

## Supporting information

### A new dipeptide as selective gelator of Cu(II), Zn(II) and Pb(II)

Santosh Kumar,<sup>a</sup> Sujay Kumar Nandi,<sup>a</sup> Saurav Suman<sup>a</sup> and Debasish Halder<sup>\*a</sup>

Department of Chemical Sciences

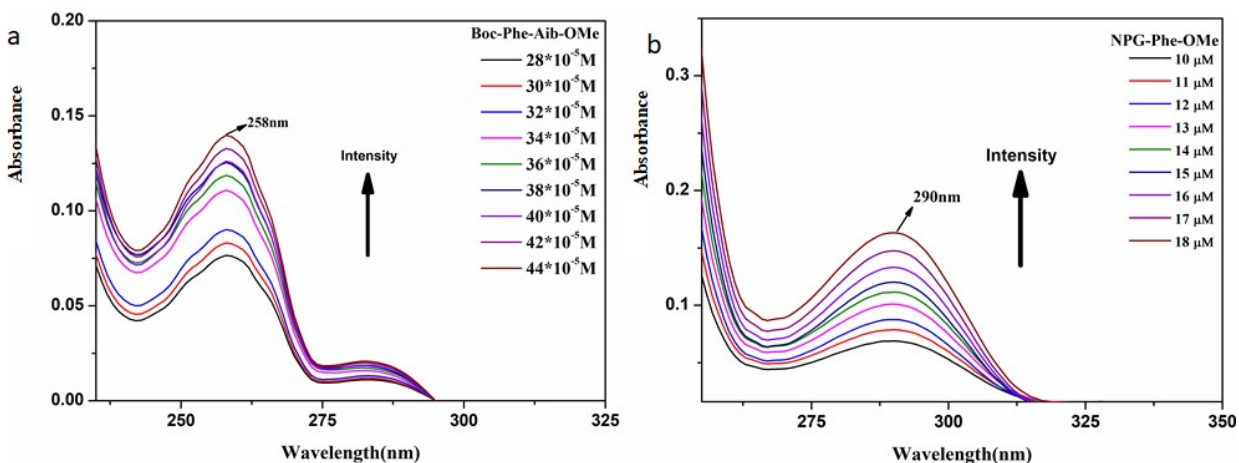
Indian Institute of Science Education and Research Kolkata

Mohanpur 741246, West Bengal, India

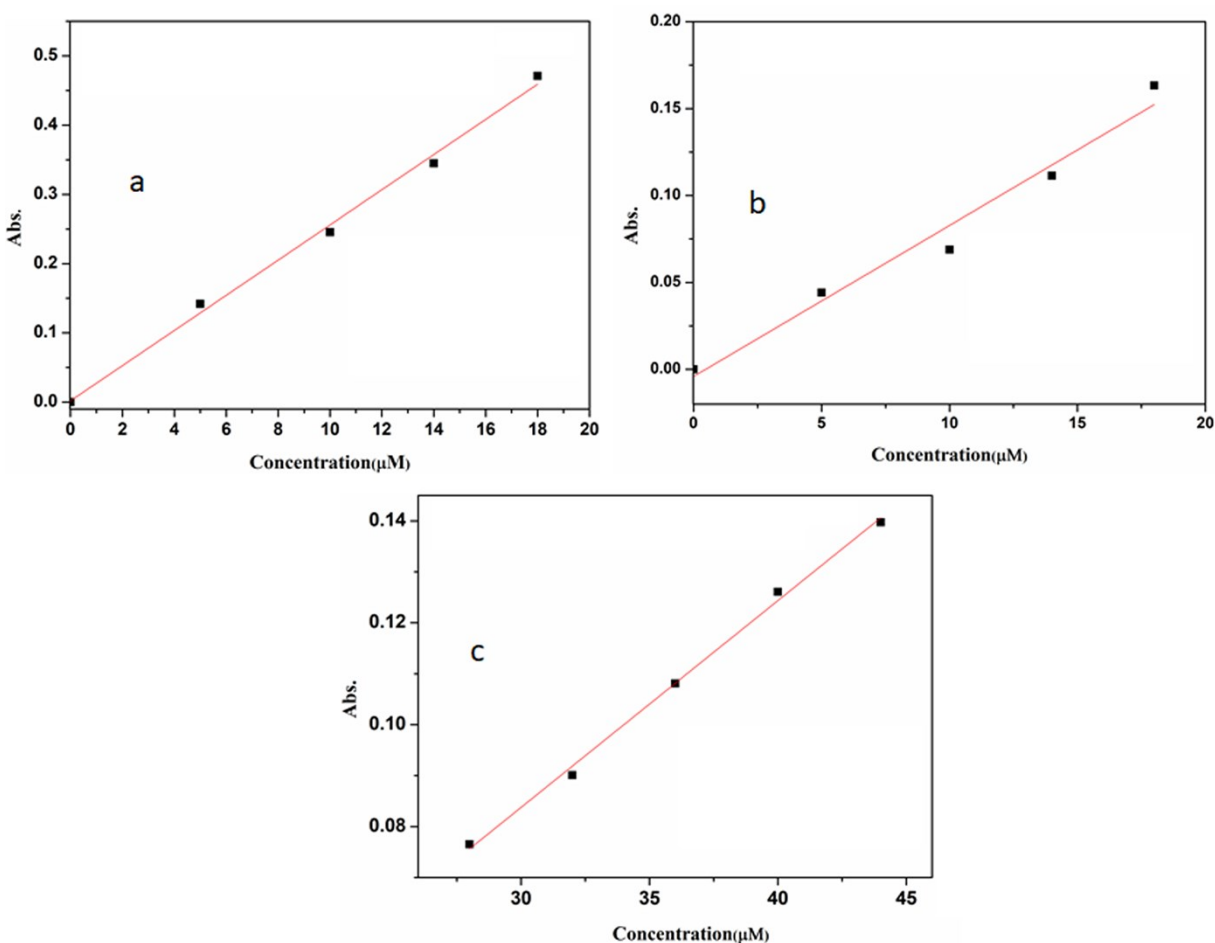
E-mail: [deba\\_h76@iiserkol.ac.in](mailto:deba_h76@iiserkol.ac.in), [deba\\_h76@yahoo.com](mailto:deba_h76@yahoo.com).

