Supplementary Information

Supramolecular tryptophan-zipper form a tripeptide as regular proton transporter

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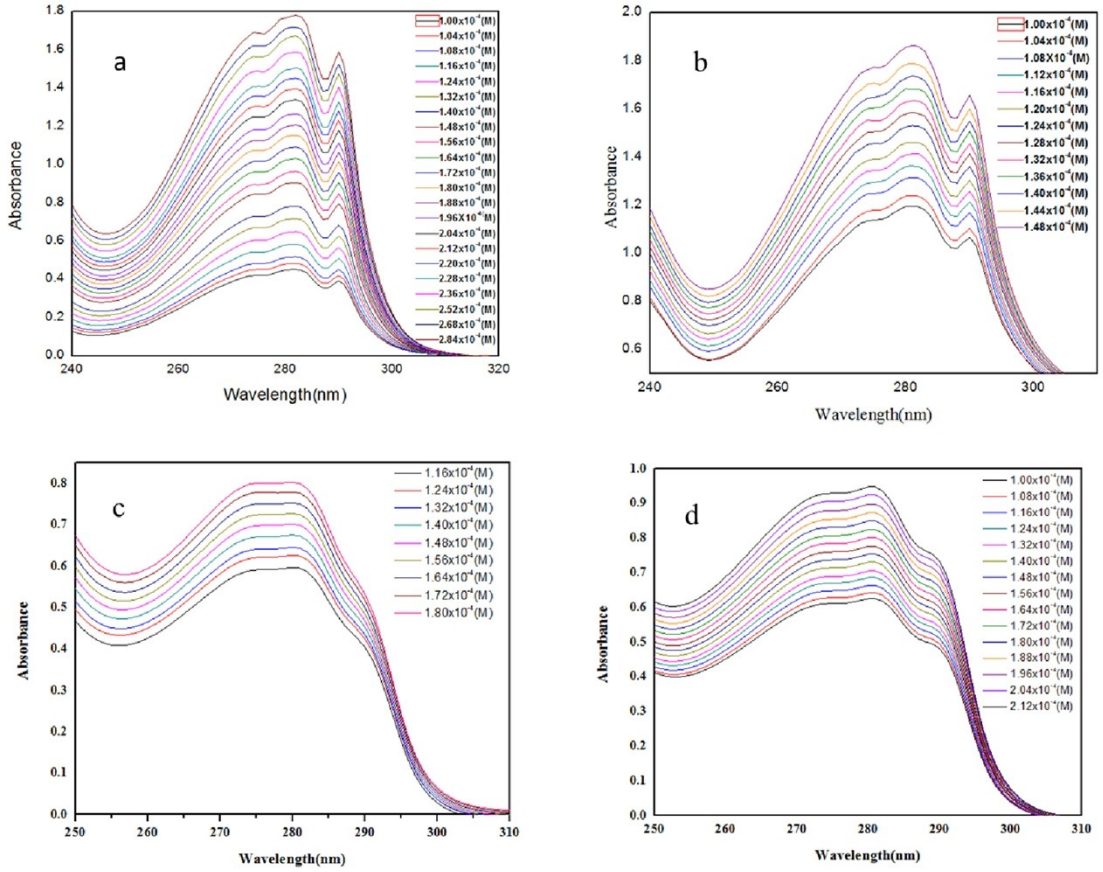
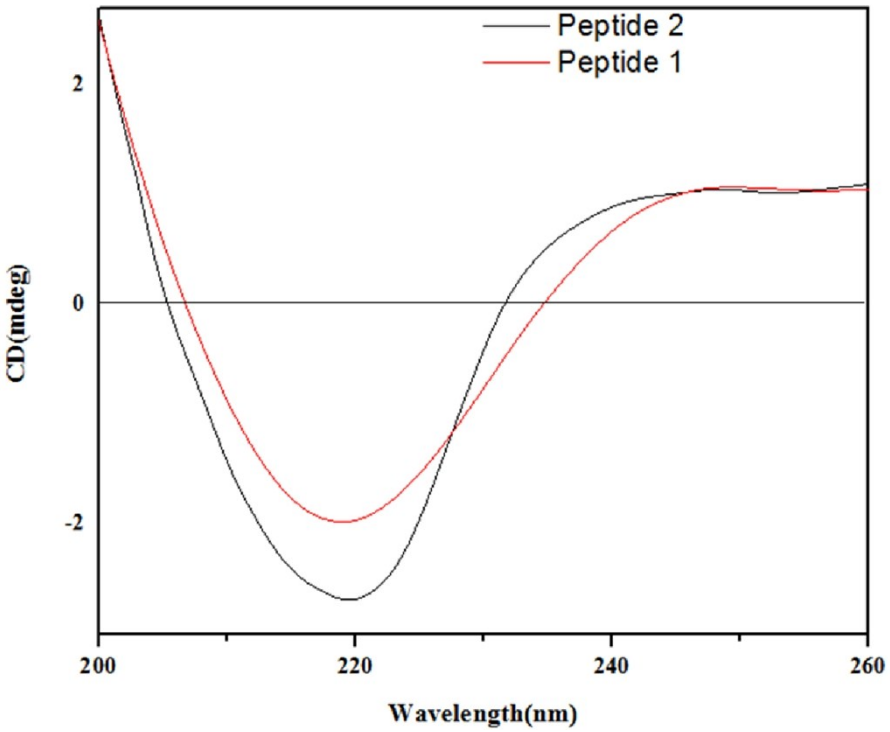
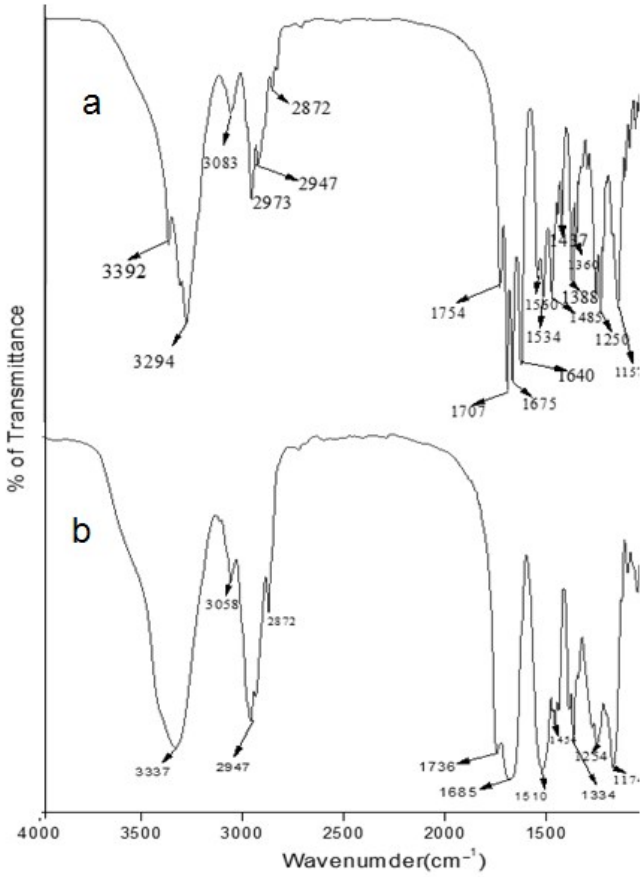


