Loss of water from protonated polyglycines; interconversion and dissociation of the product imidazolone ions

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Supporting information

Scheme S1. Mechanism for the isomerization between the $[b_5]^+_{\mathbf{I}}$ and $[b_5]^+_{\mathbf{II}}$ ions. Relative enthalpies and (free energies) both in kJ mol^{-1} are calculated at the B3LYP/6-311++G(d,p) level. The number in red denotes the highest barrier on the pathway.

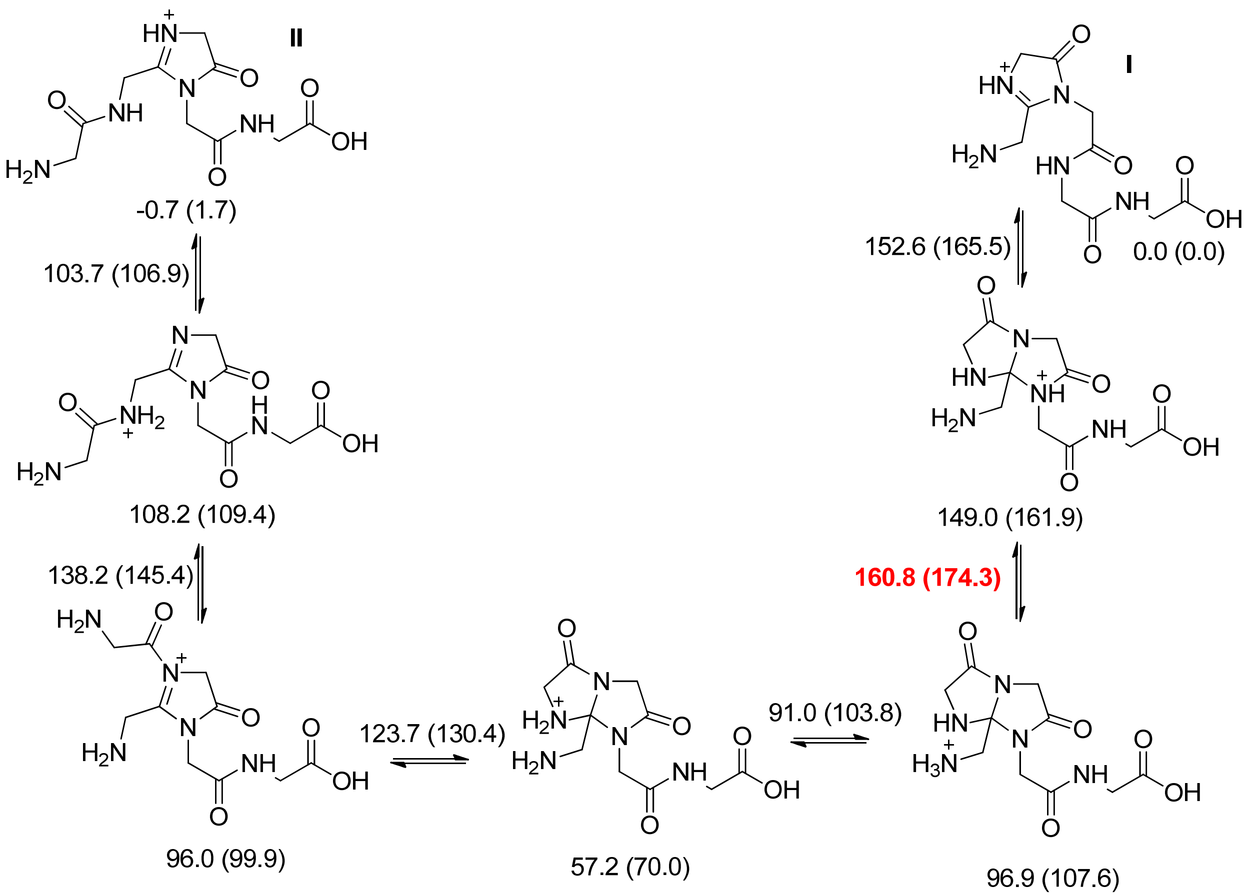

Figure S1. CID spectrum of protonated pentaglycine with ^{18}O-labeled at the first amide oxygen. The precursor ion is denoted by asterisk (*).

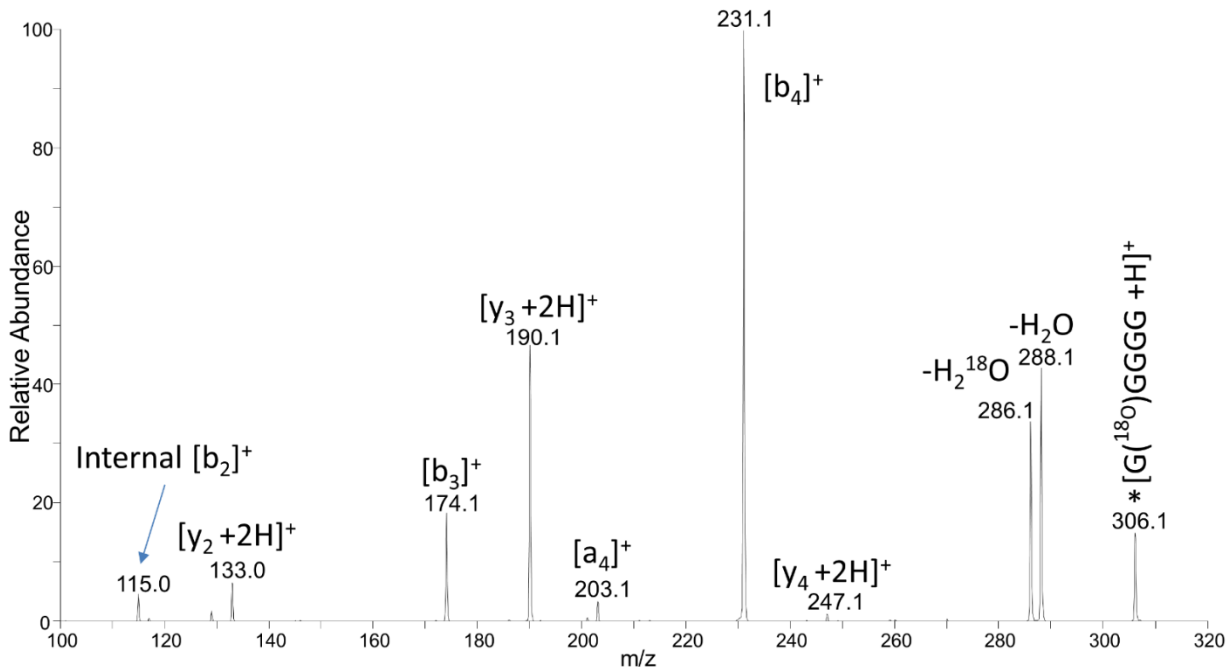

Figure S2. CID spectrum of protonated pentaglycine with ^{18}O-labeled at the second amide oxygen. The precursor ion is denoted by asterisk (*).

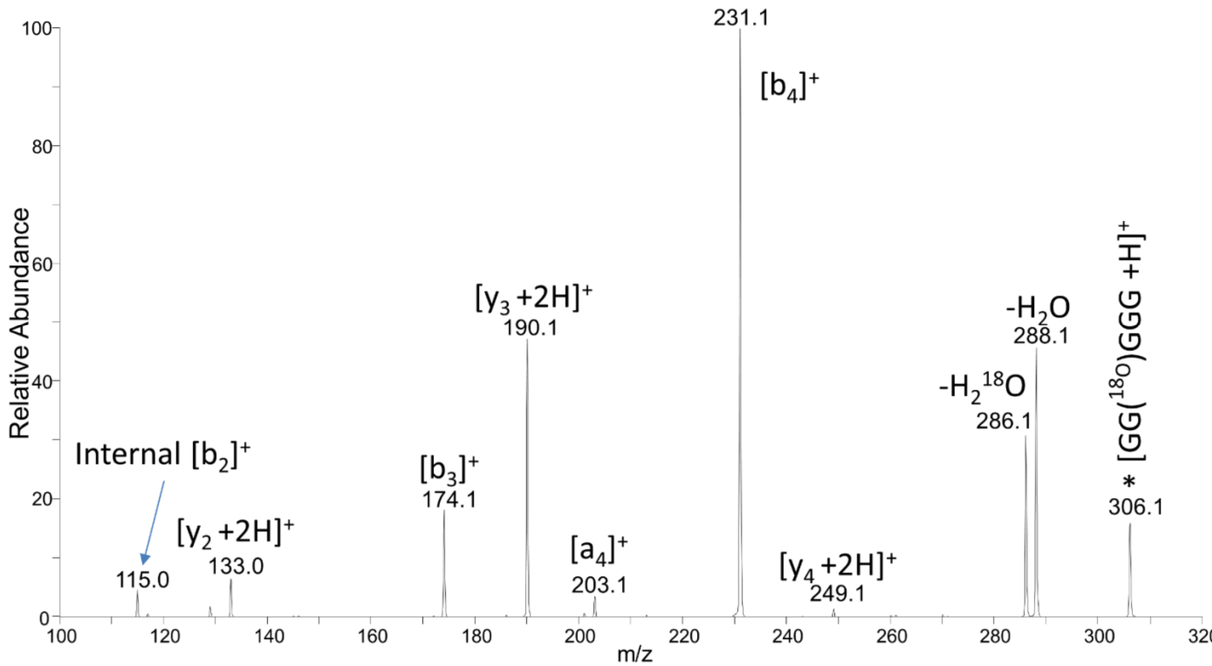

Figure S3. Energy-resolved diagram for the fragmentations of [G(^{18}O)GGGG + H]$^+$ ion

