Supplementary Material (ESI) for CrystEngComm

Electronic supplementary information (ESI)

Insights into self-assembling nanoporous peptide and in situ reducing agent

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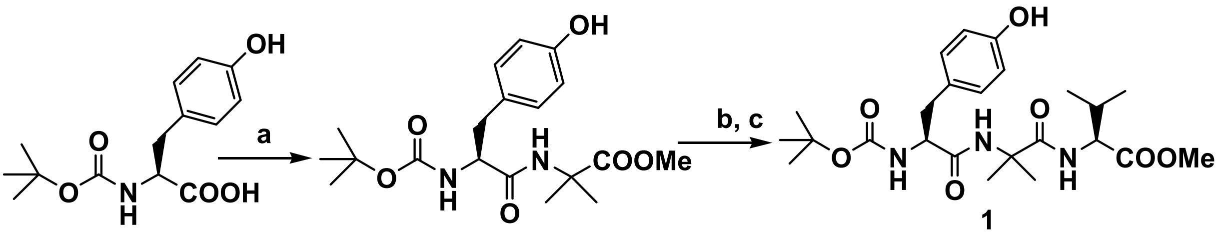
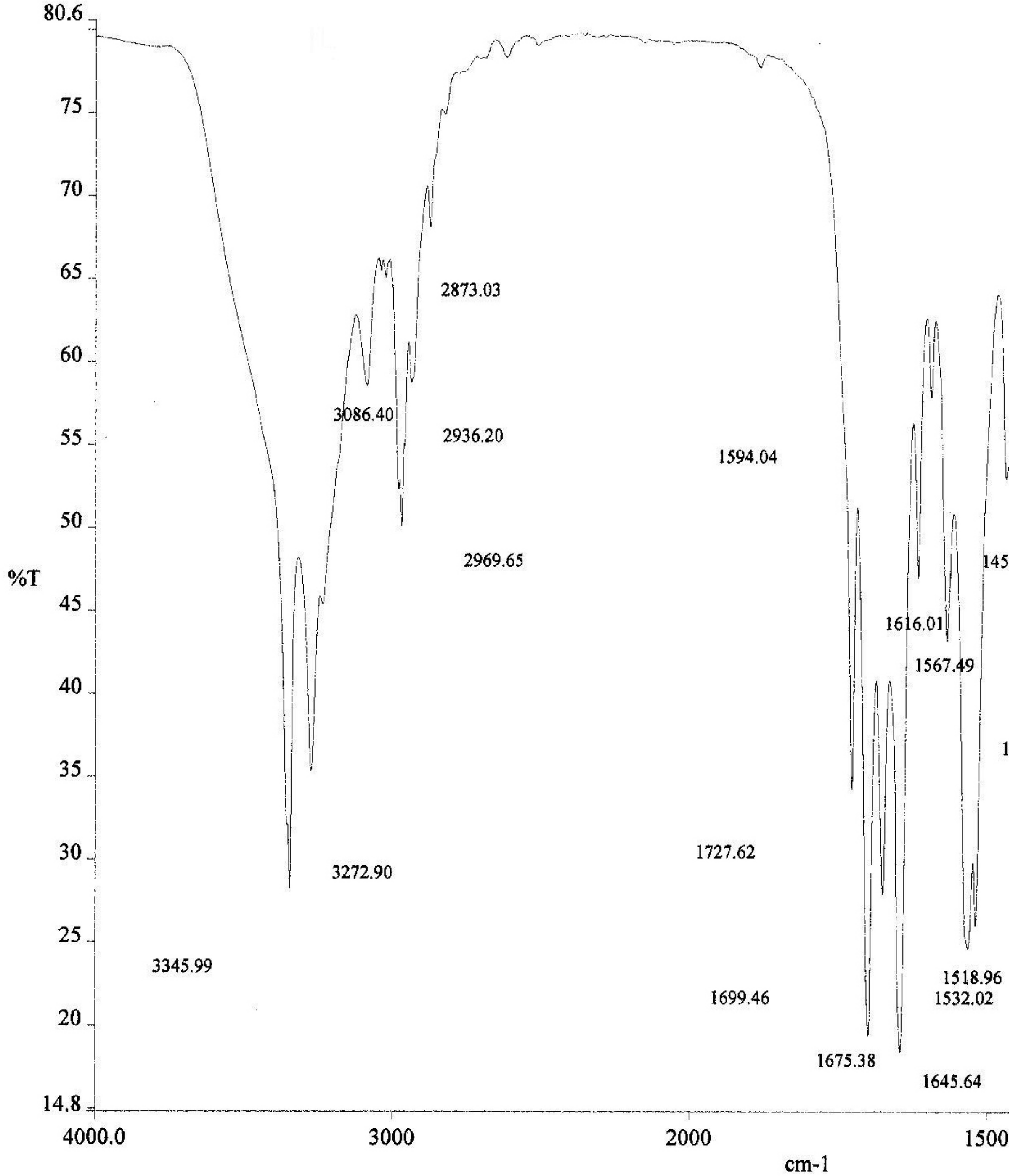
Table of contents



