

## ESI

# Photo-induced charge-transfer complex formation and organogelation by a tripeptide

Poulami Jana, Sibaprasad Maity, Suman Kumar Maity, Pradip Kumar Ghorai and Debasish Haldar\*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata,  
Mohanpur, West Bengal 741252, India,

Fax: +913325873020; Tel: +913325873119;

E-mail: [deba\\_h76@yahoo.com](mailto:deba_h76@yahoo.com); [deba\\_h76@iiserkol.ac.in](mailto:deba_h76@iiserkol.ac.in)

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Table 1. Gelation properties of peptide **1** in different organic solvents<sup>a</sup>.

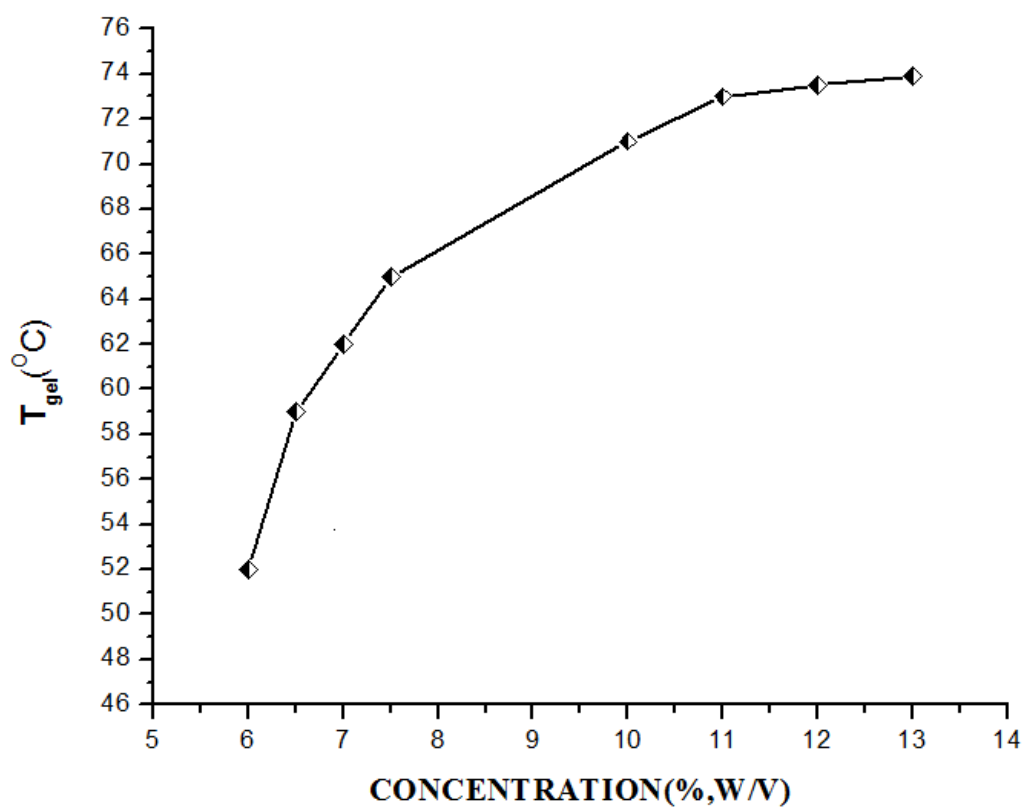
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Solvents	Peptide <b>1</b>
Benzene	g (3)
Toluene	g (2.8)
<i>o</i> -xylene	g (2.8)
<i>m</i> -xylene	g (2.8)
<i>p</i> -xylene	g(2.8)
1,2-dichlorobenzene	g (2)
DMSO	s
DMF	s
THF	s

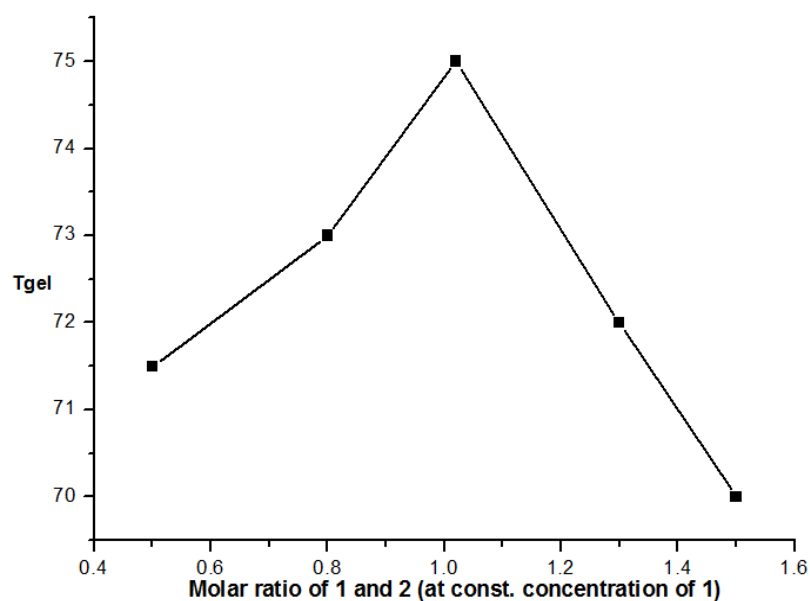
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<sup>a</sup> g = stable gel at room temperature; in parentheses: minimum gelation concentration (% w/v); s = soluble.

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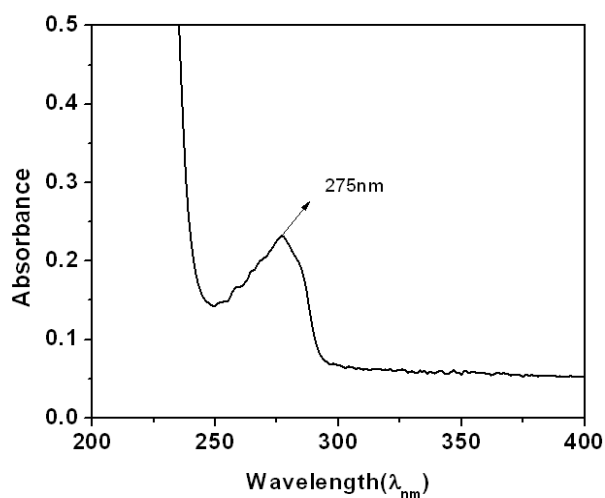
ESI Figure S1. The change of  $T_{gel}$  with increasing concentration of organogel obtained from peptide **1** in 1,2-dichlorobenzene.



