Supporting Information for:

Photoelectron Transfer Dissociation Reveals Surprising Favorability of Zwitterionic States in Large Gaseous Peptides and Proteins

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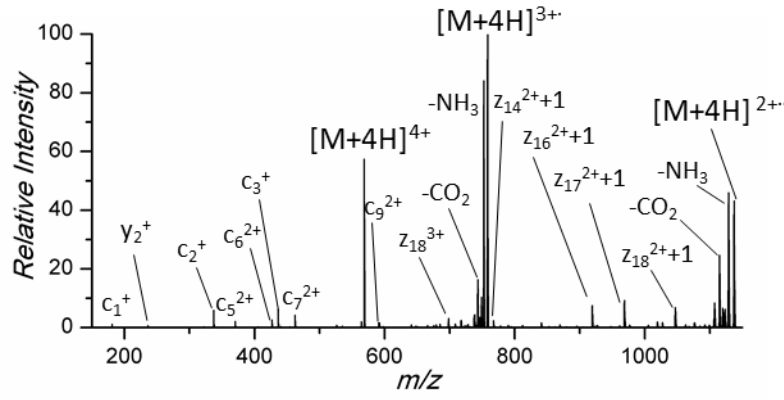


Figure S1. ETD of CD36 4+ results in several charge-reduced species as well as c/z-type fragmentation.

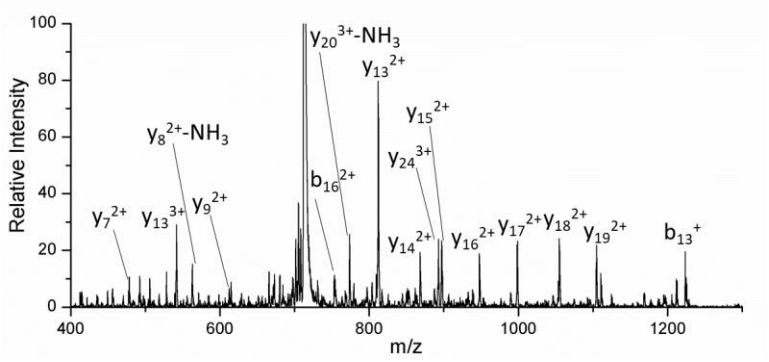
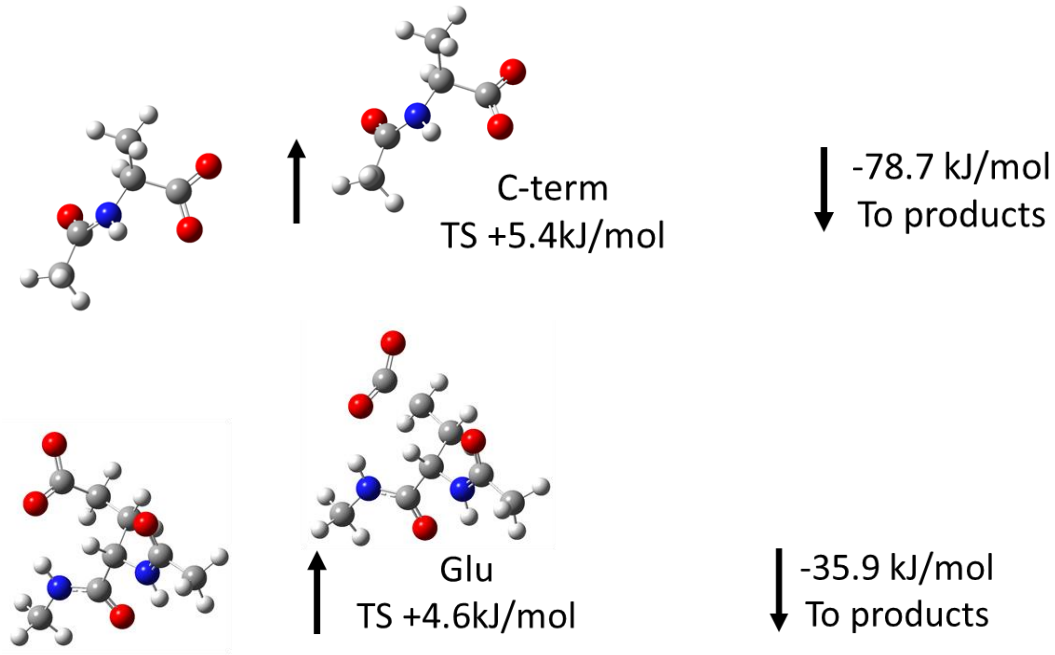


Figure S2. UVPD of melittin 4+ shows no c/z type fragmentation, but a large abundance of b/y fragmentation.