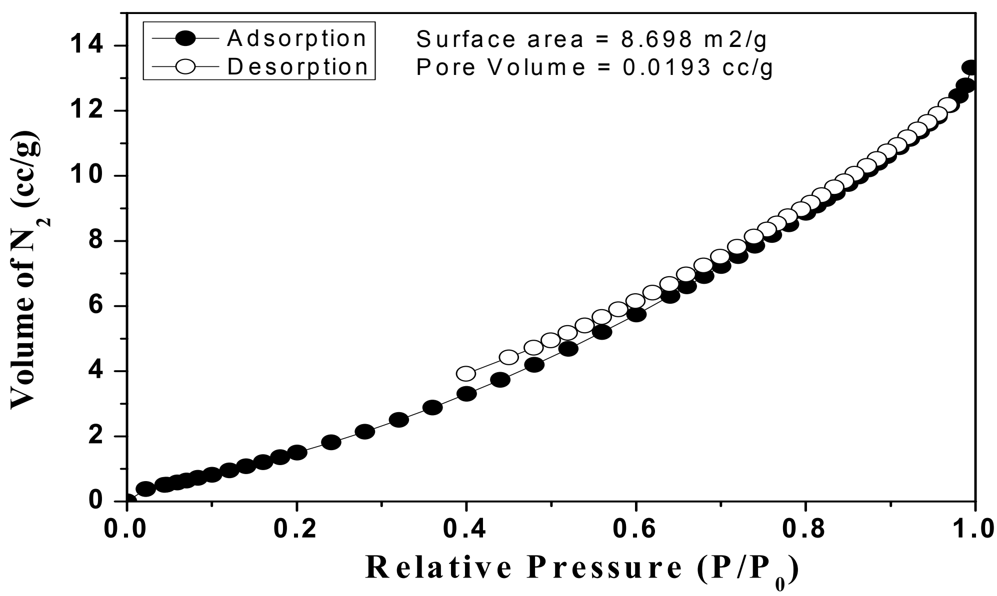
ESI Figure S1: Schematic presentation of synthesis of tripeptide **1**. Reagents and conditions: (a) DMF, H-Aib-OMe, DCC, HOBt, 0°C, 90% yield; (b) MeOH, 2M NaOH, 85% yield; (c) DMF, H-Val-OMe, DCC, HOBt, 0°C, 80% yield.



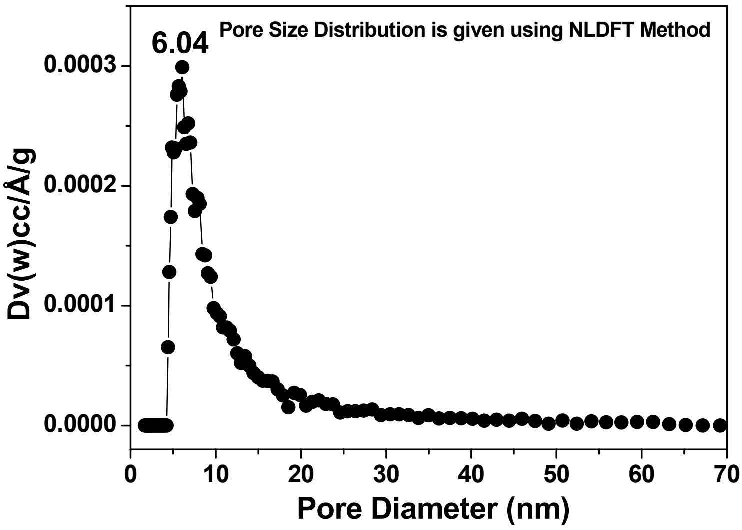
ESI Figure S2: FTIR spectra at the region 1500 – 4000 cm^{-1} of tripeptide **1** in the solid state.

N_2 gas adsorption studies. Nitrogen adsorption/desorption isotherms were obtained using a Quantachrome Autosorb Automated Gas Sorption System at 77 K. The peptide **1** crystals were degassed at 150°C for 4 h. From the N_2 gas adsorption at low P/P_0, the pore size distribution of the sample was calculated using the NLDFT(Non Local Density Functional Theory) method. The BET surface area (8.69 m^2g^-1) was calculated from the Brunauer-Emmett-Teller (BET) equation. The heating at 150°C (for degassing) may have some effect on the self-assembly and pore size of the mesoporous peptide **1**.

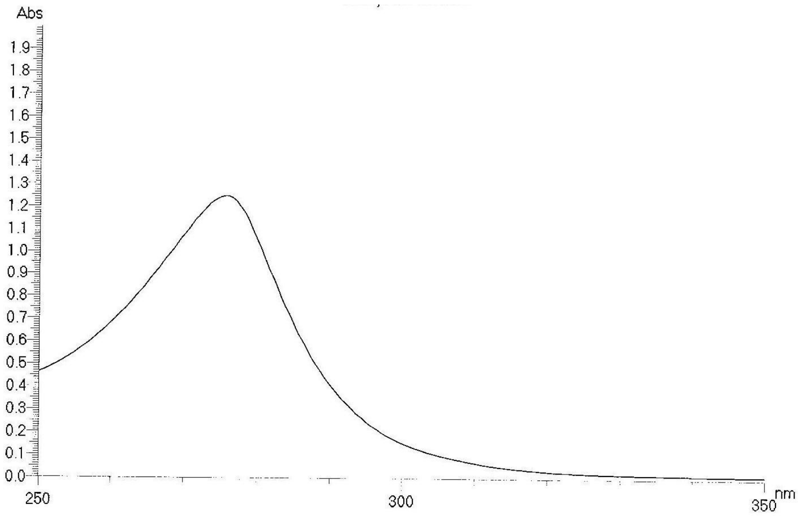
Surface area	8.68 m^2 /gm
Pore volume	0.0193 cc/gm
Pore size(diameter)	6.04 nm
Nature	mesoporous
Isotherm type	1
Max Amount of gas Ads.	13.99 cc/gm



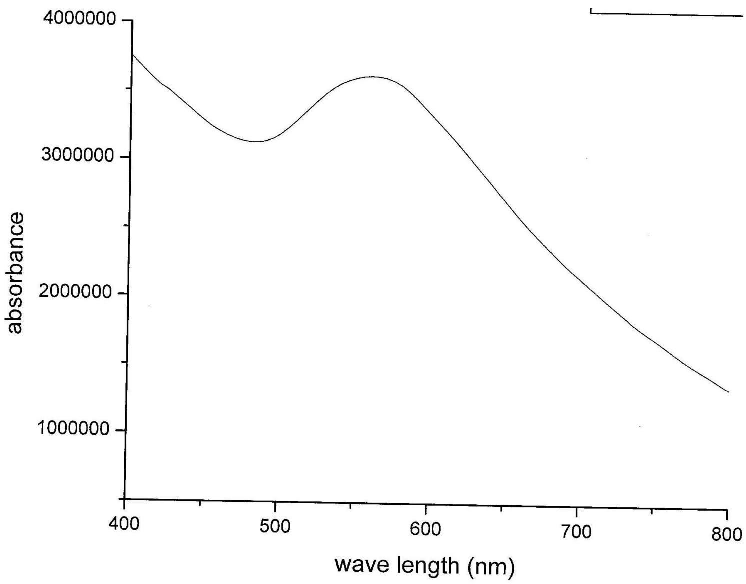
ESI Figure S3: The N_2 gas adsorption /desorption isotherms (77K) of tri-peptide **1** is close to the type 1 adsorption isotherm typical for a nanoporous material.



