

Supporting Information For:

Two-dimensional Identification and Localization of Isomers in Crystallin Peptides Using TWIM-MS

Hoi-Ting Wu, Ryan R. Julian*

Department of Chemistry, University of California, Riverside, California 92521, United States

Corresponding Author

* Correspondence should be sent to: ryan.julian@ucr.edu

Department of Chemistry, University of California, Riverside, 501 Big Spring Road, Riverside,
California 92521, United States, (951)827-3959

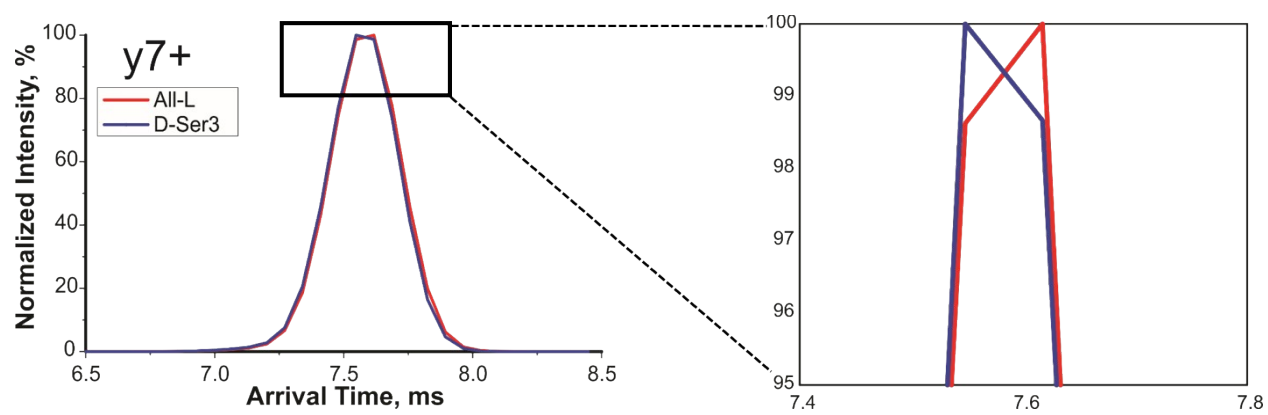


Figure S1. ATDs of y_7^+ ions for AP_{D/L} SWFDTGLSEMR and the magnified peak maxima.

Full CID spectra:

APSWFDTGLSEMR

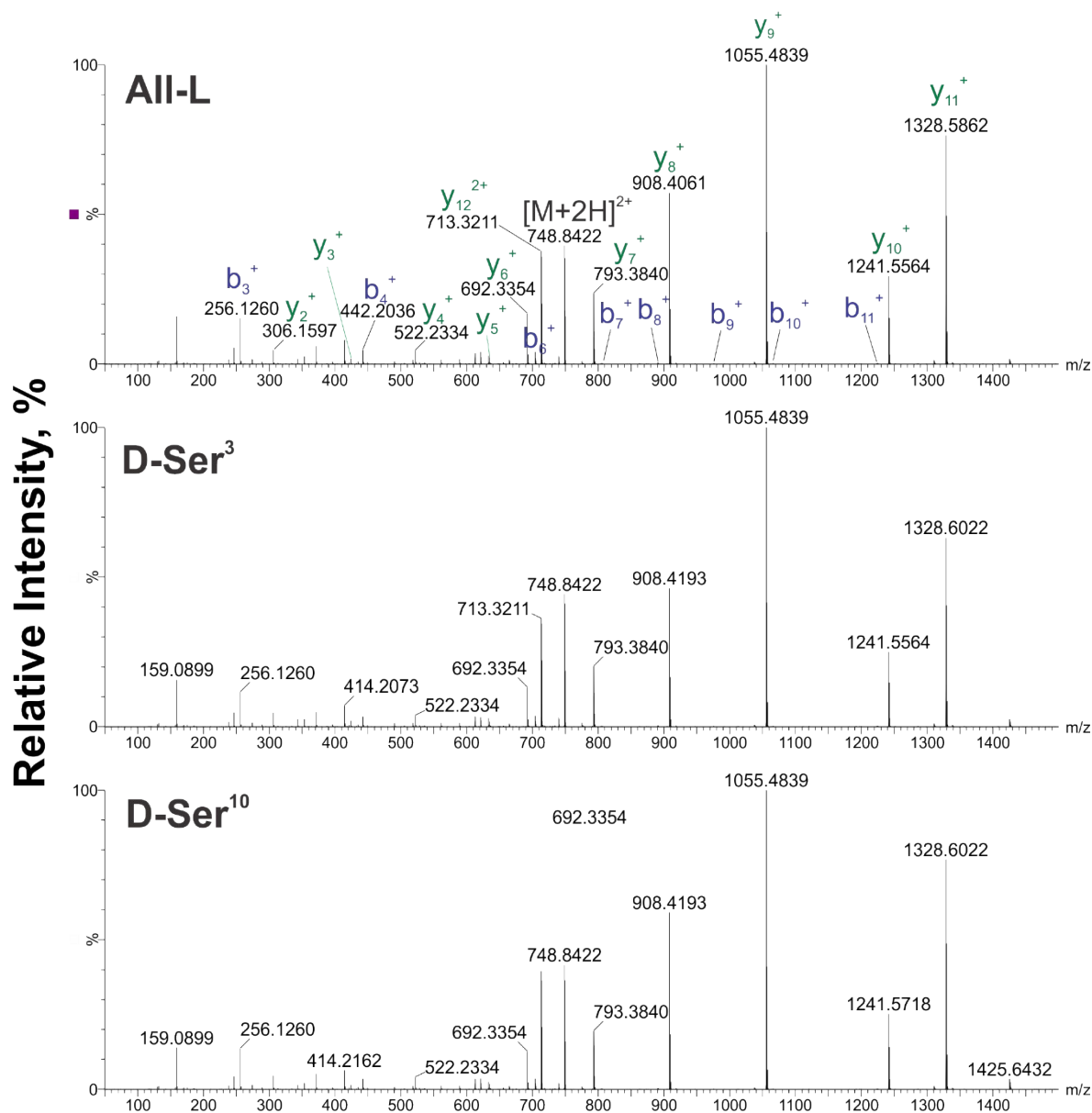


Figure S2: The CID spectra for the peptide isomers of APSWFDTGLSEMR: All-L (Top), D-Ser³ (Middle), and D-Ser¹⁰ (Bottom).