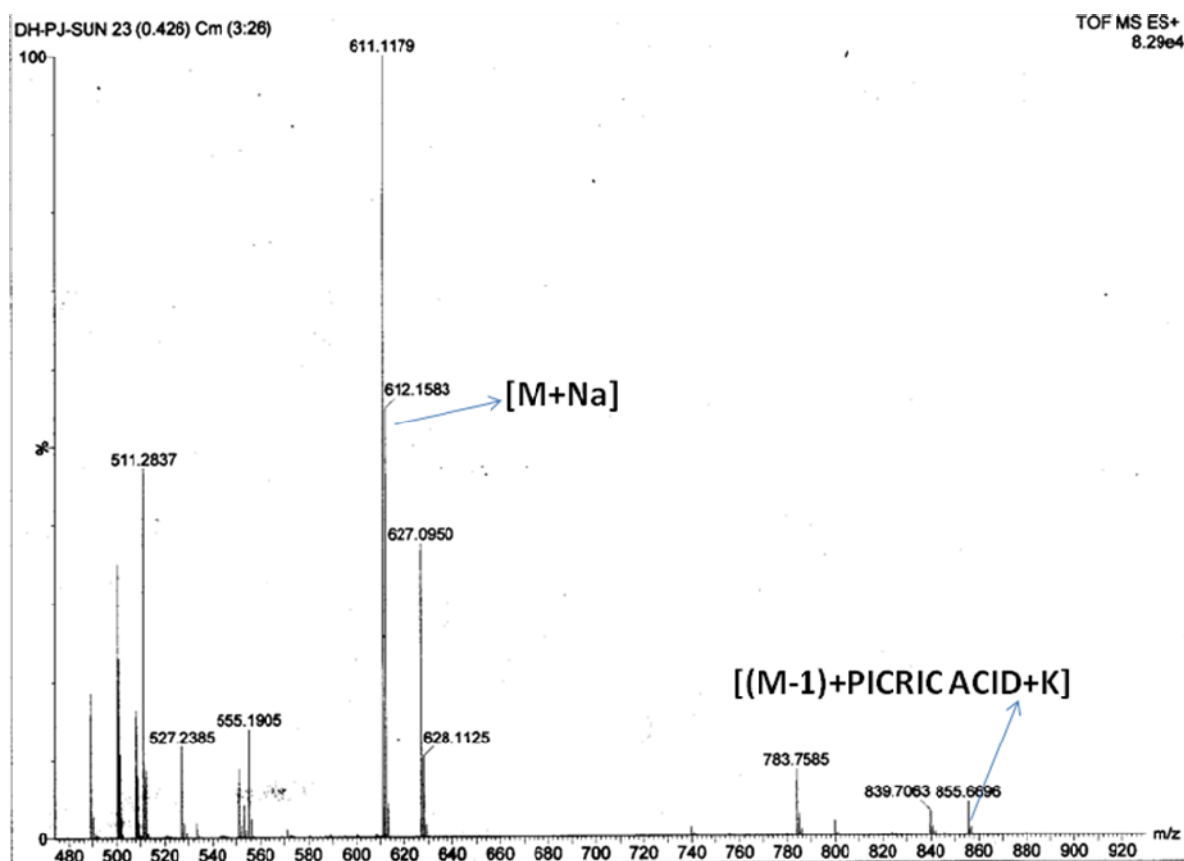
ESI Figure S2. A plot of  $T_{gel}$  vs the molar ratio of picric acid.  $T_{gel}$  is measured with increasing concentration of picric acid at a constant concentration of peptide **1** (46mM). The plot shows that the  $T_{gel}$  was maximum at a 1:1 molar ratio of peptide **1** and picric acid.

Table 2. Gelation properties of peptide **1** and picric acid in different organic solvents.

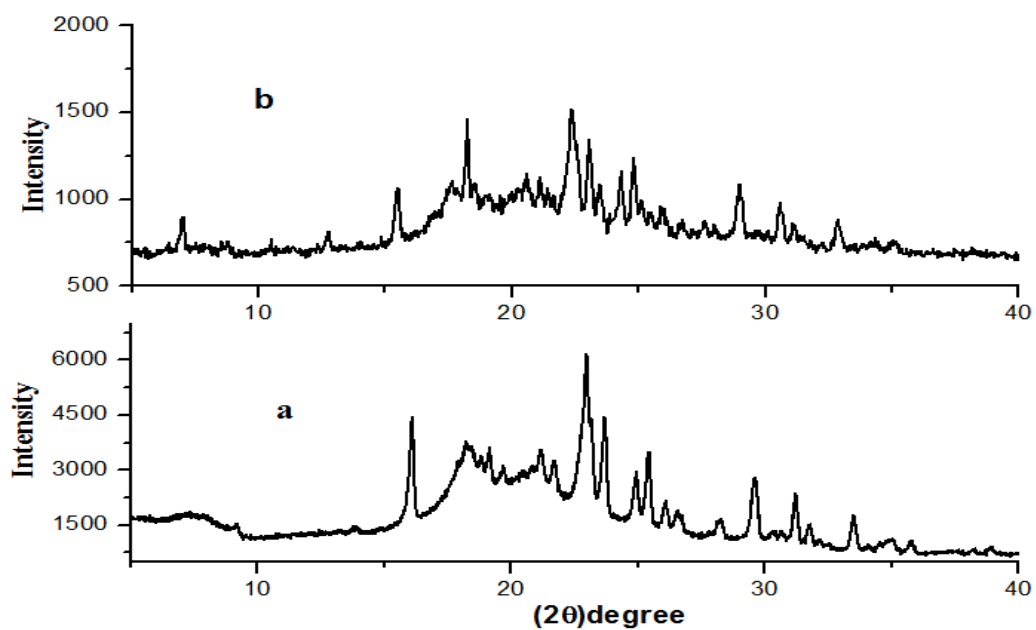
Solvent	molar ratio	MGC (% W/V)
Toluene	1:1	2.8
<i>o</i> -xylene	1:1	2.8
<i>p</i> -xylene	1:1	2.8
<i>m</i> -xylene	1:1	2.8
1,2-dichlorobenzene	1:1	1.6



ESI Figure S3 UV/visible absorption of peptide 1 in methanol ( $10^{-5}$  M).



ESI Figure S4 Mass spectra of charge transfer complex.



ESI Figure S5. PXRD spectra of peptide **1** and picric acid xerogel from 1,2-dichlorobenzene (a) after exposure to UV-light and (b) before UV-light exposure.