ESI Figure S4: The pore size distribution curve of tri-peptide **1** exhibits a peak at 6.04 nm indicating the mesoporous architecture.



(a)



(b)

ESI Figure S5. UV-VIS spectra of (a) tripeptide **1** and (b) surface Plasmon band around 548 nm of gold nanoparticle.

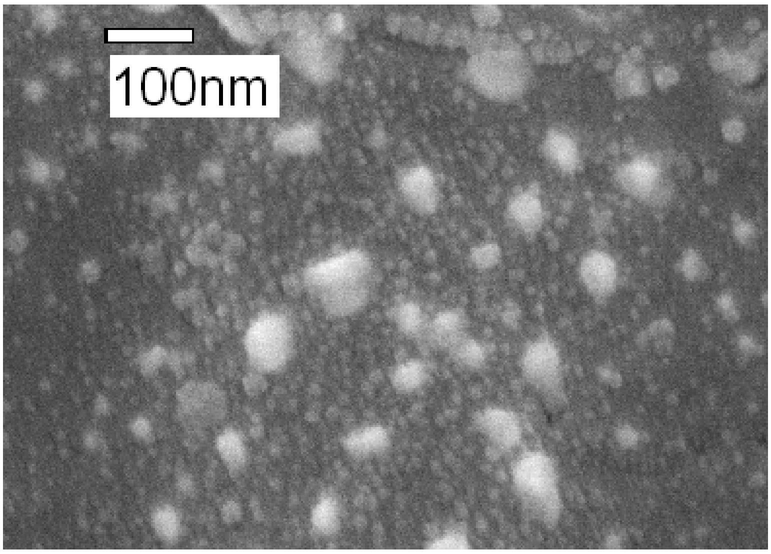
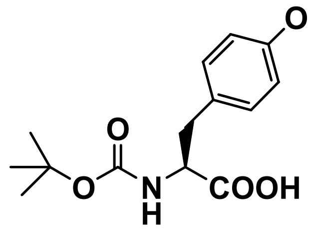


Figure S6. The formation of GNP with different size and shape from a tripeptide Boc-Phe-Phe-Tyr-OMe, which does not exhibits nanoporous structure.



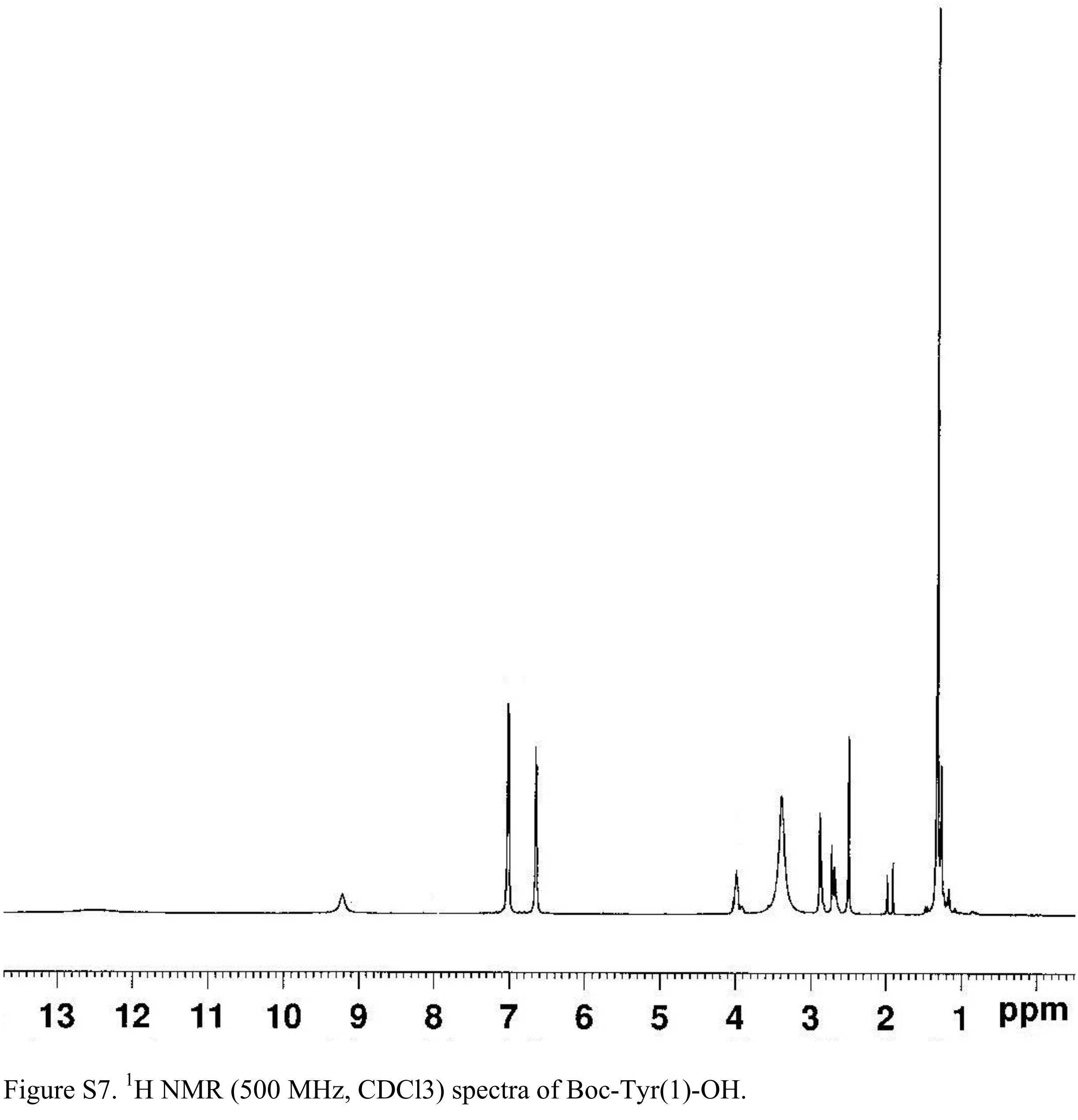
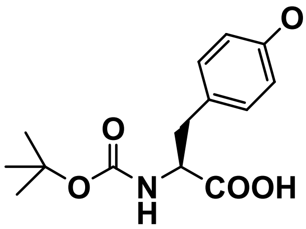


