

## Supplementary Material

### Urea-cored peptides for anion binding and vesicle formation

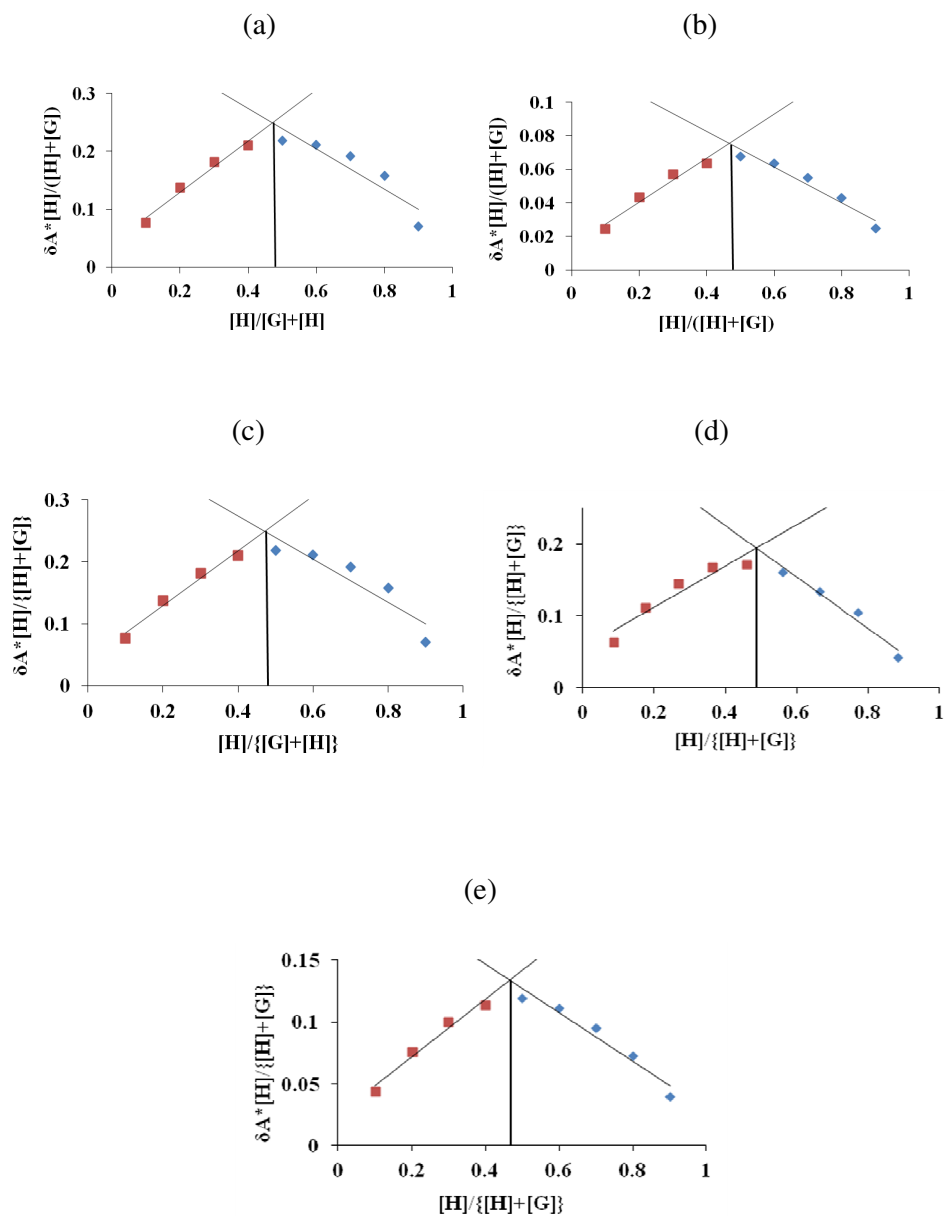
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<sup>a\*</sup>*Department of Chemistry, Indian Institute of Technology Delhi (IITD), New Delhi-110016, India.*