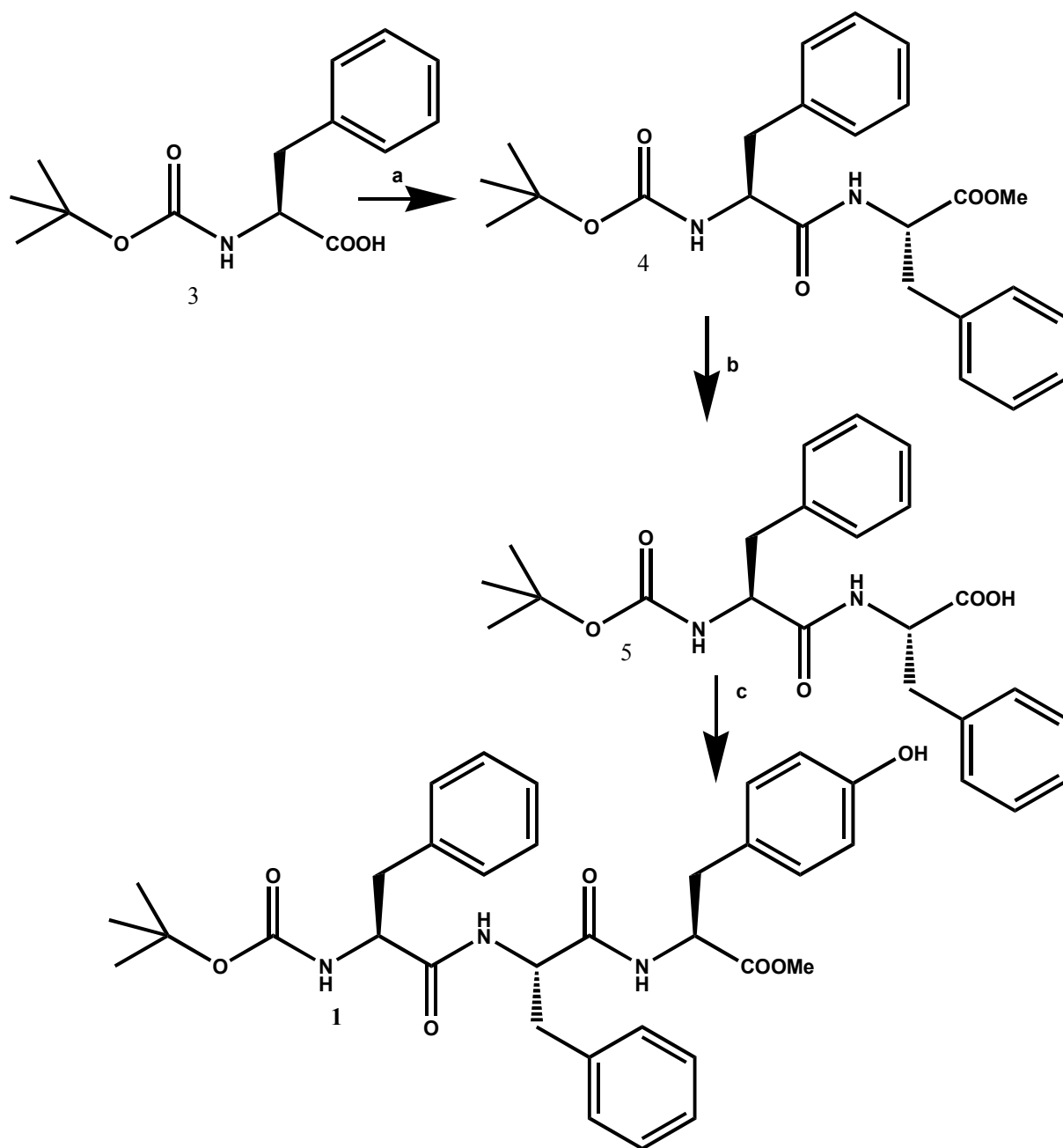


Figure S1. Schematic presentation of synthesis of peptide 1. Reagent and condition: (a) dry DCM, H-Phe-OMe, DCC, HOBT, 0°C, 24 h; (b) MeOH, 2M NaOH, 5h; (c) dry DCM, H-Tyr-OMe(1), DCC, HOBT, 0°C, 48 h.

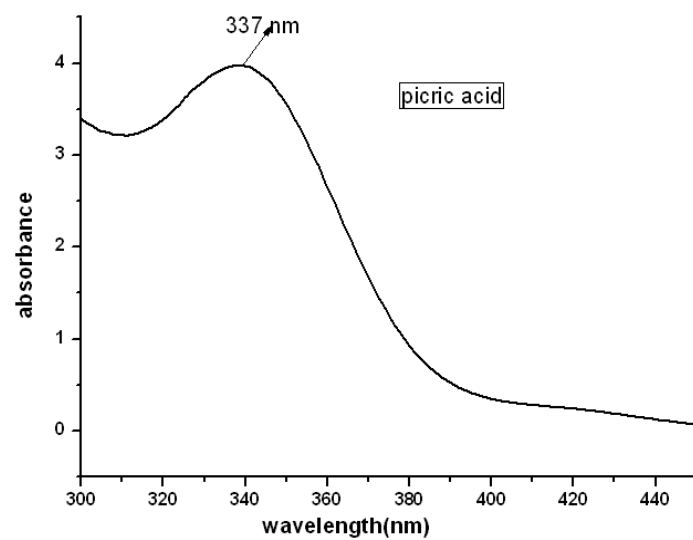


Figure S2. UV/visible absorption spectra of picric acid in 1,2 dichloro benzene (1mM).



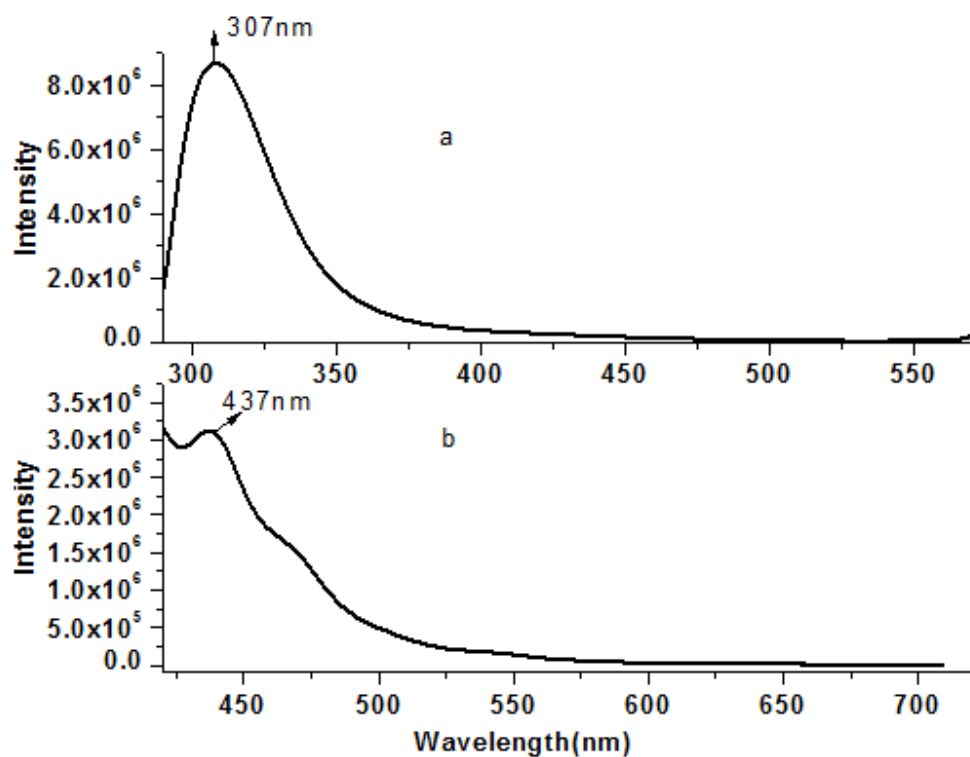


Figure S3. (a) Emission spectra of peptide 1 at 307nm (Excitation = 275nm, 0.234mM), (b) emission of picric acid at 437nm (C=0.198mM, Excitation =415nm).

