

Supporting material

UV Photo-dissociation of proline-containing peptide ions. Insights from molecular dynamics

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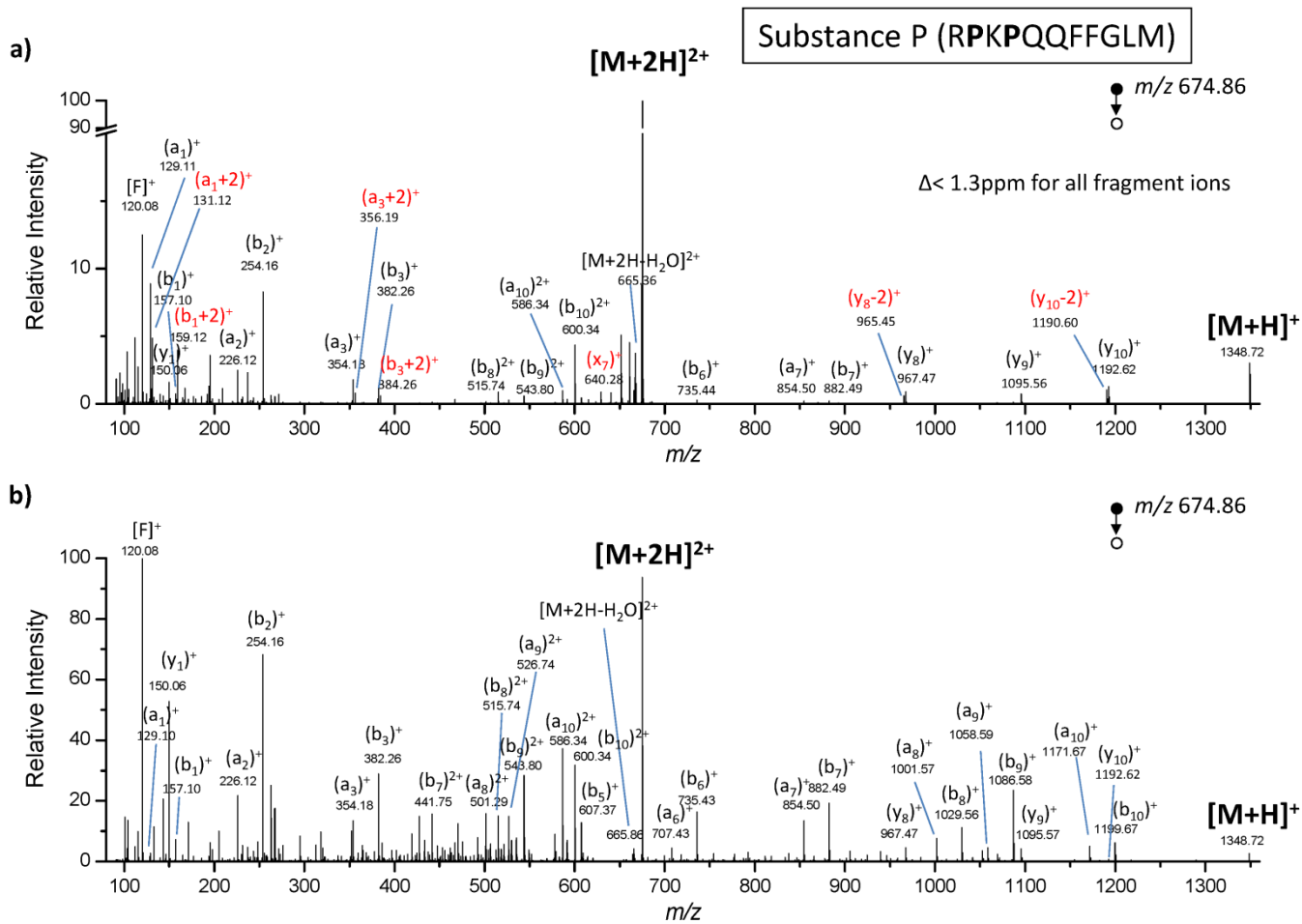


Figure S1: a) LID spectrum of doubly protonated Substance P $[M+2H]^{2+}$ ion (m/z 674.86) at 213 nm for 1000 ms (Collision energy 2 eV). b) CID spectrum of doubly protonated Substance P $[M+2H]^{2+}$ ion (m/z 674.86) under a normalized CID collision energy of 25 % for 3 ms.