Figure S7. ^{1}H NMR (500 MHz, CDCl3) spectra of Boc-Tyr(1)-OH.



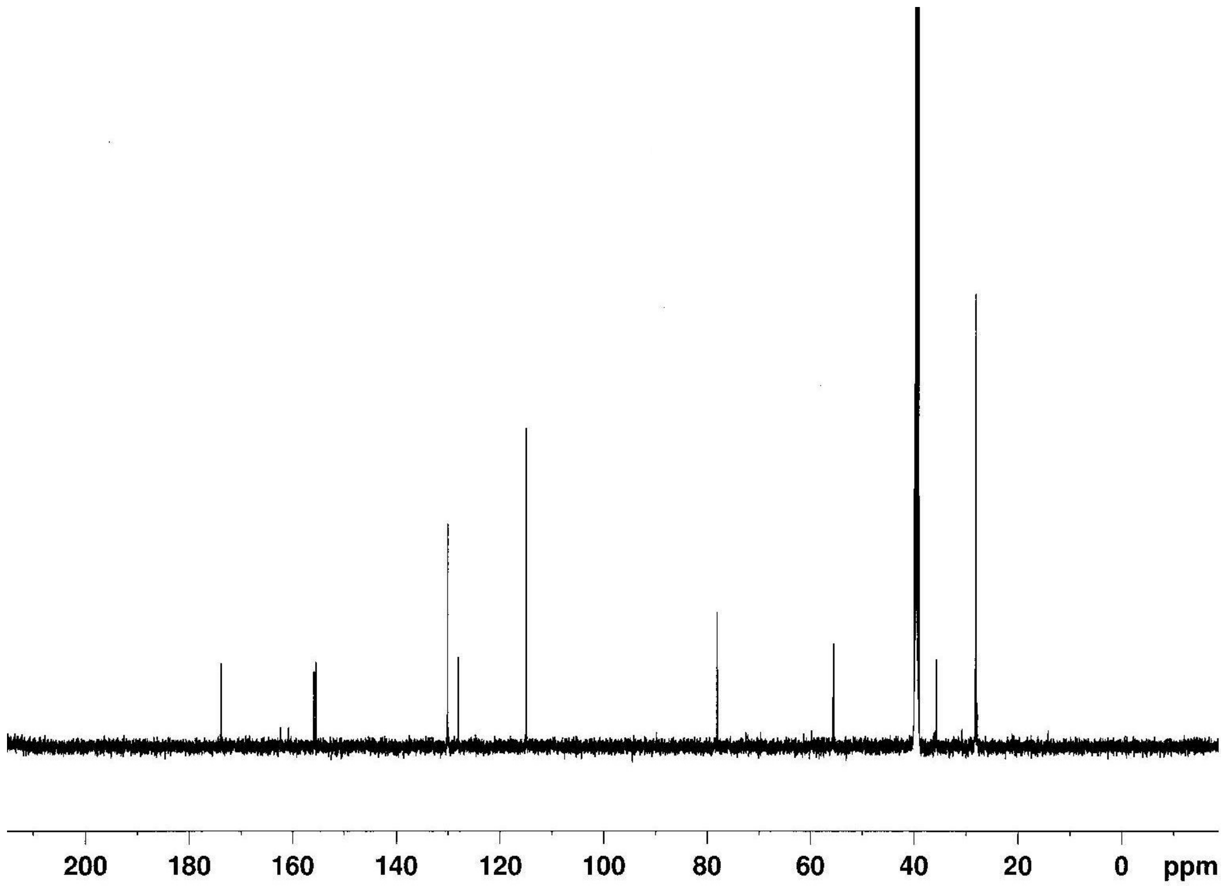
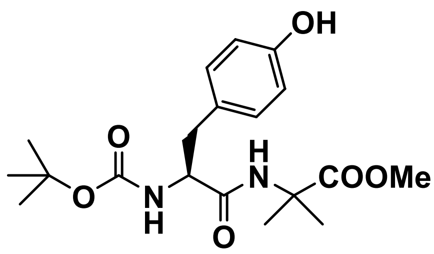


Figure S8. ^{13}C NMR (125 MHz, CDCl3) spectra of Boc-Tyr(1)-OH.