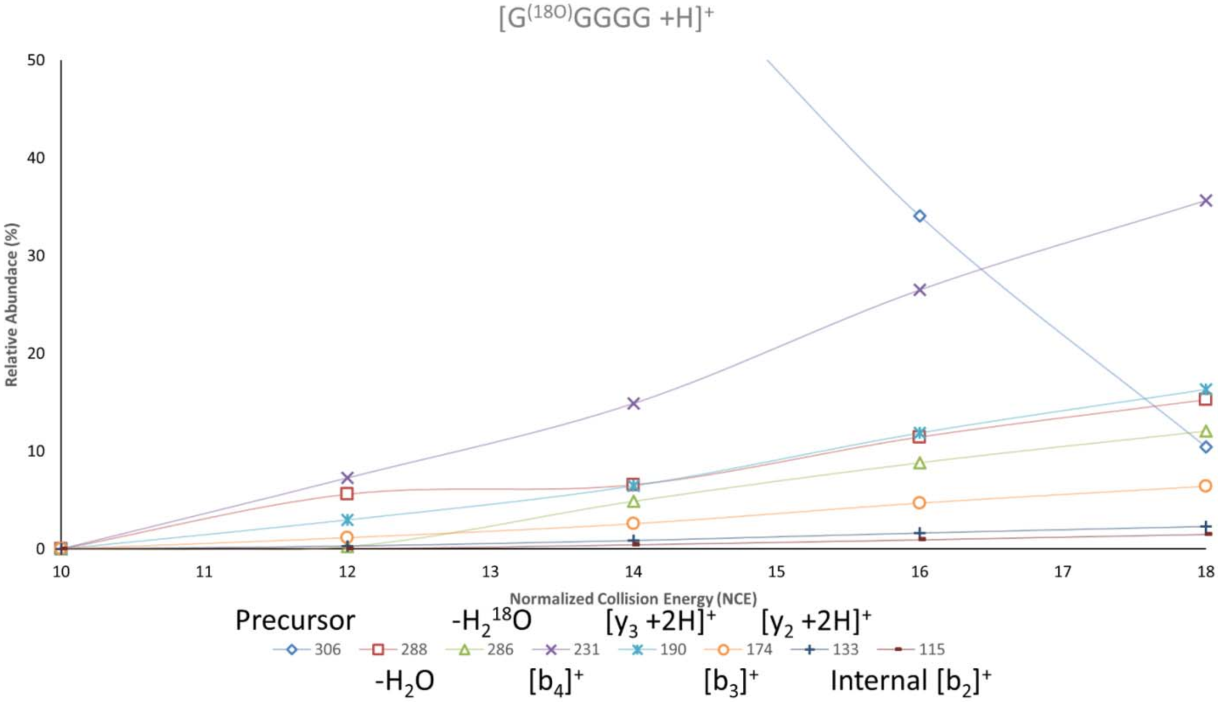

Figure S4. Energy-resolved diagram for the fragmentations of [GG(^{18}O)GGG + H]$^{+}$ ion

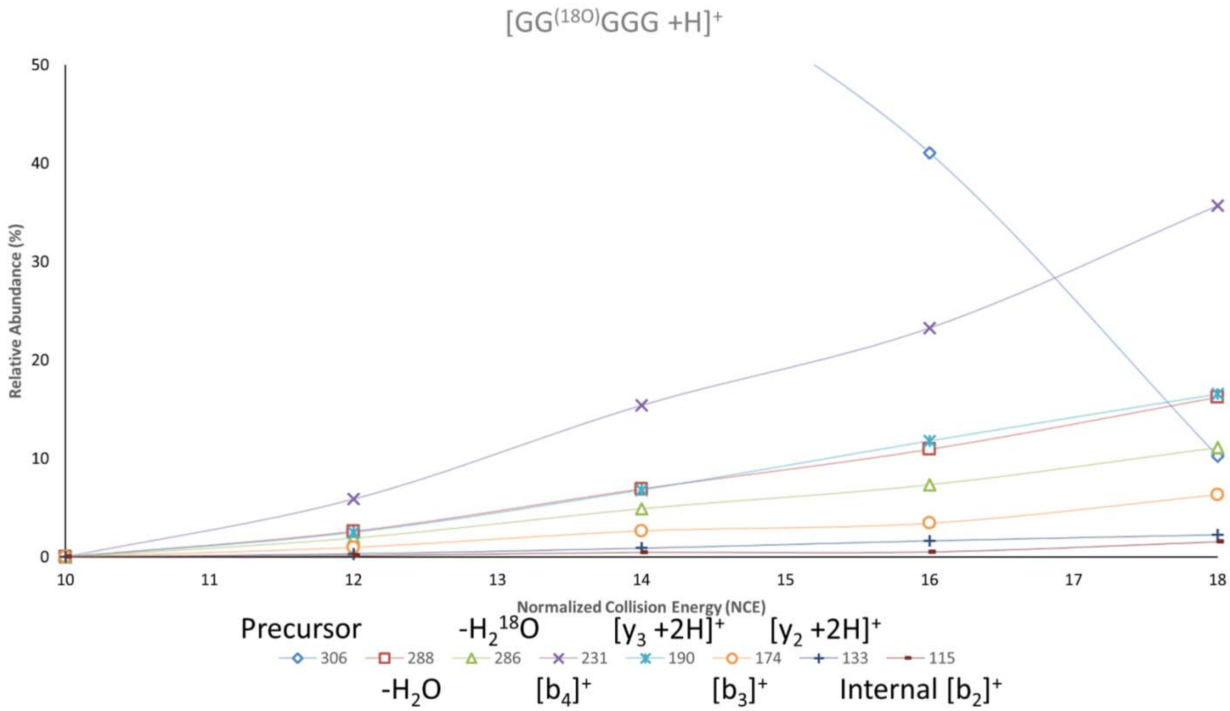

Figure S5. CID spectrum of protonated pentaglycine with ^{18}O-labeled at the third amide oxygen. The precursor ion is denoted by asterisk (*).

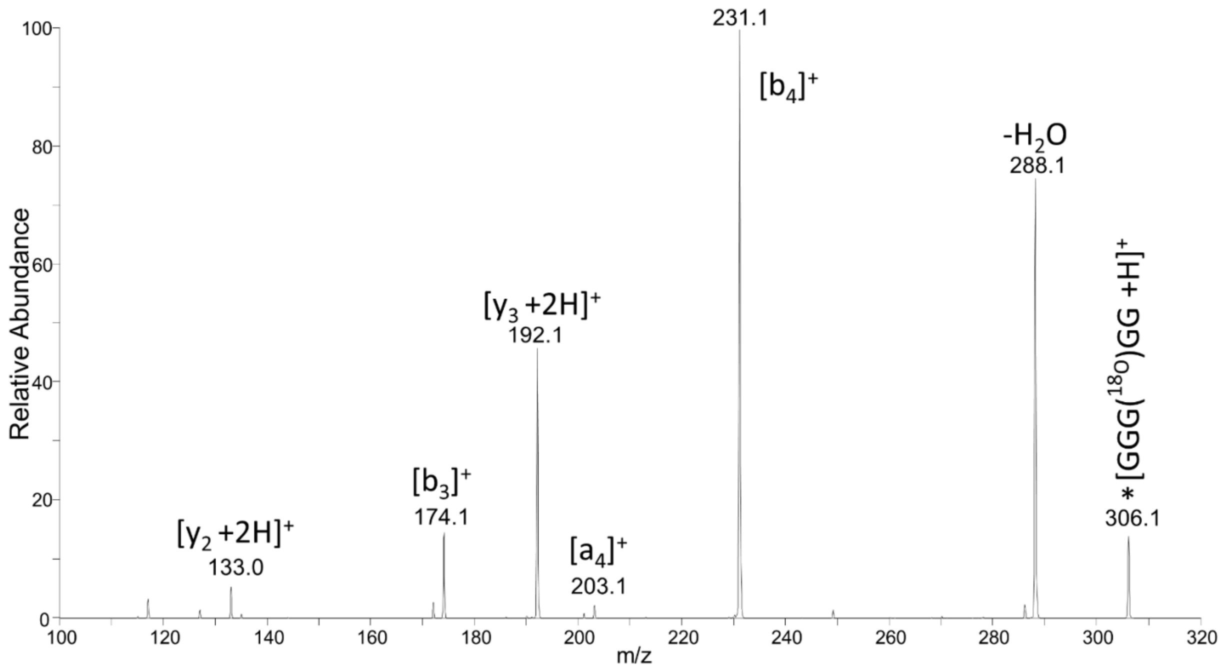

Figure S6. CID spectrum of protonated pentaglycine with ^{18}O-labeled at the fourth amide oxygen. The precursor ion is denoted by asterisk (*).

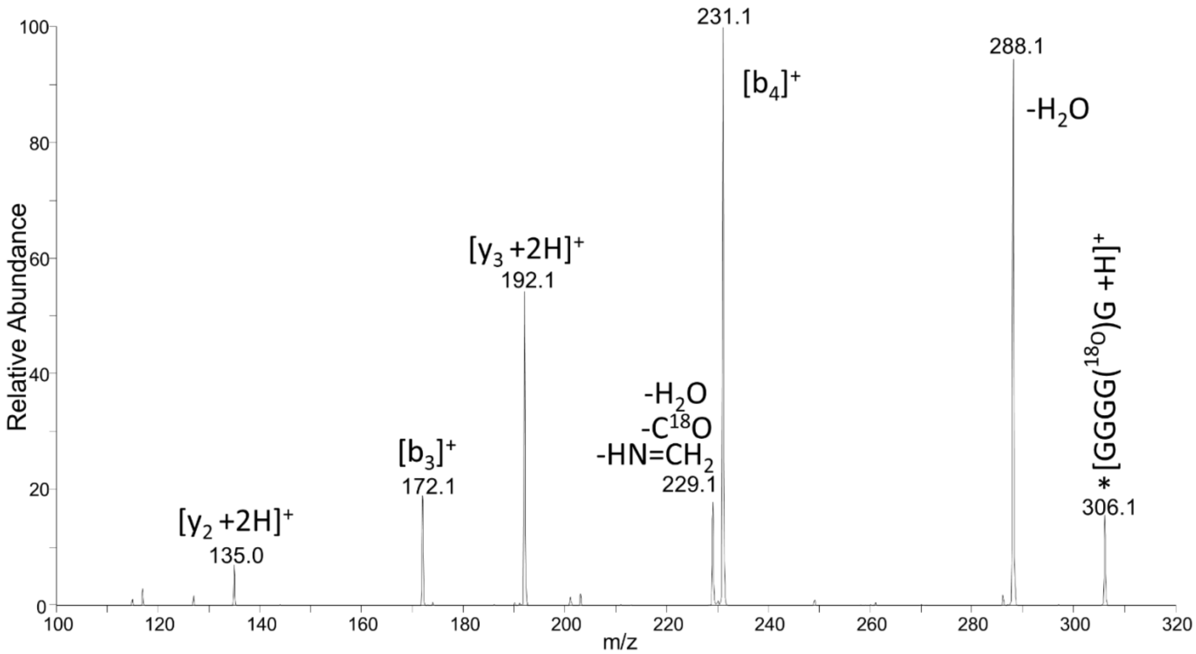

Figure S7. Energy-resolved diagram for the fragmentations of [GGG(^{18}O)GG + H]$^+$ ion.