## Table of contents

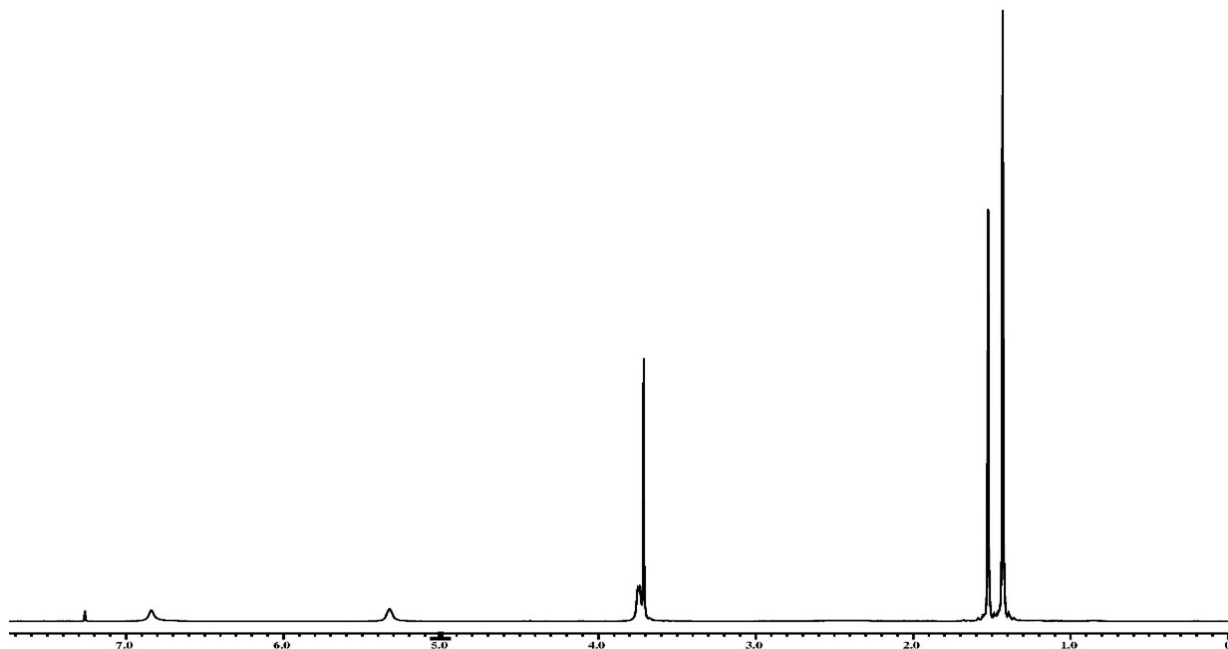
<i>1. Supporting information Figure S1</i>	3
<i>2. Supporting information Figure S2</i>	3
<i>3. Supporting information Figure S3</i>	4
<i>4. Supporting information Figure S4</i>	4
<i>5. Supporting information Figure S5</i>	5
<i>6. Supporting information Figure S6</i>	5
<i>7. Supporting information Figure S7</i>	6
<i>8. Supporting information Figure S8</i>	6
<i>9. Supporting information Figure S9</i>	7
<i>10. Supporting information Figure S10</i>	7
<i>11. Supporting information Figure S11</i>	8
<i>12. Supporting information Figure S12</i>	8
<i>13. Supporting information Figure S13</i>	9
<i>142. Supporting information Figure S14</i>	9
<i>15. Supporting information Figure S15</i>	10
<i>16. Supporting information Figure S16</i>	10
<i>17. Supporting information Figure S17</i>	11
<i>18. Supporting information Figure S18</i>	11



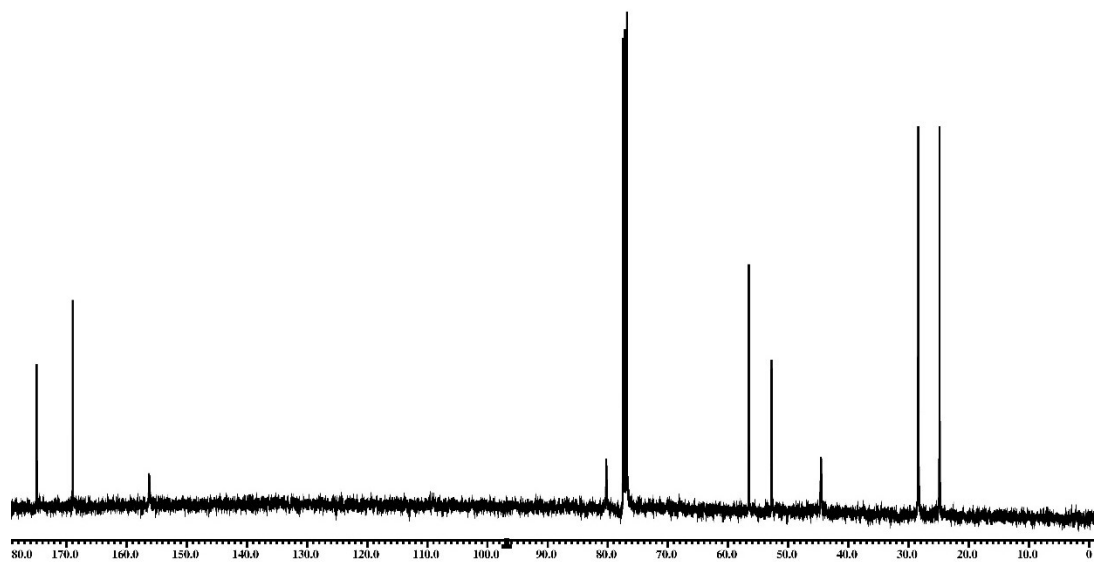
**Fig. S1.** Absorption spectra of (a) peptide 2 and (b) peptide 3 with increasing concentrations.