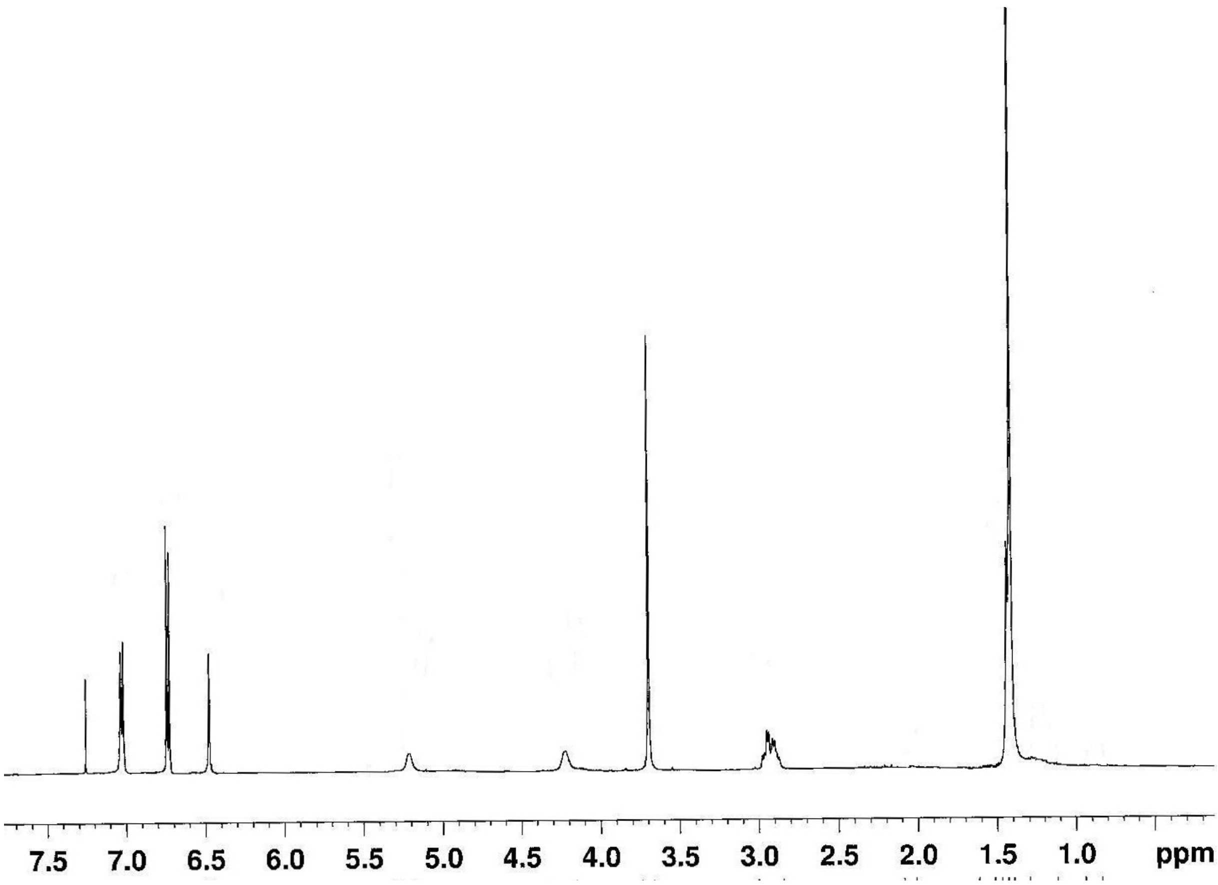


Figure S9. ^{1}H NMR (500 MHz, CDCl3) spectra of Boc-Tyr(1)-Aib(2)-OMe.