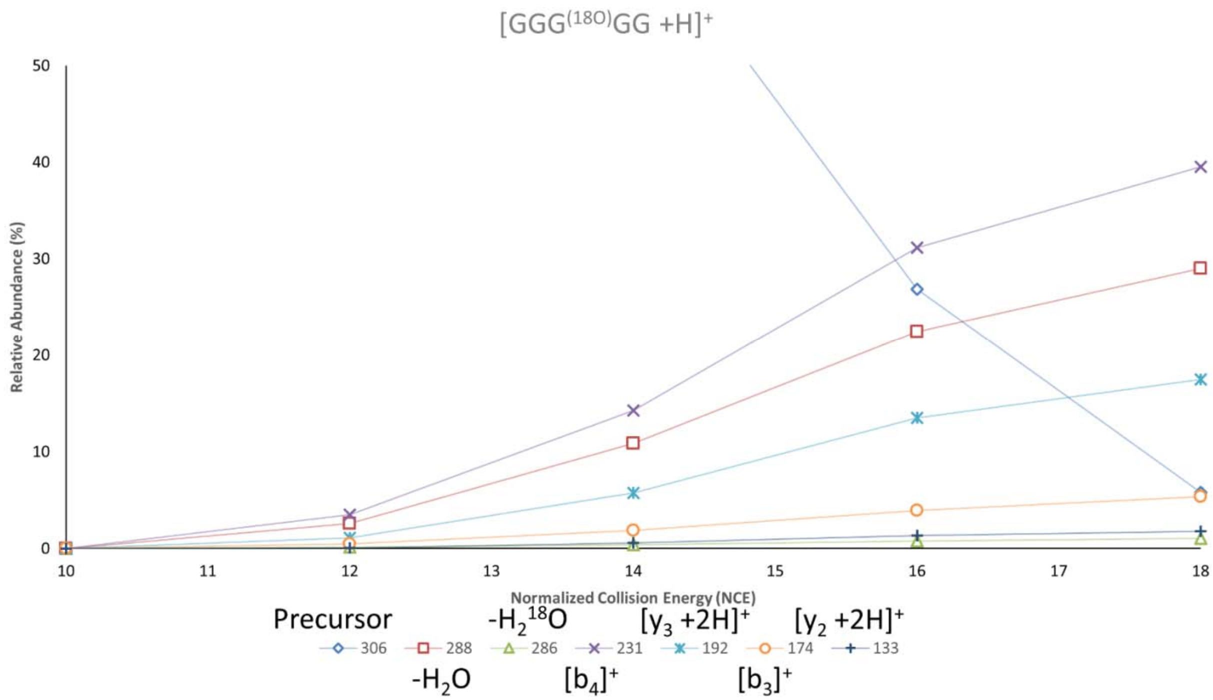

Figure S8. Energy-resolved diagram for the fragmentations of [GGGG(^{18}O)G + H]$^+$ ion.

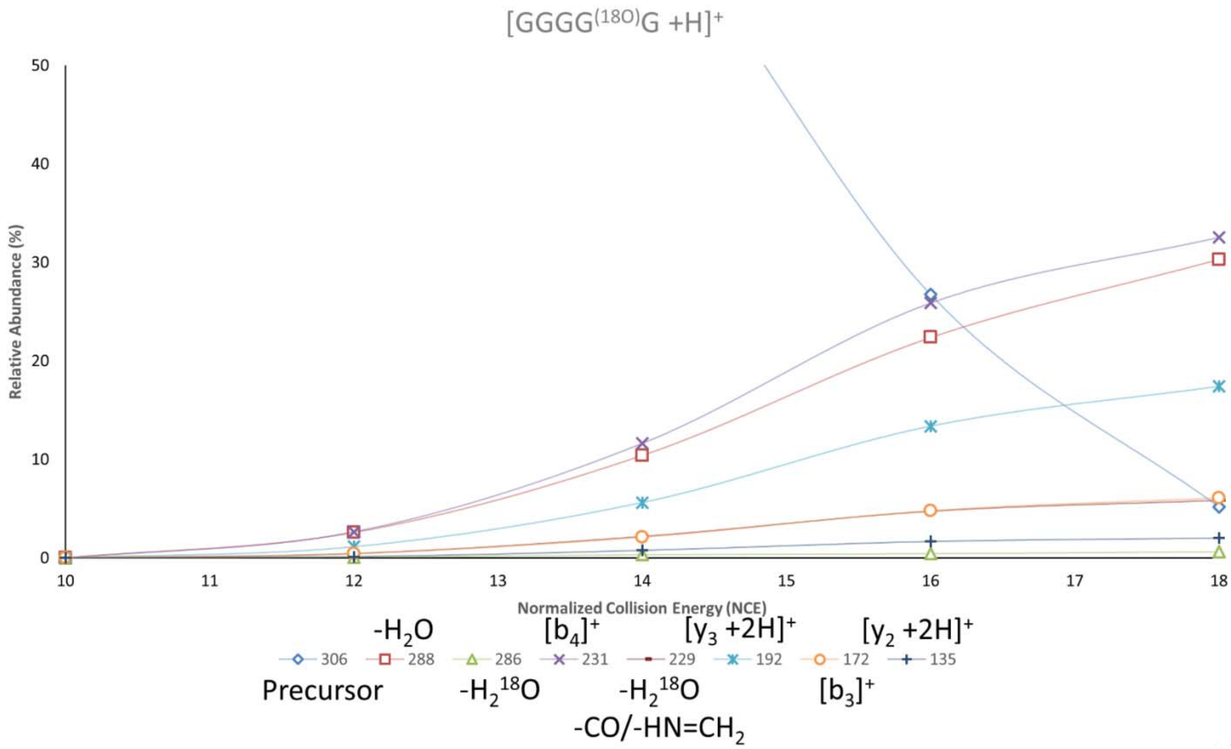

Figure S9. CID spectrum of protonated hexaglycine with ^{18}O-labeled at the first amide oxygen. The precursor ion is denoted by asterisk (*).

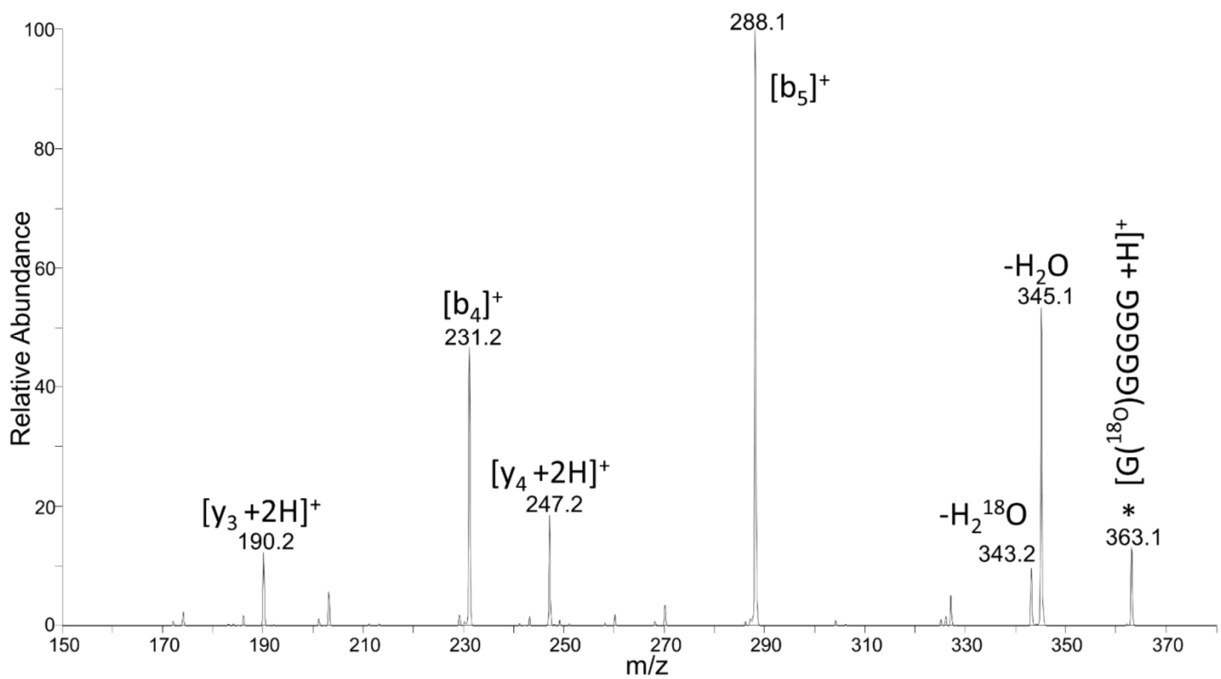

Figure S10. CID spectrum of protonated hexaglycine with ^{18}O-labeled at the second amide oxygen. The precursor ion is denoted by asterisk (*).

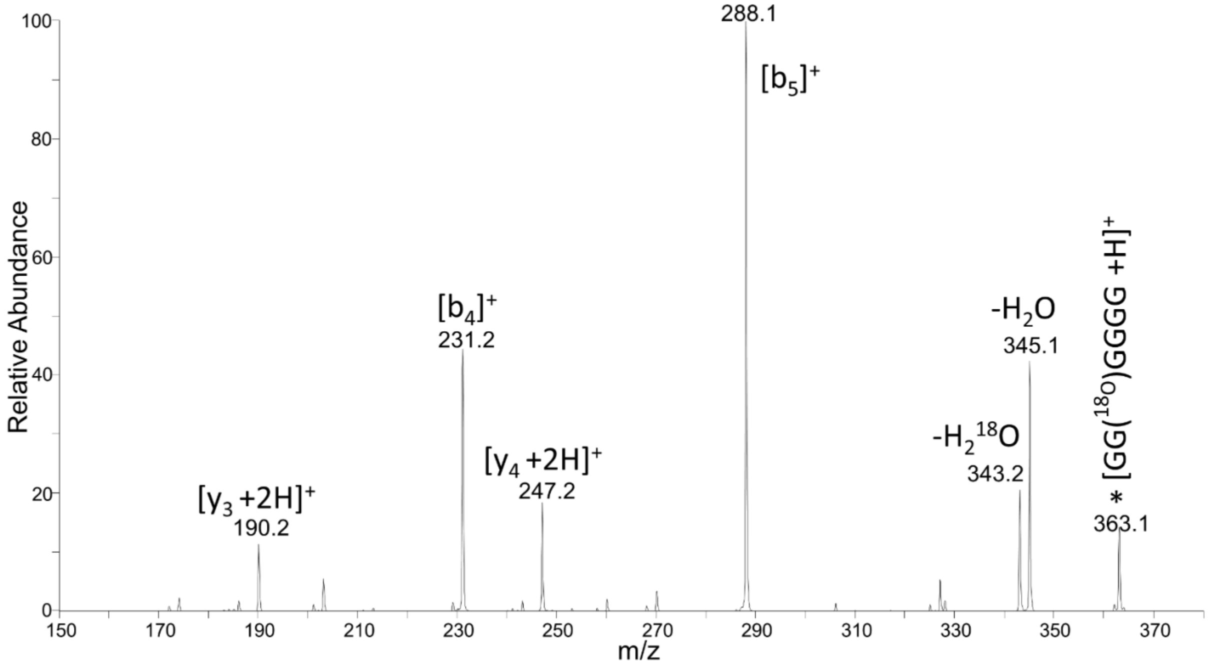

Figure S11. CID spectrum of protonated hexaglycine with ^{18}O-labeled at the third amide oxygen. The precursor ion is denoted by asterisk (*).

