

## **Supporting Information**

# **Versatility in Self-assembly and Morphology of Non-Coded Anthranilic acid and Phenylglycine based Dipeptide Stereoisomers**

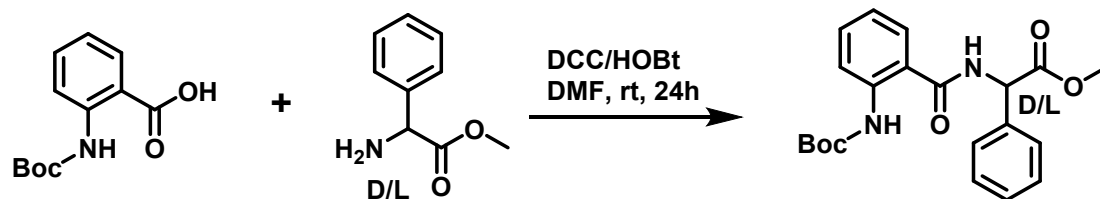
Gobinda Dolai, Rajat Subhra Giri and Bhubaneswar Mandal\*

Department of Chemistry, Laboratory of Peptide and Amyloid Research, Indian Institute of Technology Guwahati, Assam- 781039, India.

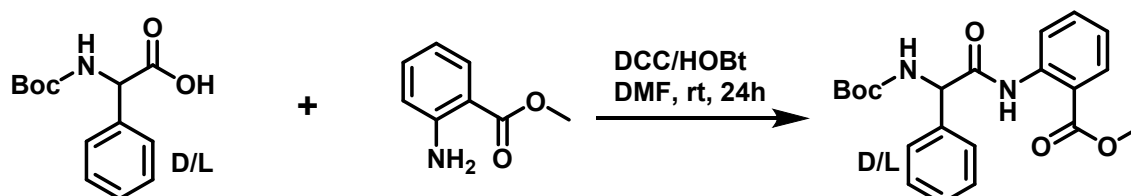
E-mail: [bmandal@iitg.ac.in](mailto:bmandal@iitg.ac.in)

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**Figure S1.** Schematic presentation of synthesis of di-peptide 1 and 2



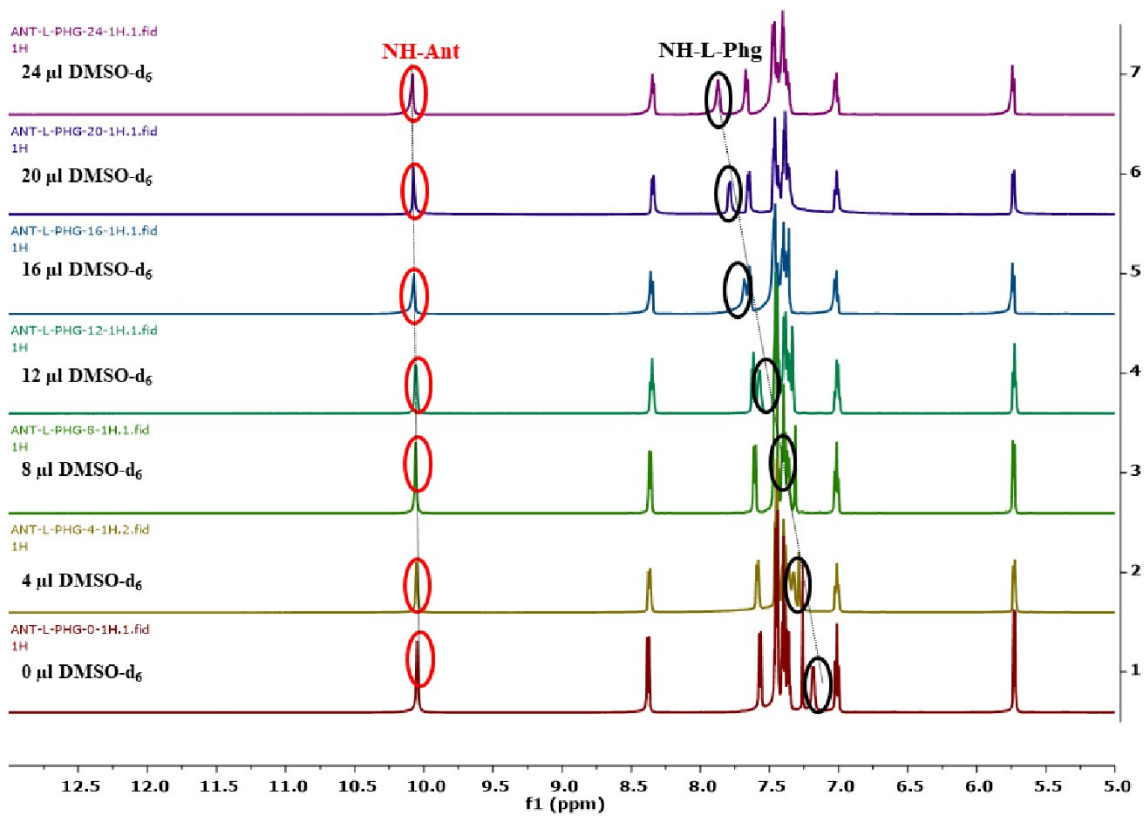
**Figure S2.** Schematic presentation of synthesis of di-peptide 3 and 4

**Table S1:** Selected backbone torsion angles ( $^{\circ}$ ) of peptide

peptide	$\omega_0$	$\omega_1$	$\phi_1$	$\phi_2$	$\psi_1$	$\psi_2$	$\theta_1$	
<b>Peptide 1</b>	N1-C5- O1-C2 = -177.0(2)	C6-N1- C5-O1 = 170.5(3)	C13-N2- C12-C11 = 178.3(3)	C11-C6- N1-C5 = -169.0(3)	C20-C13- N2-C12 = -63.9(3)	N2-C12- C11-C6 = -148.9(3)	O5-C20- C13-N2 = 156.2(3)	N1-C6- C11-C12 = -6.7(4)
<b>Peptide 2</b>	N1-C5- O1-C2 = 177.6(2)	C6-N1- C5-O1 = -170.5(2)	C13-N2- C12-C11 =- 178.4(2)	C11-C6- N1-C5 = -169.6(2)	C20-C13- N2-C12 = 63.9(2)	N2-C12- C11-C6 = -148.5(2)	O5-C20- C13-N2 = -156.4(2)	N1-C6- C11-C12 = 6.7(3)
<b>Peptide 3</b>	N1-C5- O1-C1 = -171.7(3)	C6-N1- C5-O1 = 175.4(3)	C14-N2- C13-C6 = 178.6(3)	C13-C6- N1-C5 = -108.2(3)	C19-C14- N2-C13 = 162.9(3)	N2-C13- C6-N1 = 147.3(3)	O5-C20- C19-C14 =- 177.2(3)	N2-C14- C19-C20 = 4.0(5)
<b>Peptide 4</b>	N1-C5- O1-C1 = 171.8(3)	C6-N1- C5-O1 = -175.4(2)	C14-N2- C13-C6 = -178.6(2)	C13-C6- N1-C5 = 108.4(3)	C19-C14- N2-C13 = -162.9(3)	N2-C13- C6-N1 = -147.4(2)	O5-C20- C19-C14 = 177.0(2)	N2-C14- C19-C20 = -4.0(4)

**Table S2:** Chemical shift  $\delta$  (ppm) of hydrogen bonded protons with addition of DMSO- $d_6$ 

<b>Peptide 1</b>							
<b>DMSO-<math>d_6</math> (<math>\mu</math>L)</b>	<b>0</b>	<b>4</b>	<b>8</b>	<b>12</b>	<b>16</b>	<b>20</b>	<b>24</b>
NH-Phg	7.189	7.332	7.434	7.580	7.682	7.794	7.873
NH-Ant	10.049	10.053	10.060	10.063	10.072	10.075	10.081
<b>Peptide 2</b>							
NH-Phg	7.183	7.328	7.433	7.611	7.732	7.850	7.934
NH-Ant	10.048	10.055	10.060	10.063	10.071	10.081	10.086
<b>Peptide 3</b>							
NH-Phg	5.814	5.832	5.861	5.883	5.919	5.968	6.005
NH-Ant	11.500	11.507	11.518	11.522	11.526	11.539	11.543
<b>Peptide 4</b>							
NH-Phg	5.813	5.836	5.864	5.879	5.906	5.940	5.962
NH-Ant	11.500	11.510	11.521	11.524	11.529	11.538	11.539



**Figure S3:** Partial titration spectra of peptide 1 in CDCl<sub>3</sub> with DMSO-d<sub>6</sub>.

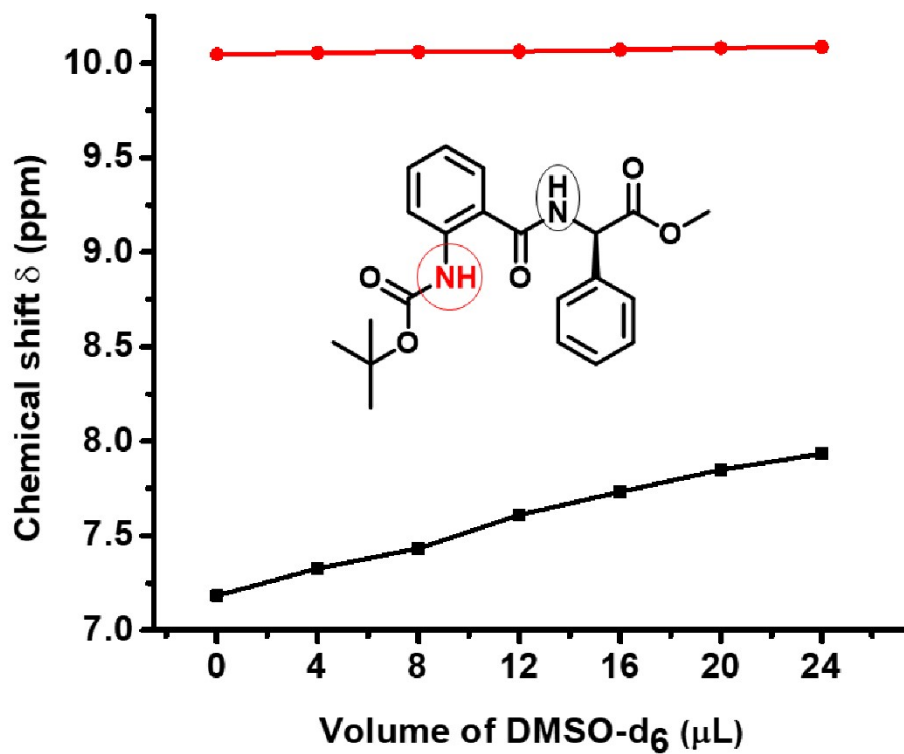


Figure S4: Solvent dependent <sup>1</sup>H-NMR titration of peptide 2.