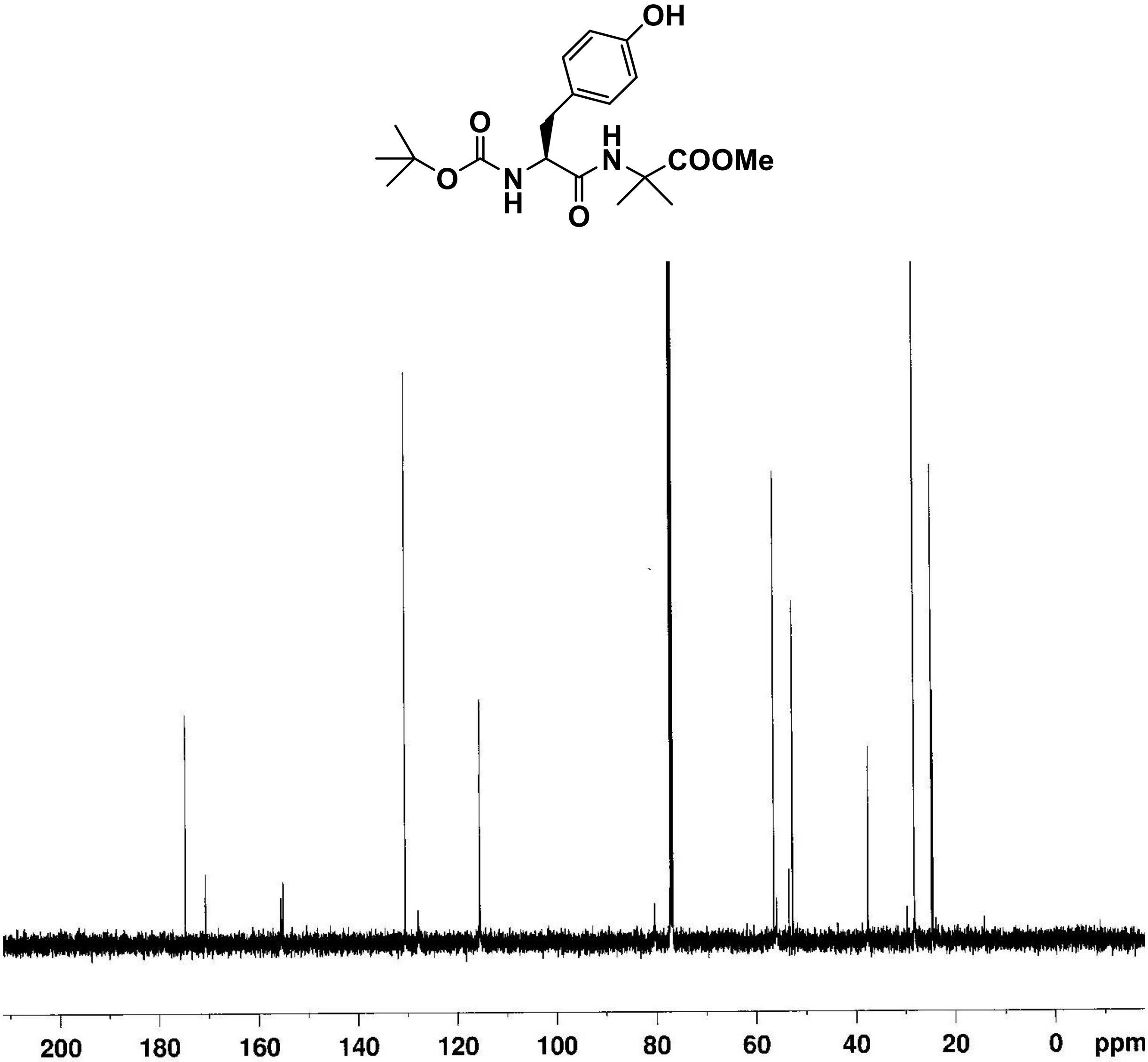


Figure S10. ^{13}C NMR (125 MHz, CDCl3) spectra of Boc-Tyr(1)-Aib(2)-OMe.

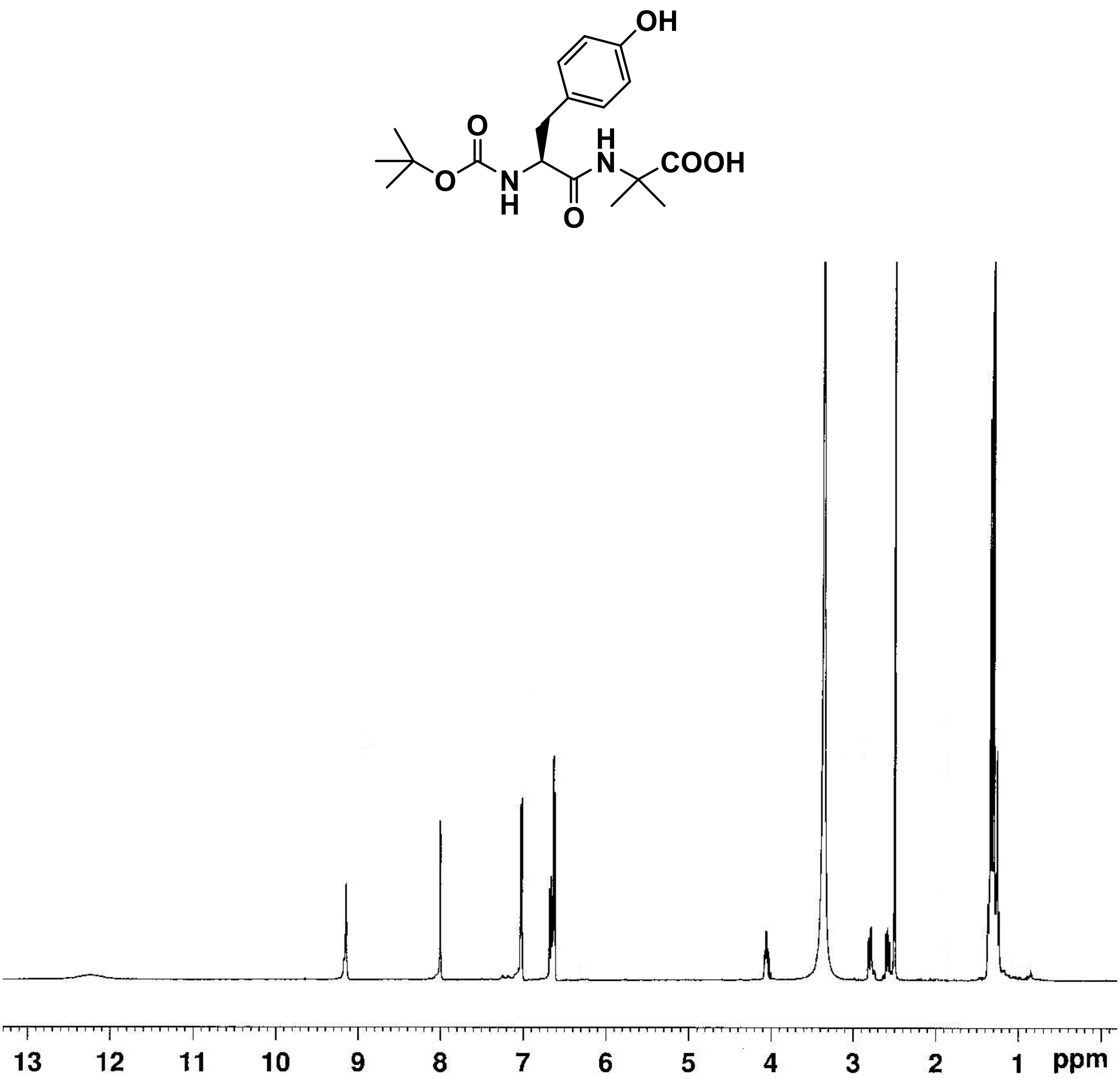
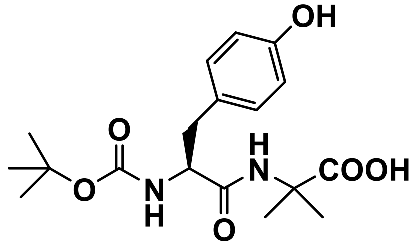


Figure S11. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of Boc-Tyr(1)-Aib(2)-OH.