Scheme S1. Structures of radical and transition state for model of the c-terminus and glutamic acid.

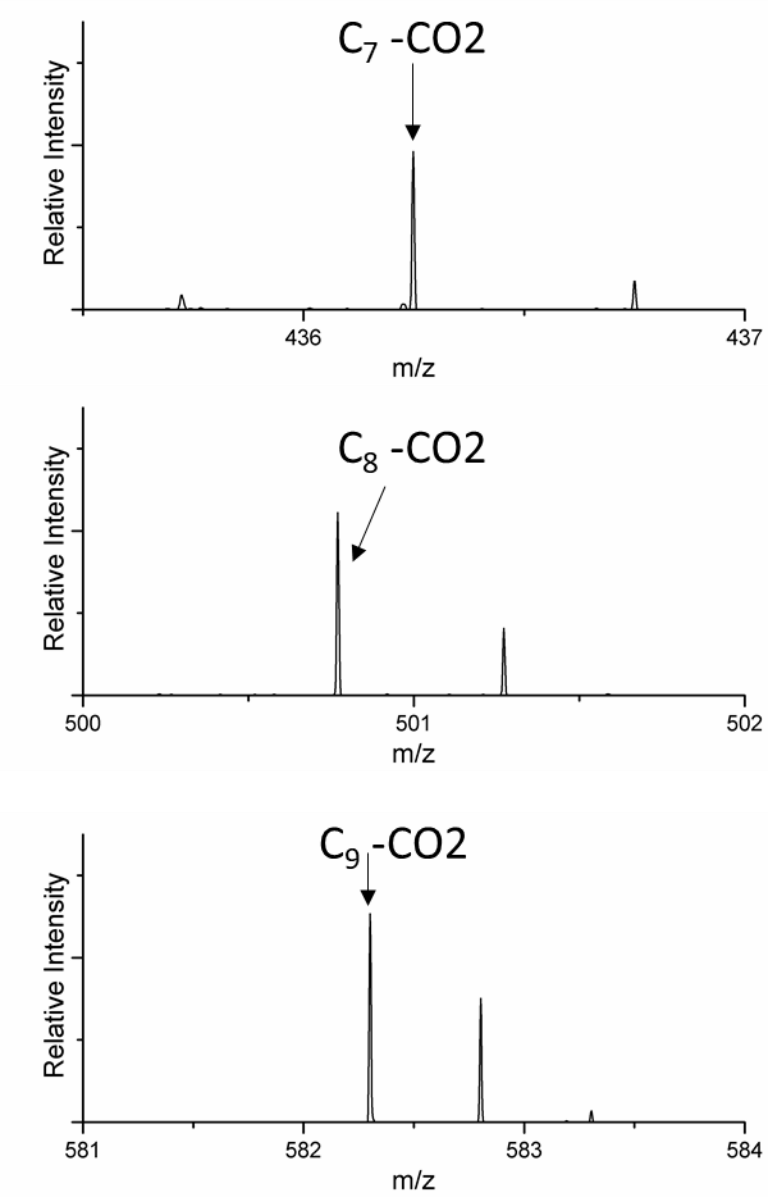


Figure S3. Zooms of several c-CO_2 ions for Figure 2c. Note the lack of a -45 Da peak in all spectra. The small -1 Da peak in the c_7-CO_2 ion is outside the mass error expected for a confident match on our orbitrap instrument.