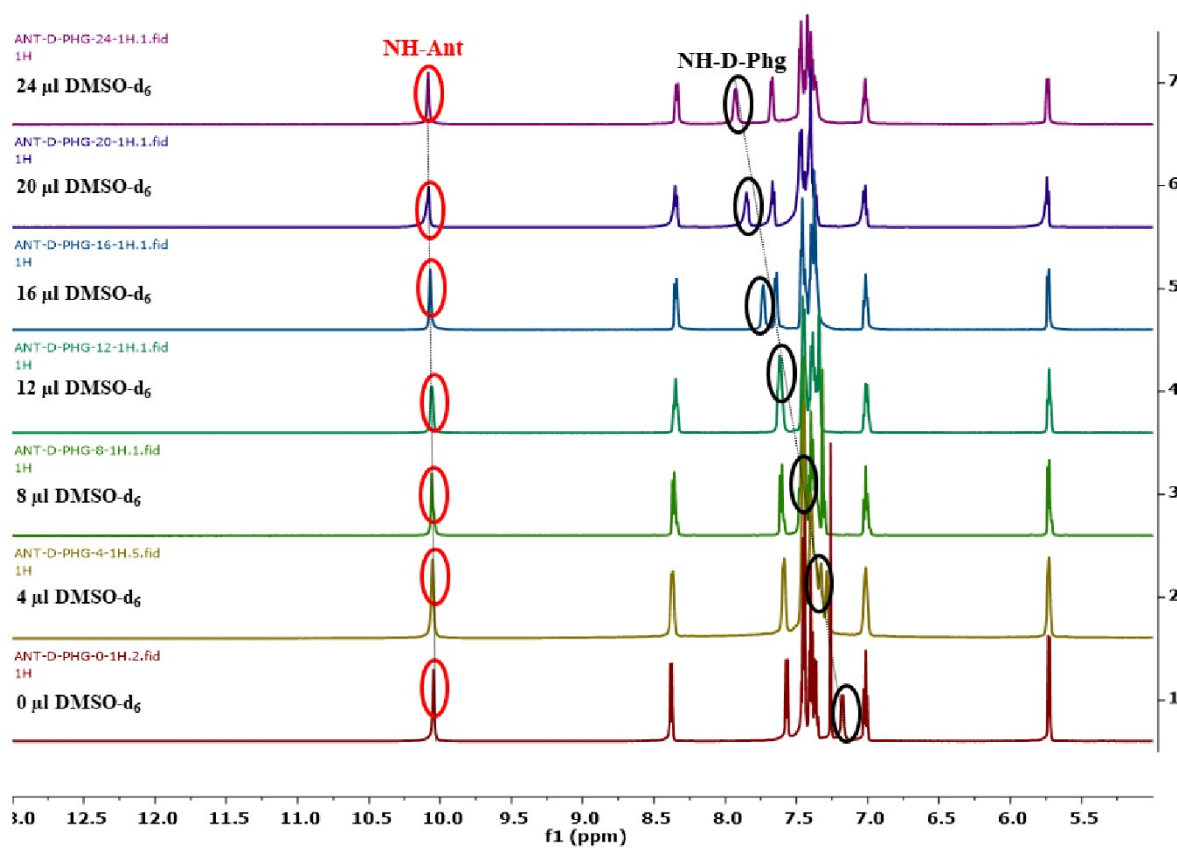
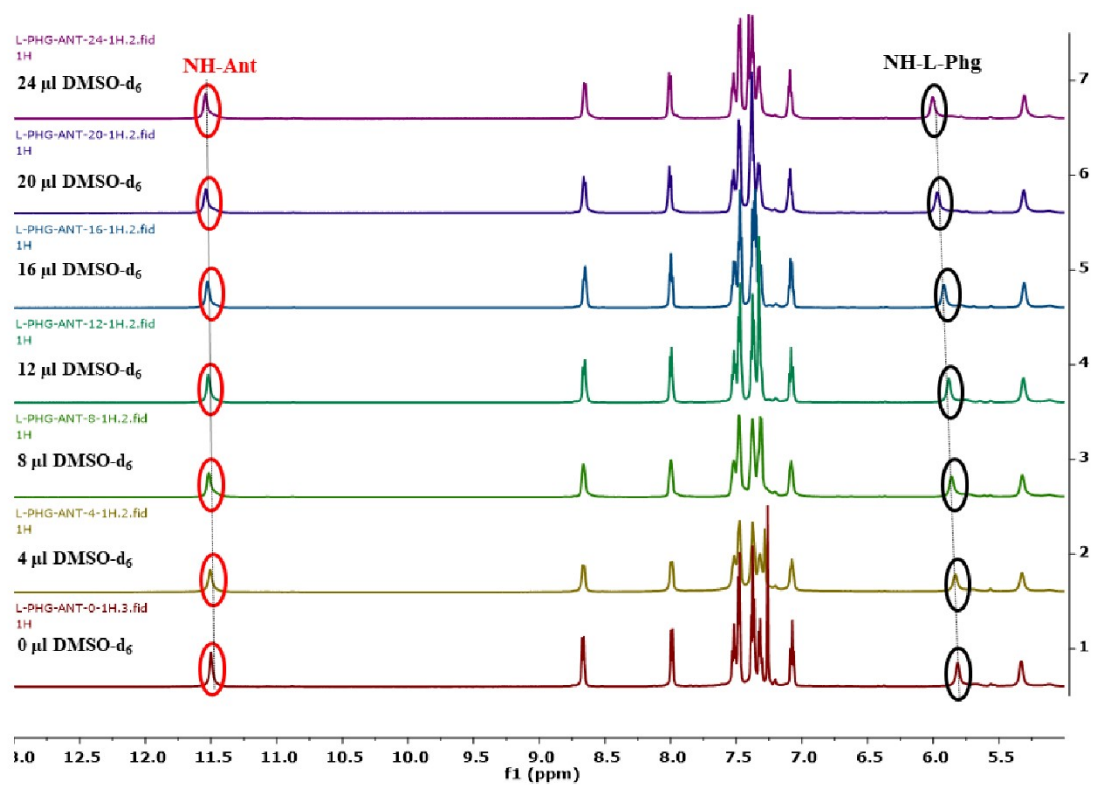


Figure S5: Partial titration spectra of peptide 2 in CDCl<sub>3</sub> with DMSO-d<sub>6</sub>.



**Figure S6:** Partial titration spectra of peptide **3** in  $\text{CDCl}_3$  with  $\text{DMSO-}d_6$ .

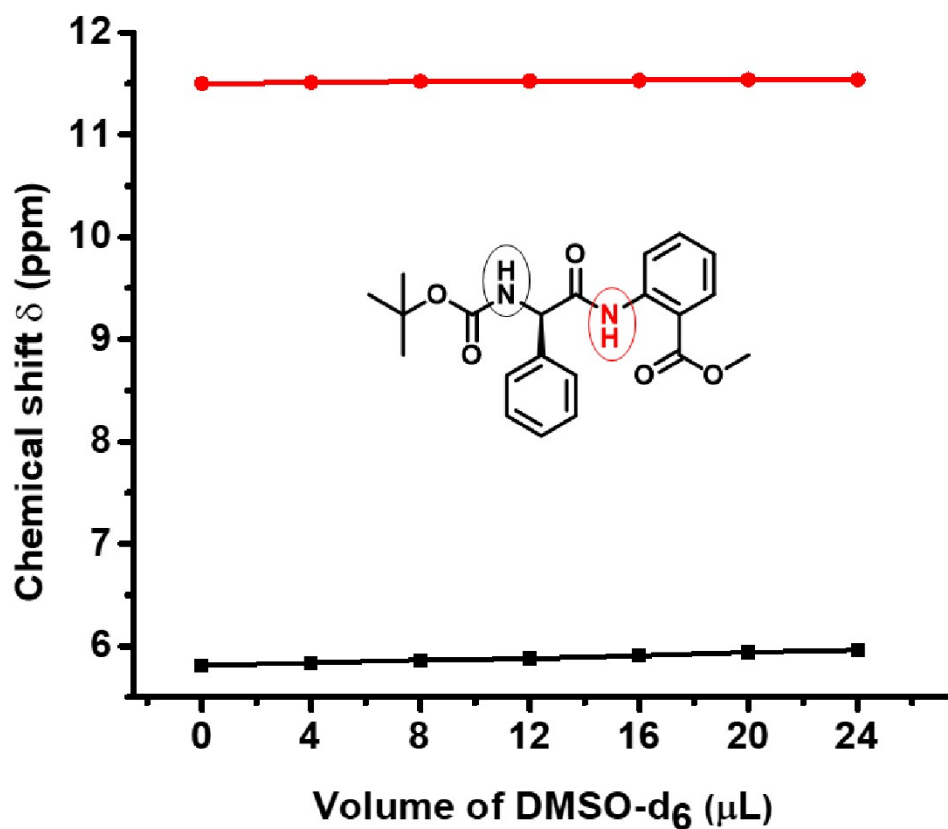


Figure S7: Solvent dependent  $^1\text{H-NMR}$  titration of peptide 4.

