

Supporting Data for

Side Chain Chemistry Mediates Backbone Fragmentation
in Hydrogen Deficient Peptide Radicals

Table of Contents

Supplementary Figures

Figure S1a: CID of [RYLGYL+H] ⁺	S2
S1b: CID of [RRPWIL+H] ⁺	S2
S1c: CID of [[RRPWIL+2H] ⁺²	S2
Figure S2a: CID of [RPPGFSPFR+2H] ⁺²	S3
S2b: CID of [DRVYIHPF+2H] ⁺²	S3
S2c: PD/CID of [DRVYIHPF•-44+2H] ⁺²	S3
Figure S3a: PD/CID of [MEHFRWG•+H] ⁺	S4
S3b: CID of [MEHFRWG+H] ⁺	S4
S3c: CID of [MEHFRWG+2H] ⁺²	S4
Figure S4a: CID of [KKPYIL+H] ⁺	S5
S4b: CID of [KKPYIL+2H] ⁺²	S5
Figure S5a: PD/CID of [RPPGFSPFR+2H] ⁺²	S6
S5b: Mechanism of backbone fragmentation at Ser/Thr...	S6
Figure S6. Scheme of the isodesmic reaction used for all βC-H BDE calculations.....	S7

Figure S1

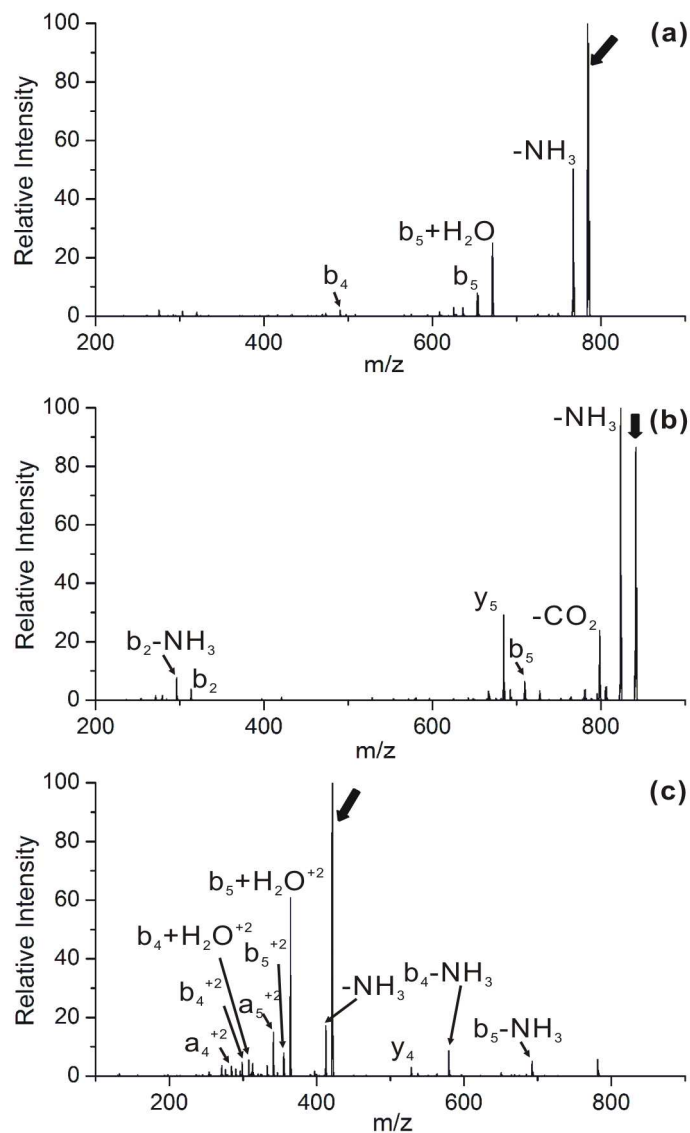


Figure S1a: CID of $[[\text{RYLGYL}+\text{H}]^+]$
S1b: CID of $[[\text{RRPWIL}+\text{H}]^+]$
S1c: CID of $[[\text{RRPWIL}+2\text{H}]^{+2}]$