Full CID Spectra

GYQYLLEPGDFR

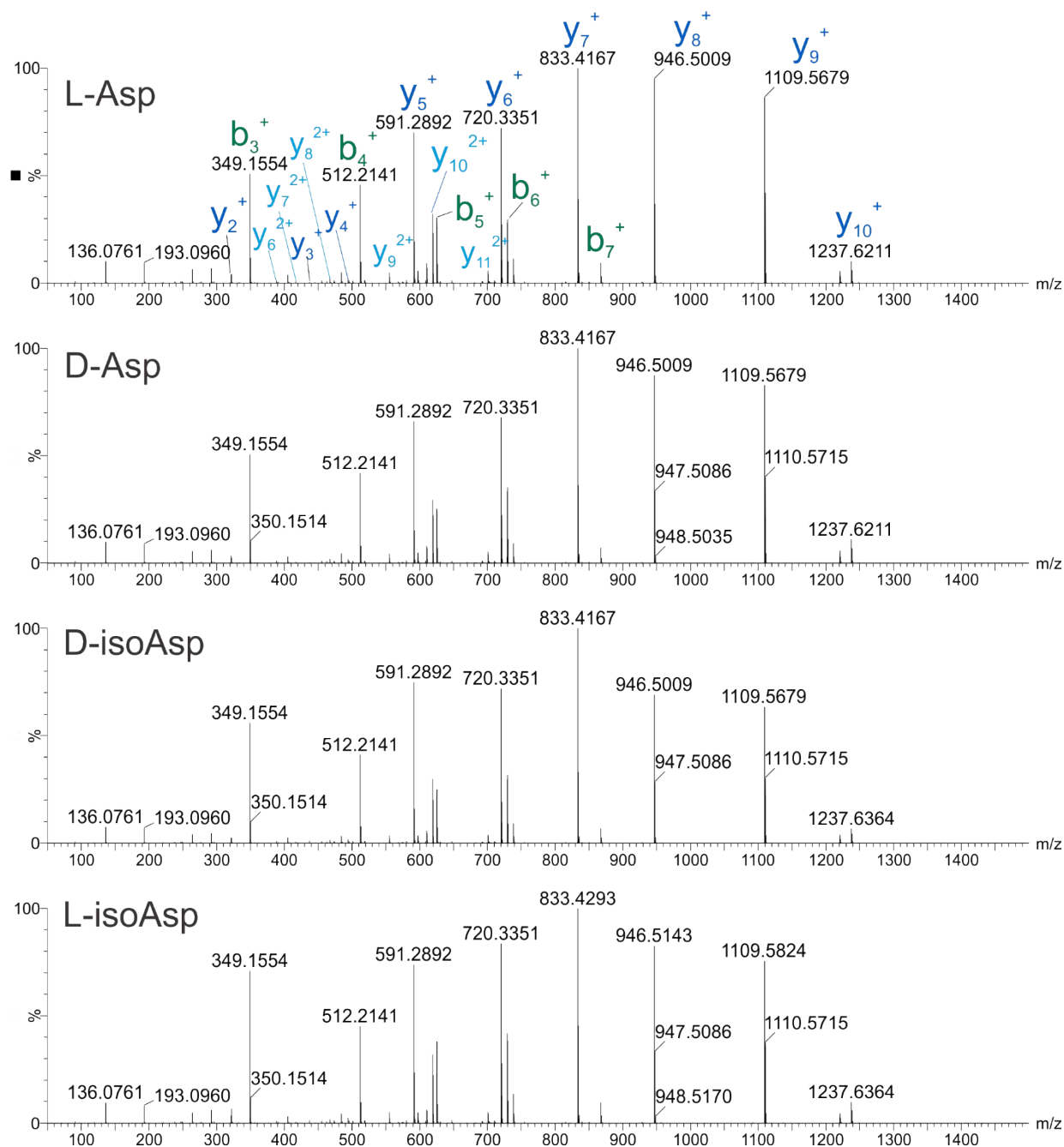


Figure S3: The CID spectra for the peptide isomers of GYQYLLEPGDFR: L-Asp (Top), D-Asp (Second), D-isoAsp (Third), and L-isoAsp (Bottom).

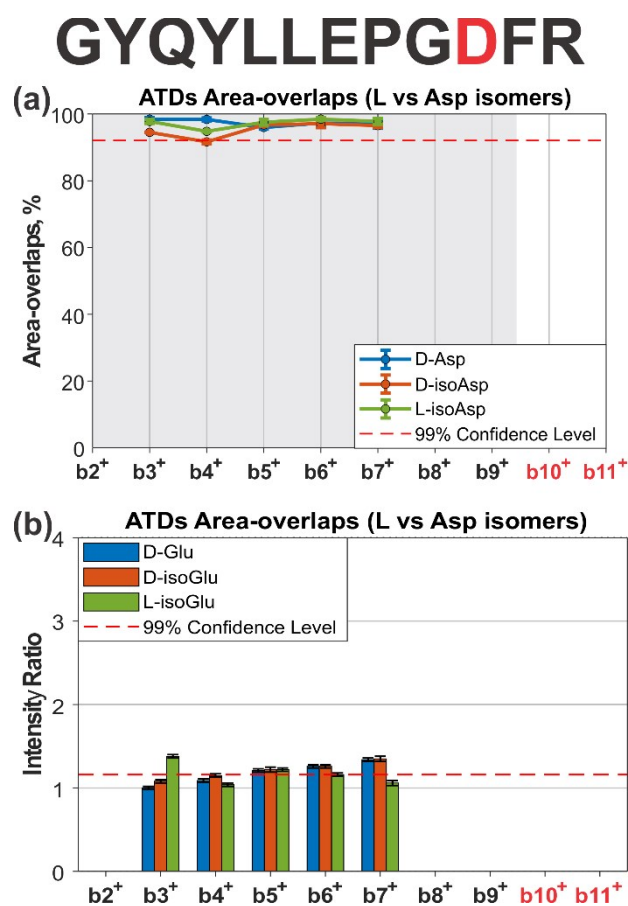


Figure S4: Result summary for peptide isomers GYQYLLEPGDFR. **(a)** ATD area-overlaps between L-Asp and D-Asp (blue), D-isoAsp (orange), or L-isoAsp (green) for b-ions. **(b)** CID intensity ratios of the isomeric b-ions.