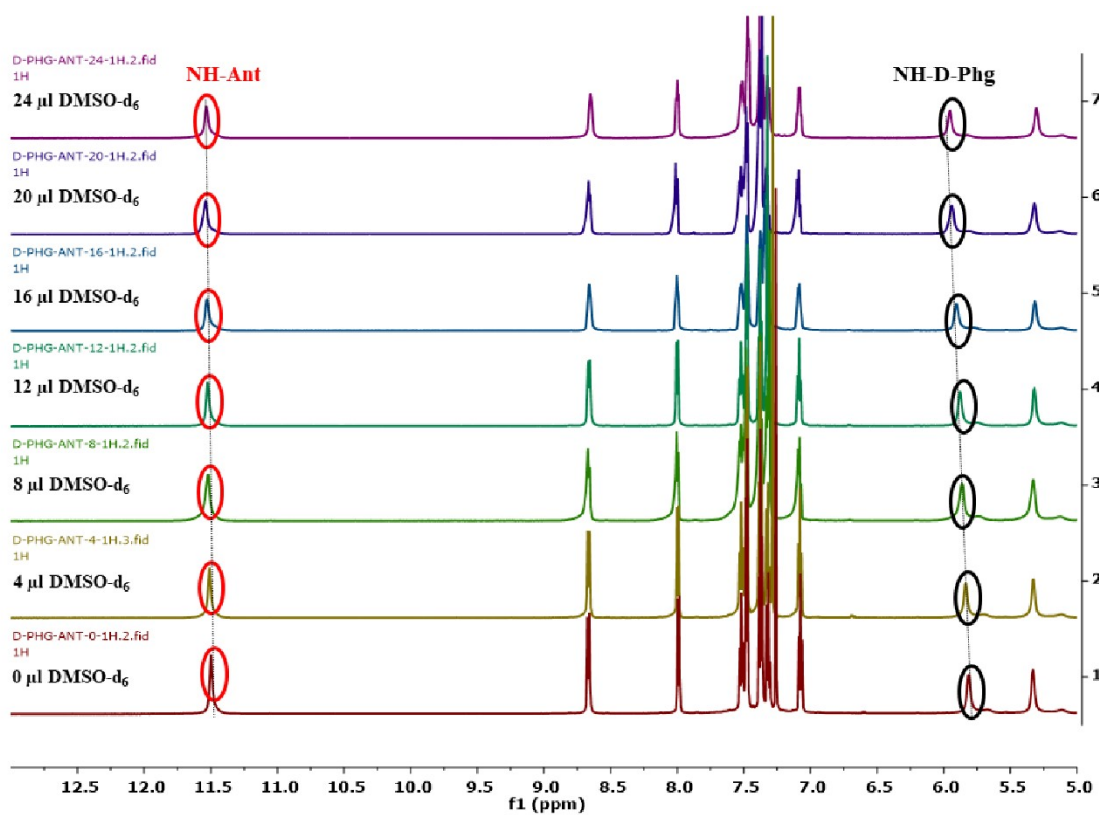
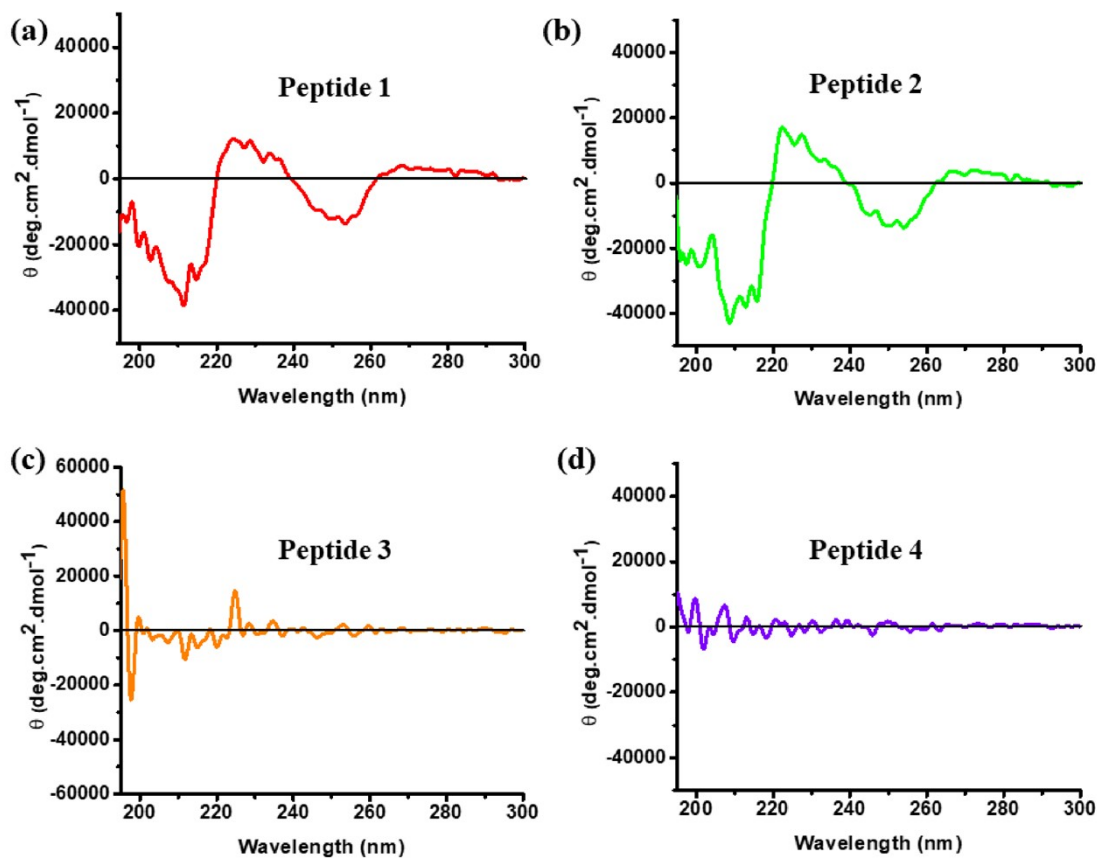
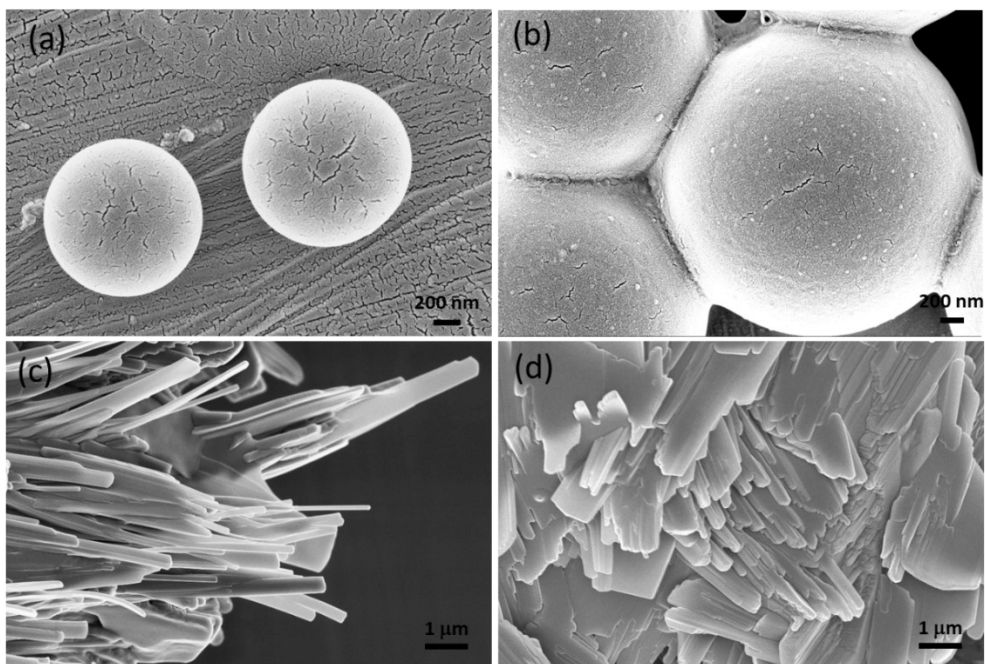


Figure S8: Partial titration spectra of peptide 4 in  $\text{CDCl}_3$  with DMSO- $d_6$ .