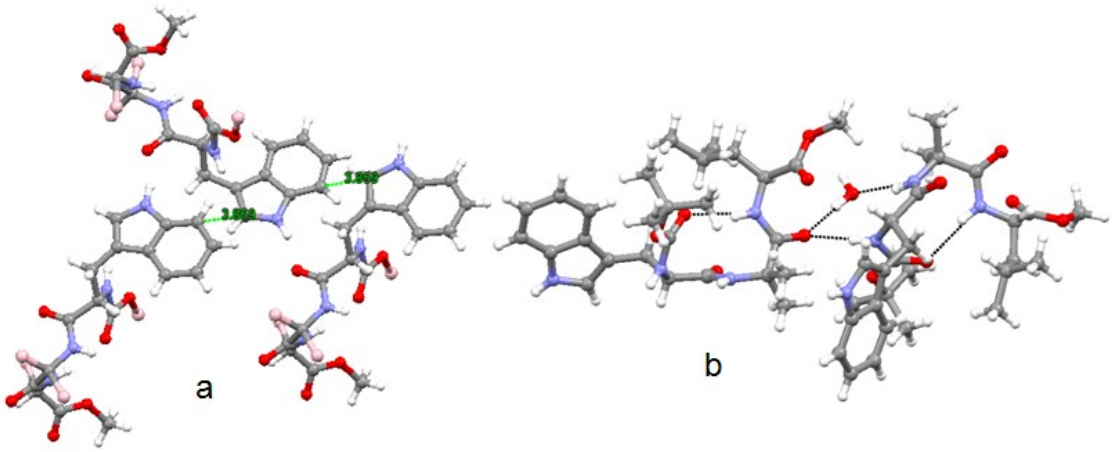
ESI Figure 1. UV-Vis absorption spectra of (a) peptide **1** in methanol (b) peptide **2** in methanol (c) peptide **1** in chloroform and (d) peptide **2** in chloroform.



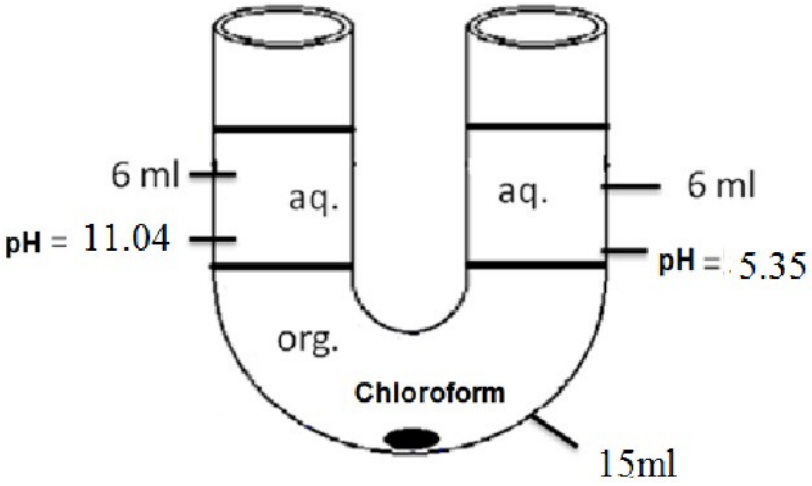
ESI Figure 2. The CD spectra of tripeptides **1** and **2** in methanol.



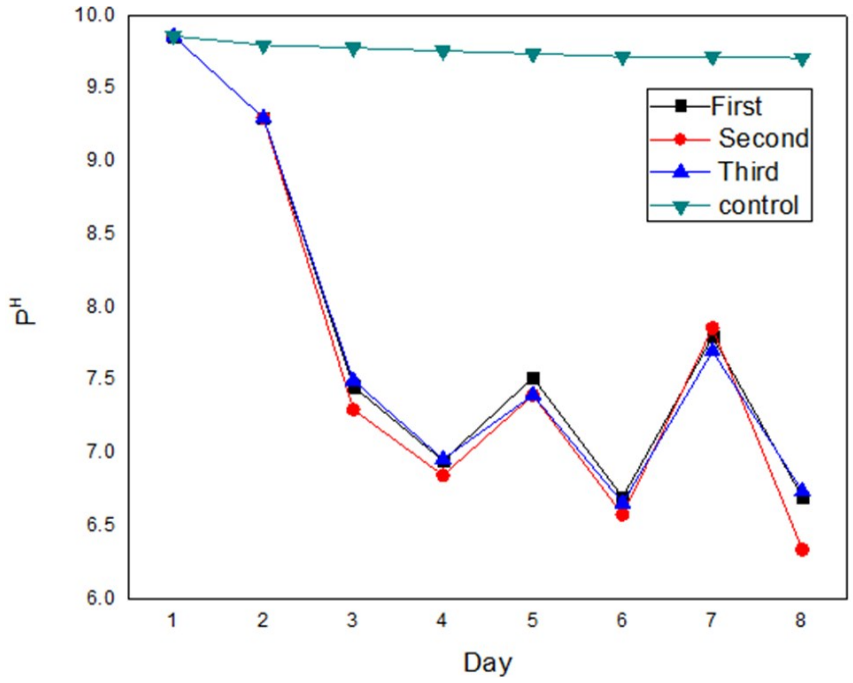
ESI Figure 3. The solid state FT-IR spectra of (a) Peptide **1** and (b) Peptide **2**.