Full CID Spectra:

HFSPEDLTVK

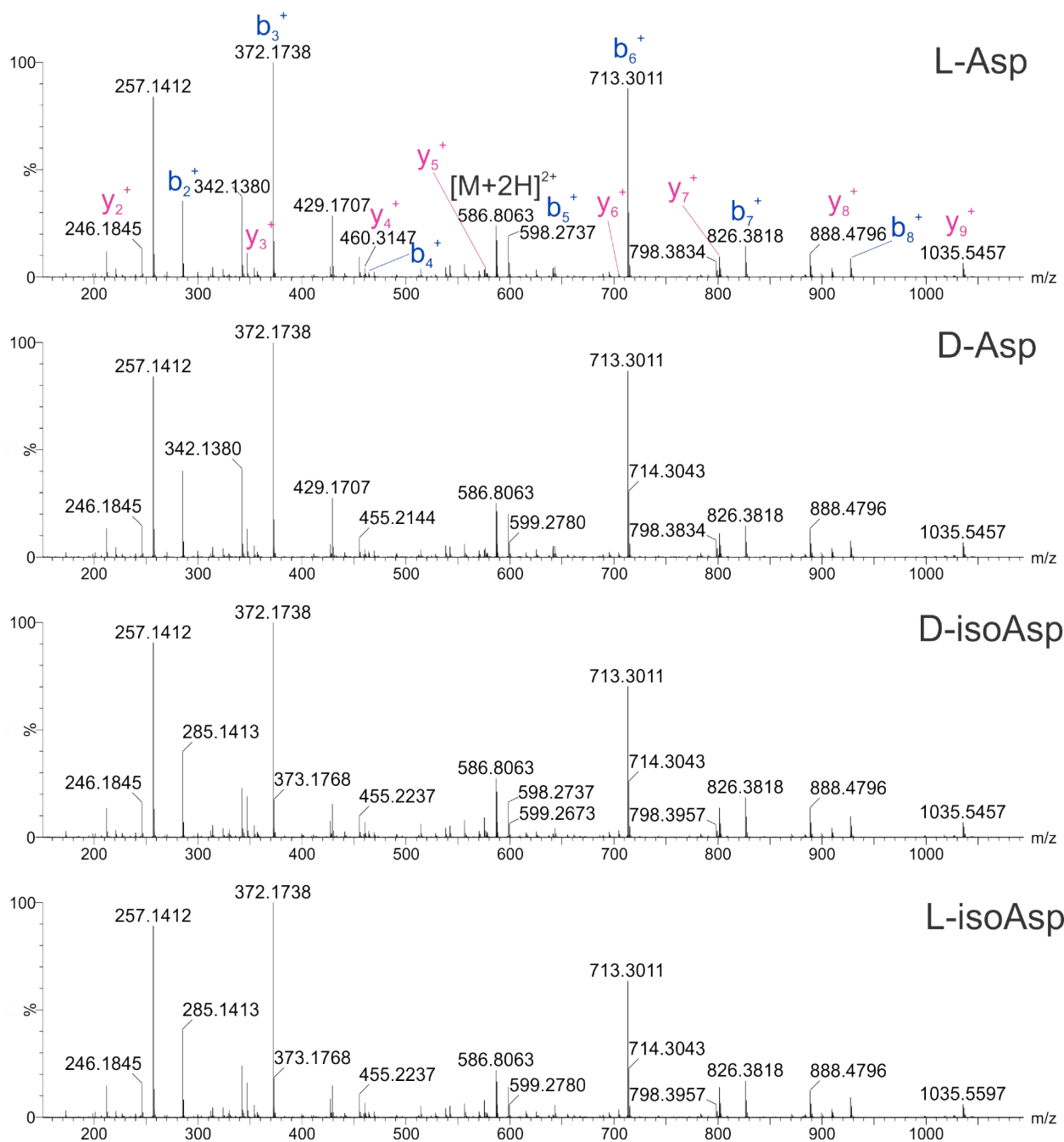


Figure S5: The CID spectra for the peptide isomers of HFSPEDLTVK: L-Asp (Top), D-Asp (Second), D-isoAsp (Third), and L-isoAsp (Bottom).