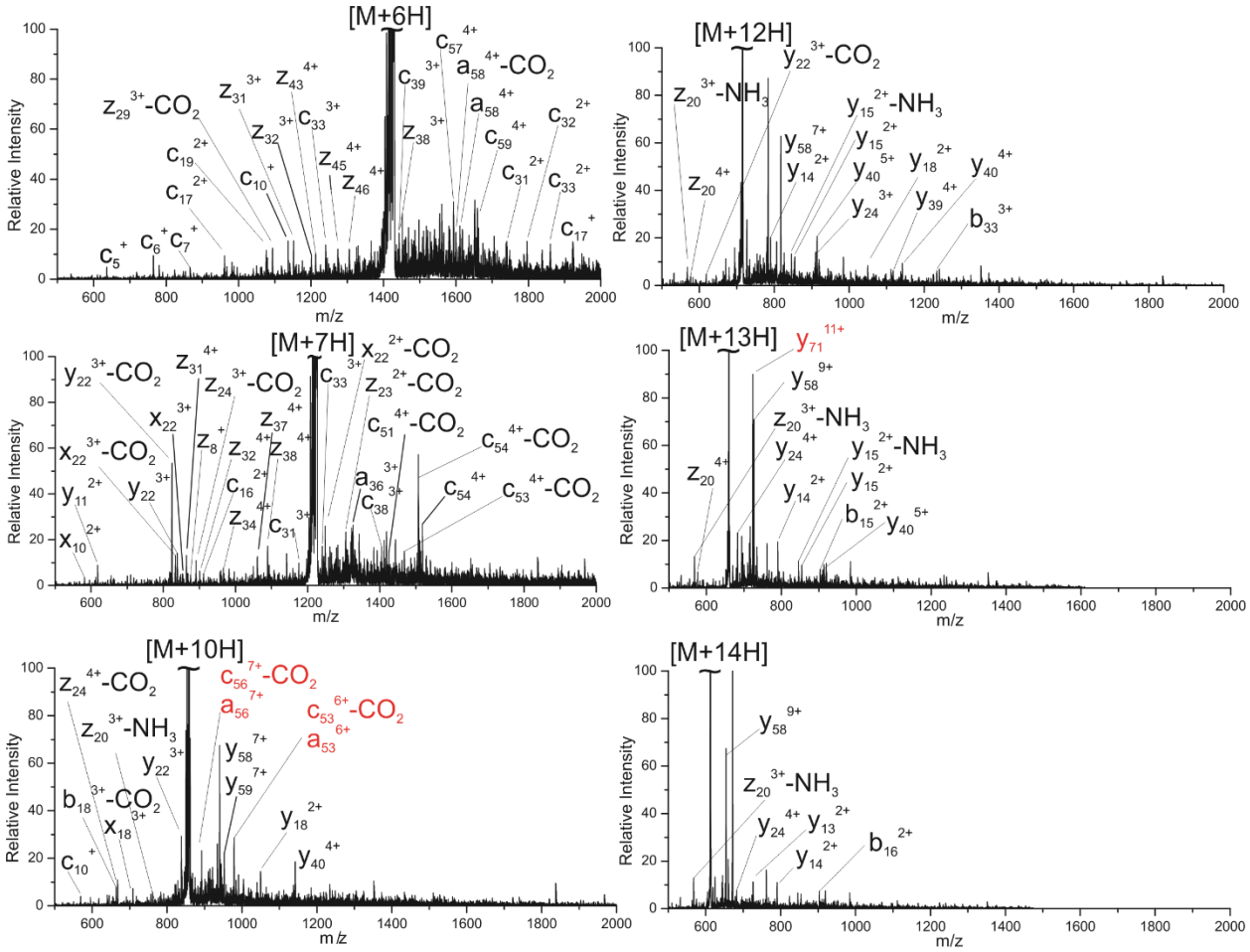


Figure S4. Mass spectra resulting from PETD experiments on Ubiquitin 6+, 7+, 10+, 12+, 13+ and 14+ ions.