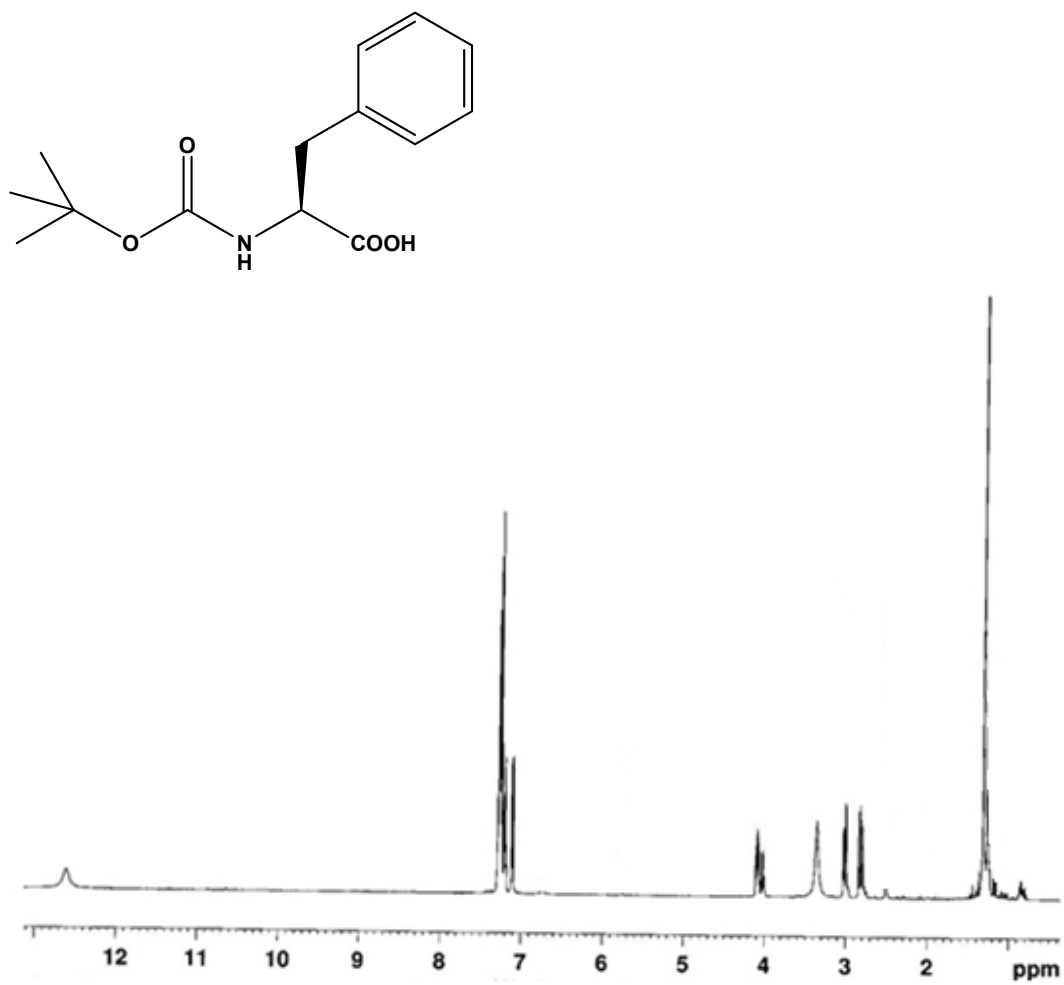


Figure S4. <sup>1</sup>H NMR (500MHz, DMSO-d<sub>6</sub>) spectra of Boc-Phe-OH 3.

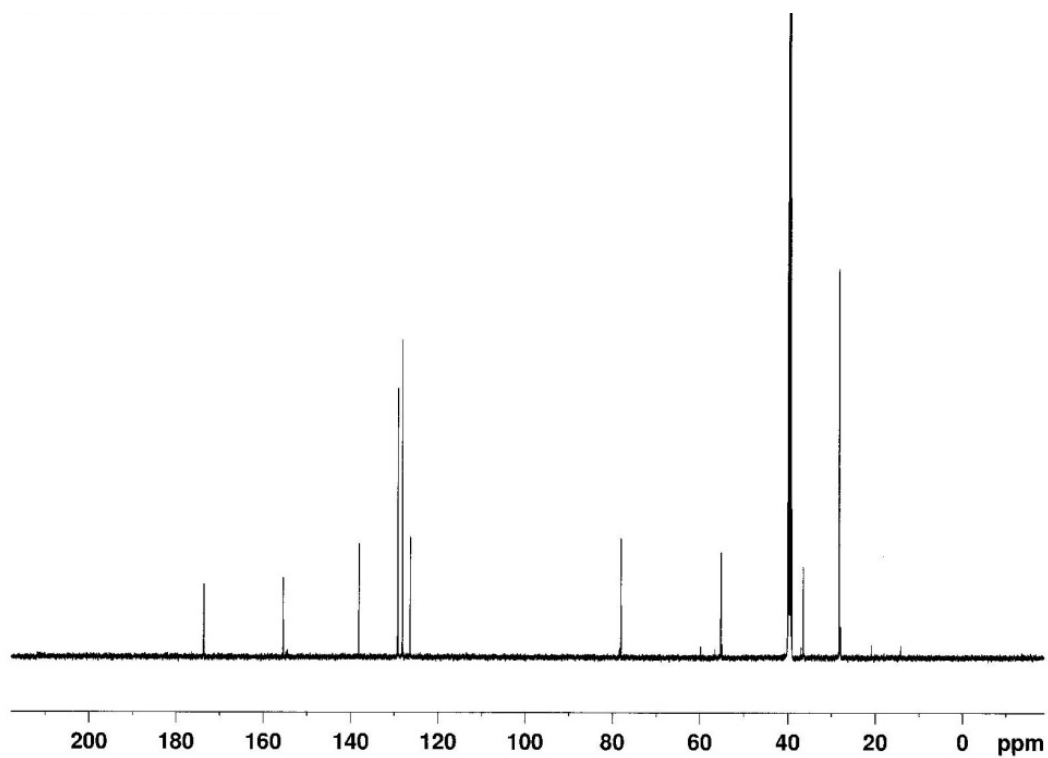


Figure S5.  $^{13}\text{C}$  NMR (125MHz, DMSO- $\text{d}_6$ ) spectra of Boc-Phe-OH 3.