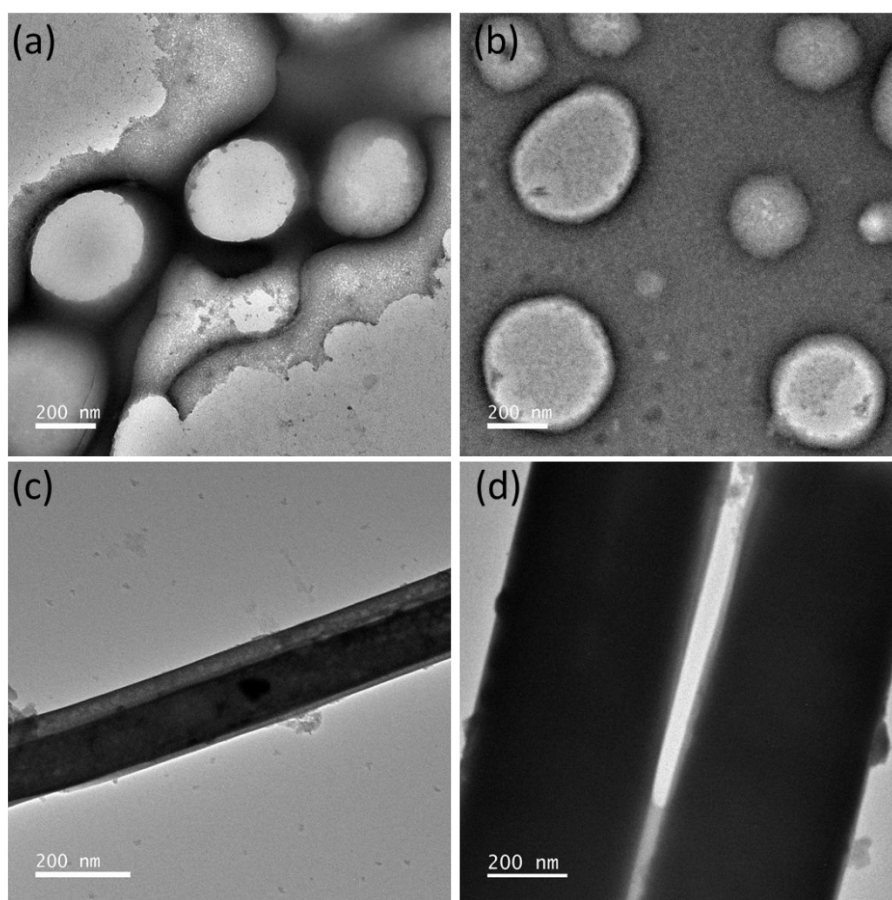




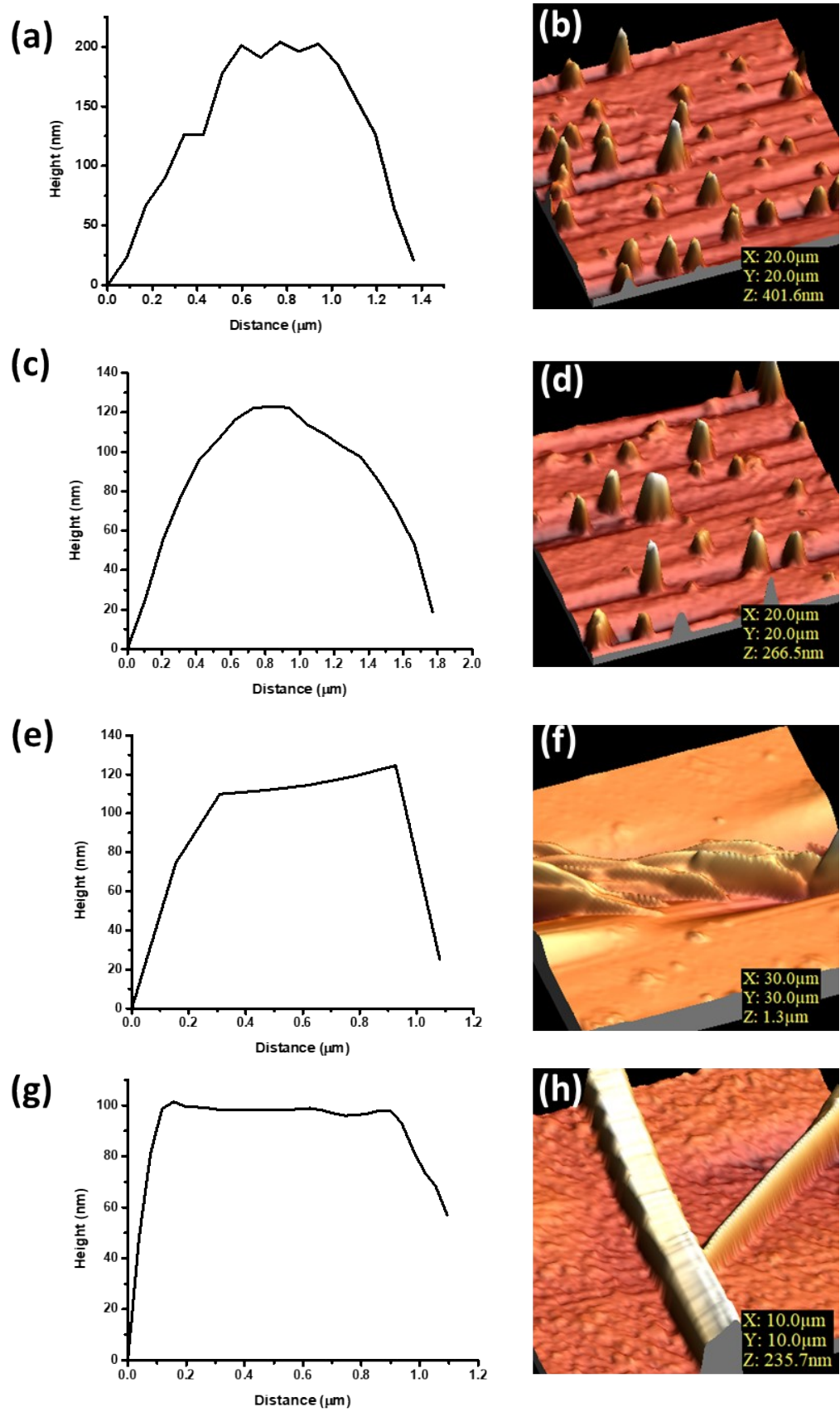
**Figure S9:** (a, b, c, d) represents CD spectra of 375  $\mu\text{M}$  peptide solution of 1, 2, 3 and 4, respectively in methanol.



**Figure S10.** a, b, c, and d displays high-resolution FE-SEM images of peptides 1, 2, 3, and 4, respectively.



**Figure S11.** a, b, c, and d exhibits high-resolution FETEM images of peptides 1, 2, 3, and 4, respectively.



**Figure S12.** (a, b), (c, d), (e, f), and (g, h) represent corresponding height to distance plot and 3D image in AFM of peptide 1, 2, 3, and 4, respectively.

## Spectra of Peptide Boc-Ant-L-Phg-OMe (1):

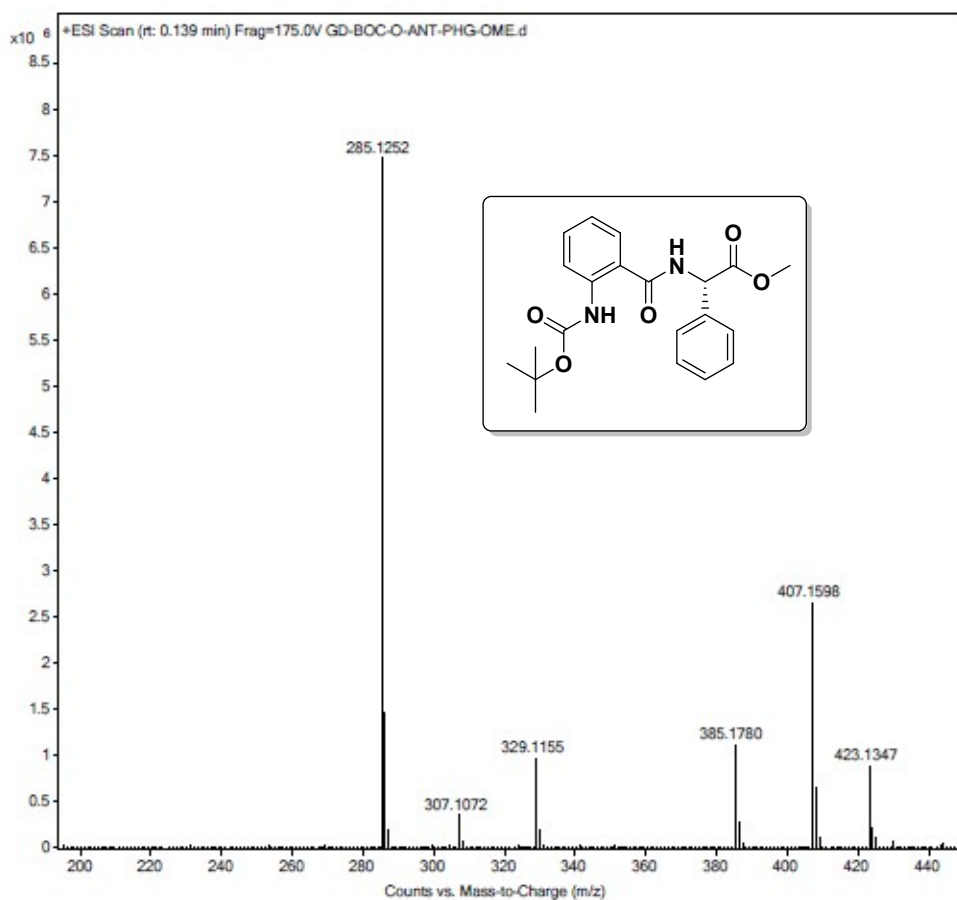


Figure S13. MS spectra of peptide Boc-Ant-L-Phg-OMe (1)

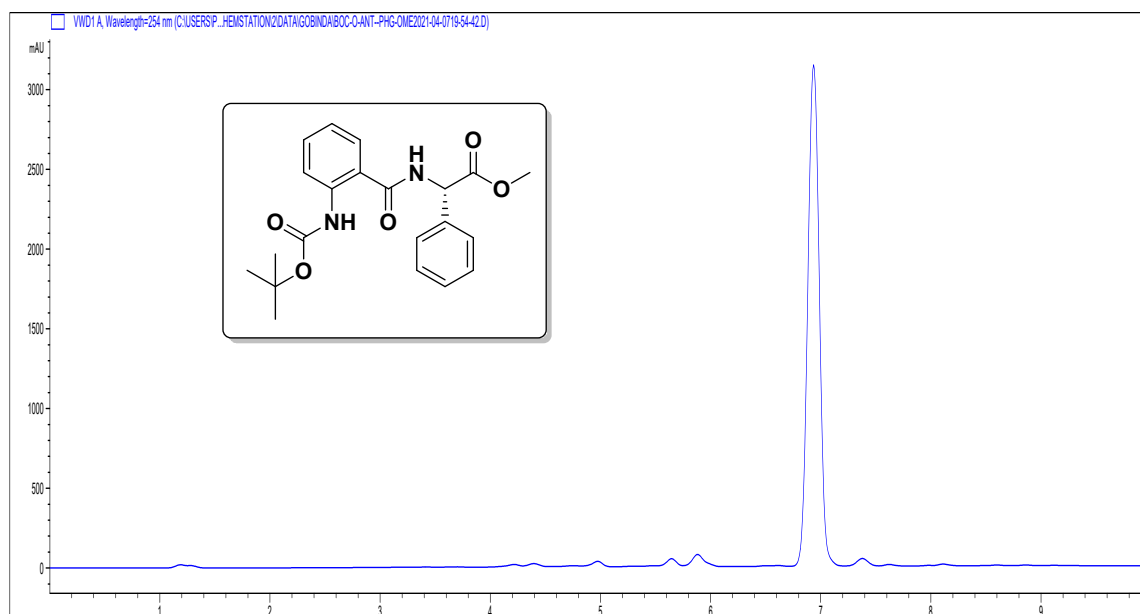


Figure S14. HPLC profile picture of purified peptide Boc-Ant-L-Phg-OMe (1)