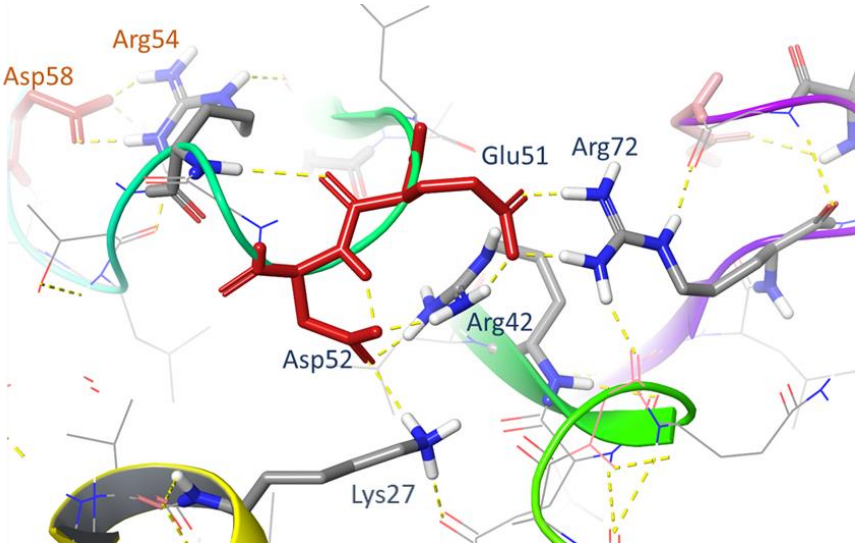


Figure S5. The Lys27-Asp52-Arg42-Glu51-Arg72 salt cluster which persists in all charge isomers evaluated by MD for the UBQ 6+ ion.

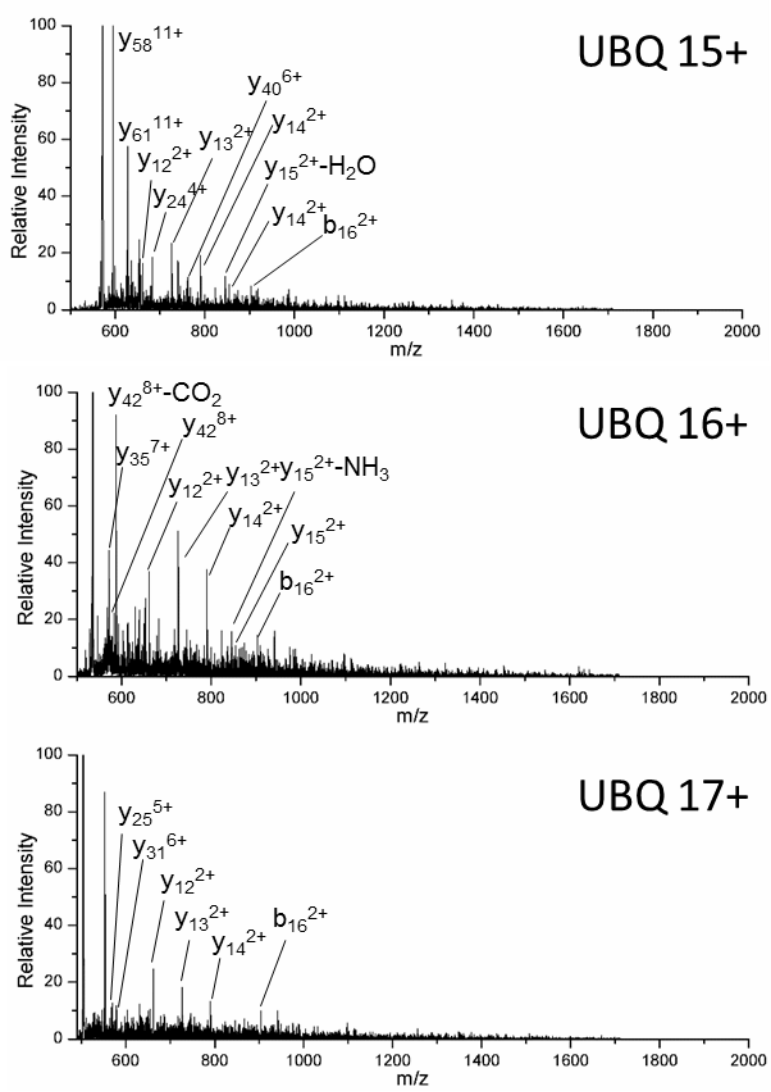


Figure S6. Mass spectra for UVPD of Ubiquitin 15-17+ ions. None of these charge states appear to be zwitterionic as noted by a complete lack of c/z-type ions.