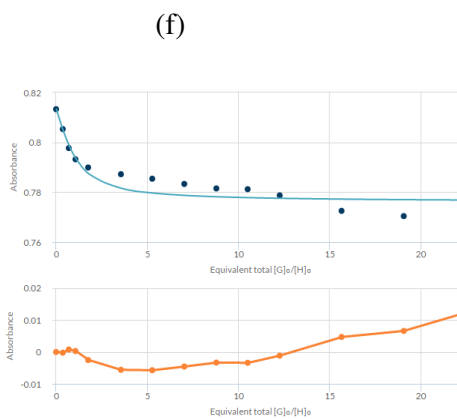
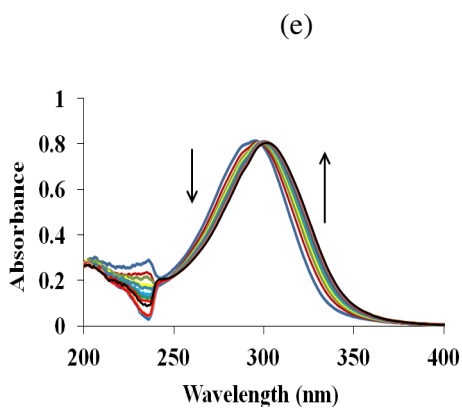
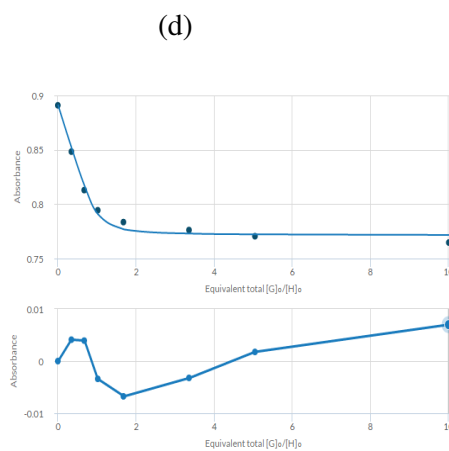
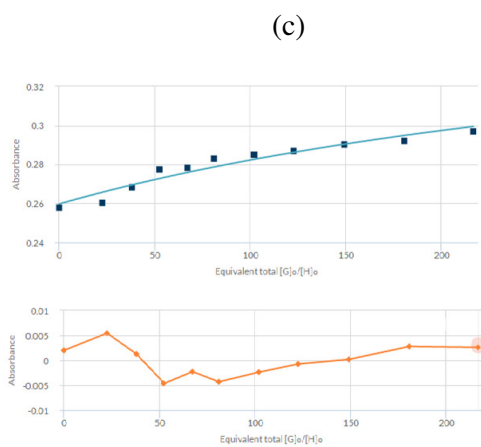
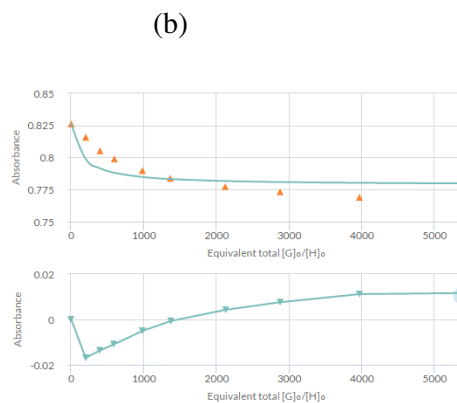
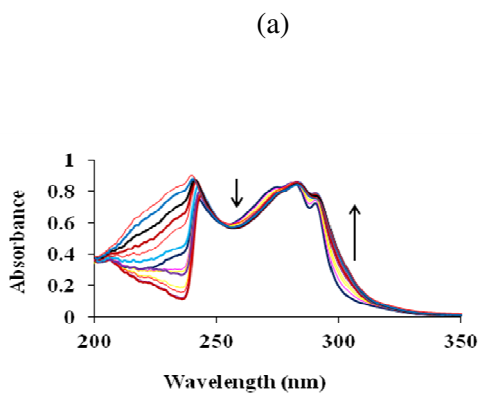
*E-mail: haridasv@chemistry.iitd.ac.in Tel: +91 01126591380.*