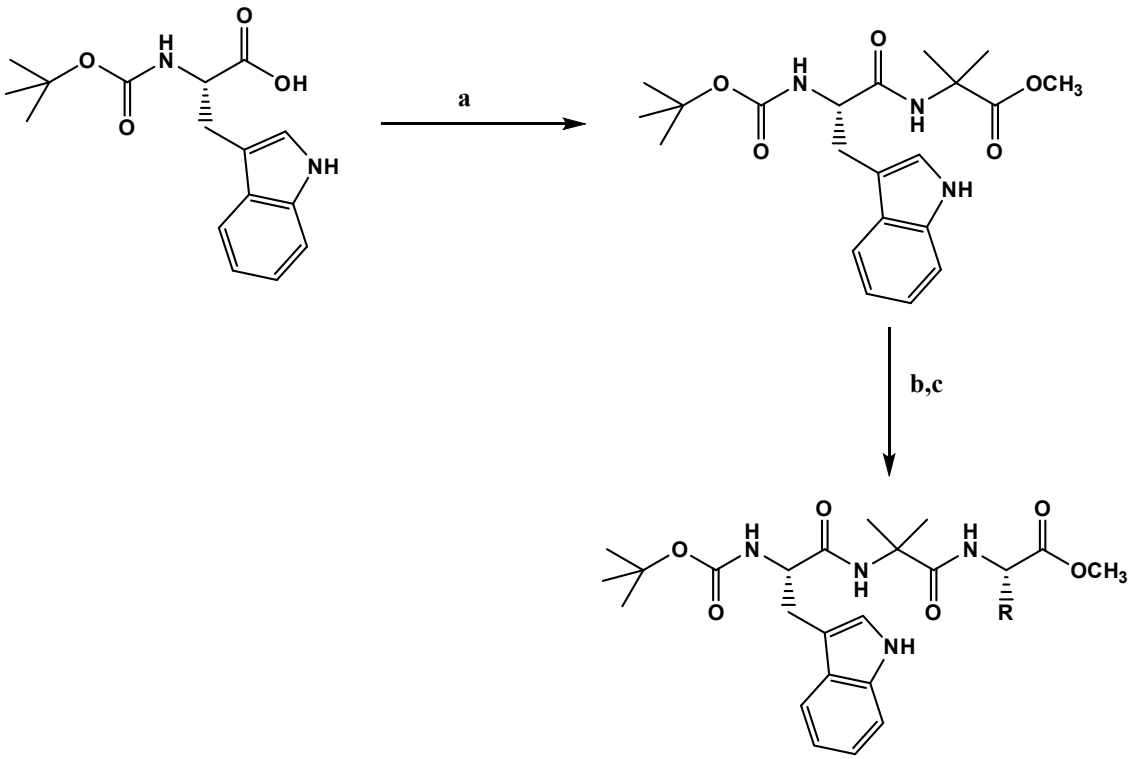
ESI Figure 4. The self-assembly of (a) tripeptide **1** through π-π interactions and (b) tripeptide **2** through intermolecular hydrogen bonding interactions.



ESI Figure 5. U-tube experiment setup for the determination of proton transport rates under pH gradients.



ESI Figure 6. The proton transport ability of the tripeptide **2** measured in U-tube experiment using pH gradient as the driving force.



Scheme1. Schematic presentation of synthesis of the tripeptides. Reagents and conditions:(a) DMF, H-Aib-OMe, DCC, HOBt, 0°C, 62% yield; (b) MeOH, 2N NaOH, 93% yield; (c) DCM, H-Val-OMe(1)/ H-Leu-OMe(2), DCC, HOBt, 0°C.

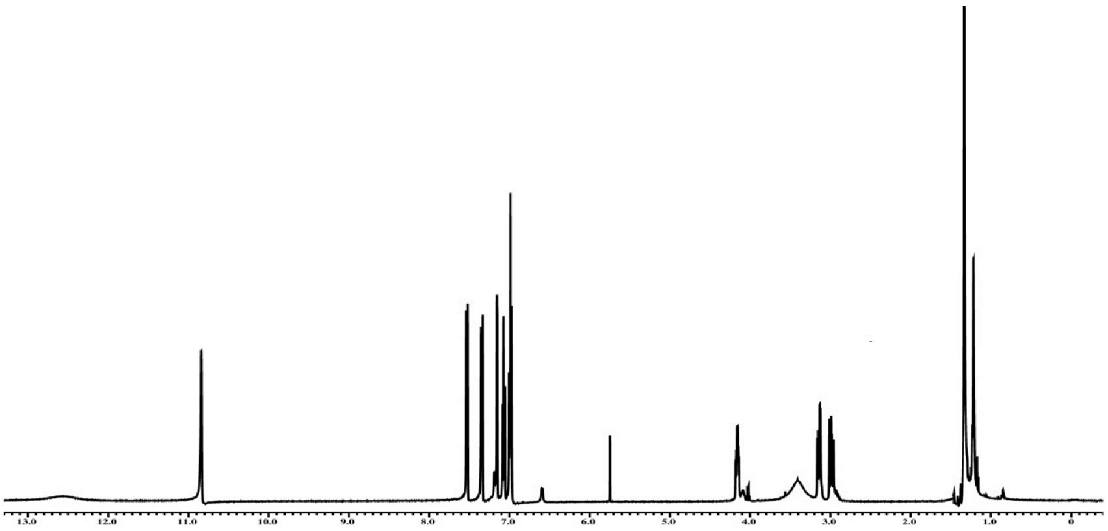


Fig S1: ^{1}H NMR (500MHz, DMSO-d_6, δ in ppm) spectra of Boc-Trp-OH.