Figure S2

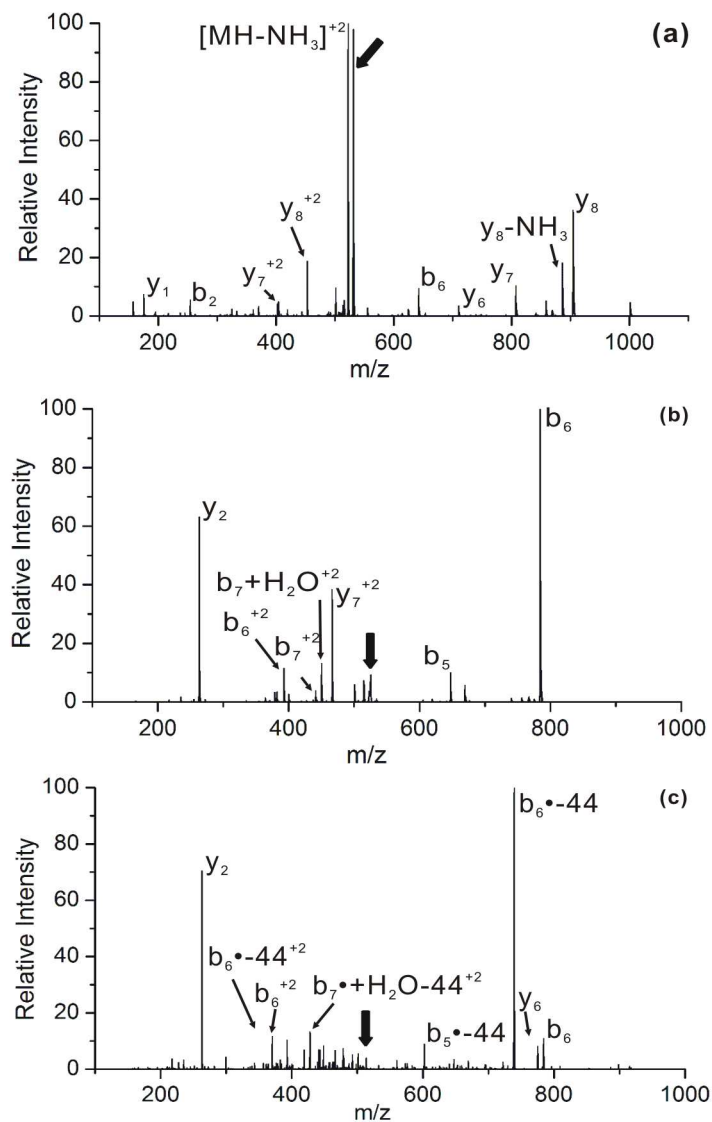


Figure S2a: CID of $[RPPGFSPFR+2H]^{+2}$

S2b: CID of $[DRVYIHPF+2H]^{+2}$

S2c: PD/CID of $[DRVYIHPF\bullet-44+2H]^{+2}$

Figure S3

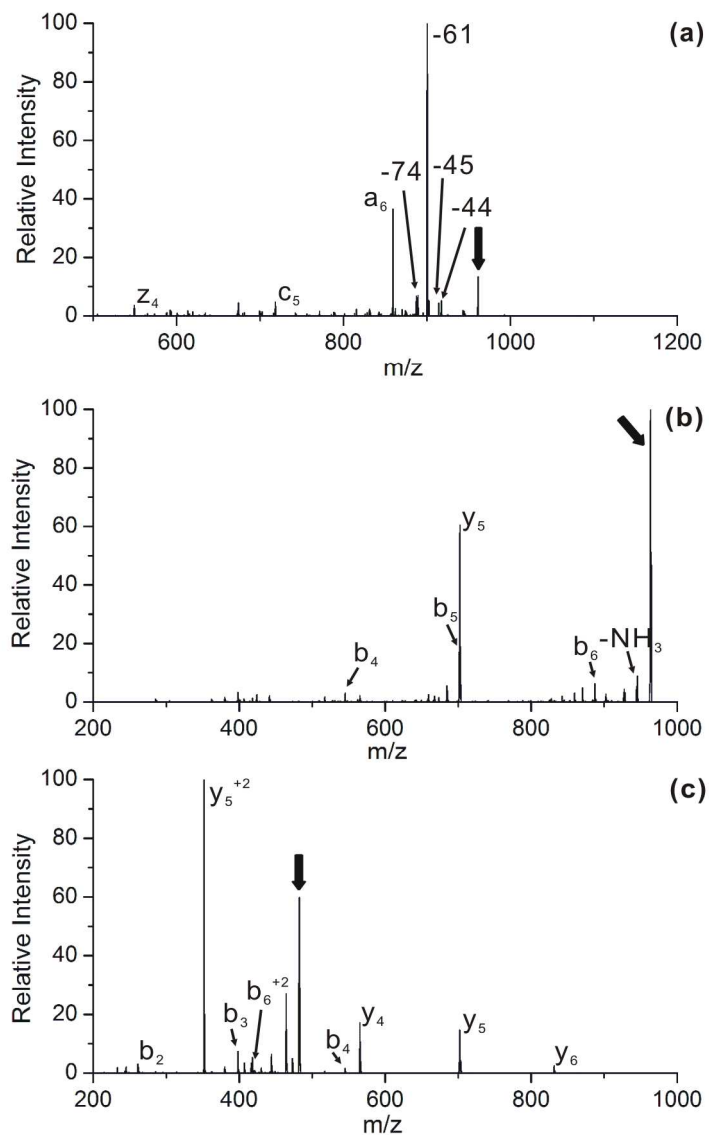