GD-BOC-ANT-PHG-1H  
GD-BOC-ANT-PHG-1H

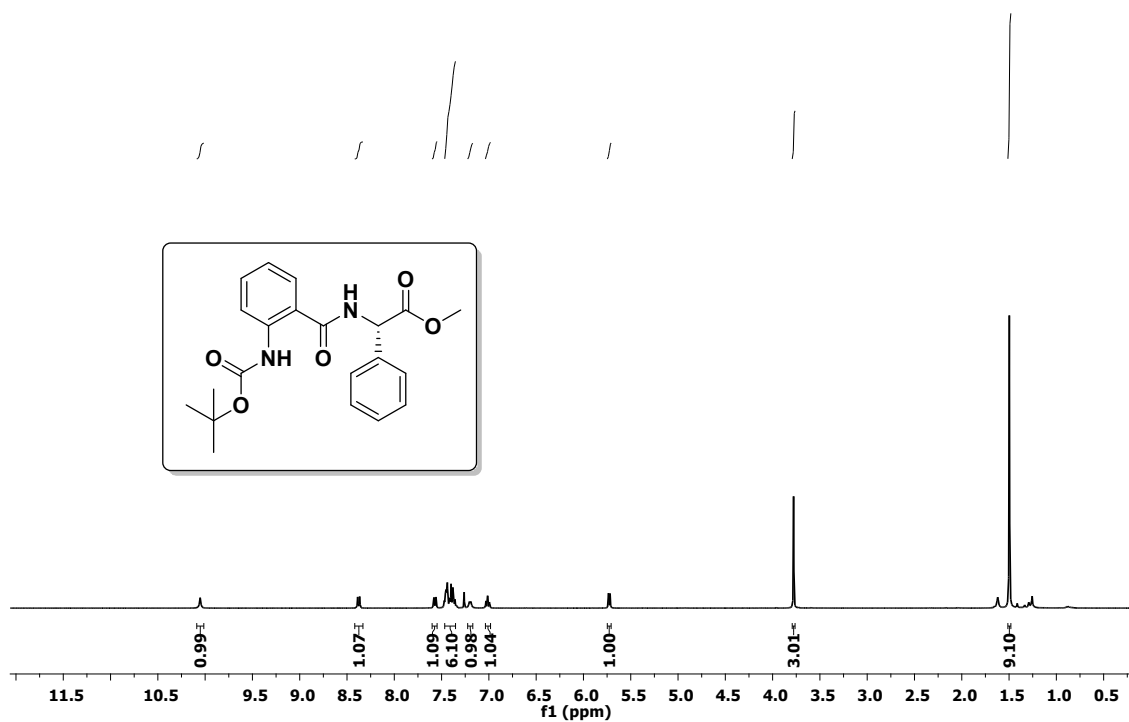


Figure S15.  $^1\text{H}$  NMR spectra of peptide **Boc-Ant-L-Phg-OMe (1)**

GD-BOC-ANT-PHG-13C  
GD-BOC-ANT-PHG-13C

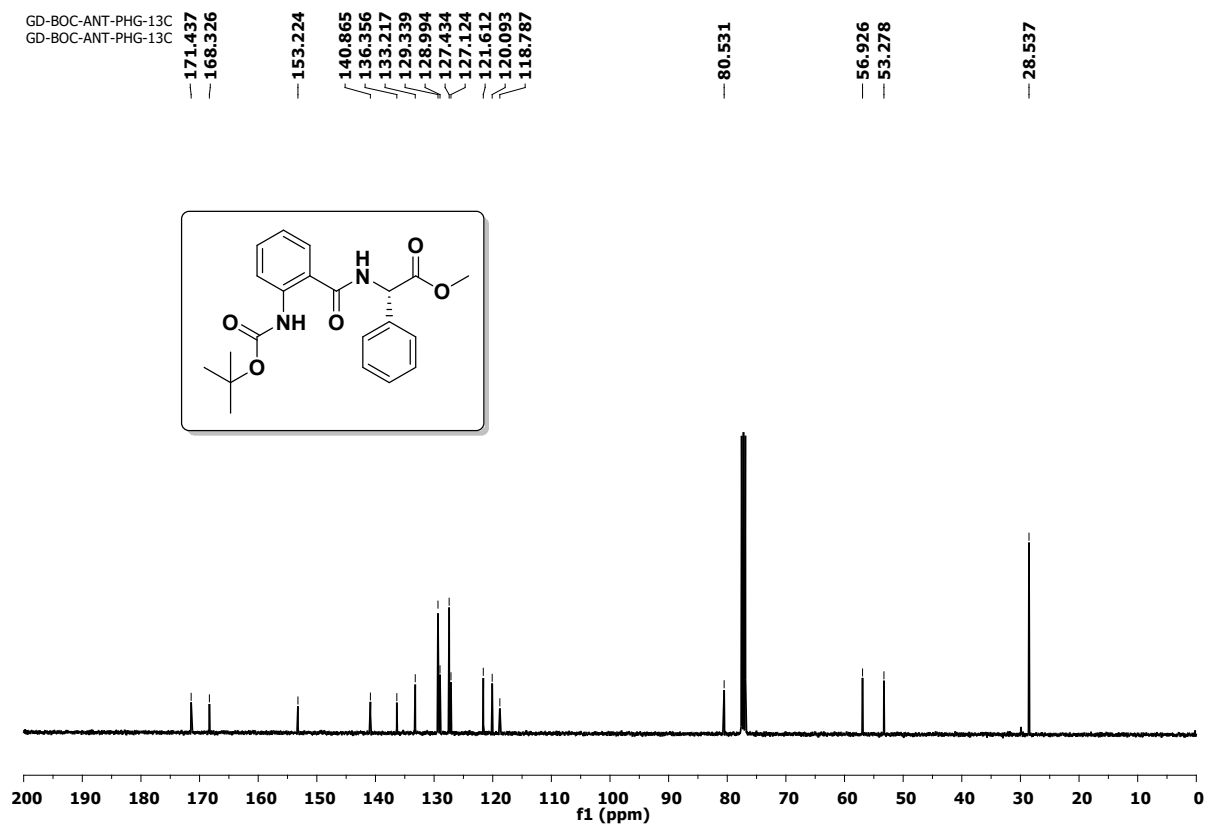


Figure S16.  $^{13}\text{C}$  NMR spectra of peptide **Boc-Ant-L-Phg-OMe (1)**

## Spectra of Peptide Boc-Ant-D-Phg-OMe (2):

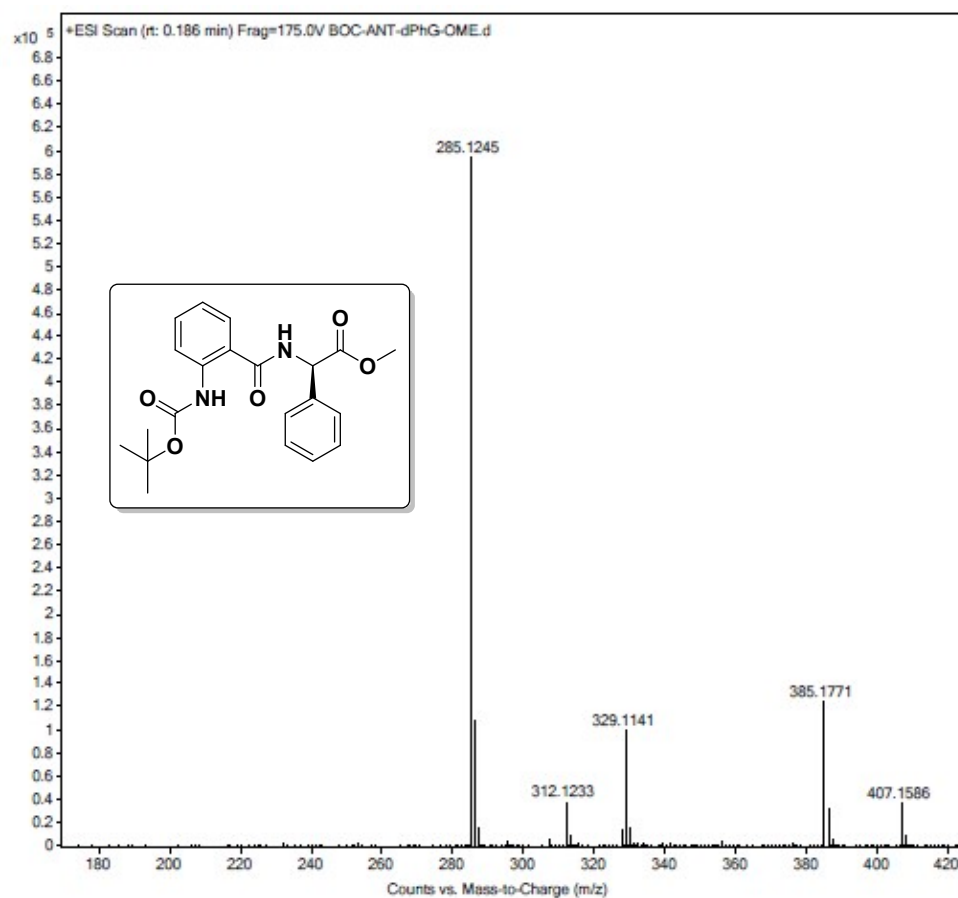


Figure S17. MS spectra of peptide Boc-Ant-D-Phg-OMe (2)