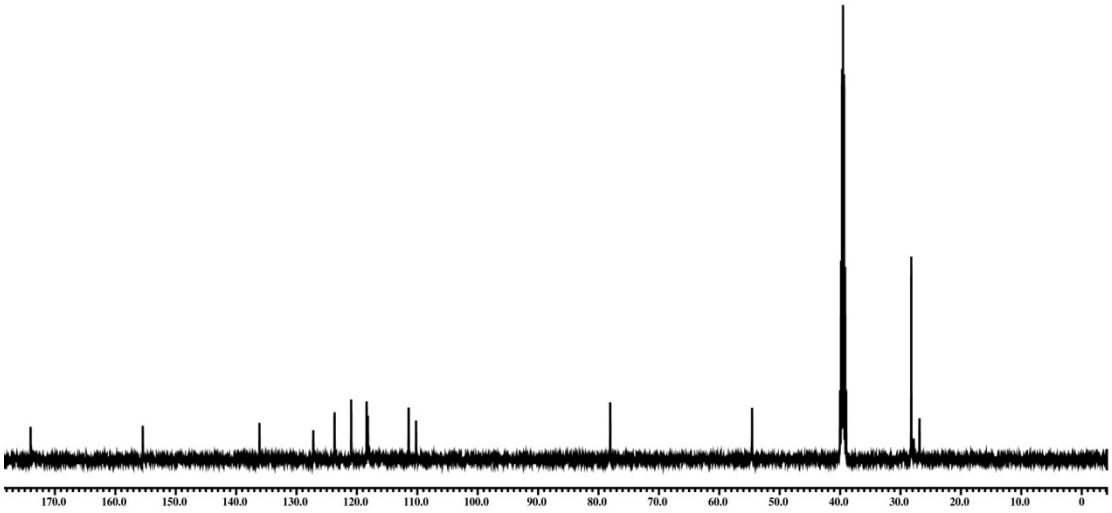


Fig S2: **^{13}C** NMR (125 MHz, DMSO-d_6, δ in ppm) spectra of Boc-Trp-OH.

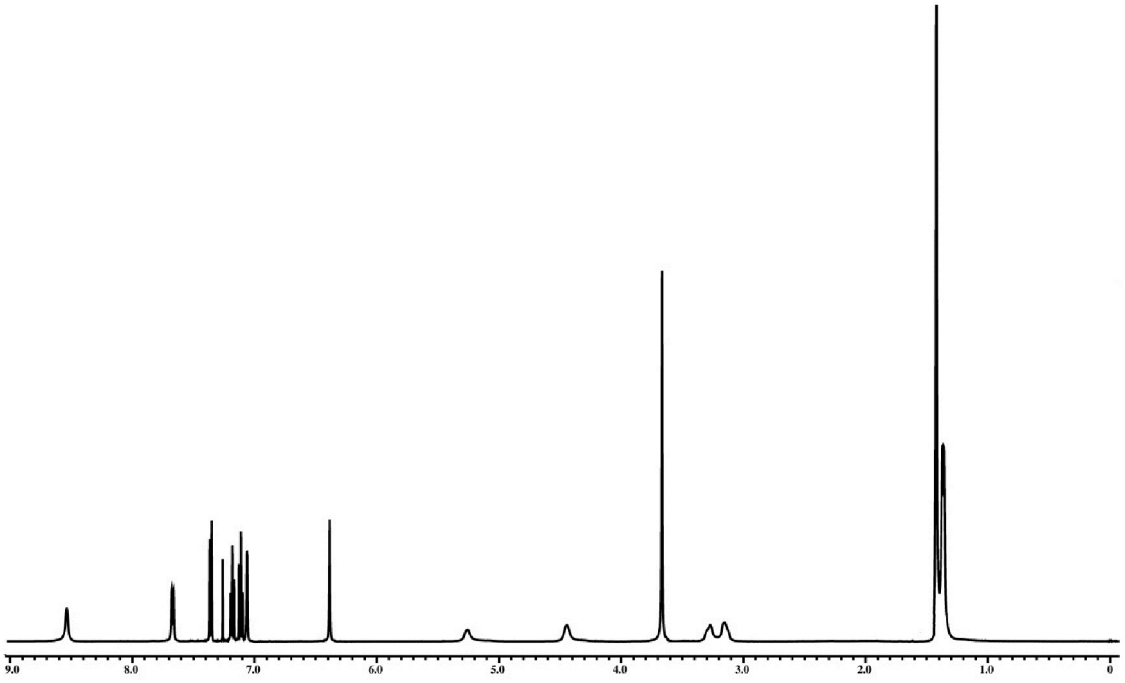


Fig S3: ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-OMe.