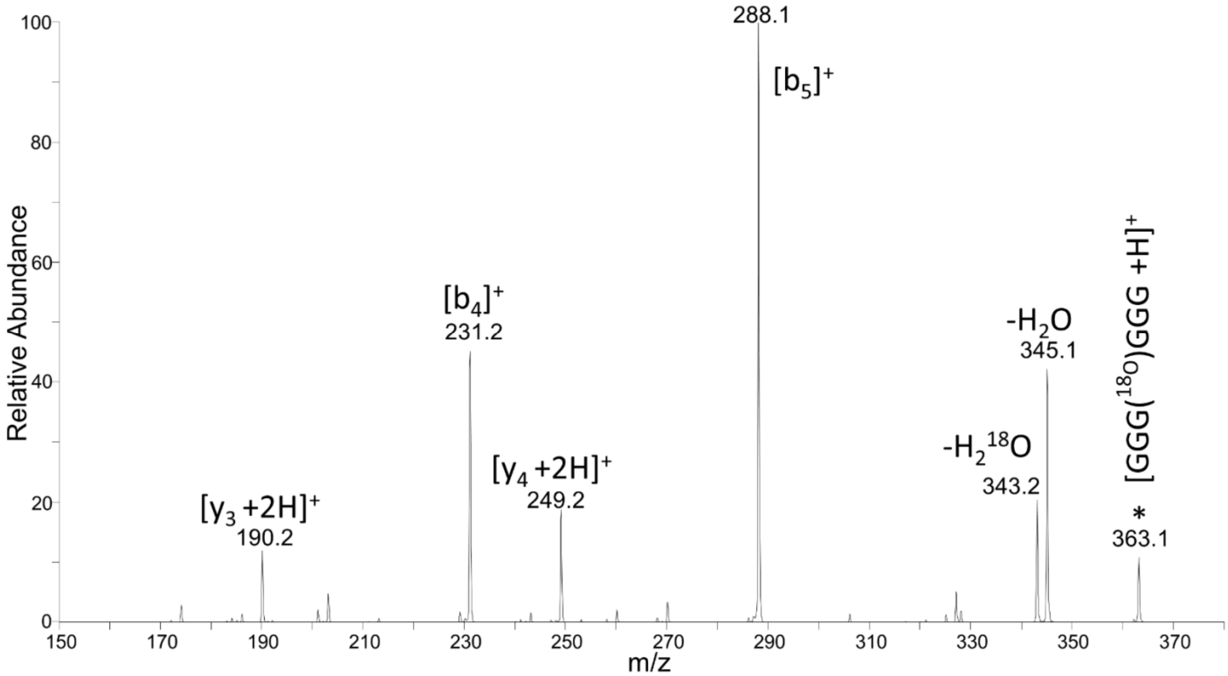

Figure S12. Energy-resolved diagram for the fragmentations of [G(^{18}O)GGGGG + H]$^+$ ion

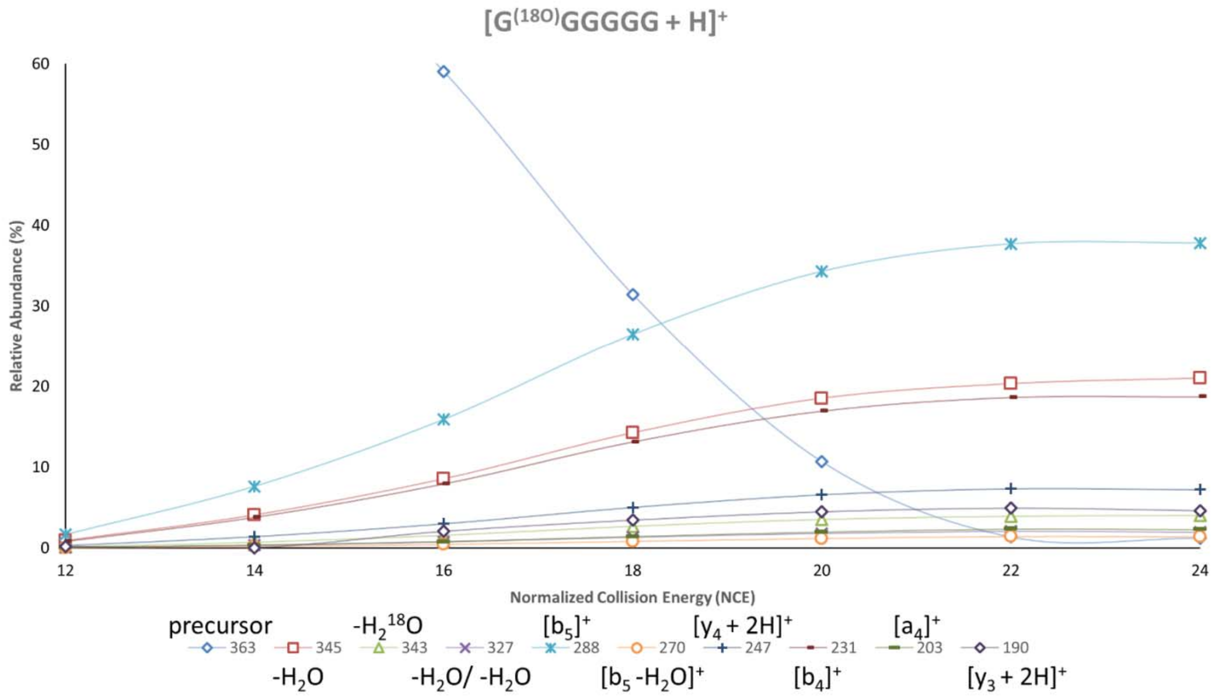

Figure S13. Energy-resolved diagram for the fragmentations of [GG(^{18}O)GGGG + H]$^+$ ion

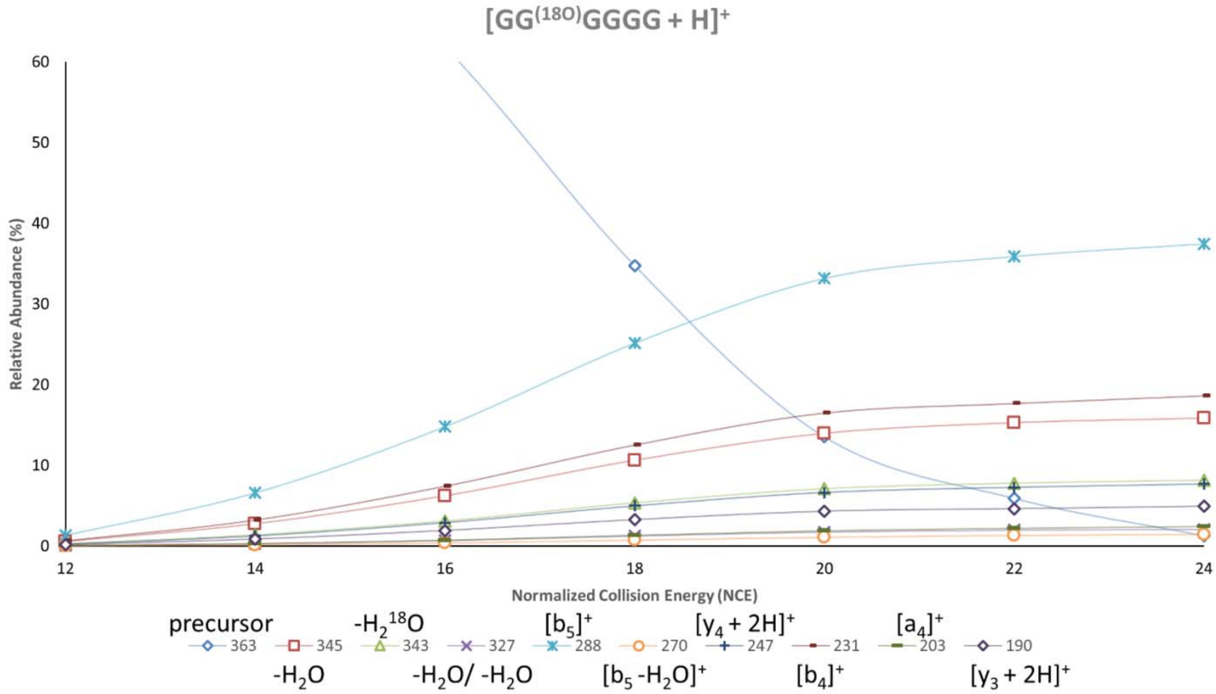

Figure S14. Energy-resolved diagram for the fragmentations of [GGG(^{18}O)GGG + H]$^+$ ion.

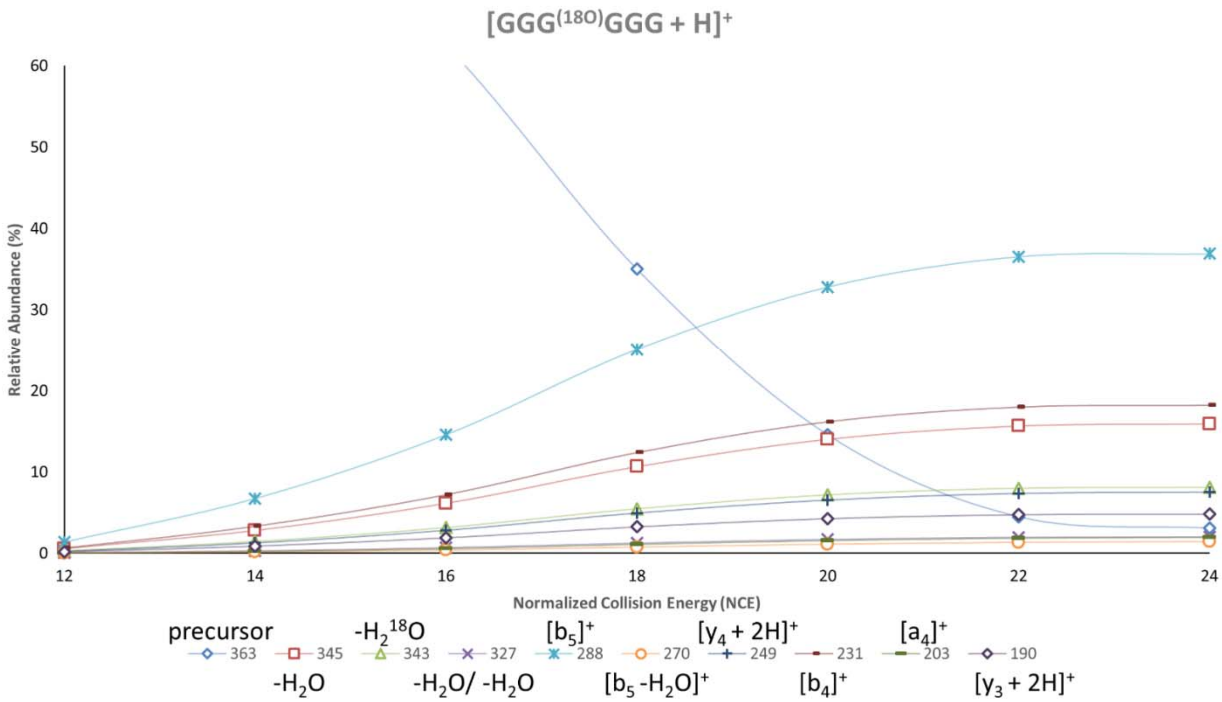

Figure S15. CID spectrum of protonated hexaglycine with ^{18}O-labeled at the fourth amide oxygen. The precursor ion is denoted by asterisk (*).