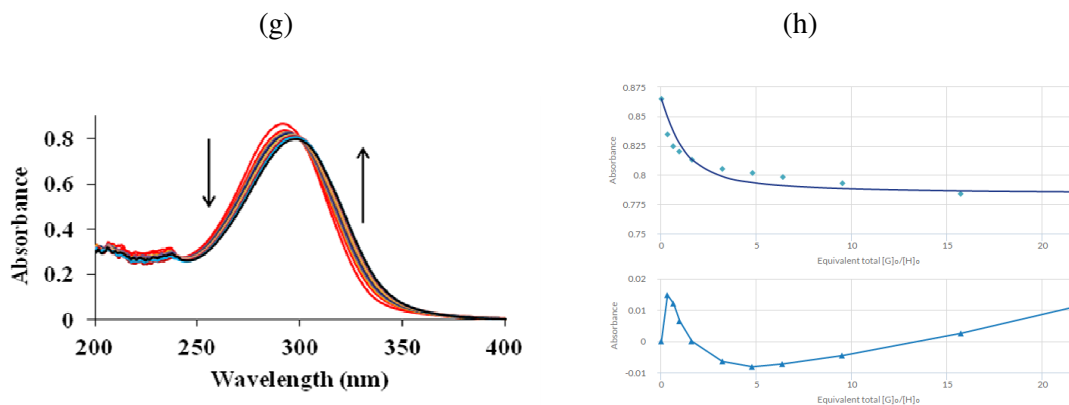
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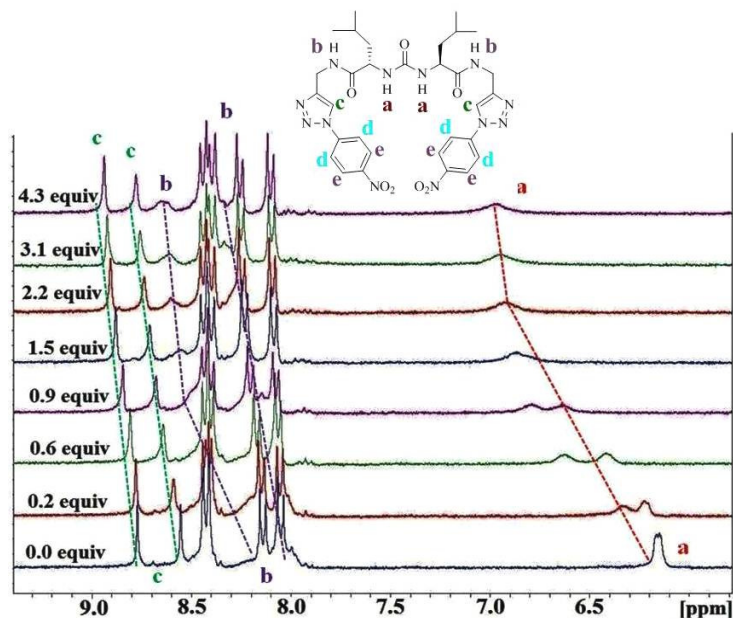
**Figure S1.** Job plot of (a) **2** ( $6.4 \times 10^{-5}$  M)- $\text{H}_2\text{PO}_4^-$  ( $6.4 \times 10^{-5}$  M) in  $\text{CHCl}_3$  (b) **4** ( $2.1 \times 10^{-5}$  M)- $\text{CH}_3\text{COO}^-$  ( $2.1 \times 10^{-5}$  M) in  $\text{CHCl}_3$  (c) **10** ( $4.3 \times 10^{-5}$  M)- $\text{F}^-$  ( $4.3 \times 10^{-5}$  M) (d) **10** ( $4.3 \times 10^{-5}$  M)- $\text{H}_2\text{PO}_4^-$  ( $4.3 \times 10^{-5}$  M) (e) **10** ( $4.3 \times 10^{-5}$  M)- $\text{HSO}_4^-$  ( $4.3 \times 10^{-5}$  M) in acetone respectively.