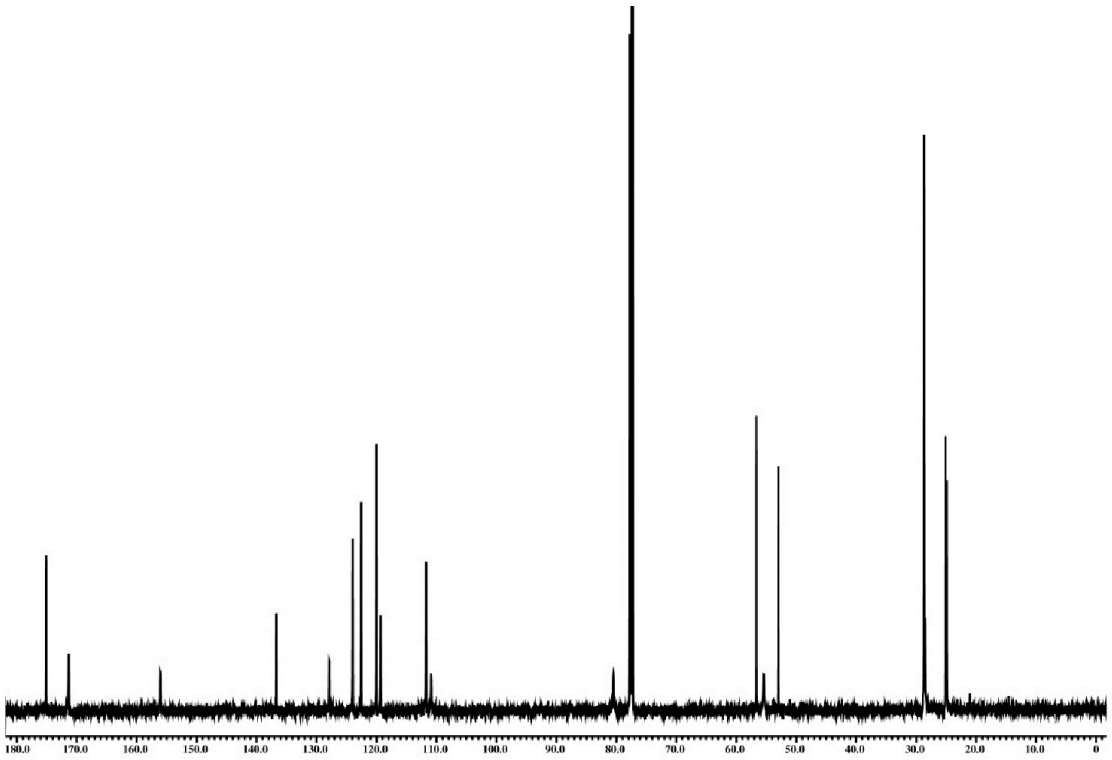


Fig S4 : ^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-OMe.

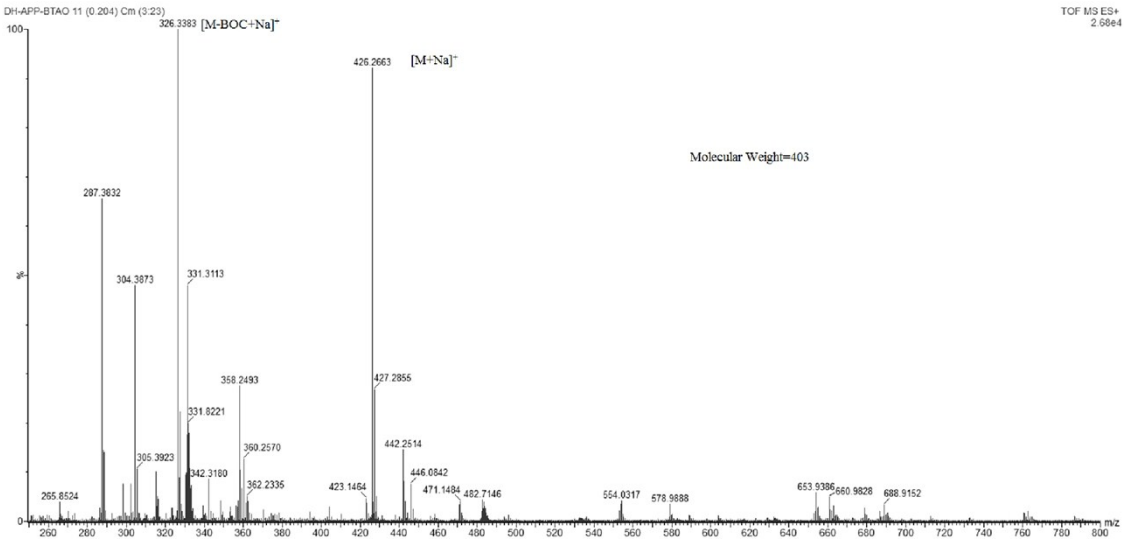


Fig S5: Mass Spectra of Boc-Trp-Aib OMe

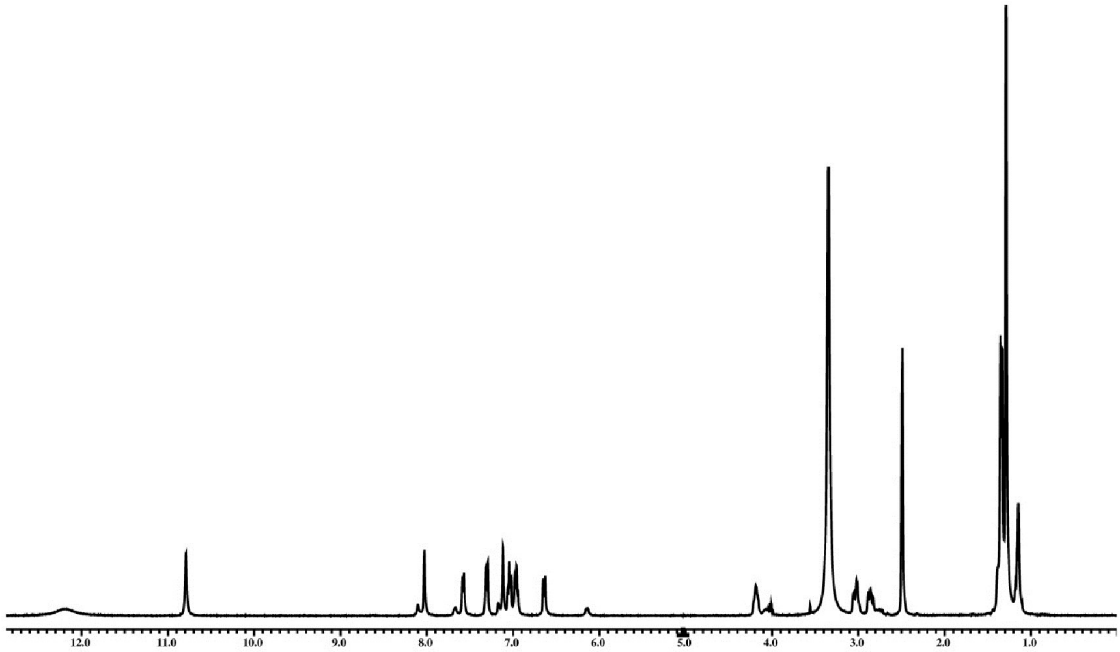


Fig S6: ^{1}H NMR (400 MHz, DMSO-d_6, δ in ppm) spectra of Boc-Trp-Aib-OH.