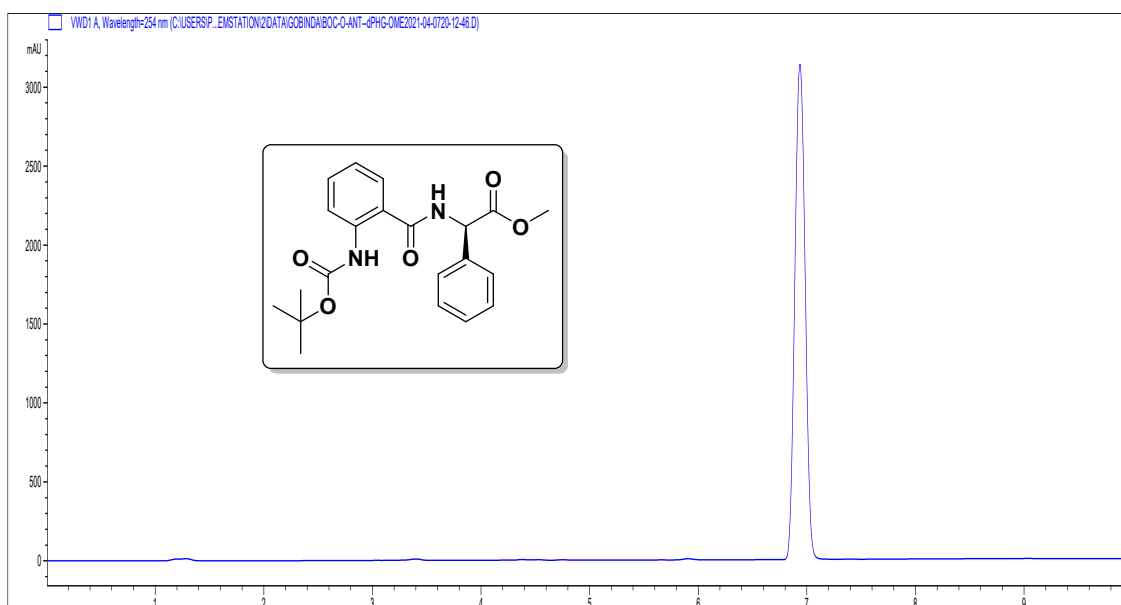


Figure S18. HPLC profile picture of purified peptide Boc-Ant-D-Phg-OMe (2)

GD-Boc-ANT-dPHG-1H  
GD-Boc-ANT-dPHG-1H

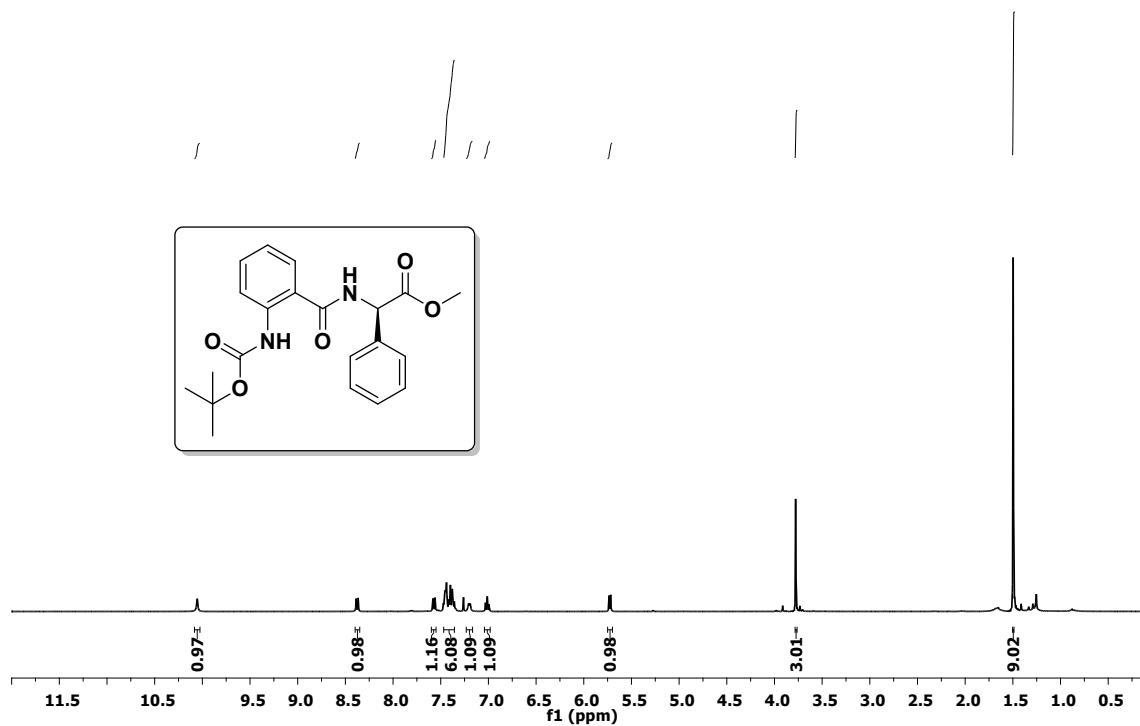


Figure S19. <sup>1</sup>H NMR spectra of peptide **Boc-Ant-D-Phg-OMe (2)**

GD-Boc-ANT-dPHG-13C  
GD-Boc-ANT-dPHG-13C

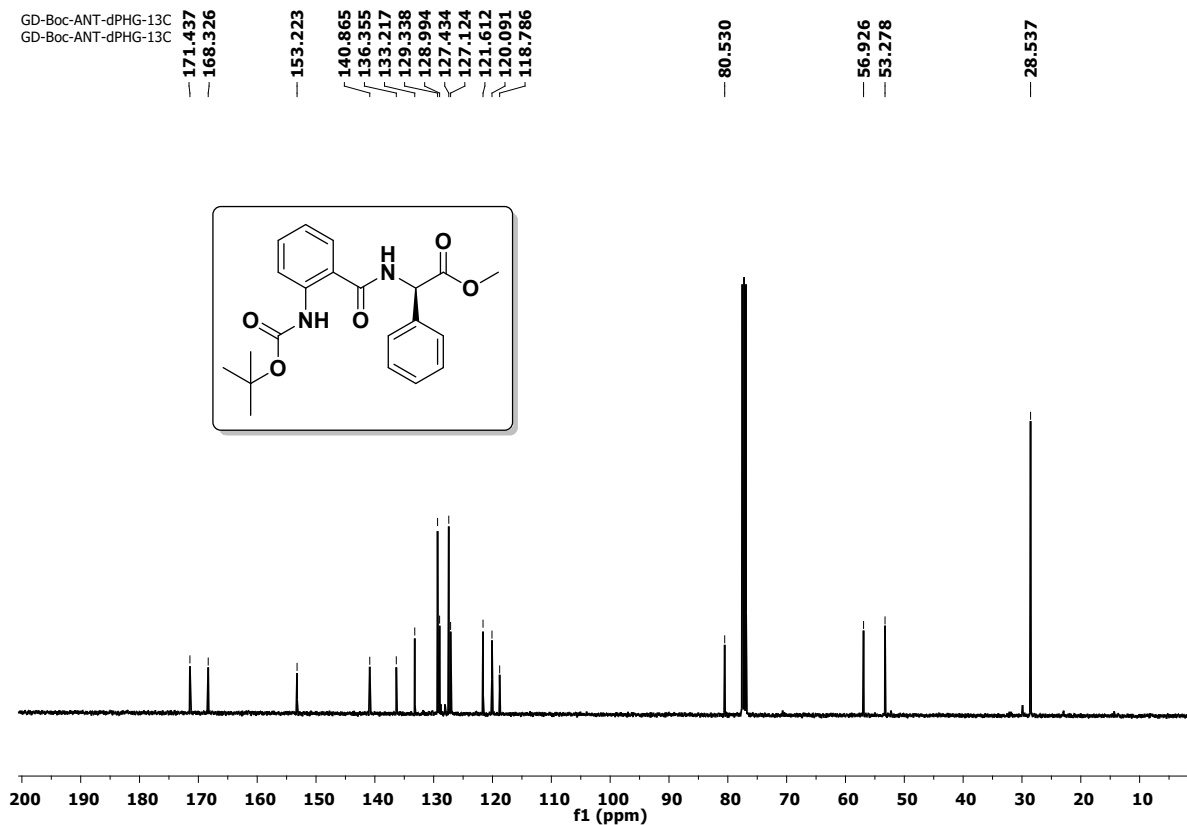


Figure S20. <sup>13</sup>C NMR spectra of peptide **Boc-Ant-D-Phg-OMe (2)**

## Spectra of Peptide Boc-L-Phg-Ant-OMe (3):

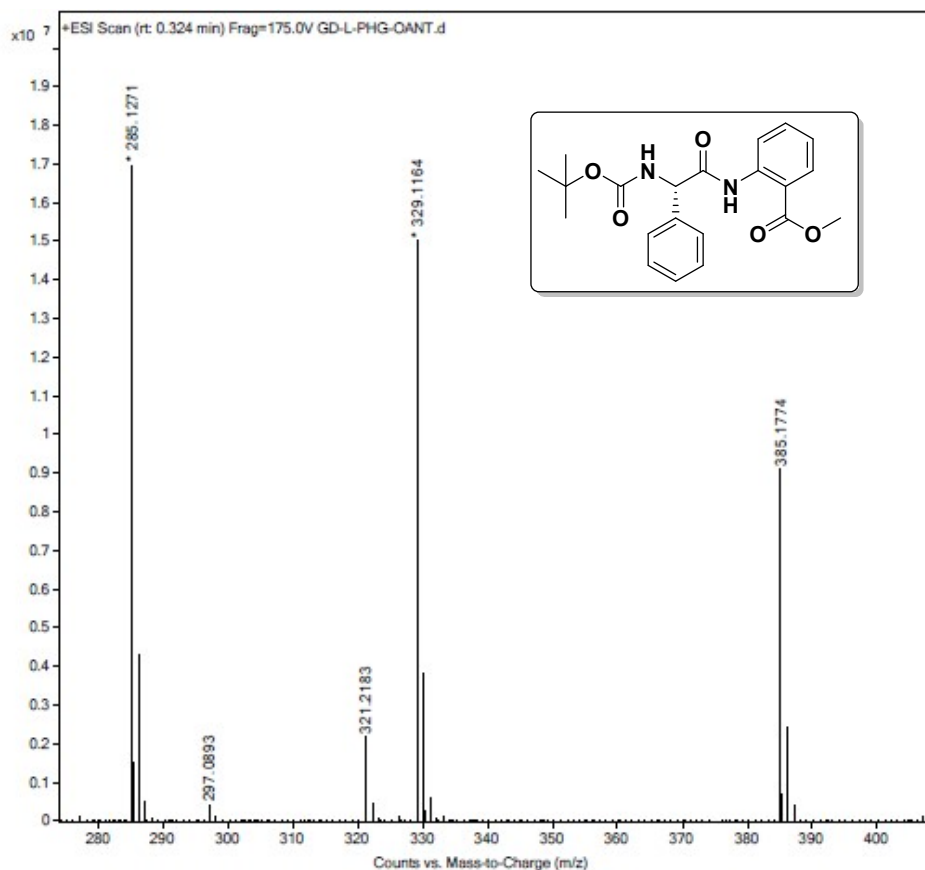


Figure S21. MS spectra of peptide Boc-L-Phg-Ant-OMe (3)

