Figure S1a. Computed structures for [Zn(Gly-H)(Gly)]^+ complexes.
Figure S1b. Computed transition structures for [Zn(Gly-H)(Gly)]⁺ complexes.
Figure S2a. Computed structures for [Zn(Pro-H)(Pro)]^+ complexes.
Figure S2b. Computed structures for [Zn(Pro-H)(Pro)]^+ complexes.
Figure S2b. Computed structures for [Zn(Pro-H)(Pro)]⁺ complexes.
Figure S2c. Computed structures for [Zn(Pro-H)(Pro)]⁺ complexes.
Figure S2d. Computed structures for [Zn(Pro-H)(Pro)]⁺ complexes.

- **r1**
  - 123.5/115.6
  - 117.7/109.9

- **r2**
  - 197.0/180.9
  - 188.1/174.2
Figure S2d. Computed transition state structures for [Zn(Pro-H)(Pro)]^+ complexes.
Figure S3. Comparison of the energetics of H₂ loss and the Pro-H₂ loss mechanisms.
Figure S4. Comparison of fragmentation induced by infrared multiphoton activation.
Figure S6. SORI/CID of m/z 180 isolated after CID of m/z 293.
Figure S7. IRMPD of m/z 295 ([$^{66}$Zn(Pro-H)(Pro)]$^+$) following its isolation.
Figure S8. a) SORI MS of m/z 178 formed SORI of ([Zn(Pro-H)(Pro)]^+) and b) SORI MS of m/z 181 formed from SORI of ([Zn(2,5,5-d_5-Pro-H)(2,5,5-d_5-Pro)]^+). The dissociation of this ion is the topic of JPCB, 2013.