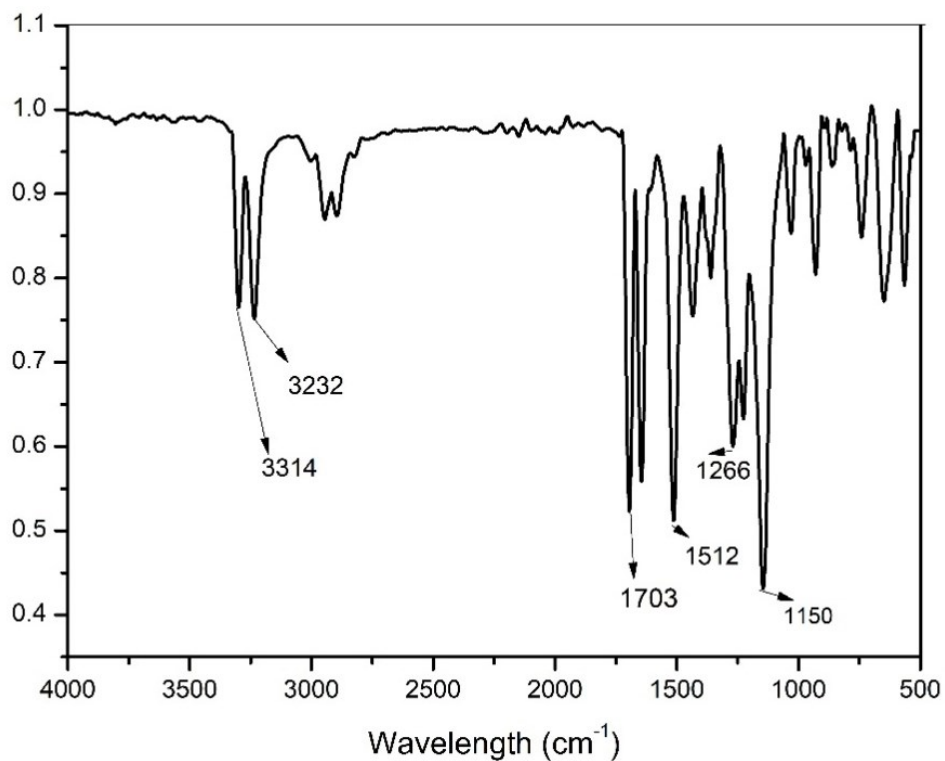
**Fig. S2.** Plots of the key absorbance intensities as a function of concentration of (a) peptide 2 at 259nm, (b) peptide 3 at 290nm and (c) peptide 4 at 282nm. The linear fitting show that the Beer-Lambert behavior have observed.



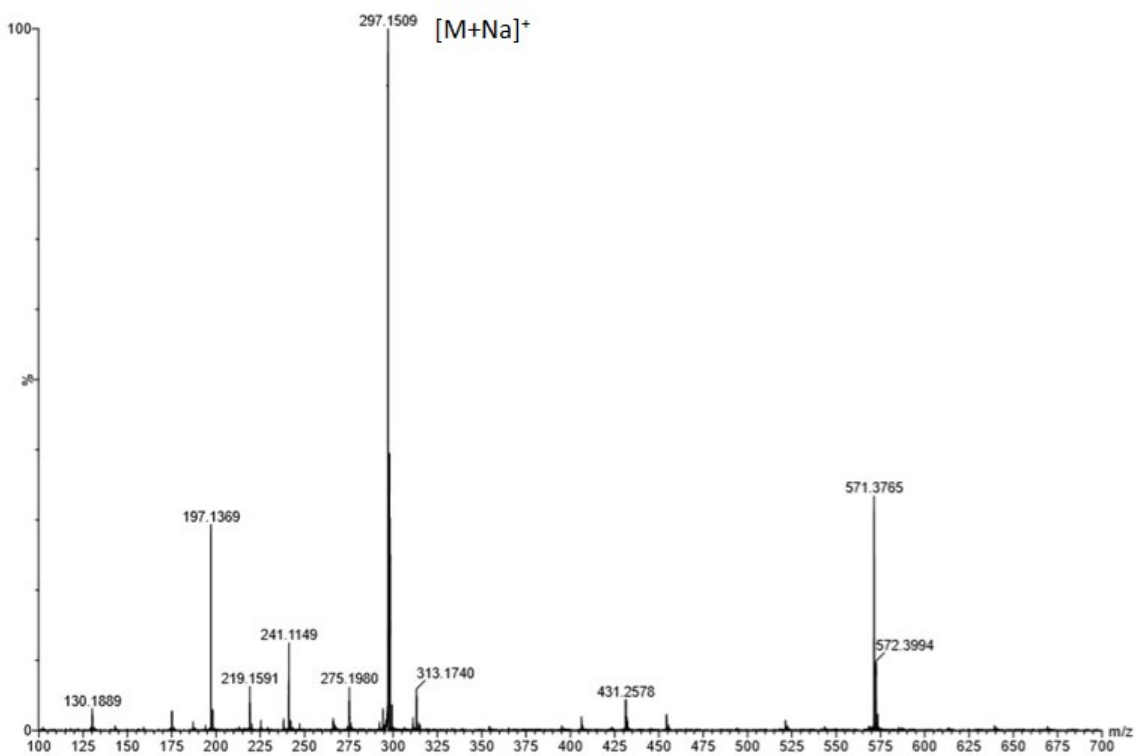
**Fig. S3:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra of BOC-Gly-Aib-OMe **1**.



