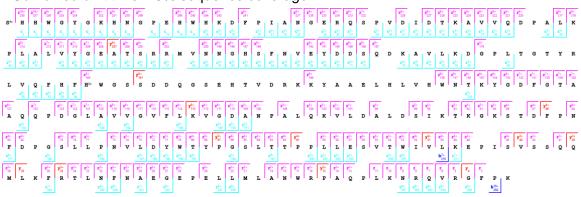


Figure S8. Product ion maps for pre-IMS ECD of 11+ bovine carbonic anhydrase II produced by a single mass spectrum of the entire drift time range combined.