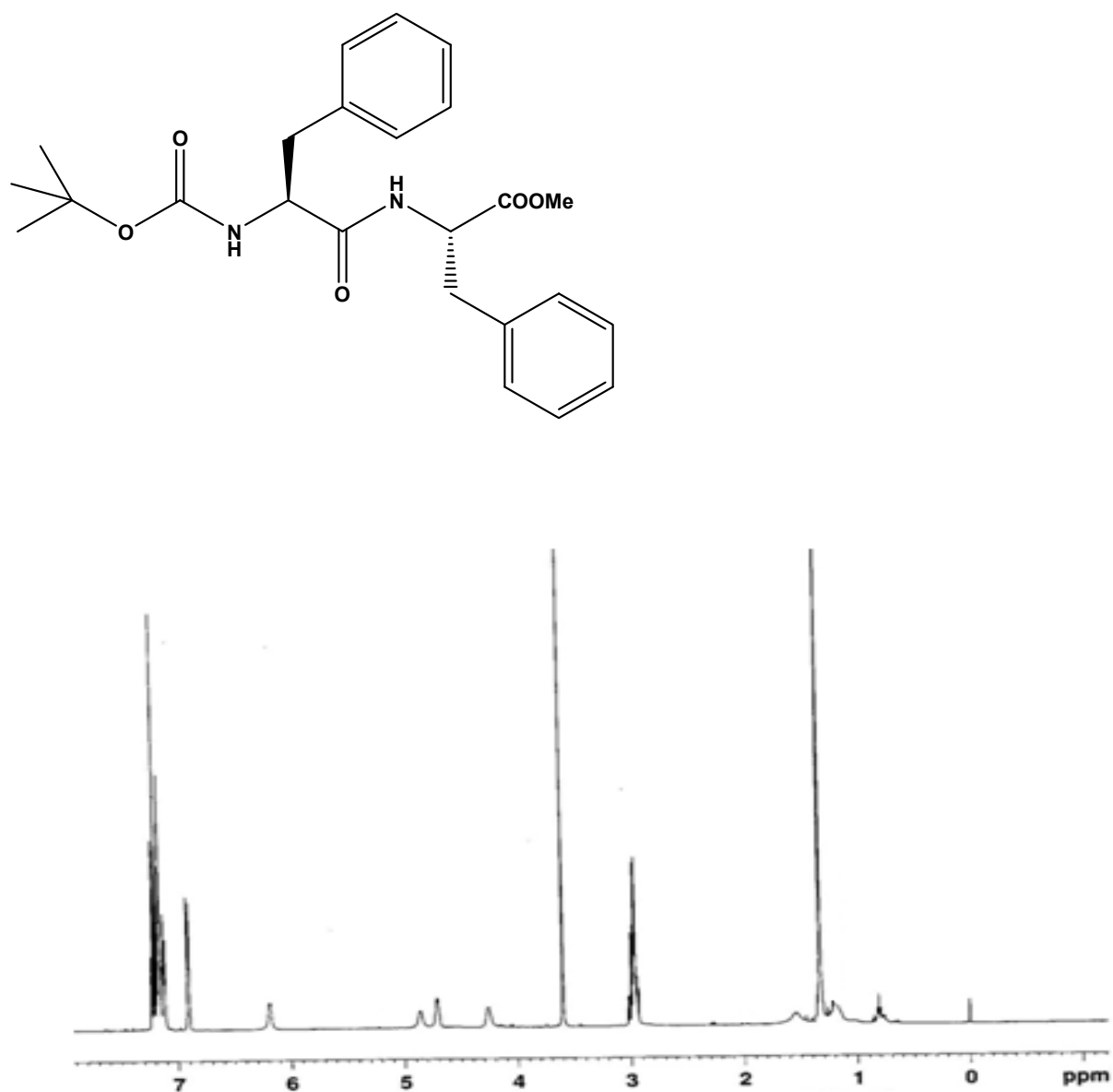


Figure S6. <sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>) spectra of Boc-Phe-Phe-OMe 4.

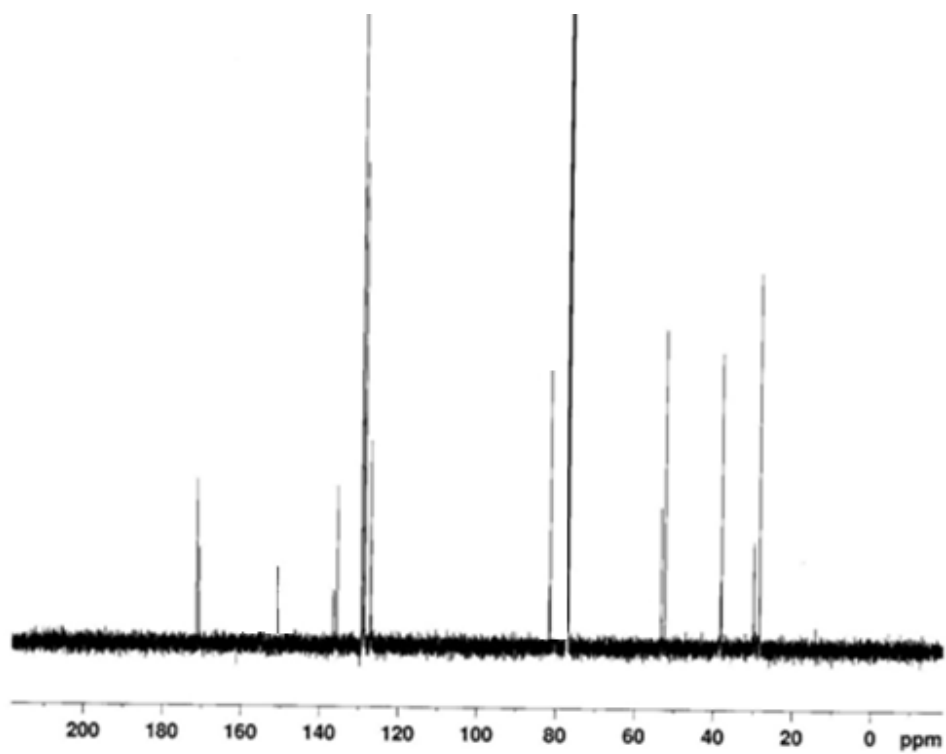


Figure S7  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) spectra of Boc-Phe-Phe-OMe 4.

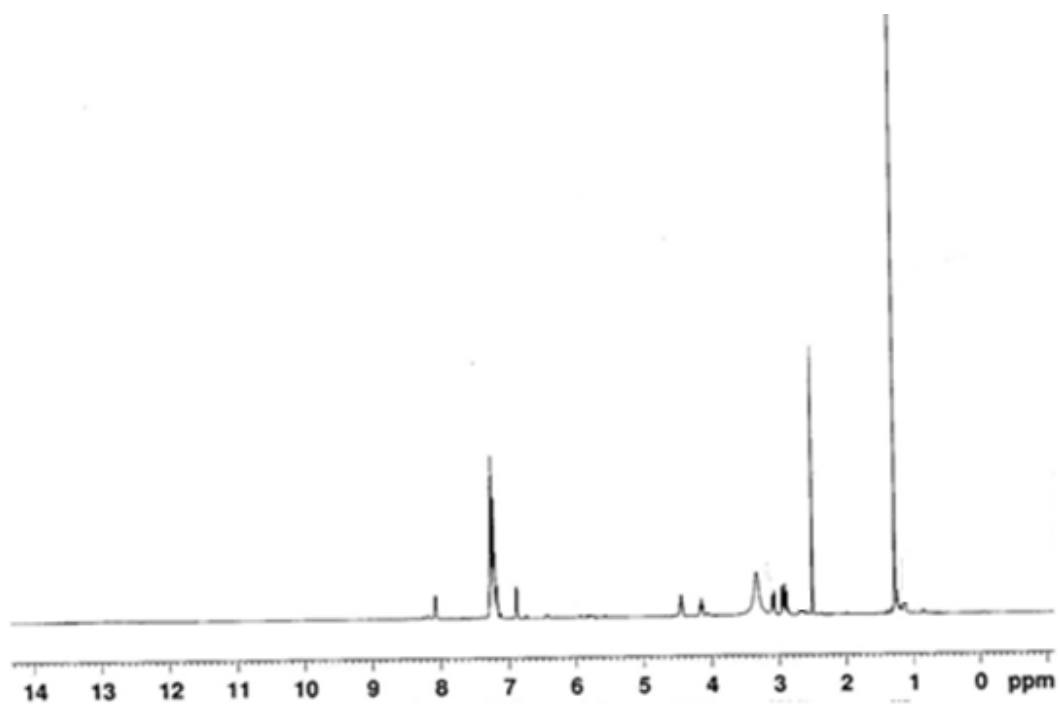
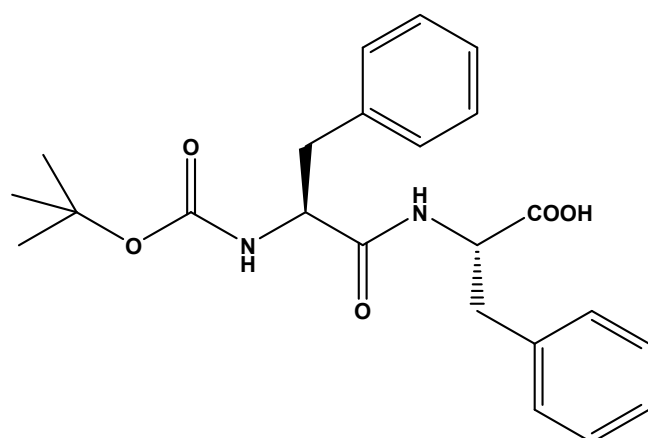


Figure S8. <sup>1</sup>H NMR (500MHz, DMSO-d<sub>6</sub>) spectra of BOC-Phe-Phe-OH **5**.