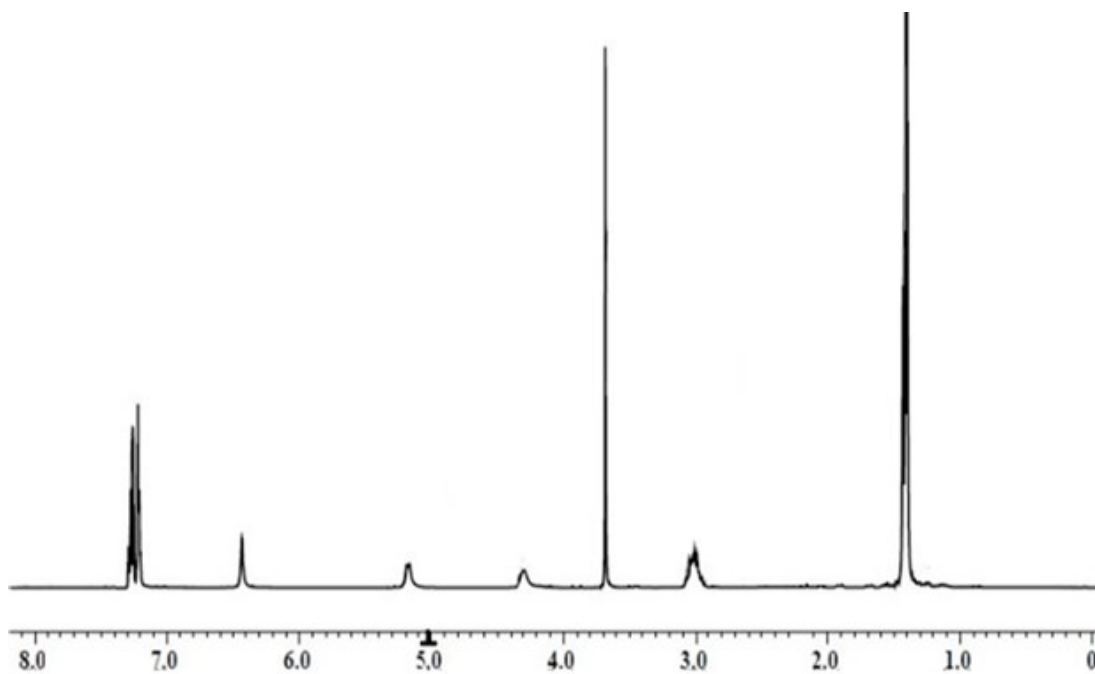
**Fig. S4:**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra of BOC-Gly-Aib-OMe **1**.



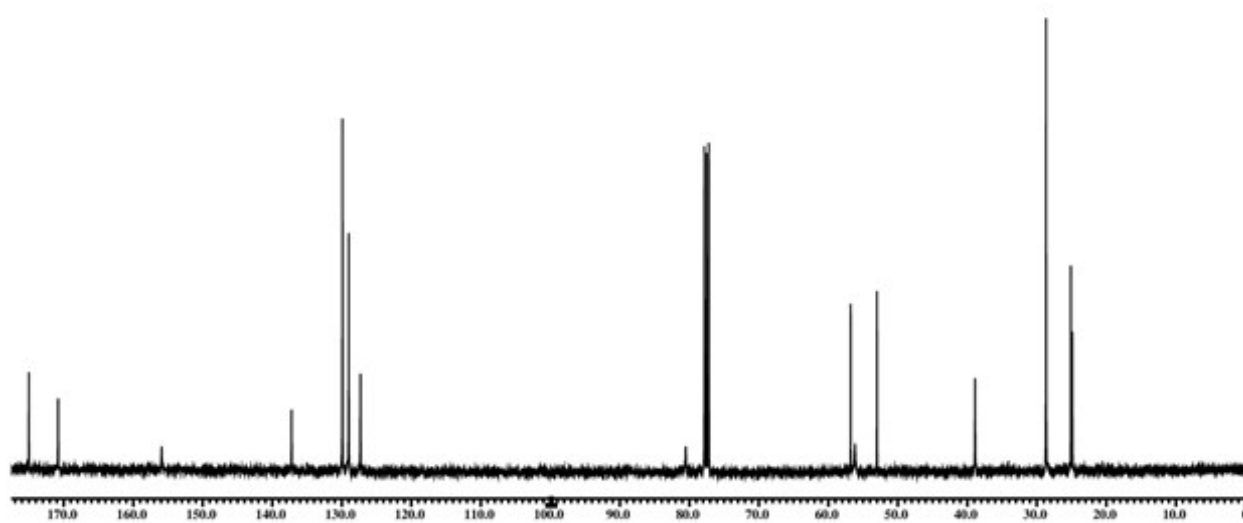
**Fig. S5:** FT-IR spectra of Boc-Gly-Aib-OMe 1.