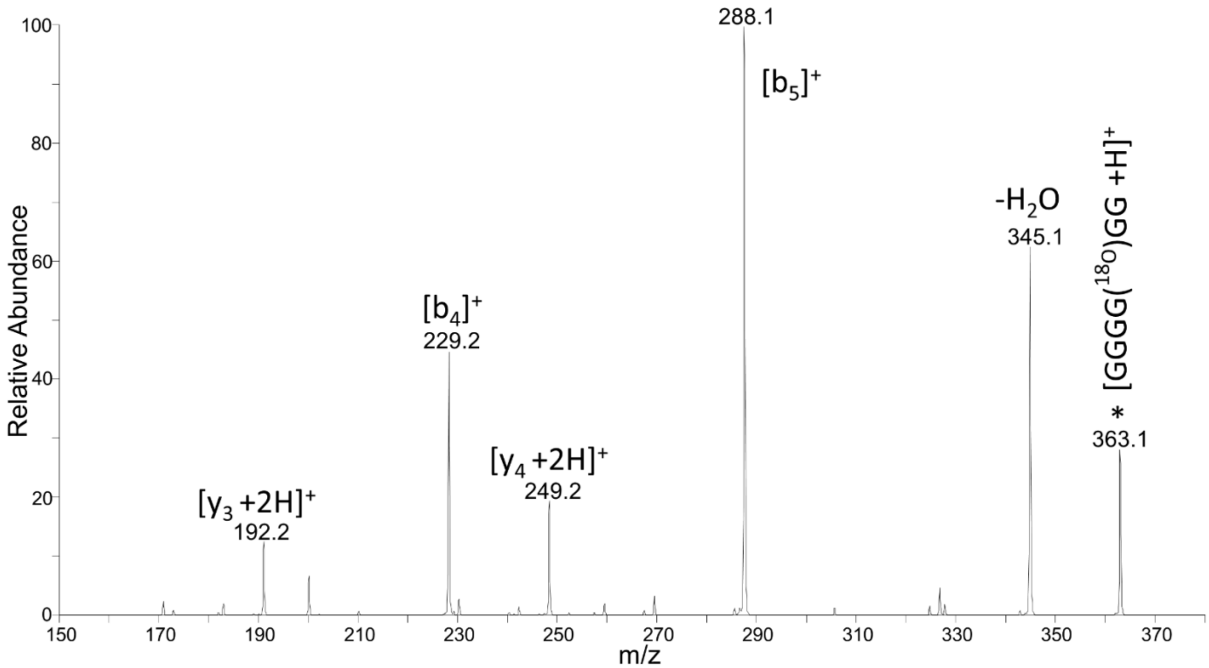

Figure S16. CID spectrum of protonated hexaglycine with ^{18}O-labeled at the fifth amide oxygen. The precursor ion is denoted by asterisk (*).

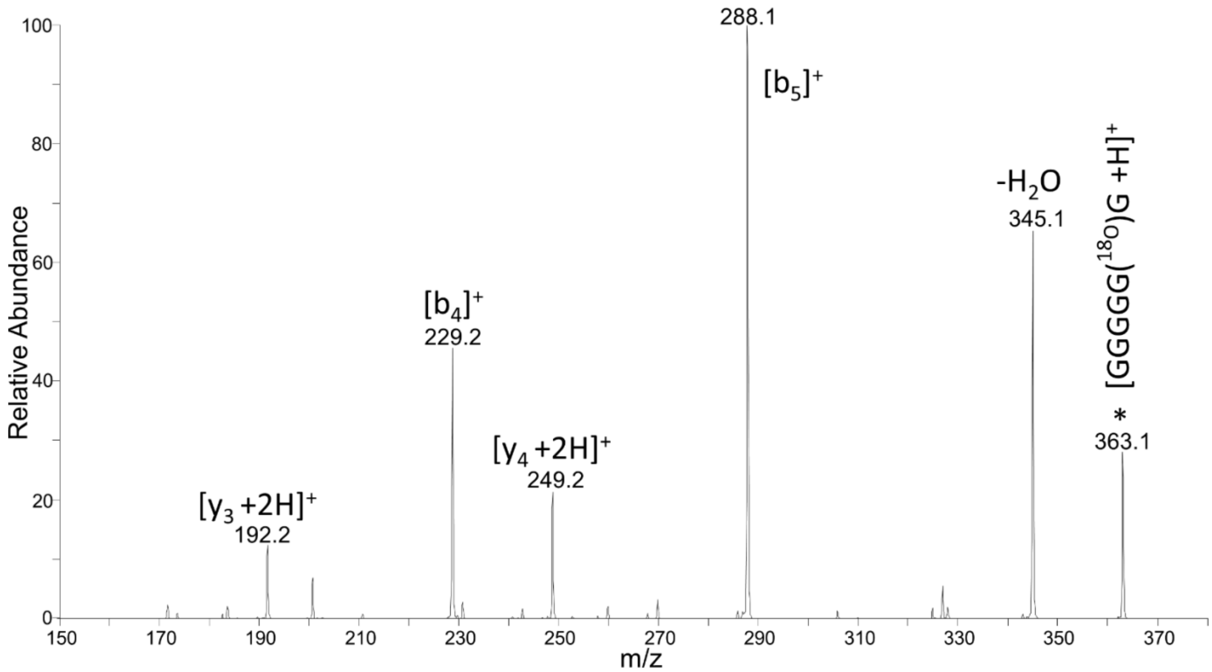

Figure S17. Energy-resolved diagram for the fragmentations of [GGGG(^{18}O)GG + H]$^+$ ion.

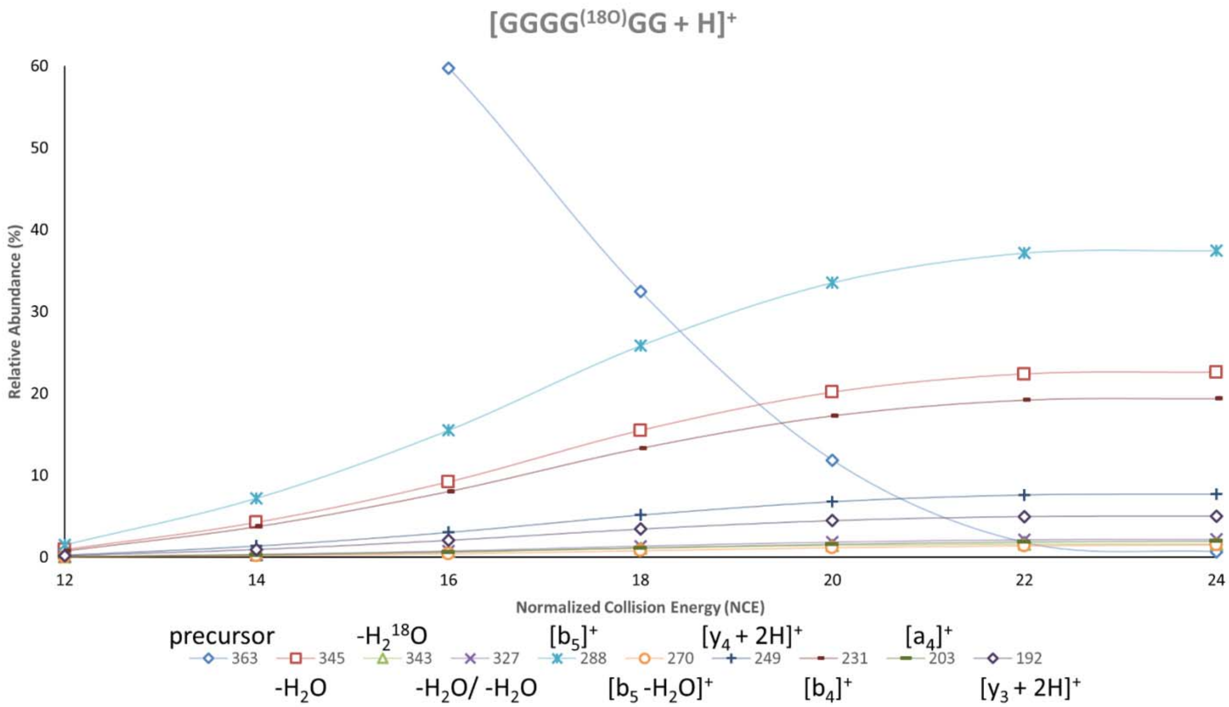

Figure S18. Energy-resolved diagram for the fragmentations of [GGGGG(^{18}O)G + H]$^+$ ion.