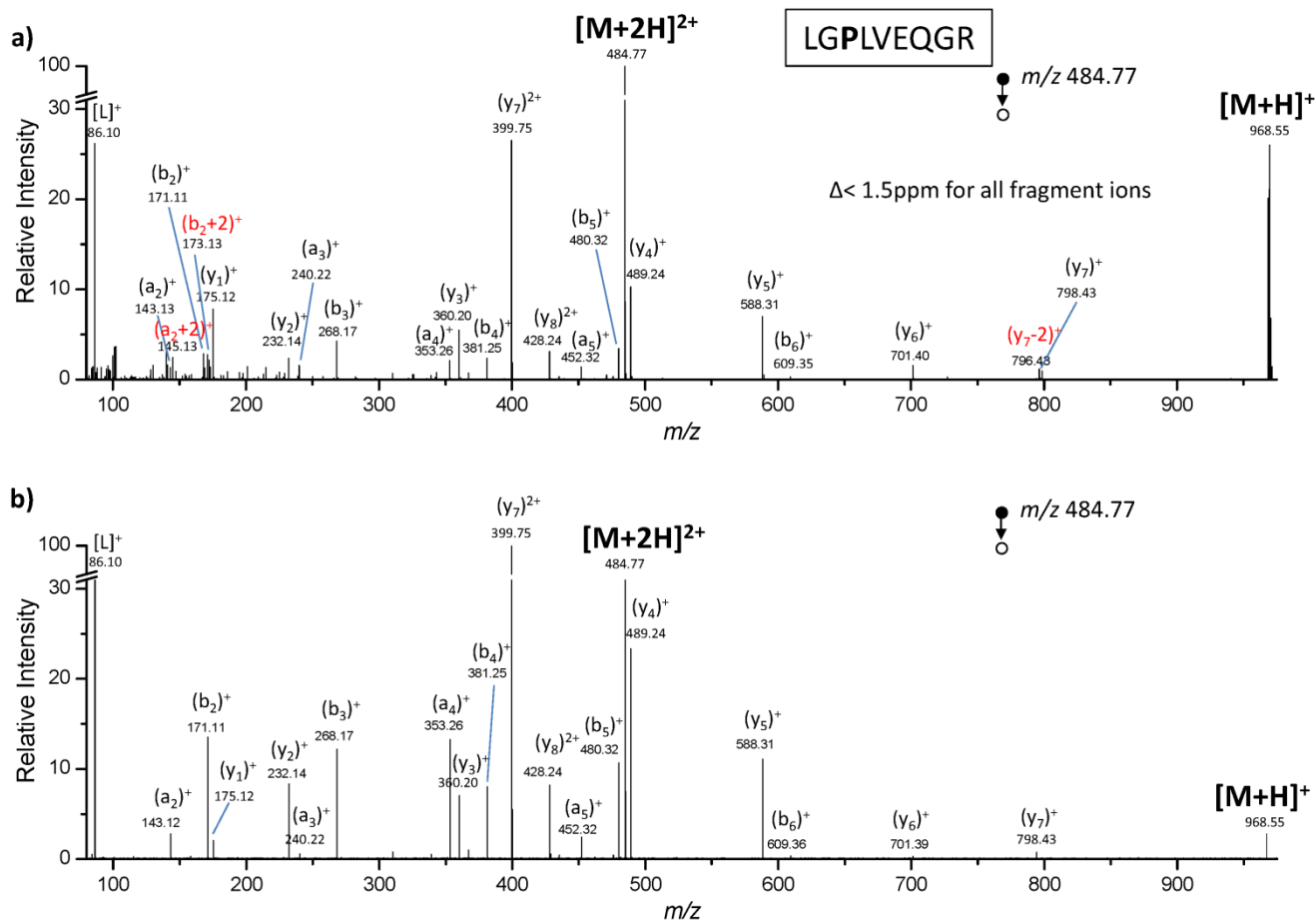


Figure S2: a) LID spectrum of doubly protonated LGPLVEQGR $[M+2H]^{2+}$ ion (m/z 484.77) at 213 nm for 1000 ms (Collision energy 2 eV). b) CID spectrum of doubly protonated LGPLVEQGR $[M+2H]^{2+}$ ion (m/z 484.77) under a normalized CID collision energy of 25 % for 3 ms.