**Fig. S6:** Mass Spectra of Boc-Gly-Aib-OMe 1.



**Fig. S7:**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra Boc-Phe-Aib-OMe **2**.



**Fig. S8:**  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra Boc-Phe-Aib-OMe **2**.

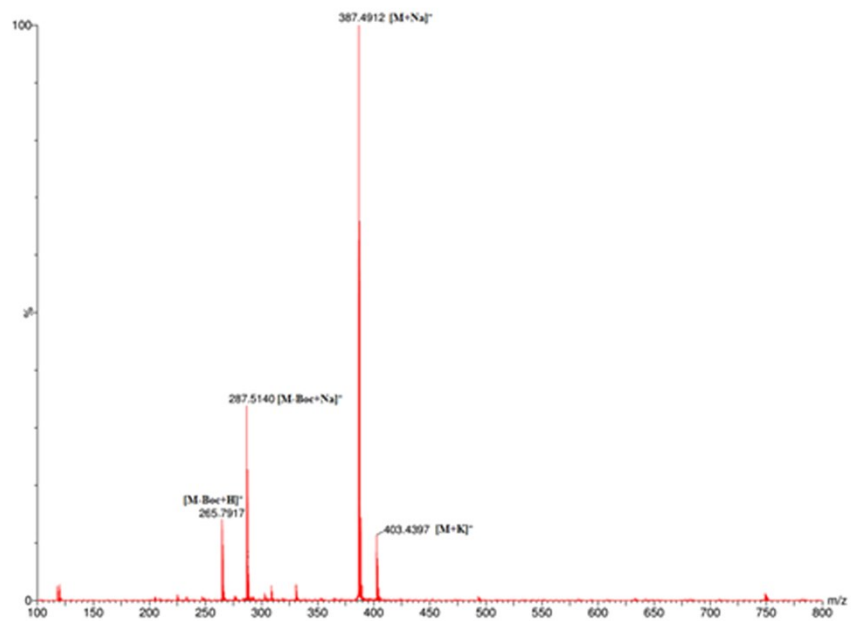


Fig. S9: Mass spectrum of Boc-Phe-Aib-OMe 2.

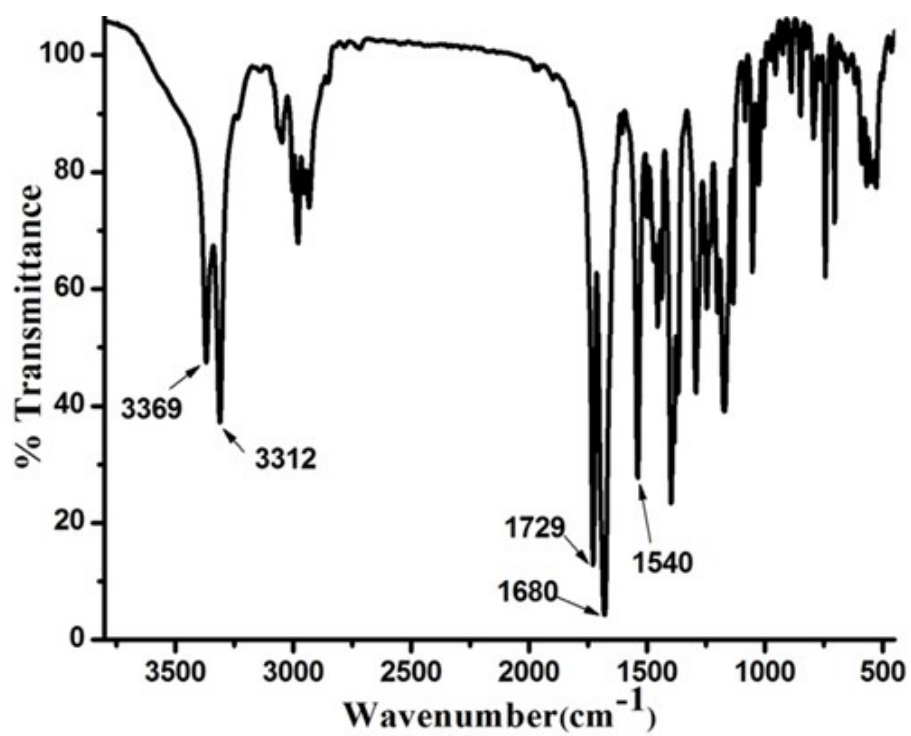
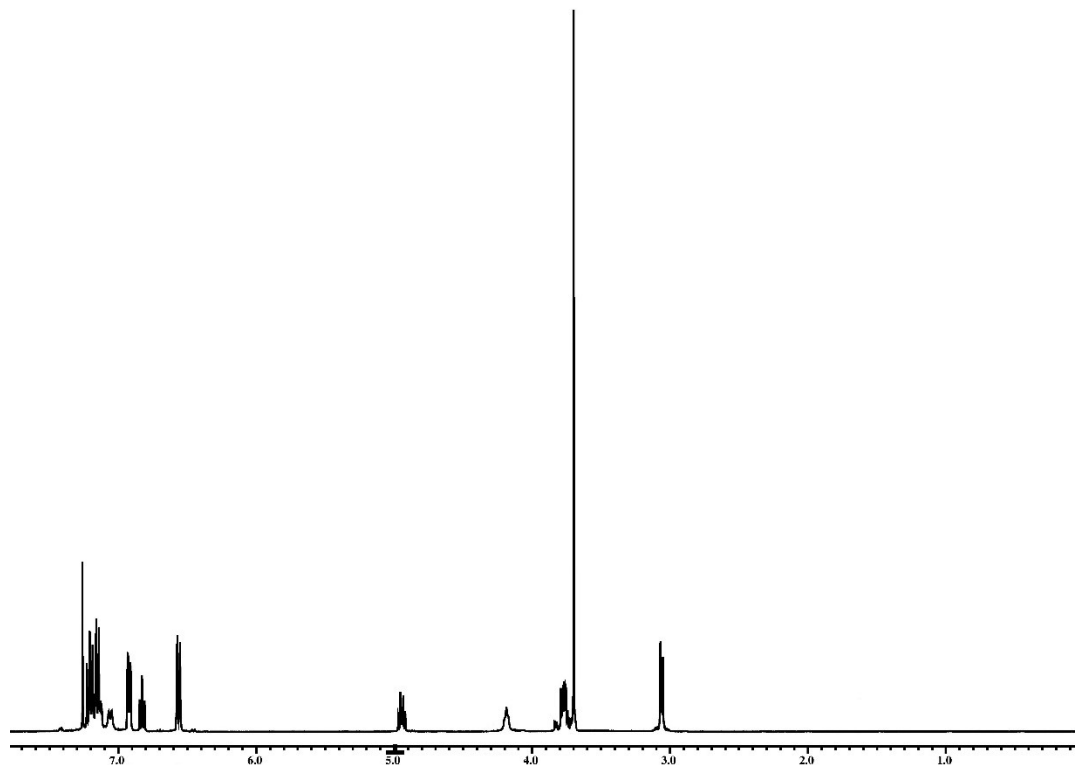
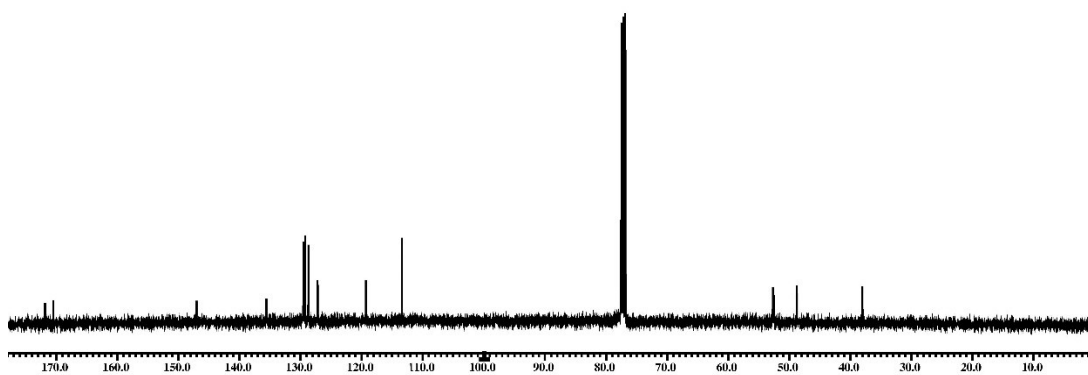