Figure S3a: PD/CID of $[\text{MEHFRWG}\bullet+\text{H}]^+$

S3b: CID of $[\text{MEHFRWG}+\text{H}]^+$

S3c: CID of $[\text{MEHFRWG}+2\text{H}]^{+2}$

Figure S4

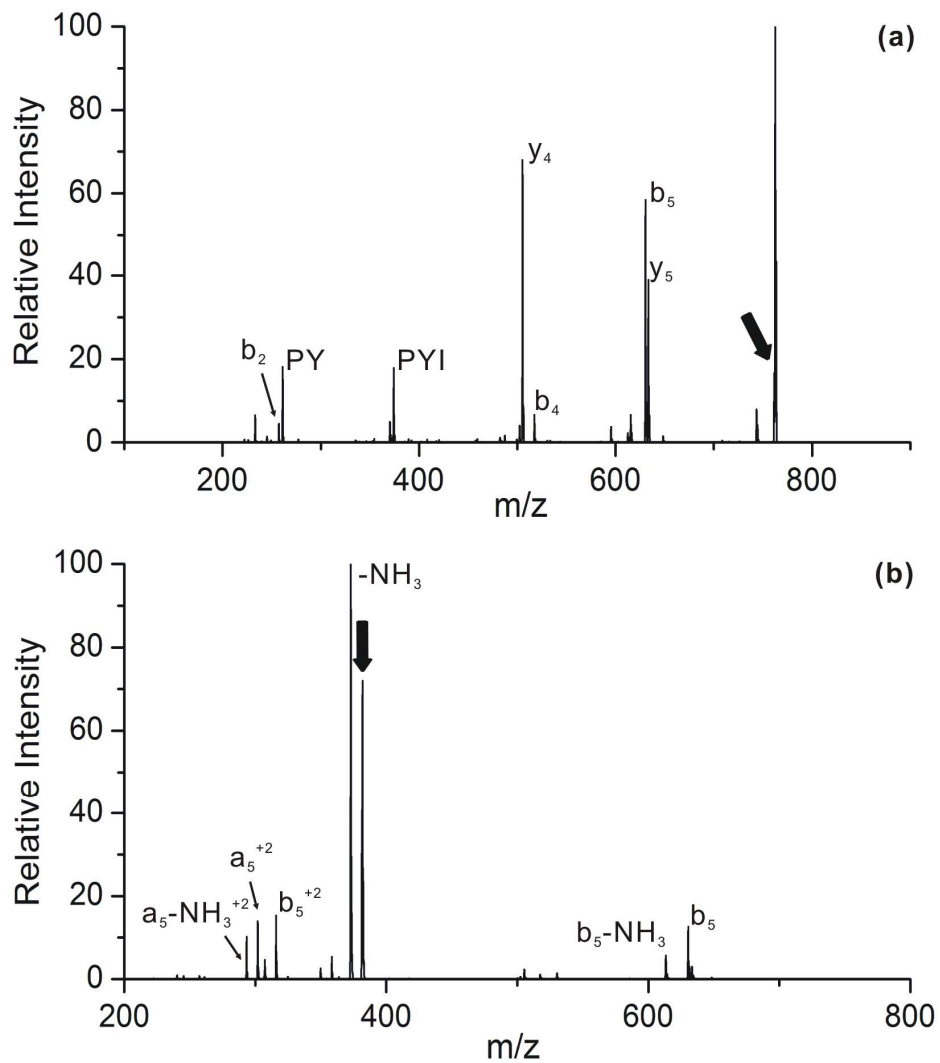


Figure S4a: CID of $[KKPYIL+H]^+$
S4b: CID of $[KKPYIL+2H]^{+2}$