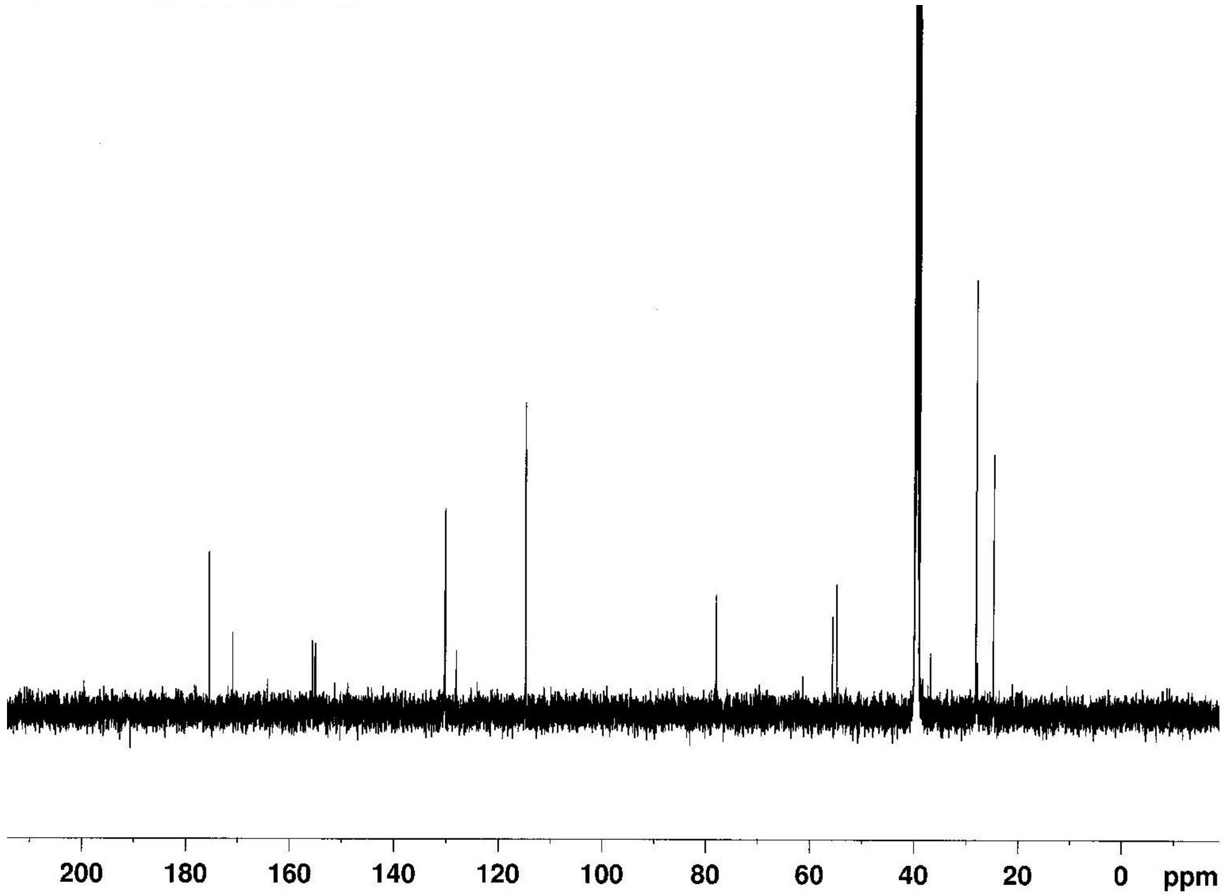
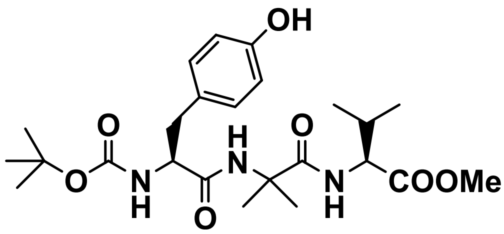


Figure S12. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of Boc-Tyr(1)-Aib(2)-OH.