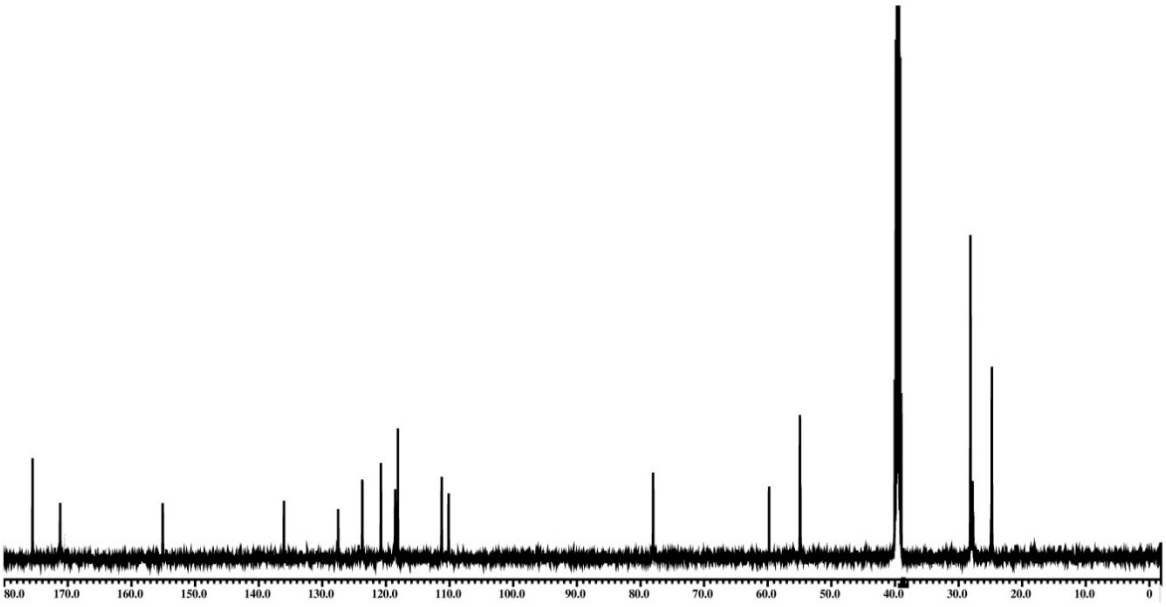


Fig S7: ^{13}C NMR (125 MHz, DMSO-d_6, δ in ppm) spectra of Boc-Trp-Aib-OH.

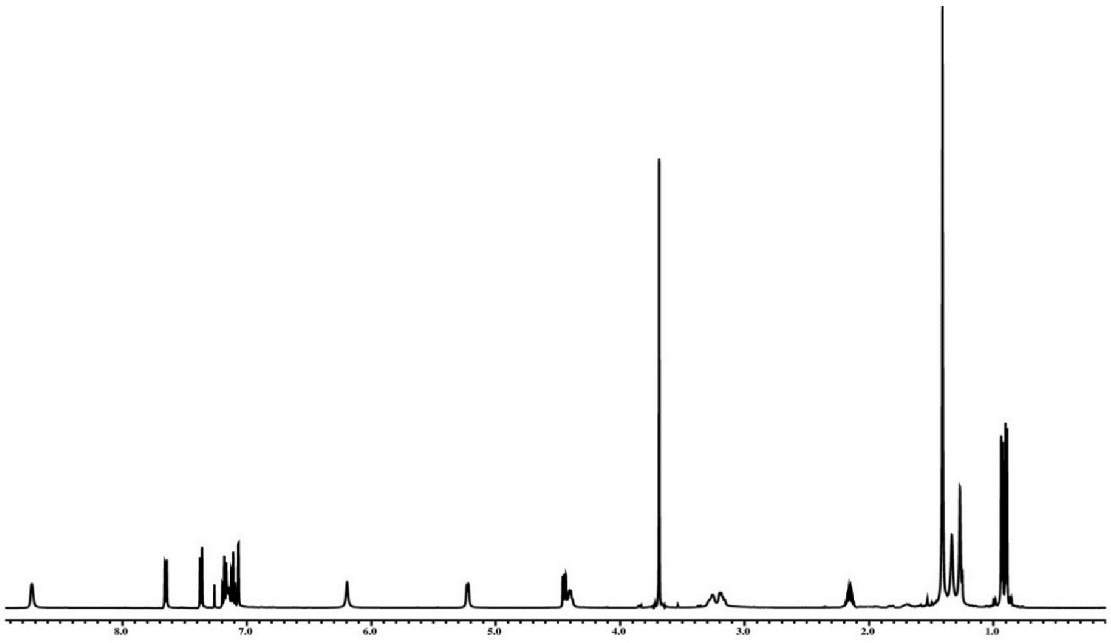


Fig S8: ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-Val-OMe 1.