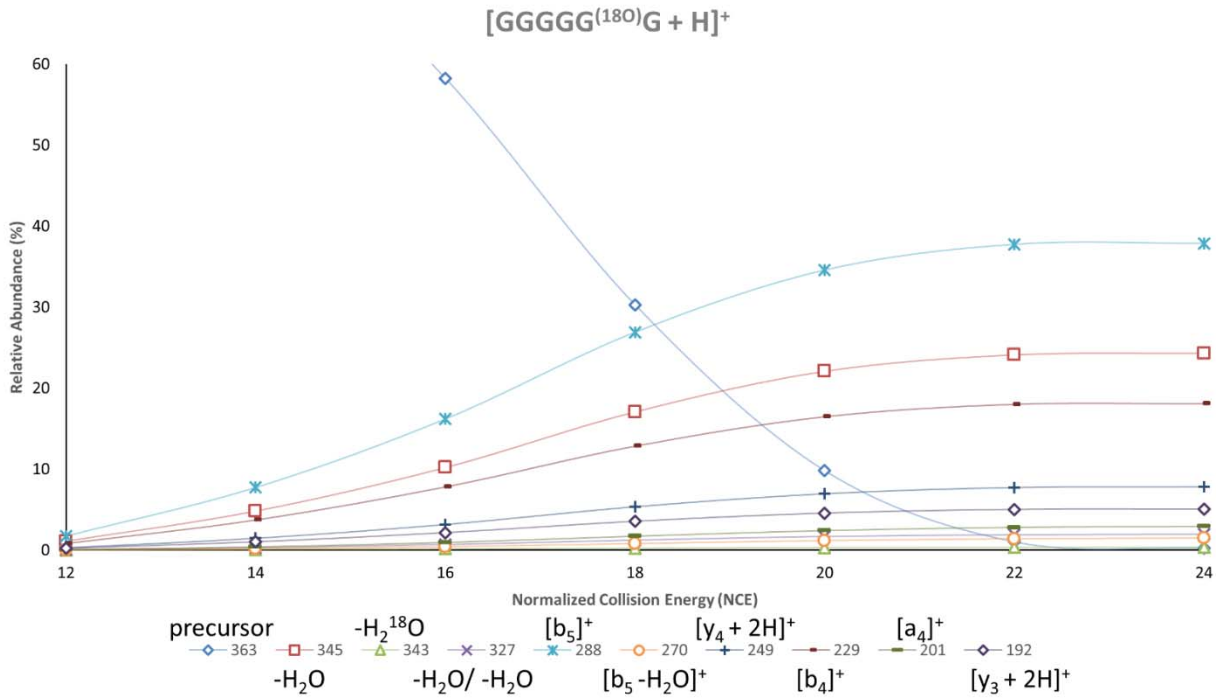

Figure S19. Energy-resolved diagram for the fragmentations of the $[b_6]^+_{\mathbf{I}}$ ion.

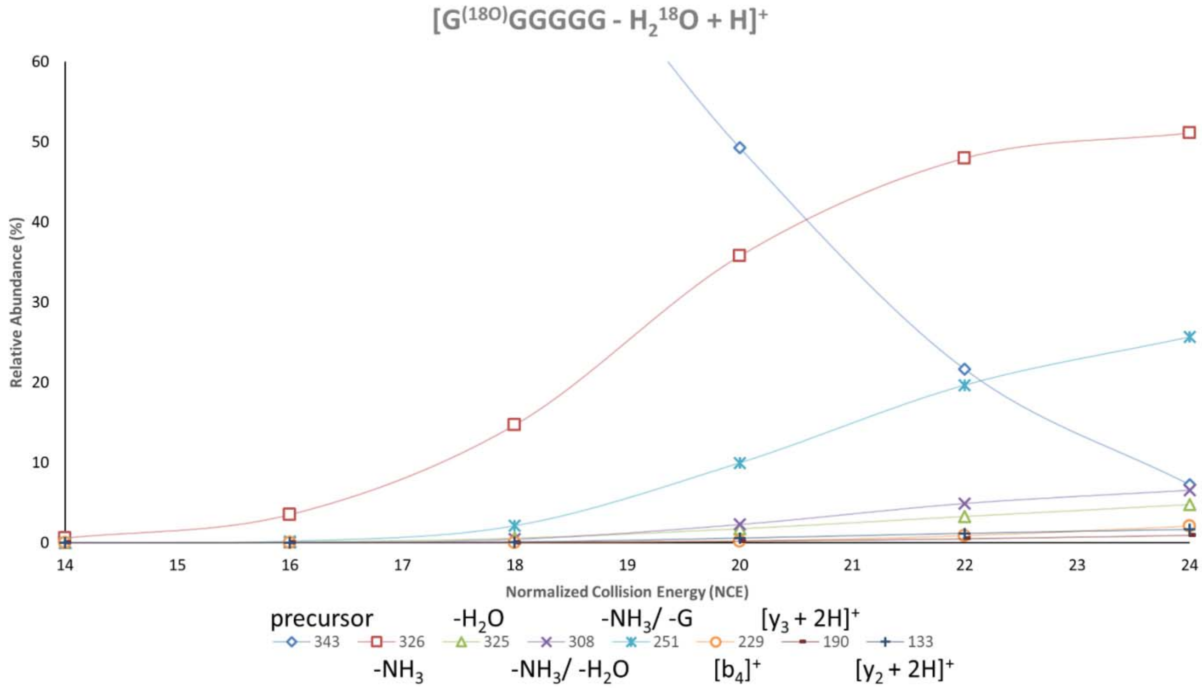

Figure S20. Energy-resolved diagram for the fragmentations of the $[b_6]^+_{II}$ ion.

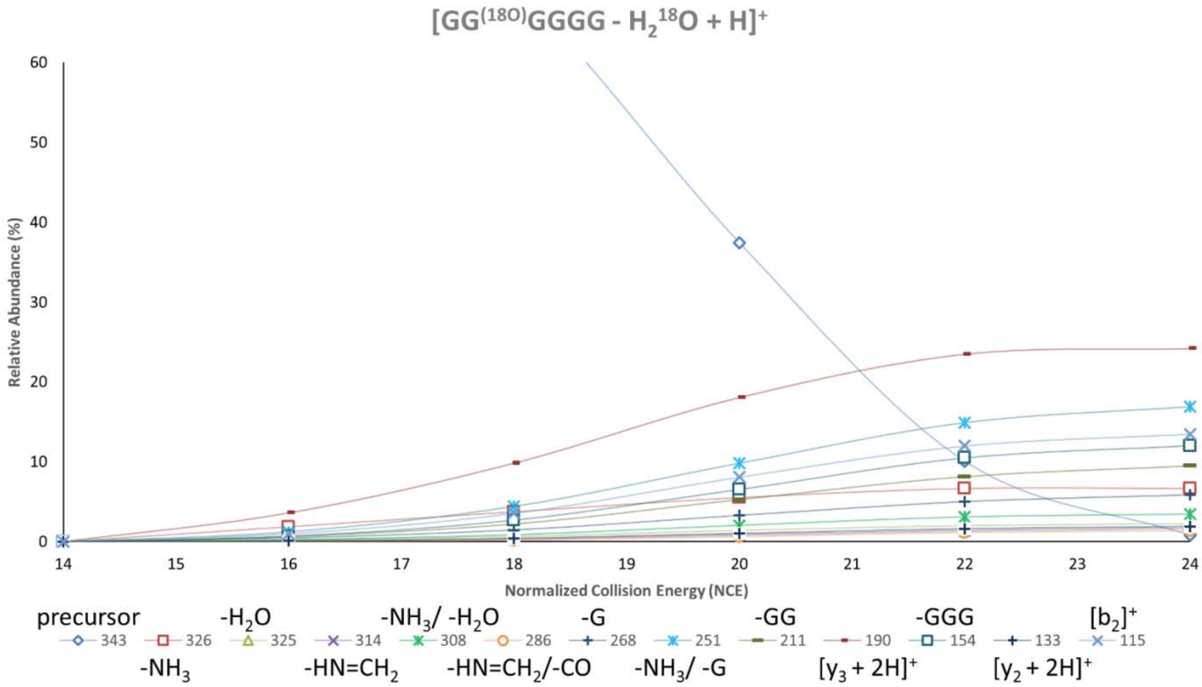

Figure S21. Energy-resolved diagram for the fragmentations of the $[b_6]^+_{III}$ ion.

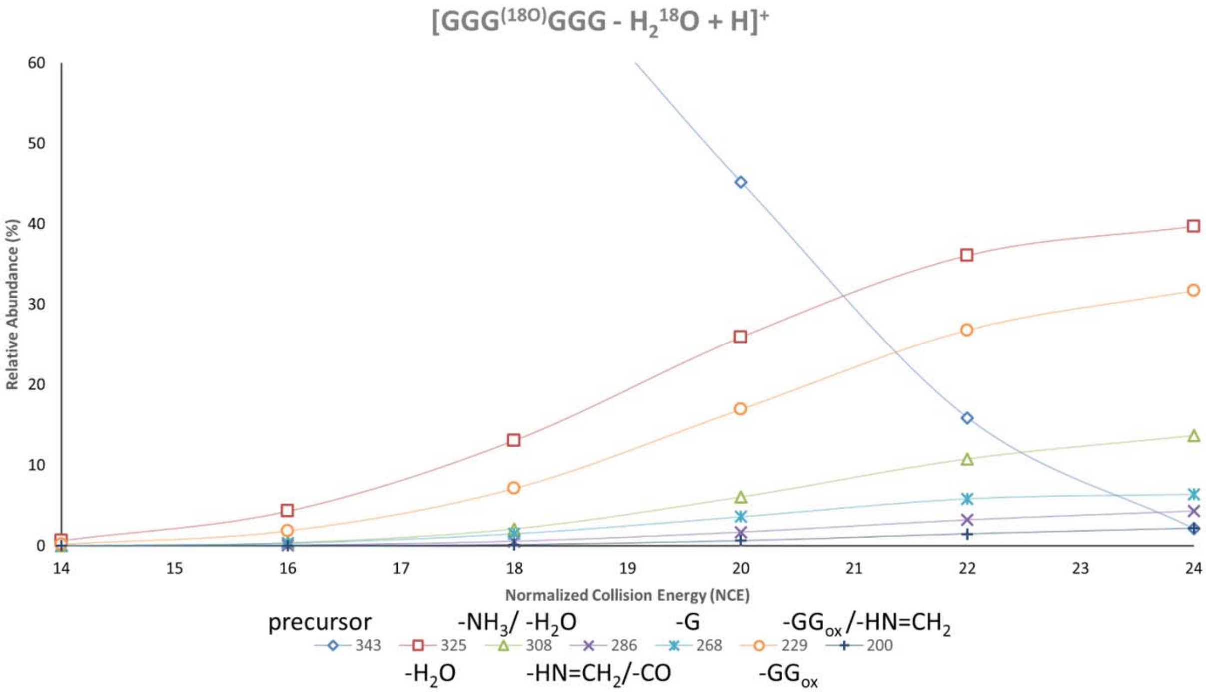

Figure S22. CID spectrum of [GGG(^{18}O,^{15}N)GGG-OMe + H – $H_2{}^{18}O$]$^+$. The precursor ion is denoted by asterisk (*)