Fig. S10: FT-IR spectrum of Boc-Phe-Aib-OMe 2.



**Fig. S11:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ,  $\delta$  ppm) spectra of NPG-Phe-OMe **3**.



**Fig. S12:**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra of NPG-Phe-OMe **3**.



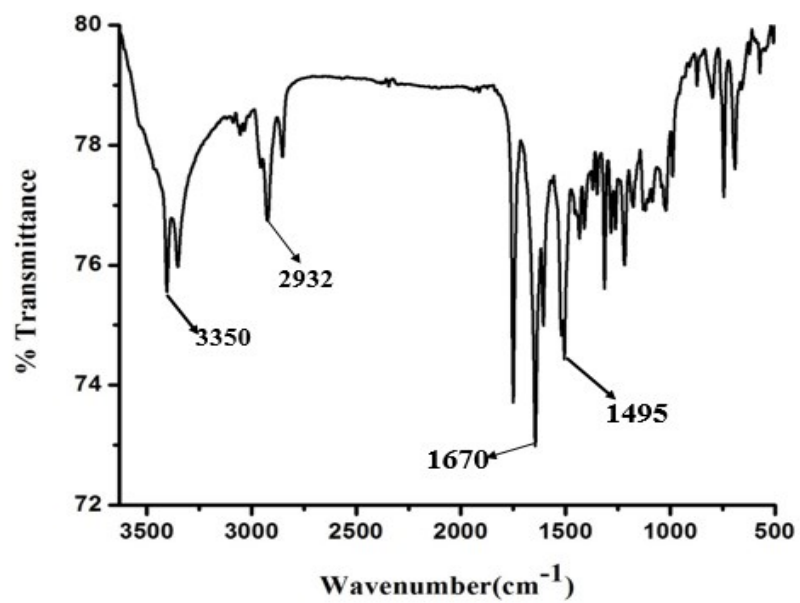


Fig. S13: IR spectra of NPG-Phe-OMe 3.