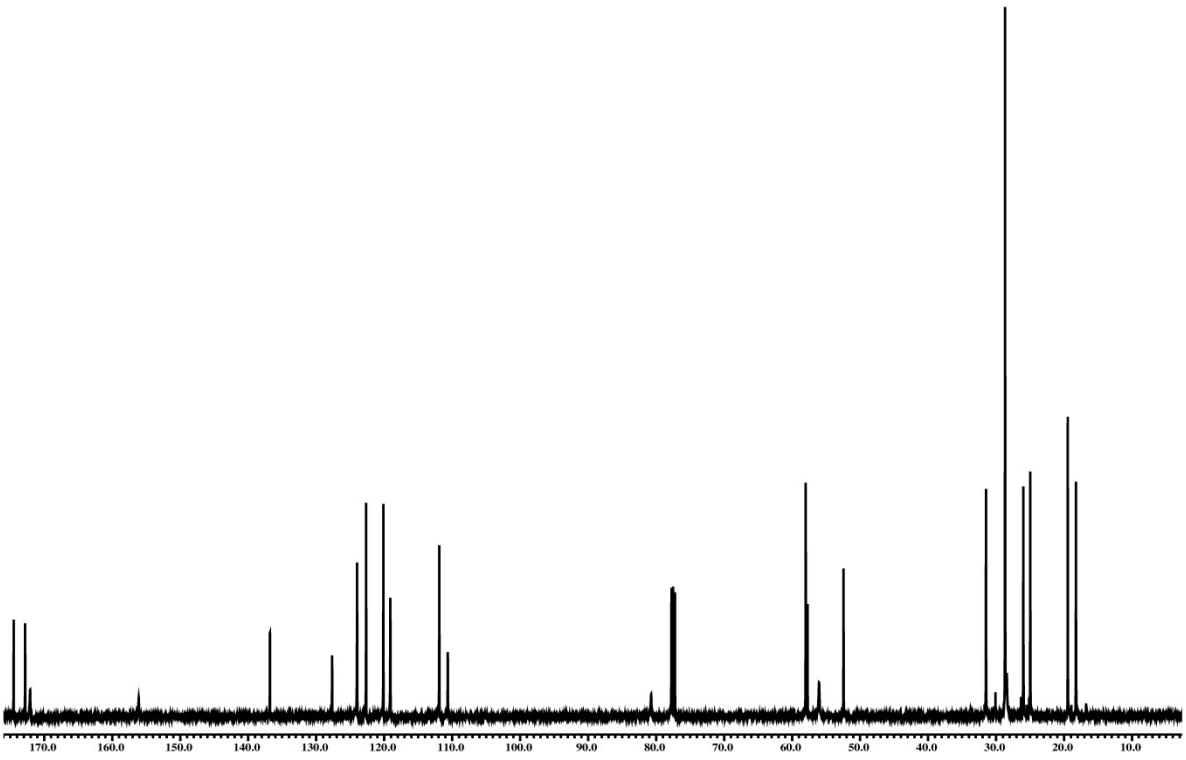


Fig S9: ^{13}CNMR (100 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-Val-OMe 1.

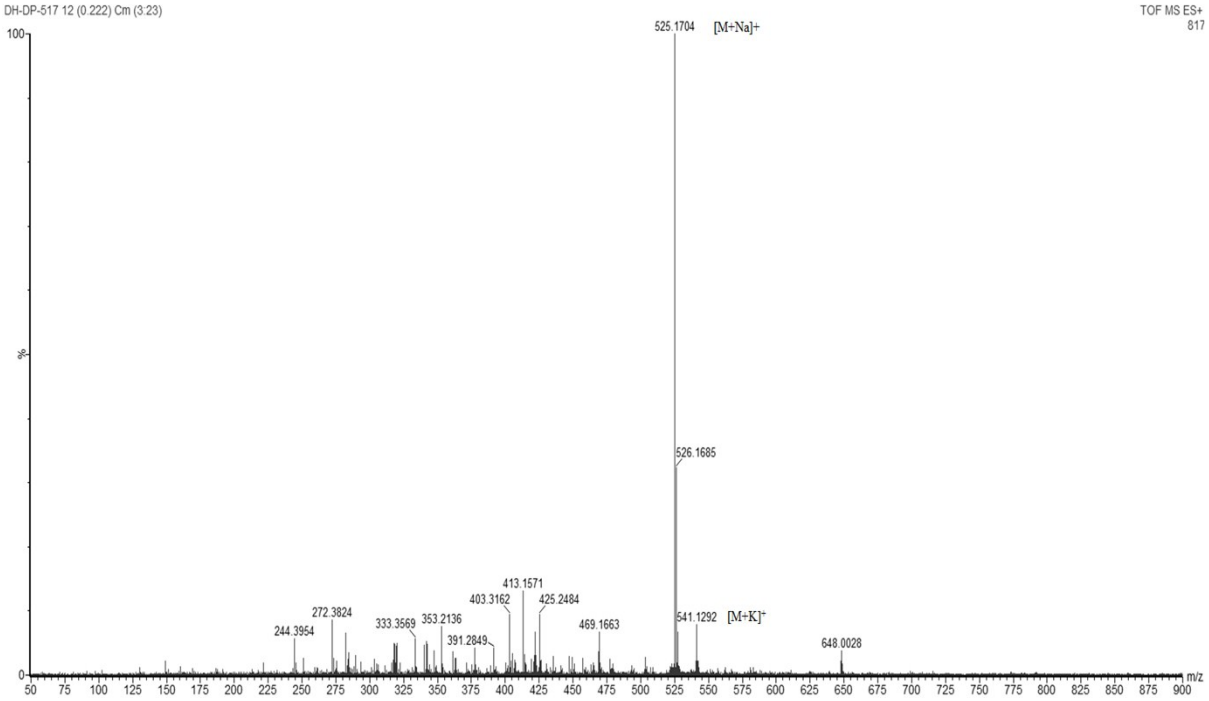


Fig S10: Mass Spectra of Boc-Trp-Aib-Val-OMe 1.

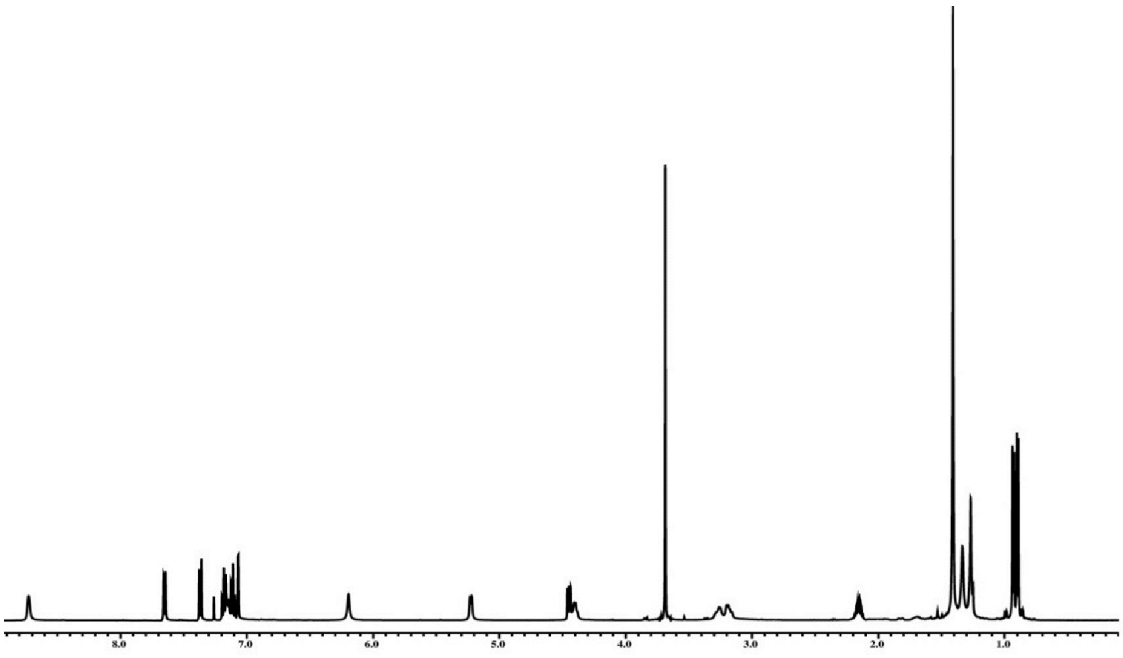


Fig S11: ^{1}H NMR (400 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-Leu-OMe 2.