Figure S5

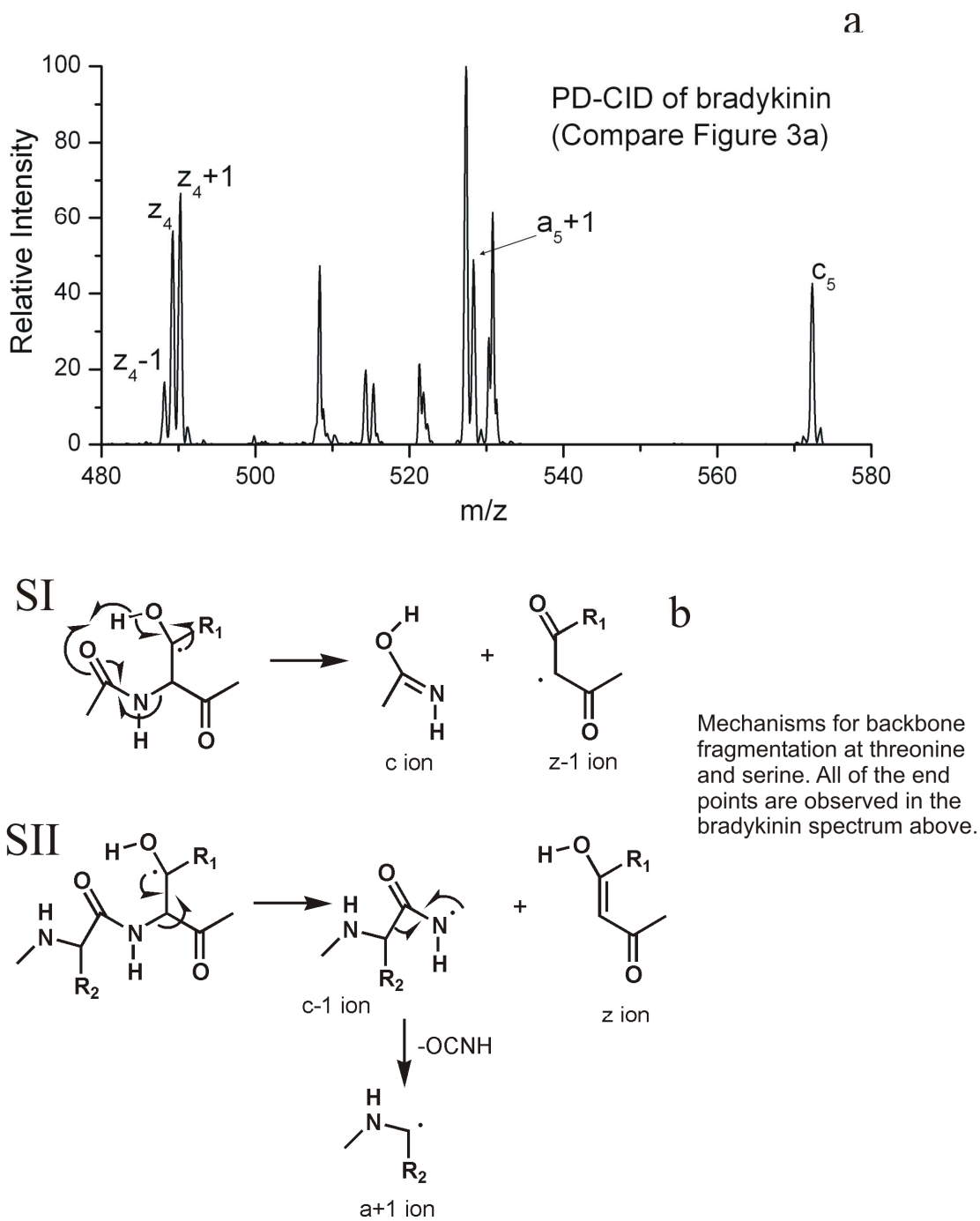


Figure S5a: PD CID of bradykinin
S5b: Mechanism

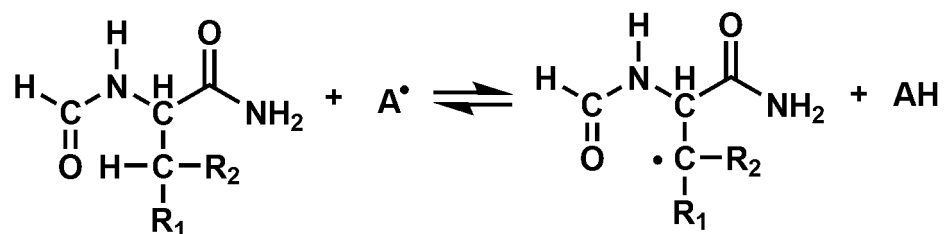
Figure S6

Fig S6. Scheme of the isodesmic reaction used for all β C-H BDE calculations