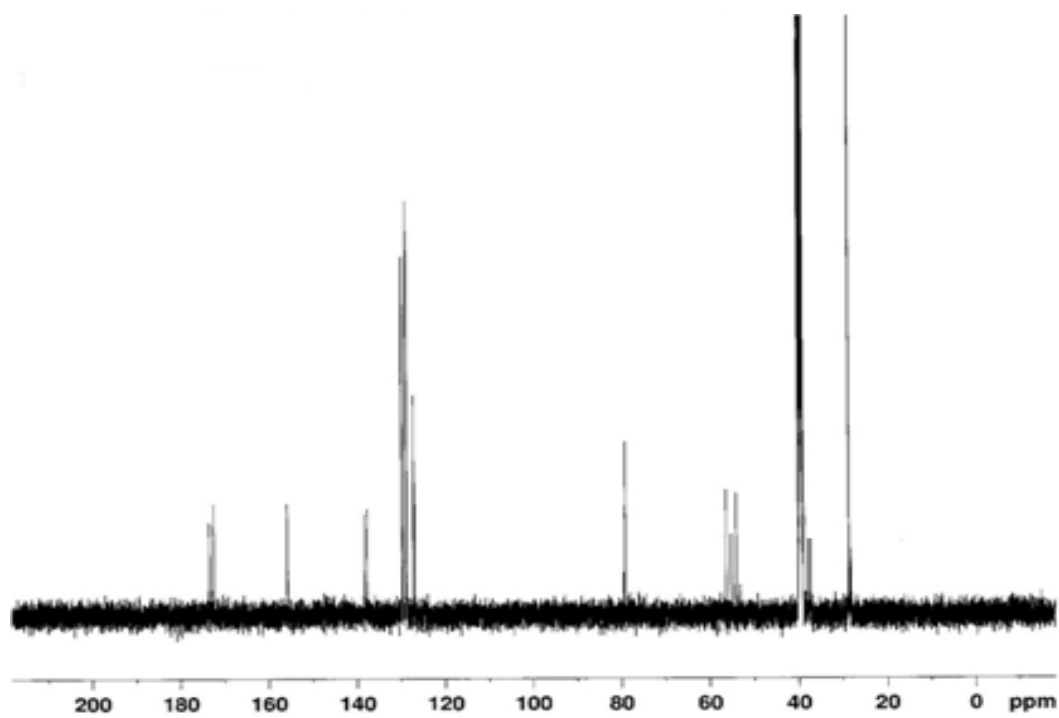


Figure S9.  $^{13}\text{C}$  NMR (125MHz,  $\text{DMSO-d}_6$ ) spectra of BOC-Phe-Phe-OH **5**.

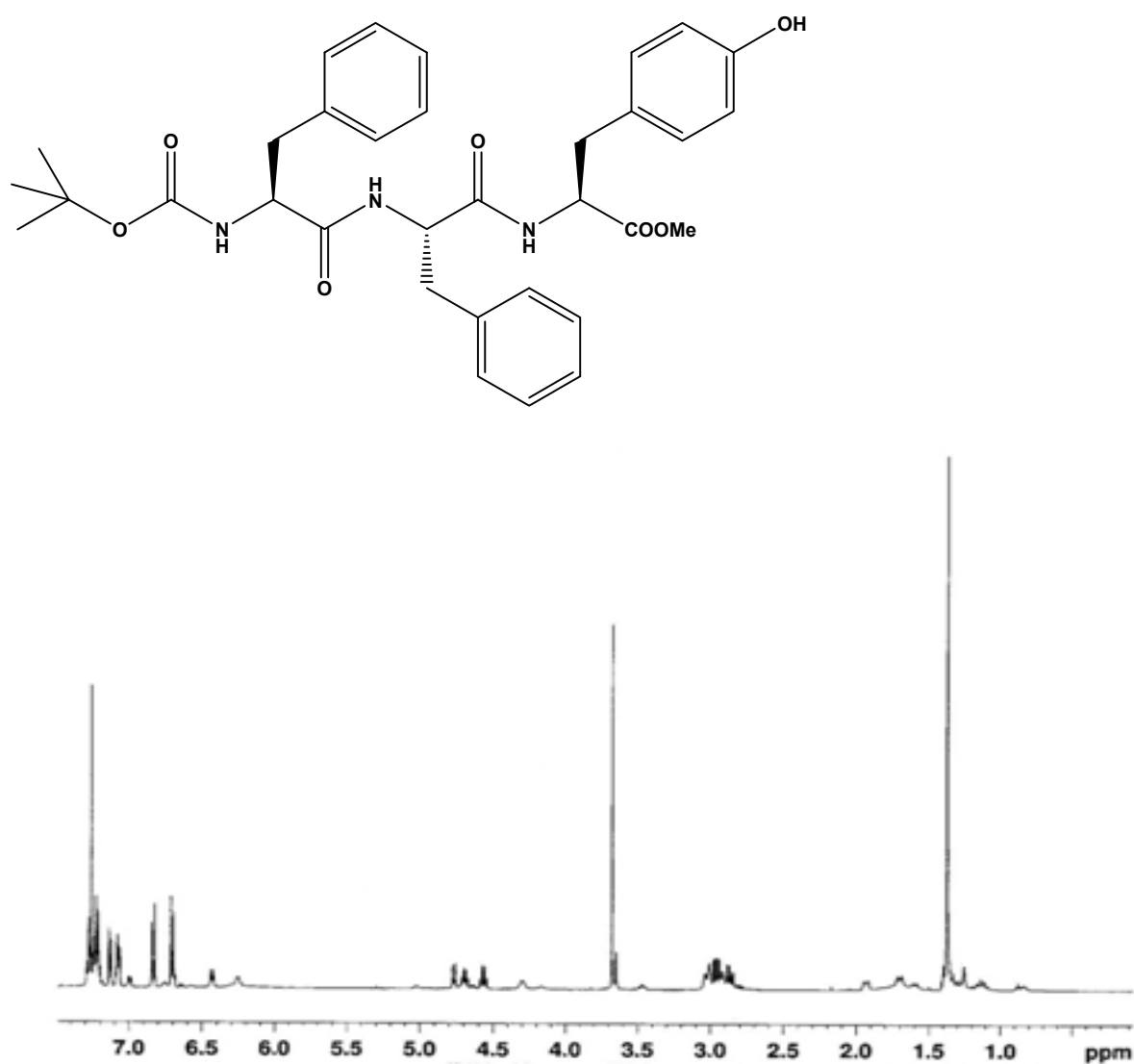


Figure S10. <sup>1</sup>H NMR (500MHz, CDCl<sub>3</sub>) spectra of Boc-Phe-Phe-Tyr-OMe **1**.