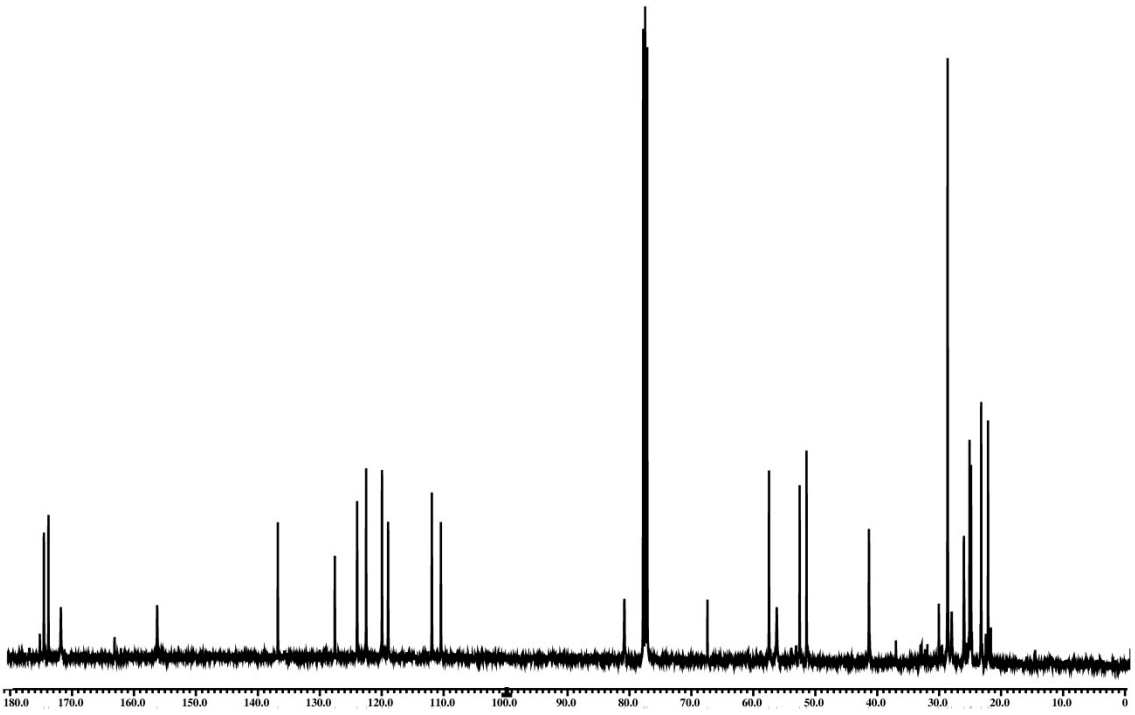


Fig S12:^{13}C NMR (100 MHz, $CDCl_3$, δ in ppm) spectra of Boc-Trp-Aib-Leu-OMe 2.

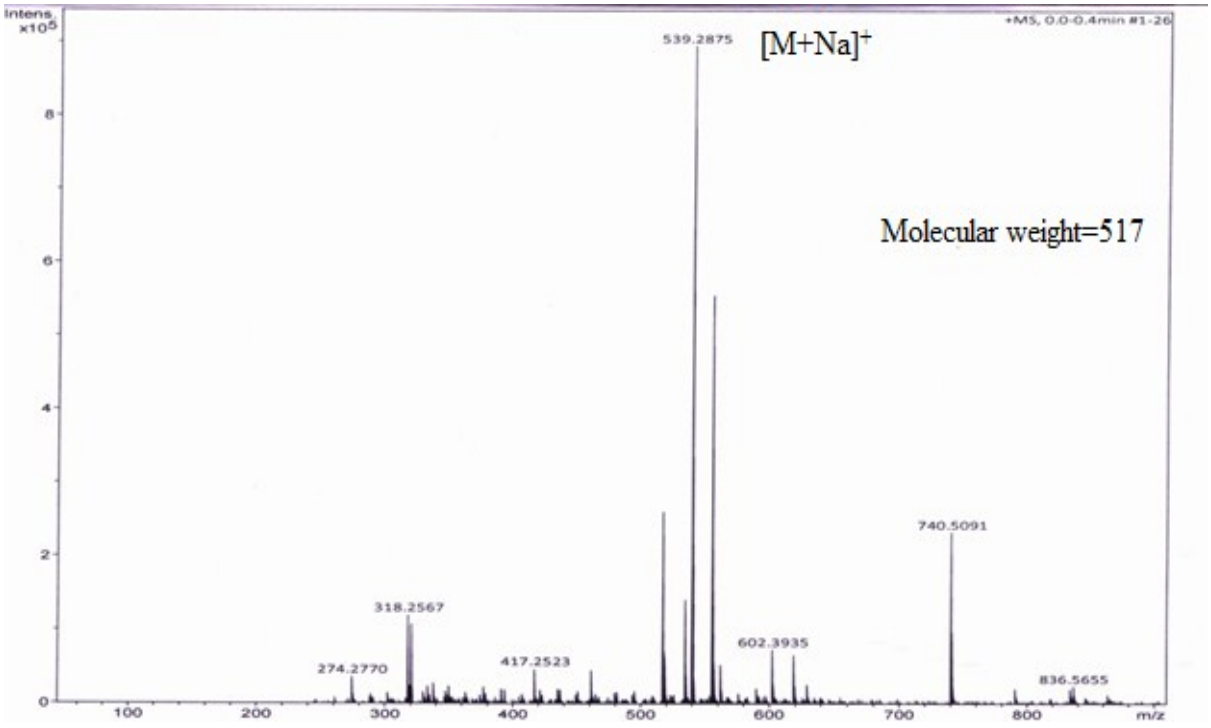


Fig S13: Mass Spectra of Boc-Trp-Aib-Leu-OMe 2.