Full CID Spectra:

HFSPEDLTVK

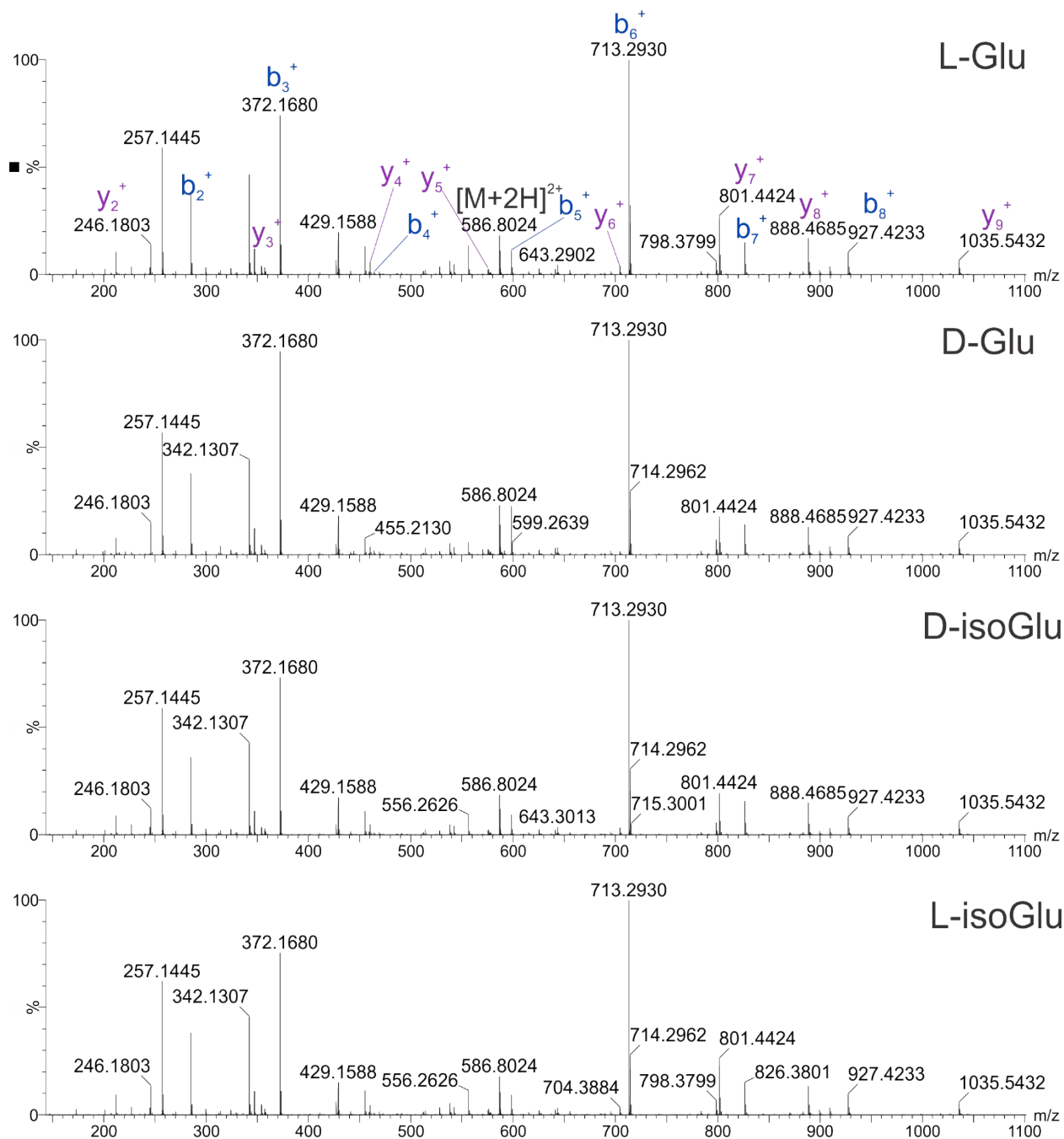


Figure S6: The CID spectra for the peptide isomers of HFSPEDLTVK: L-Glu (Top), D-Glu (Second), D-isoGlu (Third), and L-isoGlu (Bottom).