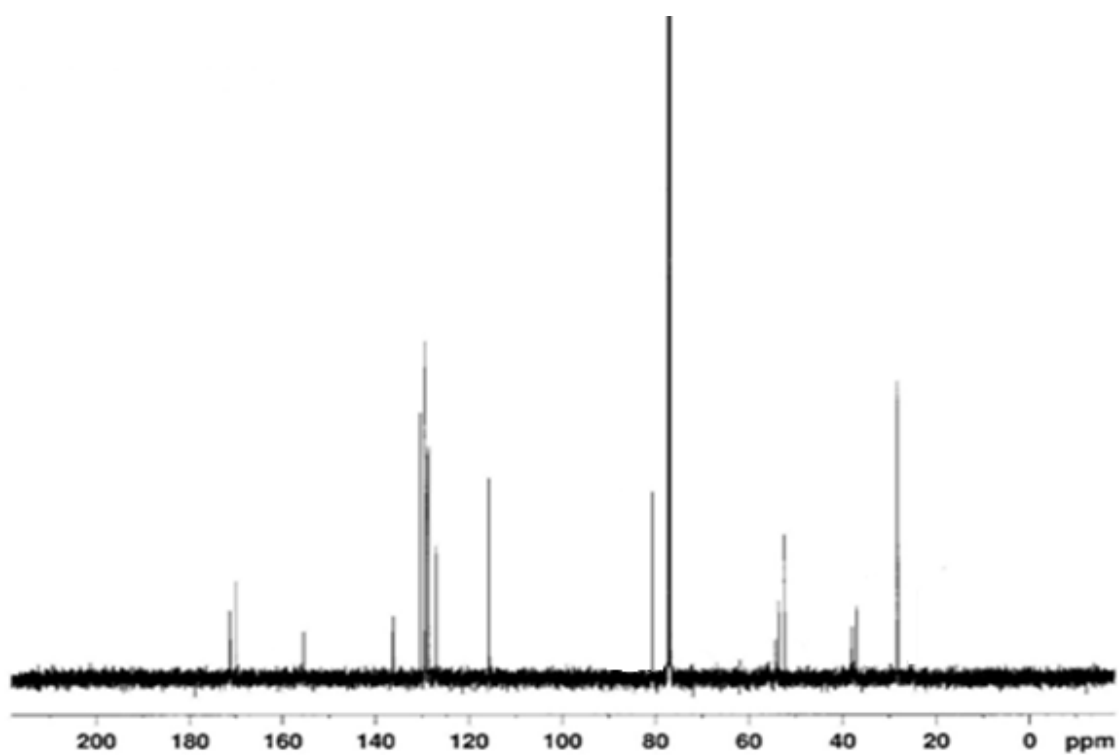


Figure S11.  $^{13}\text{C}$  NMR (125MHz,  $\text{CDCl}_3$ ) spectra of Boc-Phe-Phe-Tyr-OMe **1**.