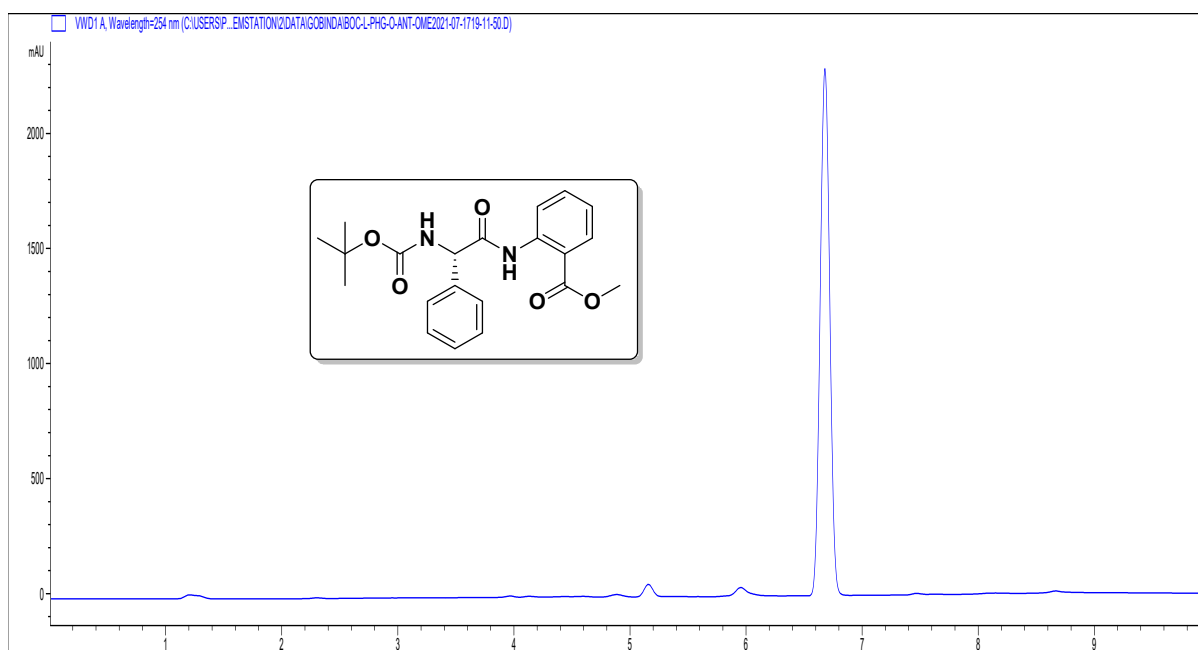


Figure S22. HPLC profile picture of purified peptide Boc-L-Phg-Ant-OMe (3)



L-PHG-OANT-1H.4.fid  
1H

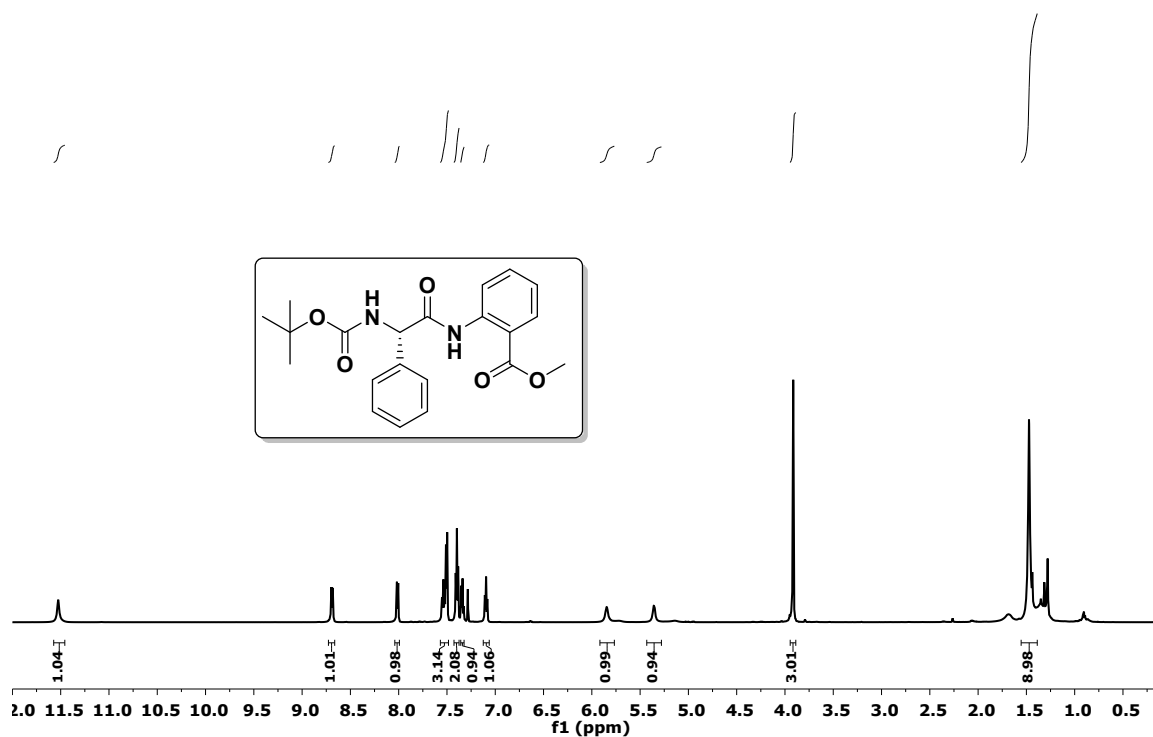


Figure S23. <sup>1</sup>H NMR spectra of peptide Boc-L-Phg-Ant-OMe (3)

L-PHG-OANT-13C.5.fid  
13C

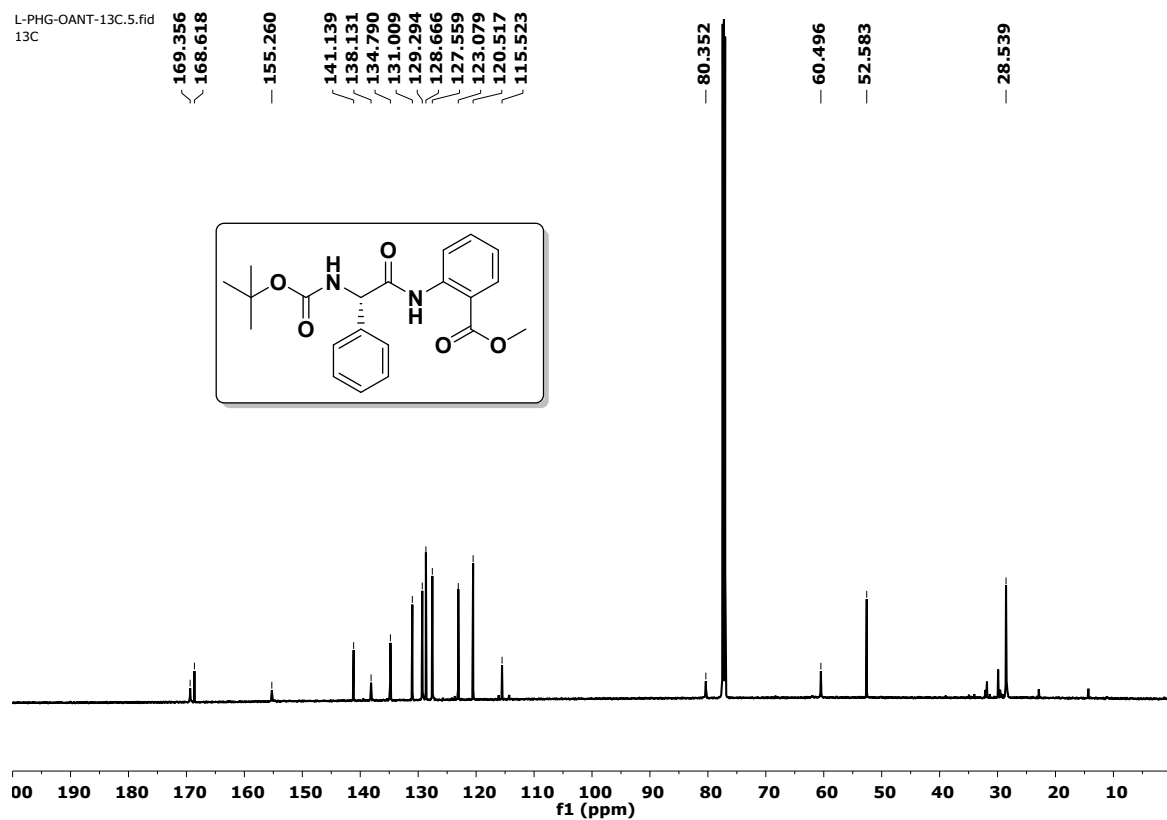


Figure S24. <sup>13</sup>C NMR spectra of peptide Boc-L-Phg-Ant-OMe (3)