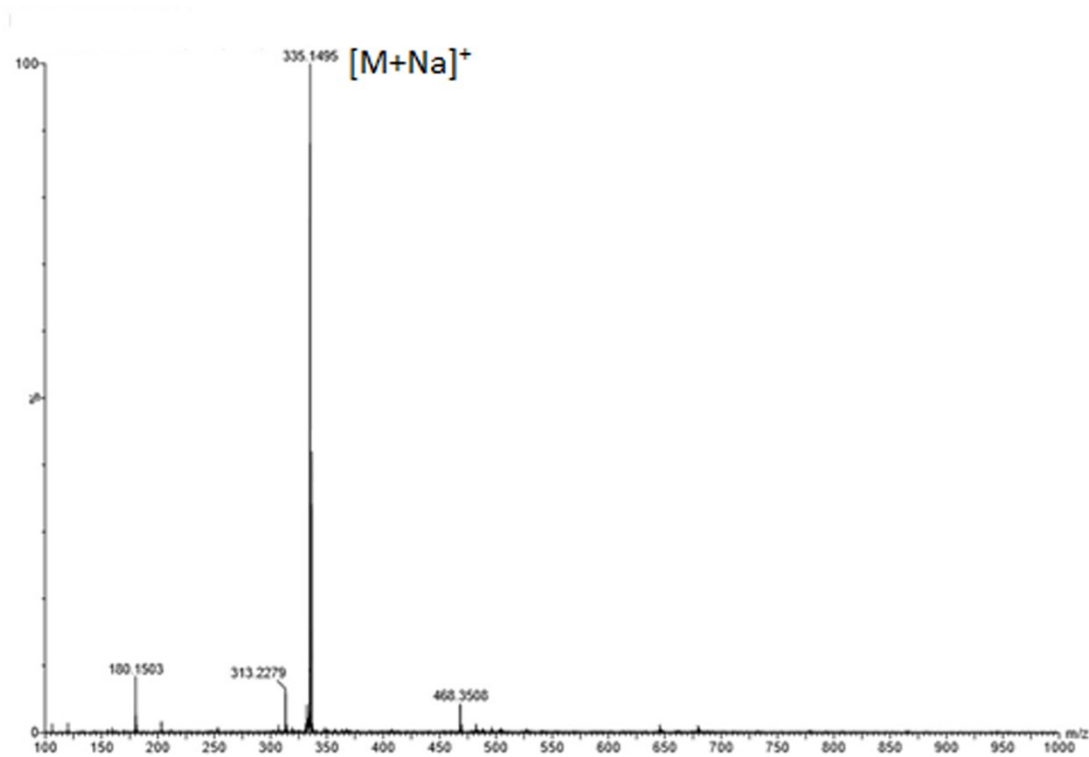
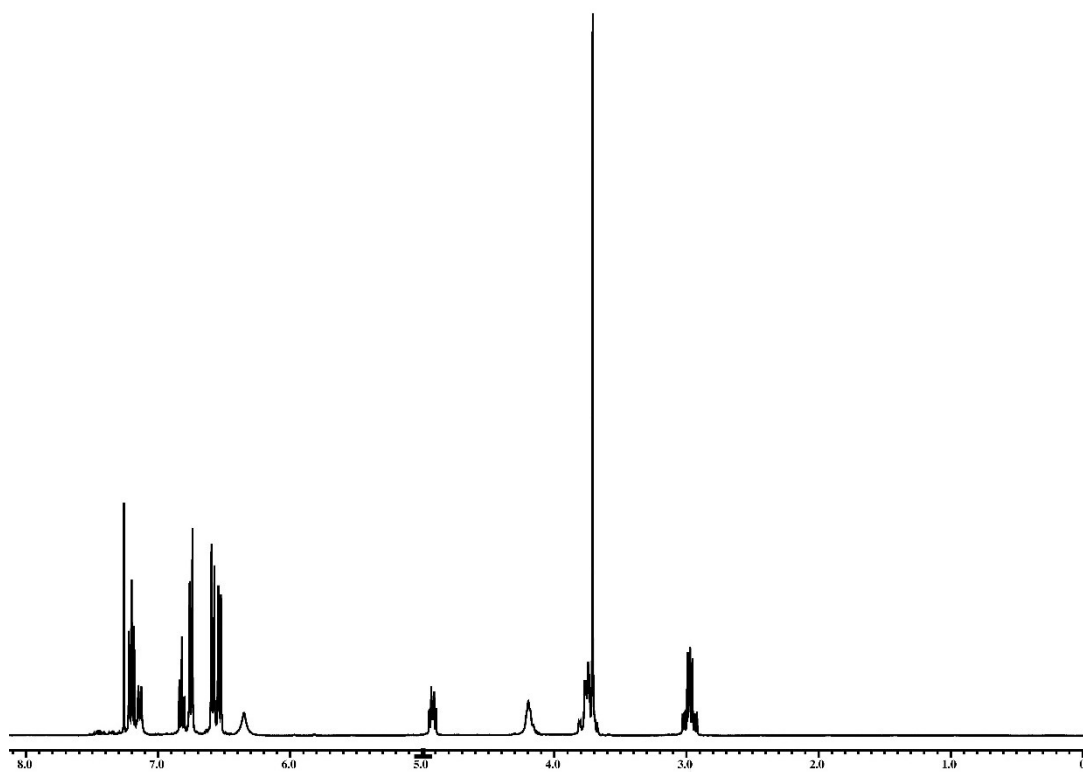
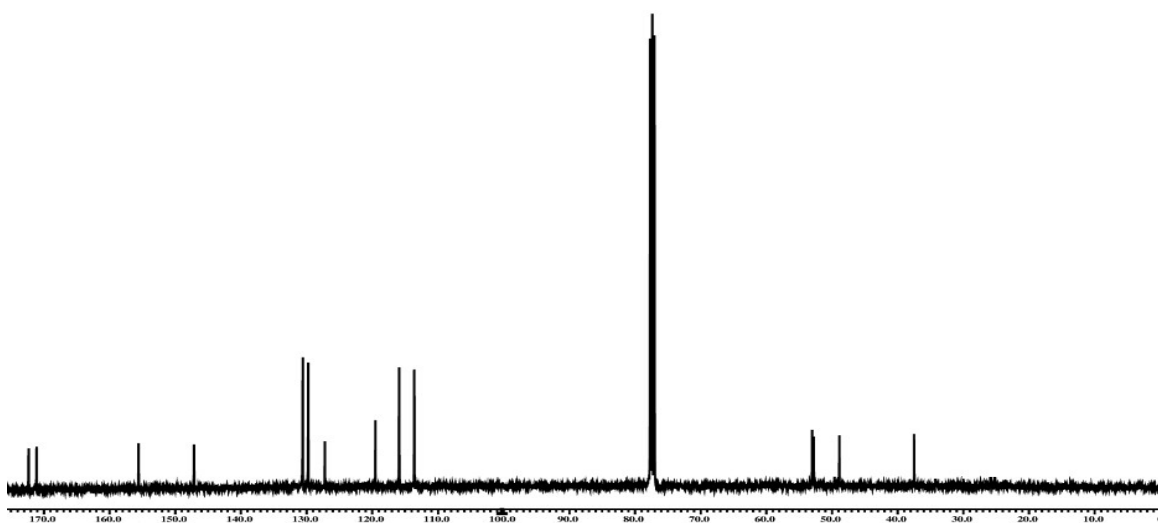


Fig. S14: Mass Spectra of NPG-Phe-OMe 3.