**Figure S2.** (a) UV-vis. titration profile for **2** ( $6.4 \times 10^{-5}$  M) with  $\text{H}_2\text{PO}_4^-$  ( $5.1 \times 10^{-2}$  M) (0.0-123.0 equiv) (b) Screenshot showing the fitting and residual plot for UV-vis titration of **2** with  $\text{H}_2\text{PO}_4^-$  (c) Screenshot showing the fitting and residual plot for UV-vis titration of **4** with  $\text{CH}_3\text{COO}^-$  (d) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with  $\text{H}_2\text{PO}_4^-$  (e) UV-vis. titration profile for **10** ( $4.35 \times 10^{-5}$  M) with  $\text{F}^-$  ( $3.1 \times 10^{-2}$  M) (0.0-22.5 equiv) in acetone (f) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with  $\text{F}^-$  (g) UV-vis. titration profile for **10** ( $4.35 \times 10^{-5}$  M) with  $\text{HSO}_4^-$  ( $2.8 \times 10^{-2}$  M) (0.0-22.0 equiv) in acetone (h) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with  $\text{HSO}_4^-$  (Temperature 296-298 K).

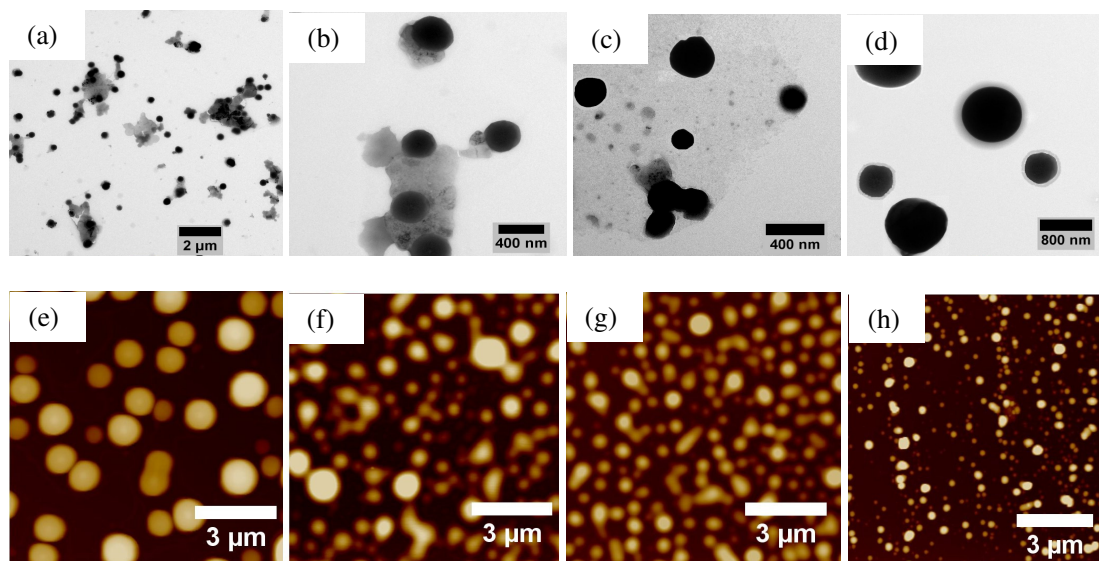




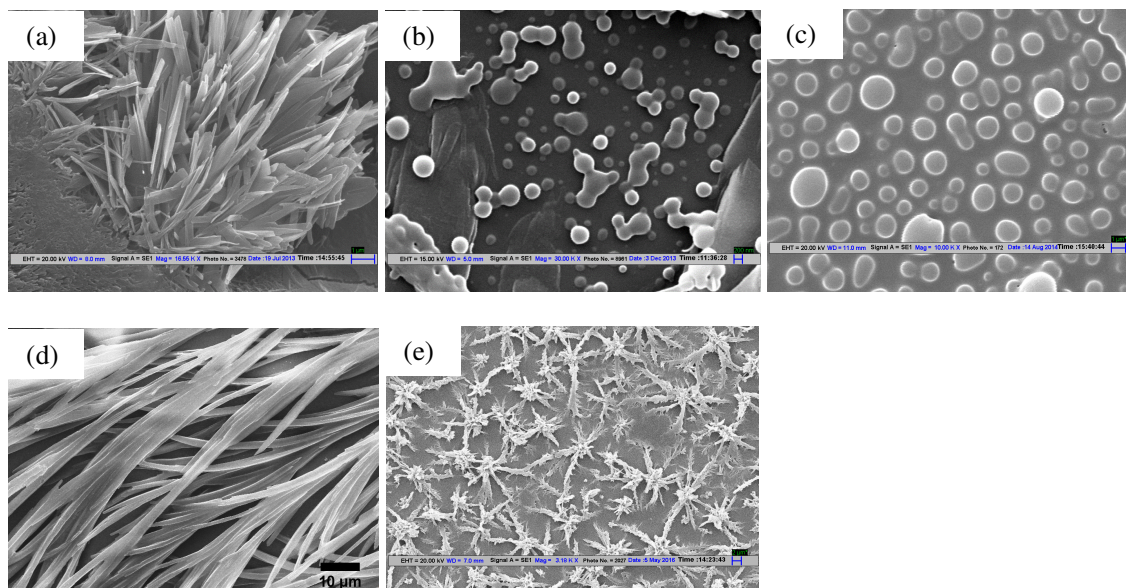
**Figure S3.** Partial  $^1\text{H}$  NMR titration profile **10** ( $4.34 \times 10^{-3}$  M) with  $\text{HSO}_4^-$  ( $4.1 \times 10^{-1}$  M) (0.0-4.3 equiv) in acetone- $d_6$ .

Compound	Urea NH	Peptide NH	Triazole CH	Indole NH
<b>4</b> + $\text{CH}_3\text{COO}^-$	2.40	~ 0.0	NA	1.78
<b>10</b> + $\text{H}_2\text{PO}_4^-$	2.00	1.0	0.80	NA
<b>10</b> + $\text{HSO}_4^-$	0.80	0.35	0.20	NA