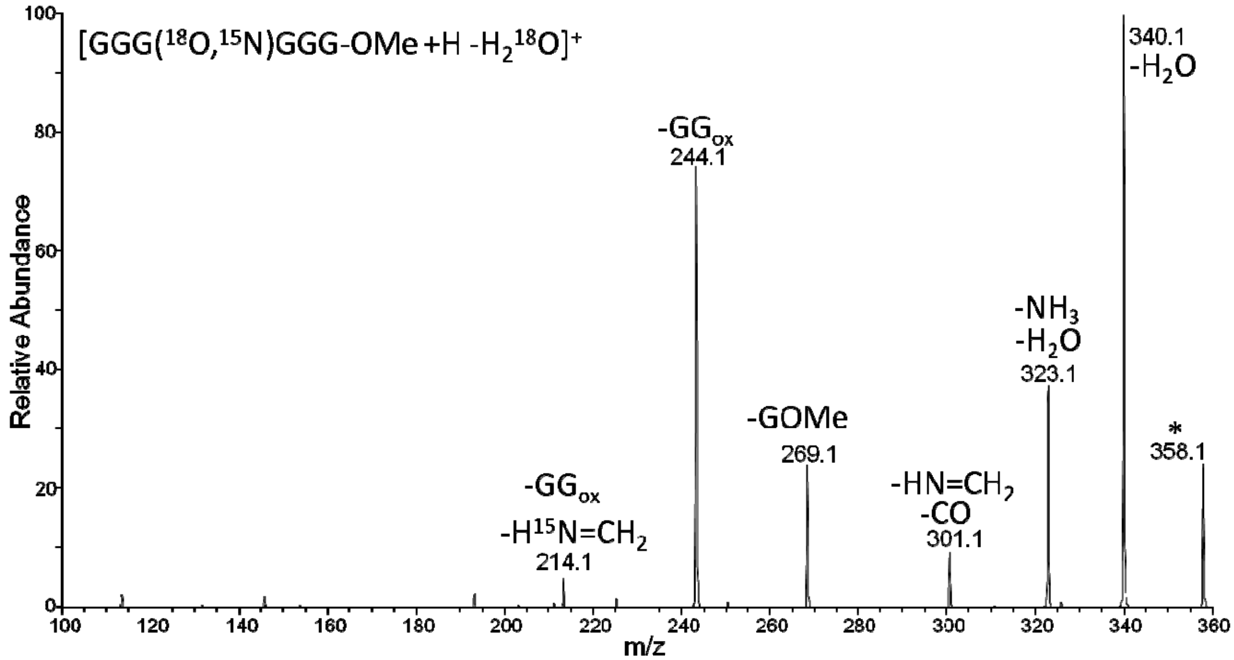

Figure S23. CID specta of (a) $[Gly_7 + H]^+$, (b) $[Gly_8 + H]^+$, and (c) $[Gly_9 + H]^+$. The precursor ion is denoted by asterisk (*)

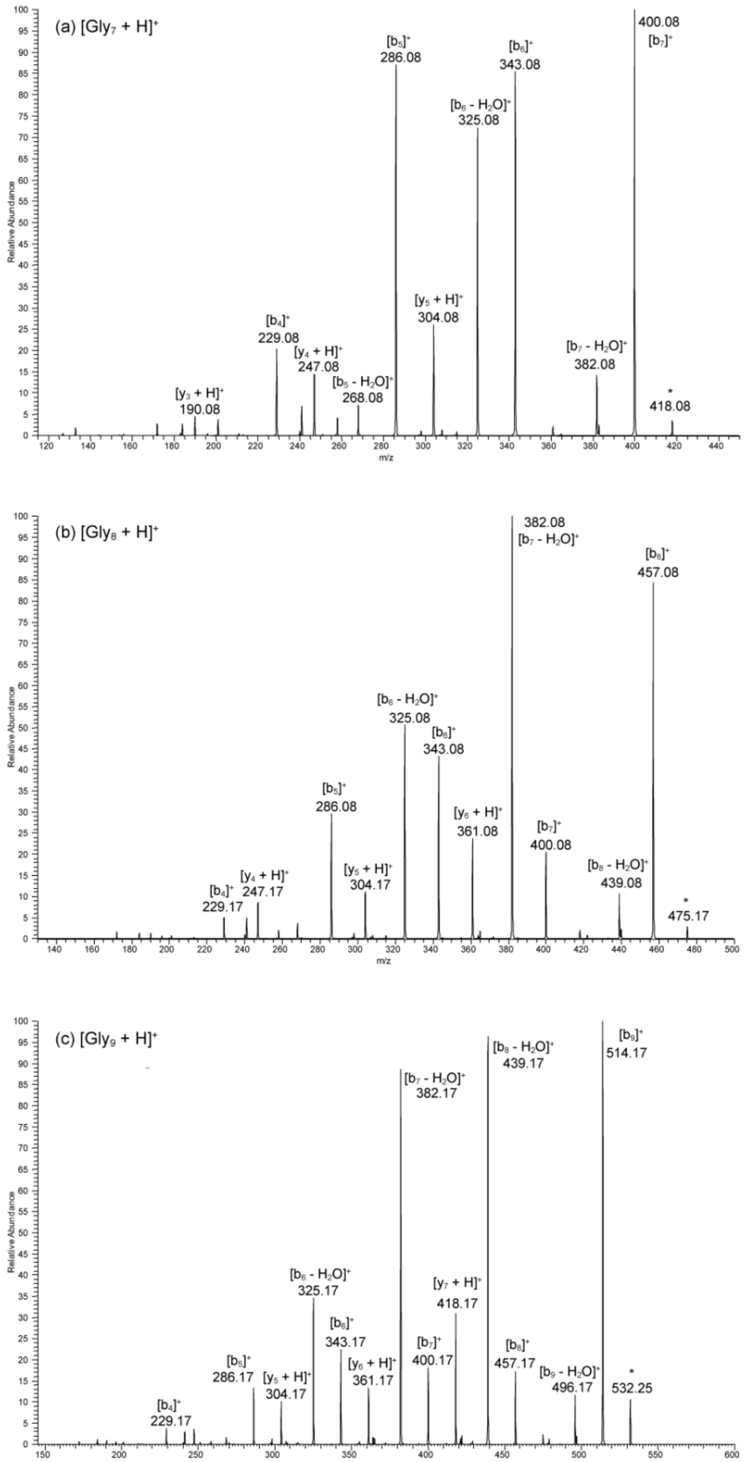

Figure S24. CID spectrum of [Gly$_7$ + H – H_2O]$^+$. The precursor ion is denoted by asterisk (*)

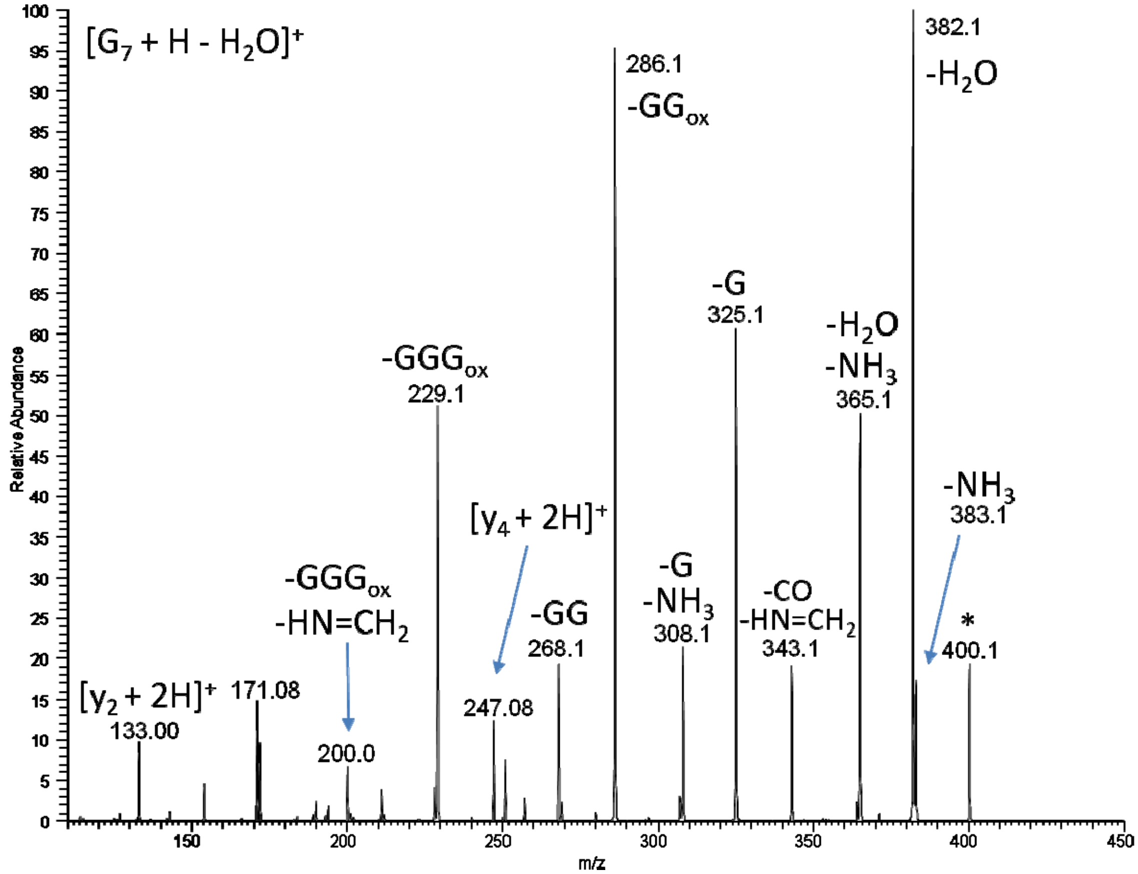

Figure S25. CID spectrum of $[Gly_8 + H – H_2O]^+$. The precursor ion is denoted by asterisk (*)