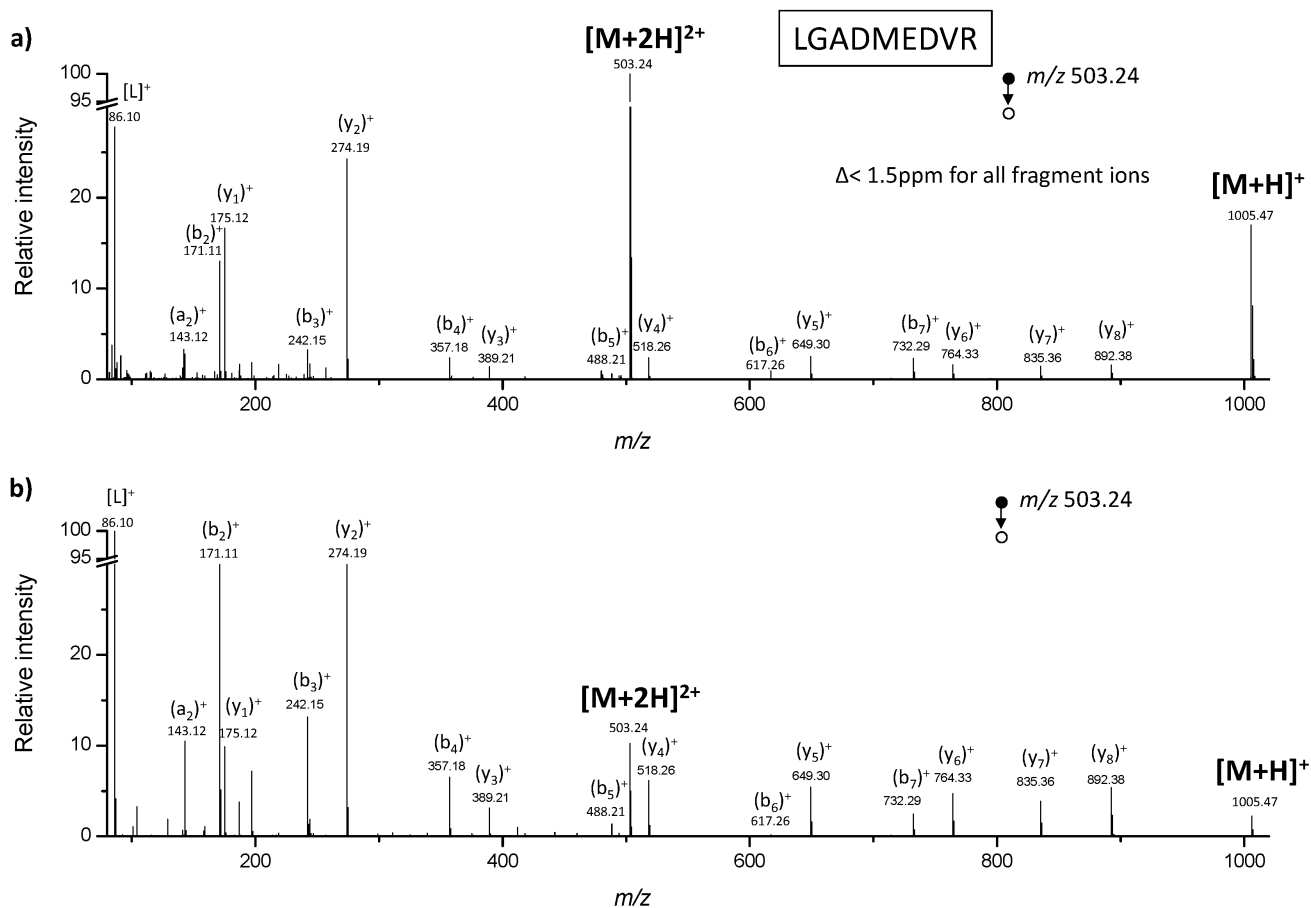


Figure S3: a) LID spectrum of doubly protonated LGADMEDVR $[M+2H]^{2+}$ ion (m/z 503.24) at 213 nm for 1000 ms (Collision energy 2 eV). b) CID spectrum of doubly protonated LGADMEDVR $[M+2H]^{2+}$ ion (m/z 503.24) under a normalized CID collision energy of 25 % for 3 ms.