**Fig. S15:**  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra of NPG-Tyr-OMe **4**.



**Fig. S16:**  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ,  $\delta$  in ppm, 298K) spectra NPG-Tyr-OMe **4**.

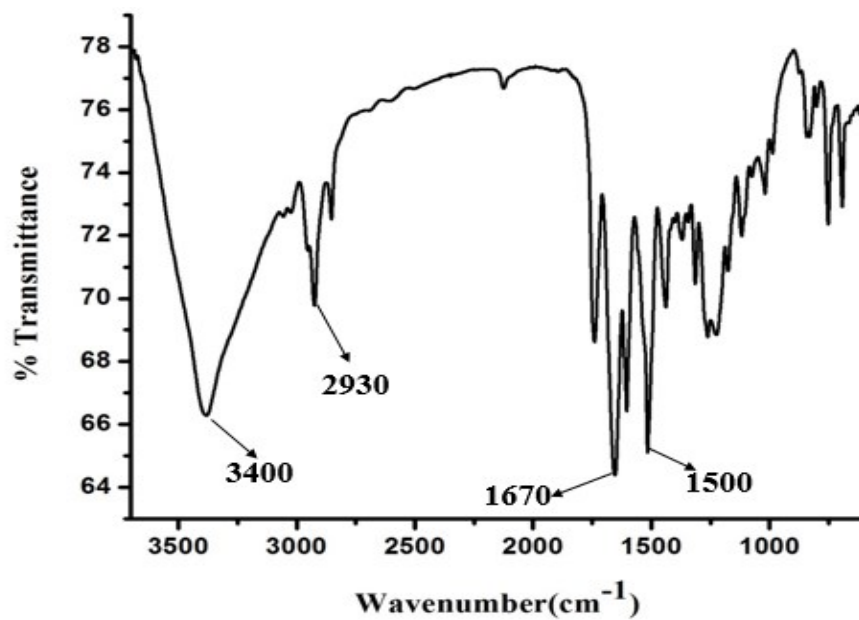


Fig. S17: IR spectra of NPG-Tyr-OMe 4.

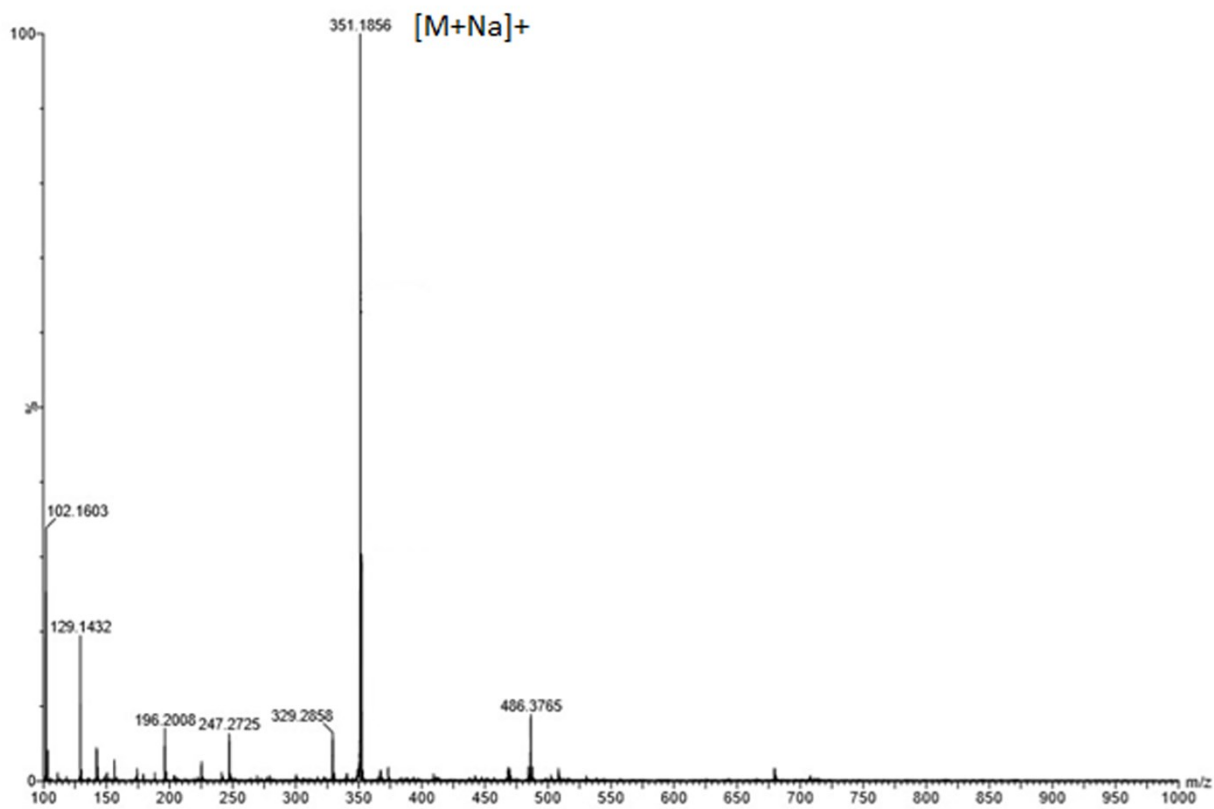


Fig. S18: Mass Spectra of NPG-Tyr-OMe 4.