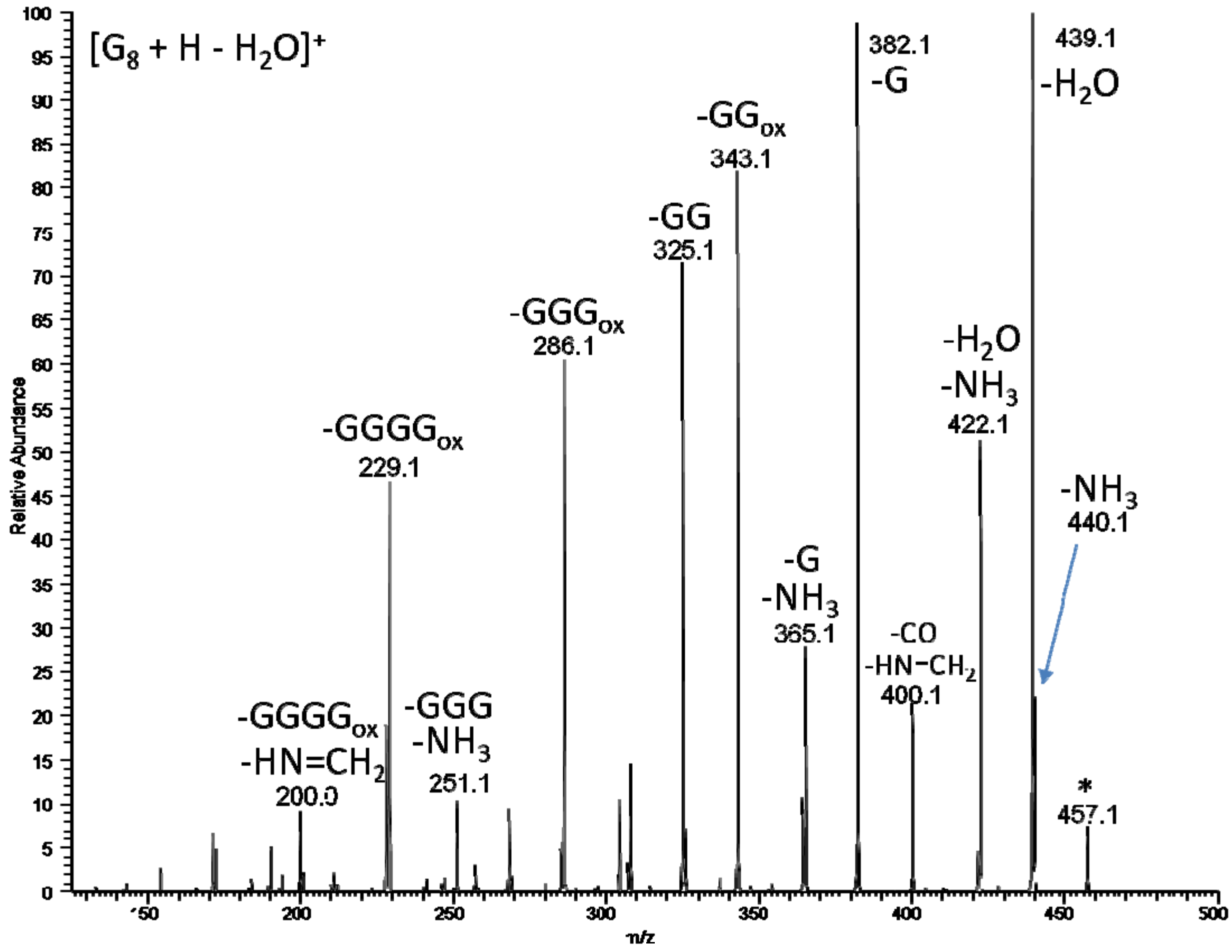

Figure S26. CID spectrum of $[Gly_9 + H - H_2O]^+$. The precursor ion is denoted by asterisk (*)

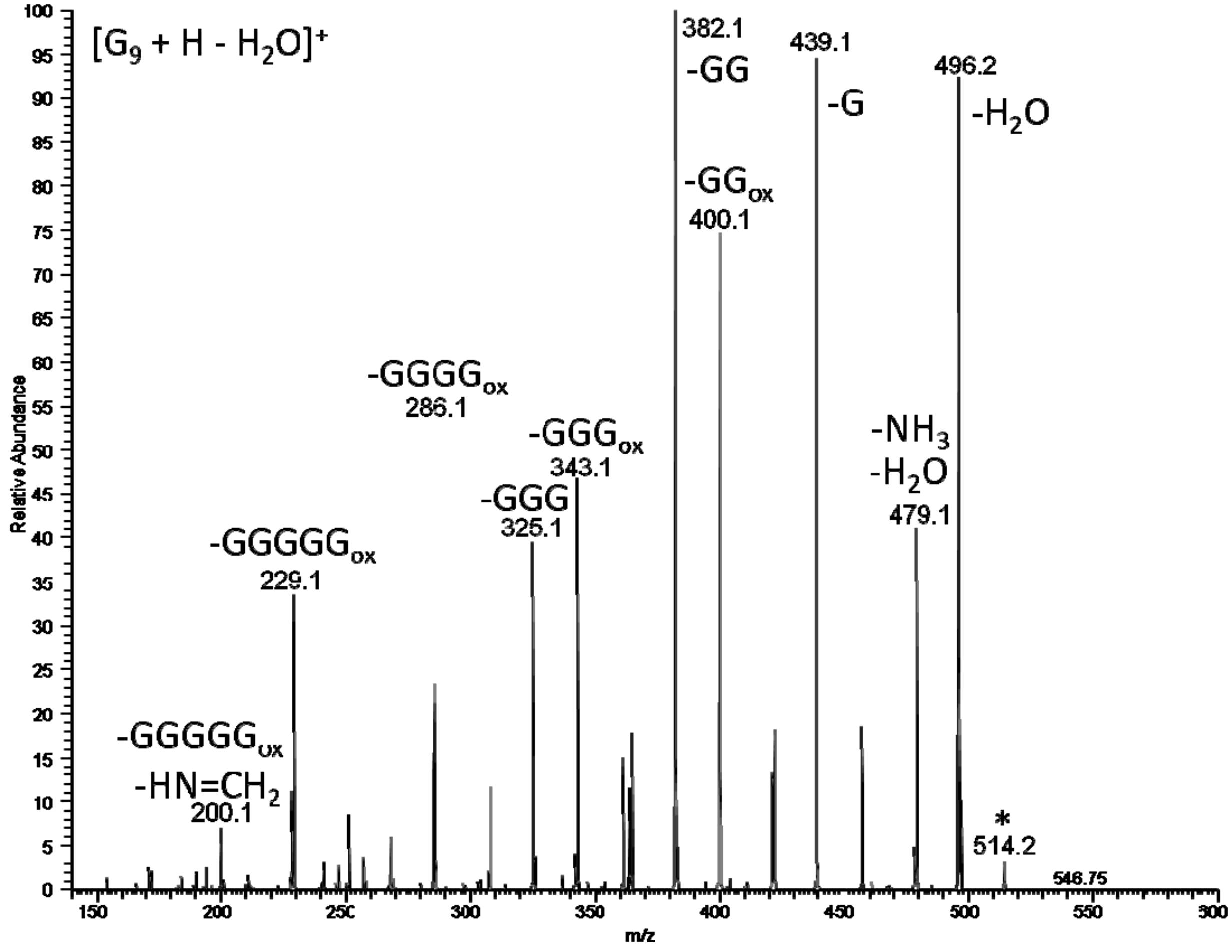

Figure S27. CID spectrum of [Gly_{10} + H – H_2O]$^+$. The precursor ion is denoted by asterisk (*)

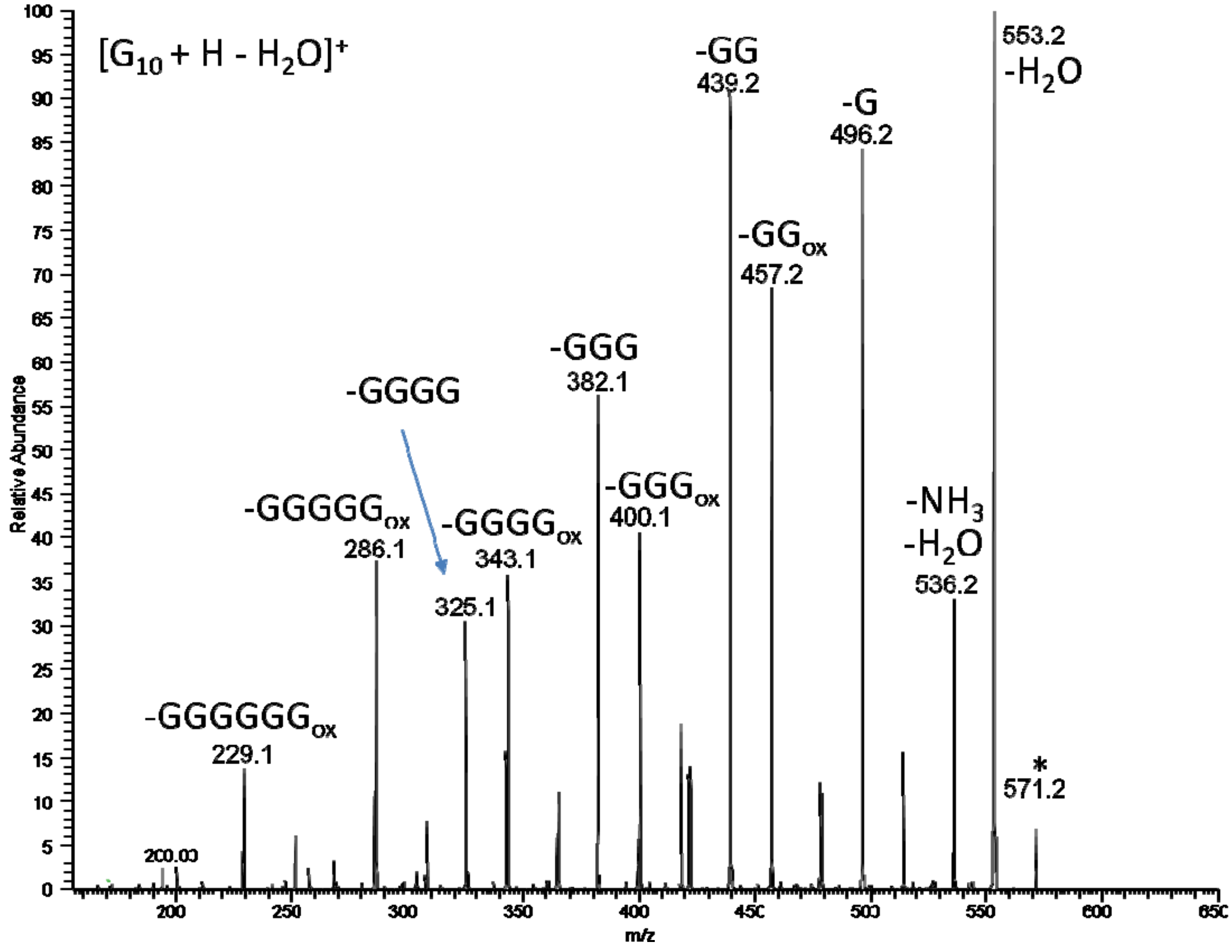

Figure S28. CID spectrum of (A) [AGGG + H]+, (B) [GAGG + H]$^+$, (C) [GGAG + H]$^+$, and (D) [P(^{18}O)GGG + H]$^+$. The precursor ion is denoted by asterisk (*)