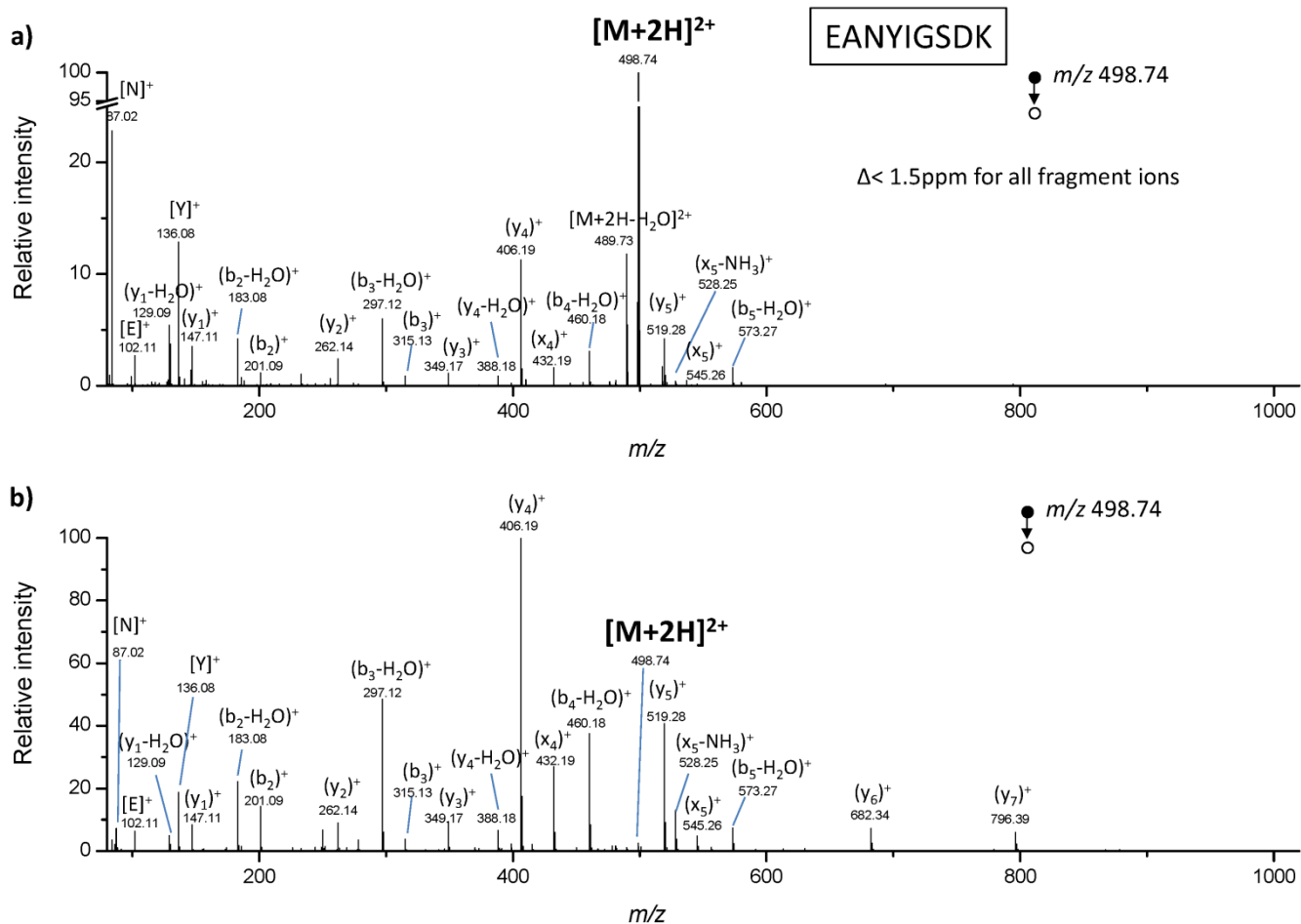


Figure S4: a) LID spectrum of doubly protonated EANYIGSDK $[M+2H]^{2+}$ ion (m/z 498.74) at 213 nm for 1000 ms (Collision energy 2 eV). b) CID spectrum of doubly protonated EANYIGSDK $[M+2H]^{2+}$ ion (m/z 498.74) under a normalized CID collision energy of 25 % for 3 ms.