## Spectra of Peptide Boc-D-Phg-Ant-OMe (4):

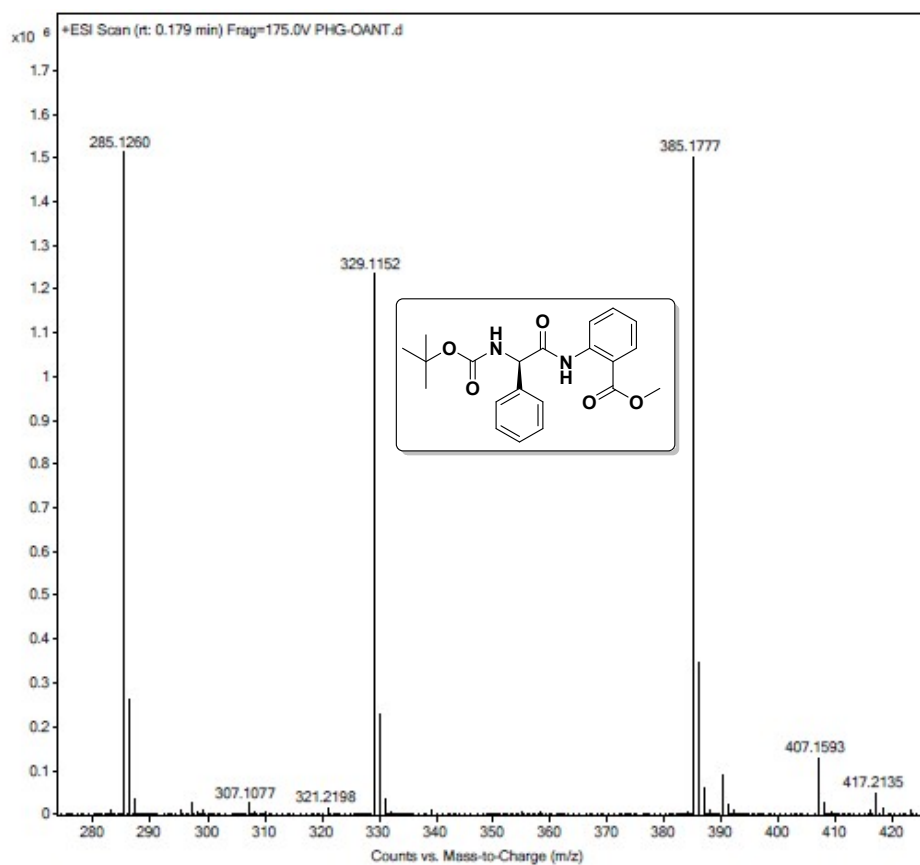


Figure S25. MS spectra of peptide **Boc-D-Phg-Ant-OMe (4)**

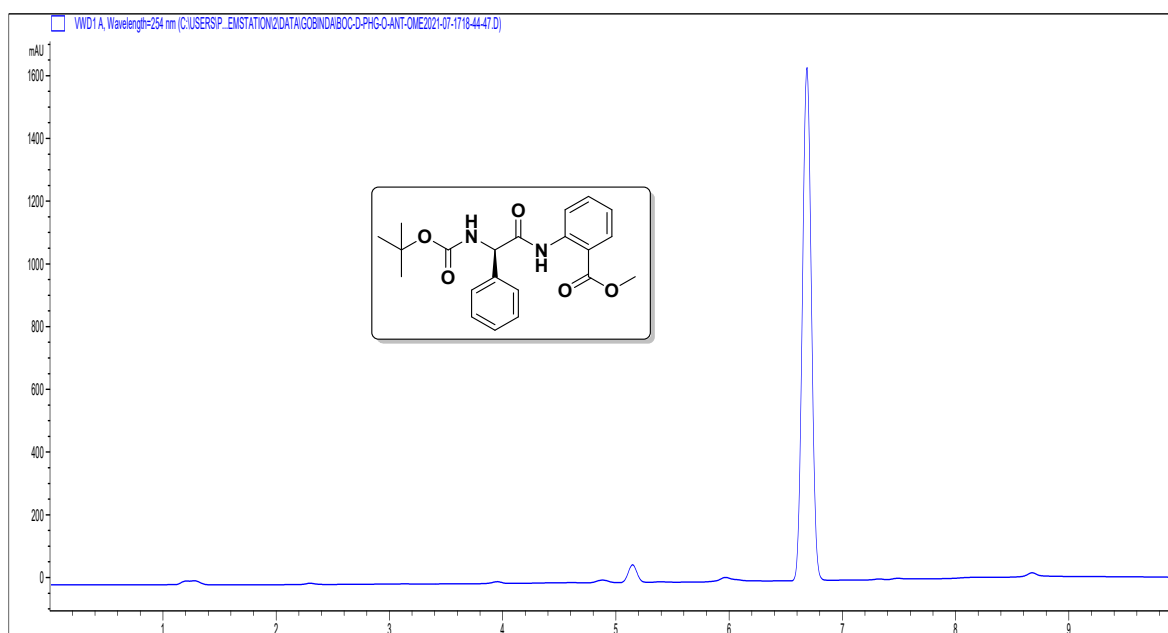


Figure S26. HPLC profile picture of purified peptide **Boc-D-Phg-Ant-OMe (4)**

GD-PHG-OANT-1H  
GD-PHG-OANT-1H

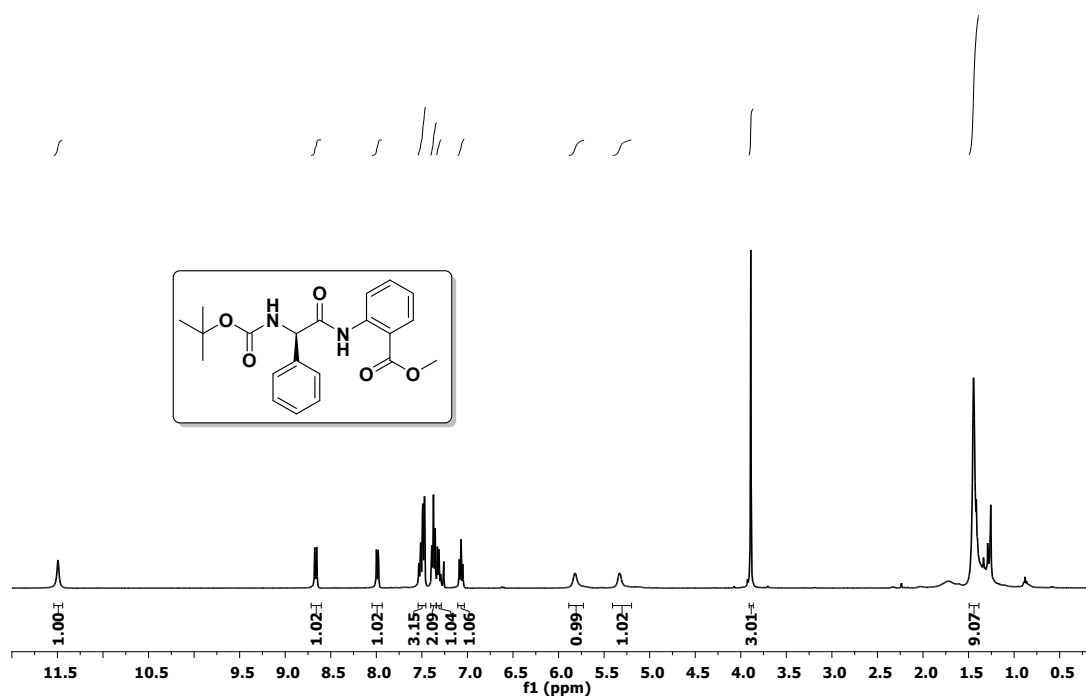


Figure S27. <sup>1</sup>H NMR spectra of peptide **Boc-D-Phg-Ant-OMe (4)**

GD-PHG-OANT-13C  
GD-PHG-OANT-13C

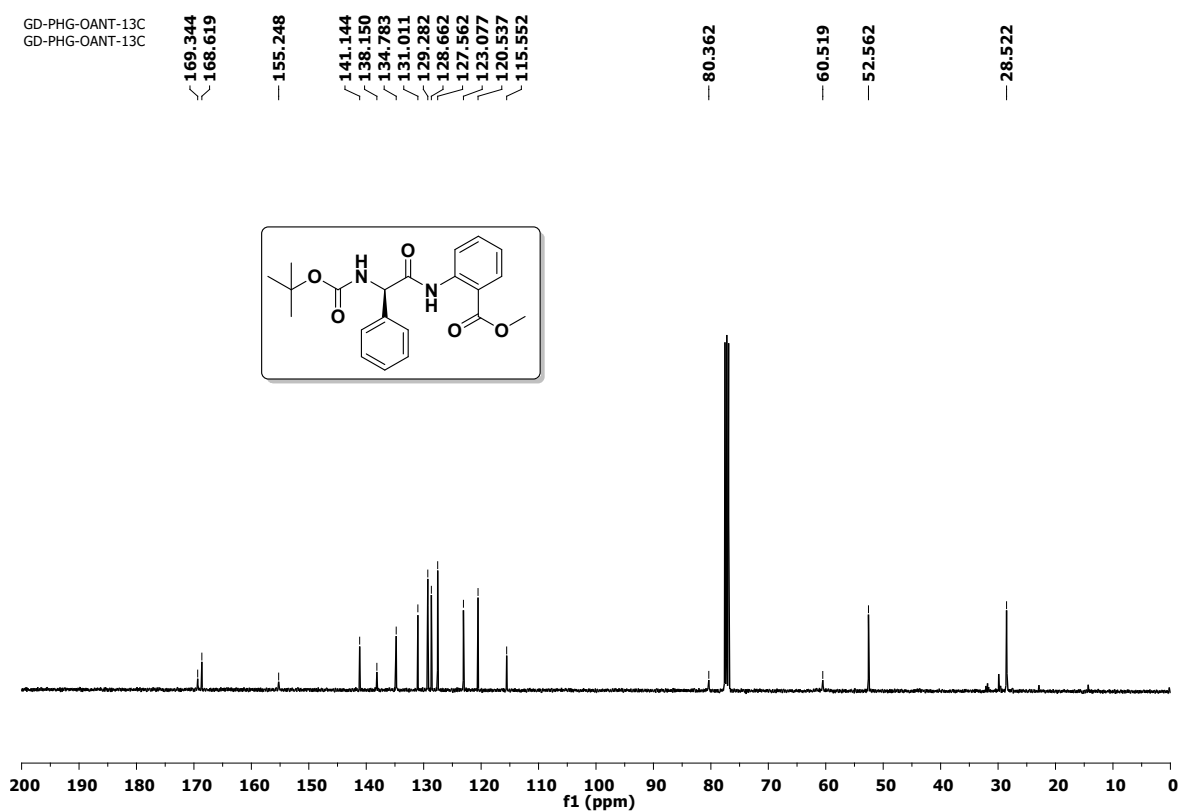


Figure S28. <sup>13</sup>C NMR spectra of peptide **Boc-D-Phg-Ant-OMe (4)**