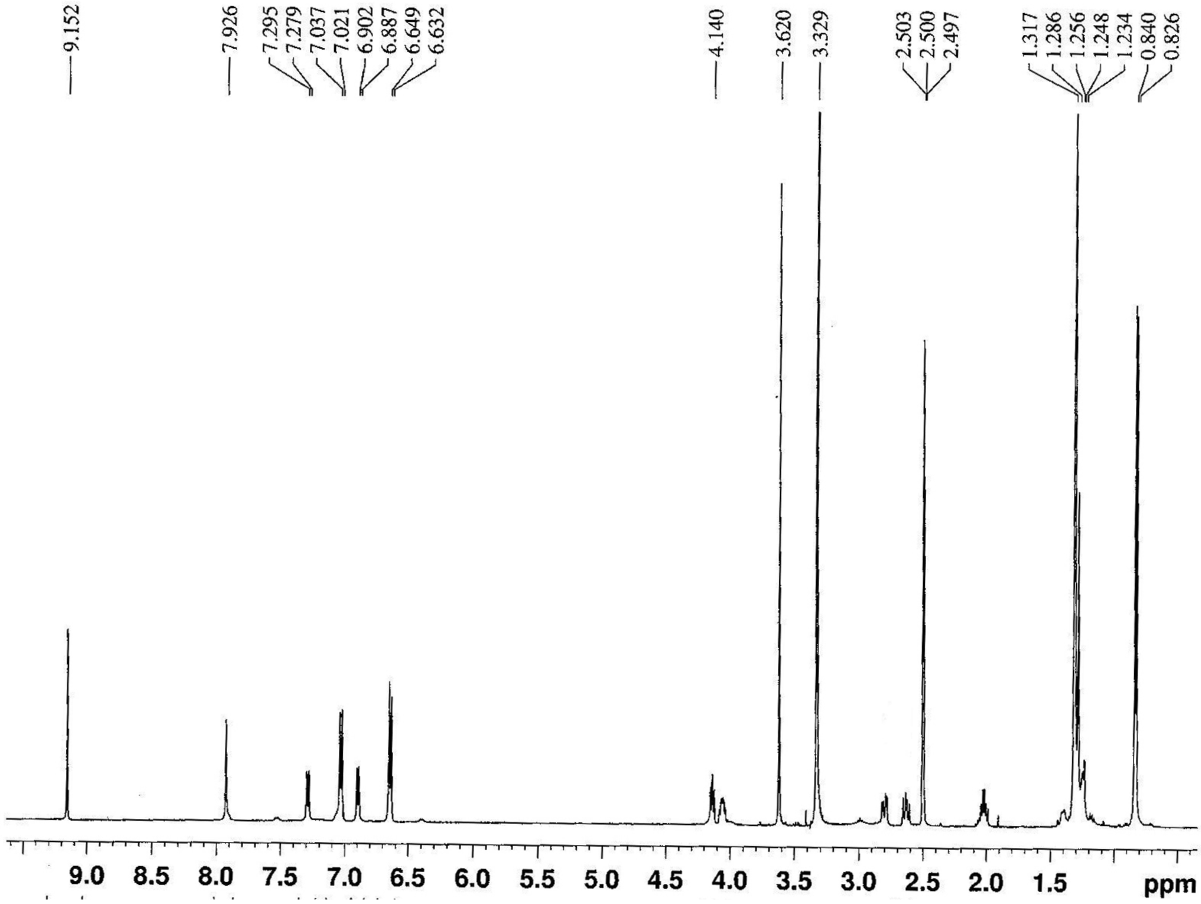


Figure S13. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of Boc-Tyr(1)-Aib(2)-Val(3)-OMe.

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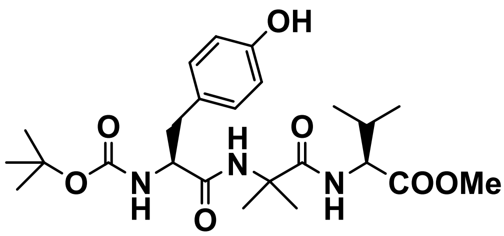

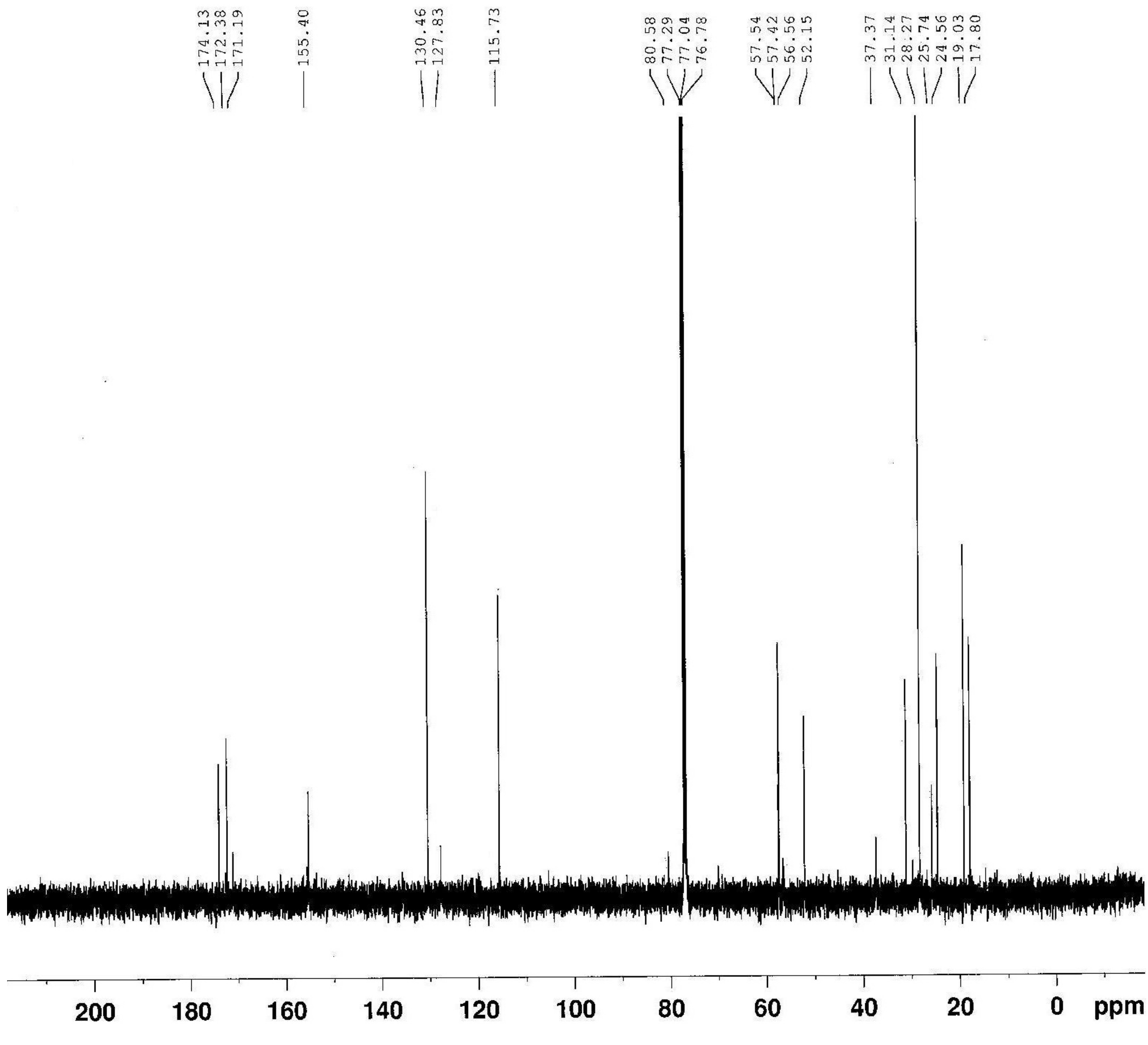

Figure S14. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of Boc-Tyr(1)-Aib(2)-Val(3)-OMe.