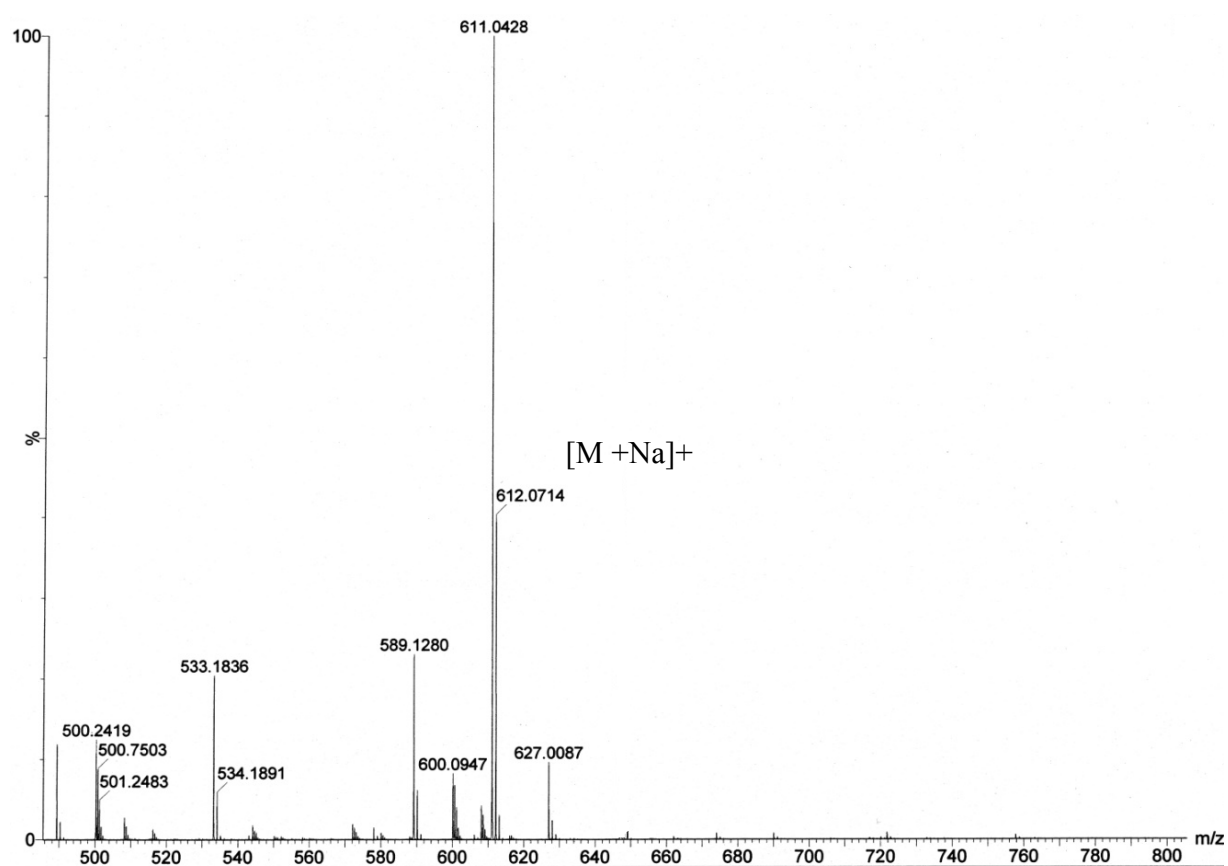


Figure S12. Mass spectra of Boc-Phe-Phe-Tyr-OMe 1

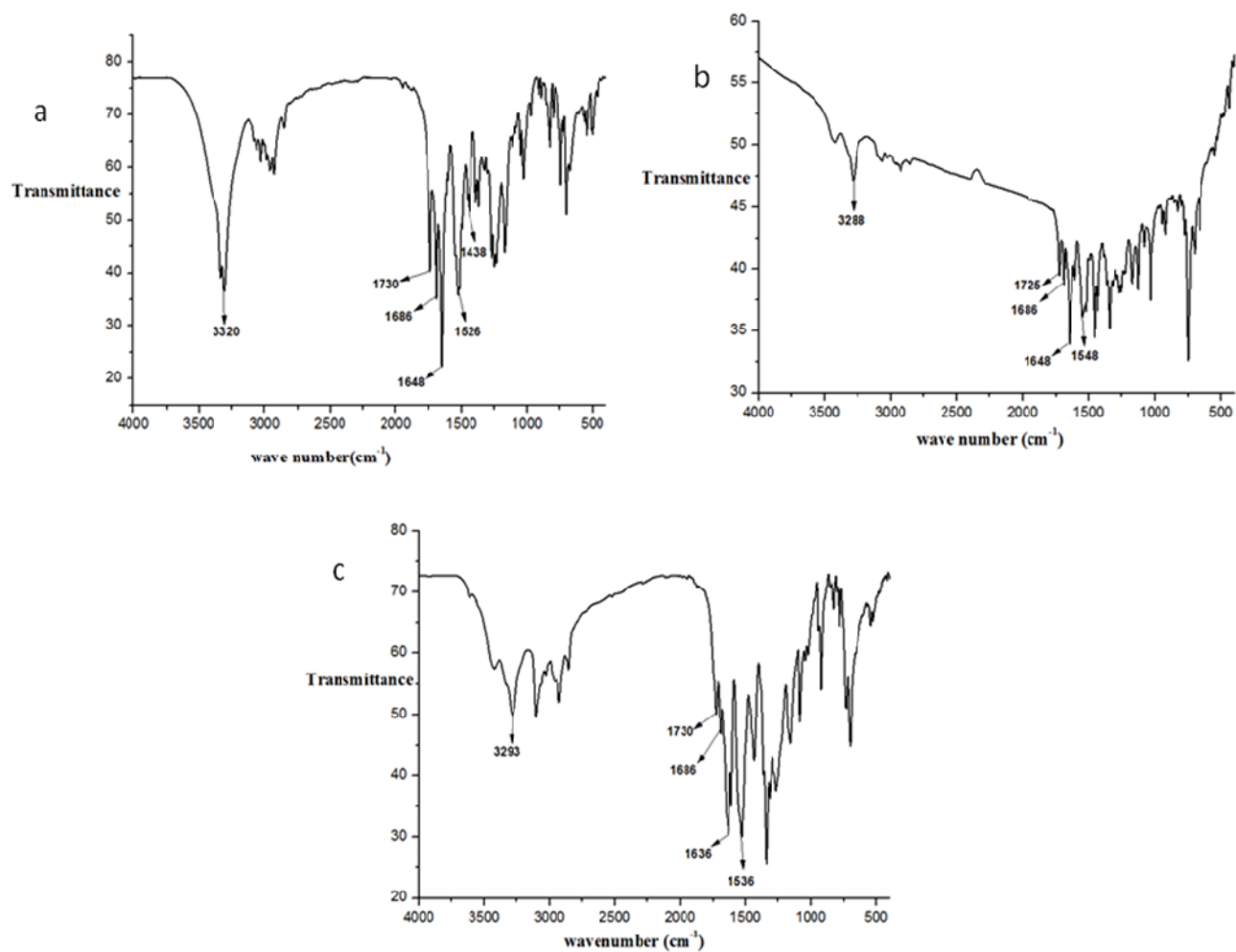


Figure S13. FT-IR spectra of (a) tripeptide Boc-Phe-Phe-Tyr-OMe **1** in the solid state; (b) xerogel from 1:1 mixture of peptide **1** and picric acid in 1,2-dichlorobenzene before UV-light exposure; (c) xerogel from 1:1 mixture of peptide **1** and picric acid in 1,2-dichlorobenzene after UV-light exposure.

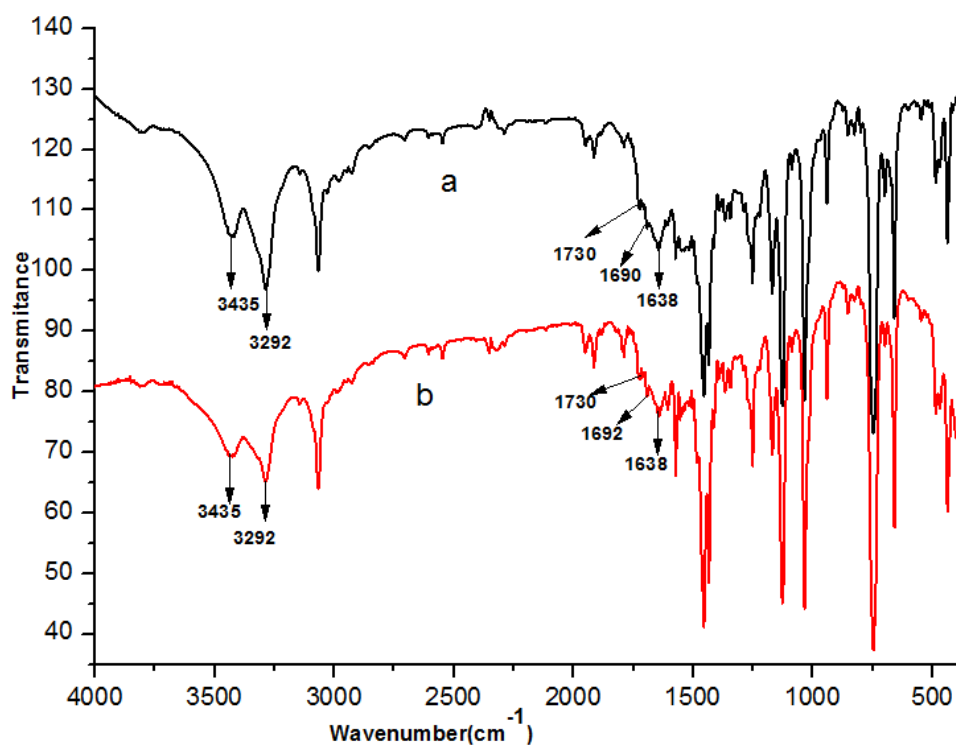


Figure S14: Comparison of FT-IR spectra of peptide **1** in (a) solution state and (b) gel state which shows that in both state the structure of peptide **1** is same.

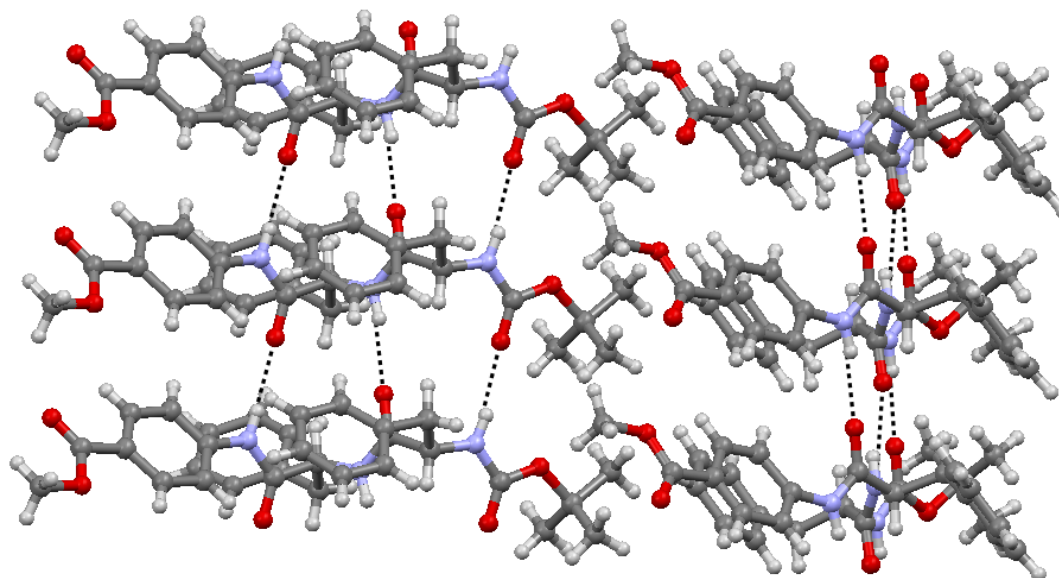


Figure S15: The ball and stick presentation of intermolecular hydrogen bonded parallel  $\beta$ -sheet like structure of Boc-Phe-Phe-Paba-OMe along crystallographic *a* direction. Hydrogen bonds are shown as dotted lines.