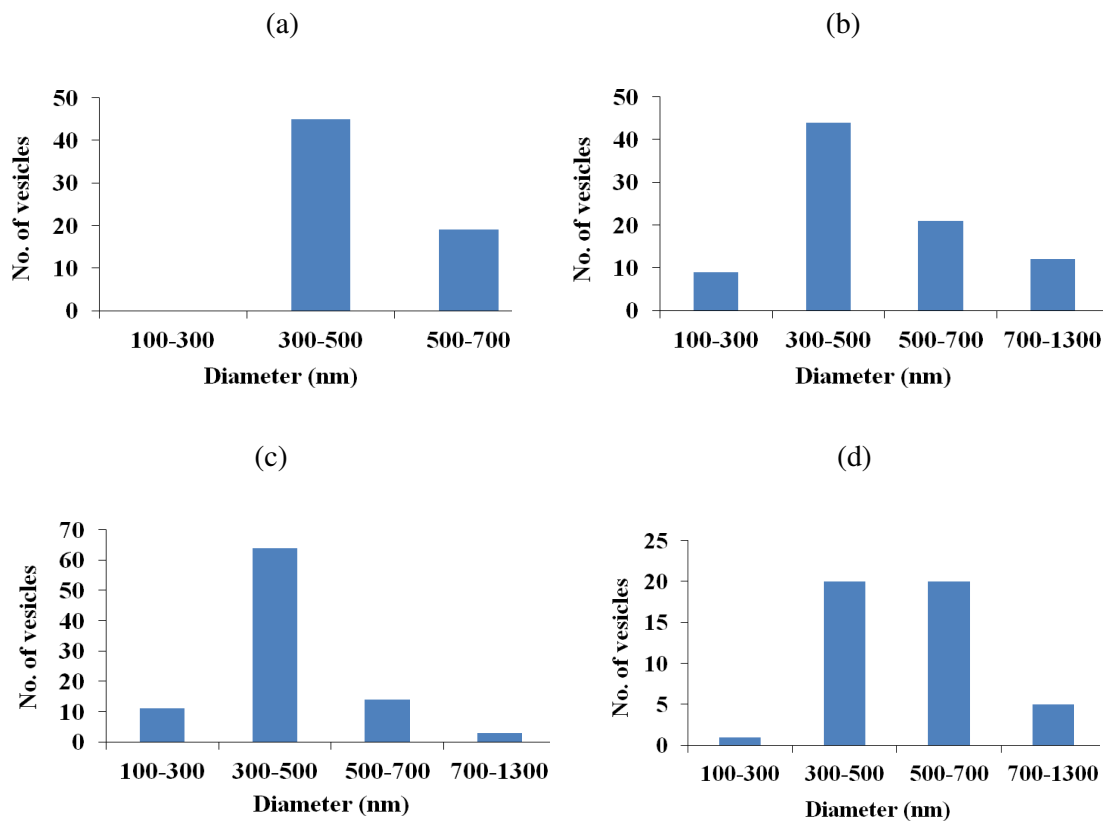
**Table S1.** Change in the chemical shift values for different protons on the basis of  $^1\text{H}$  NMR titration experiments for **4** and **10** (NA= not applicable).



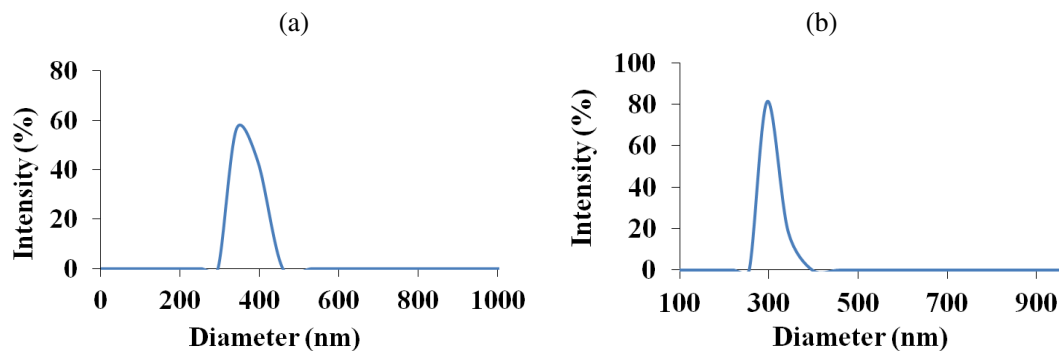
**Figure S4.** TEM images (stained with 0.2 % phosphotungstic acid) of (a) **2** (3.2 mM) (b) **4** (2.9 mM) (c) **6** (2.8 mM) (d) **10** (2.8 mM). AFM images (tapping mode) of (e) **2** (3.2 mM) (f) **4** (2.9 mM) (g) **6** (2.8 mM) (h) **10** (2.8 mM) in 1:1 CH<sub>3</sub>OH/CHCl<sub>3</sub> respectively.

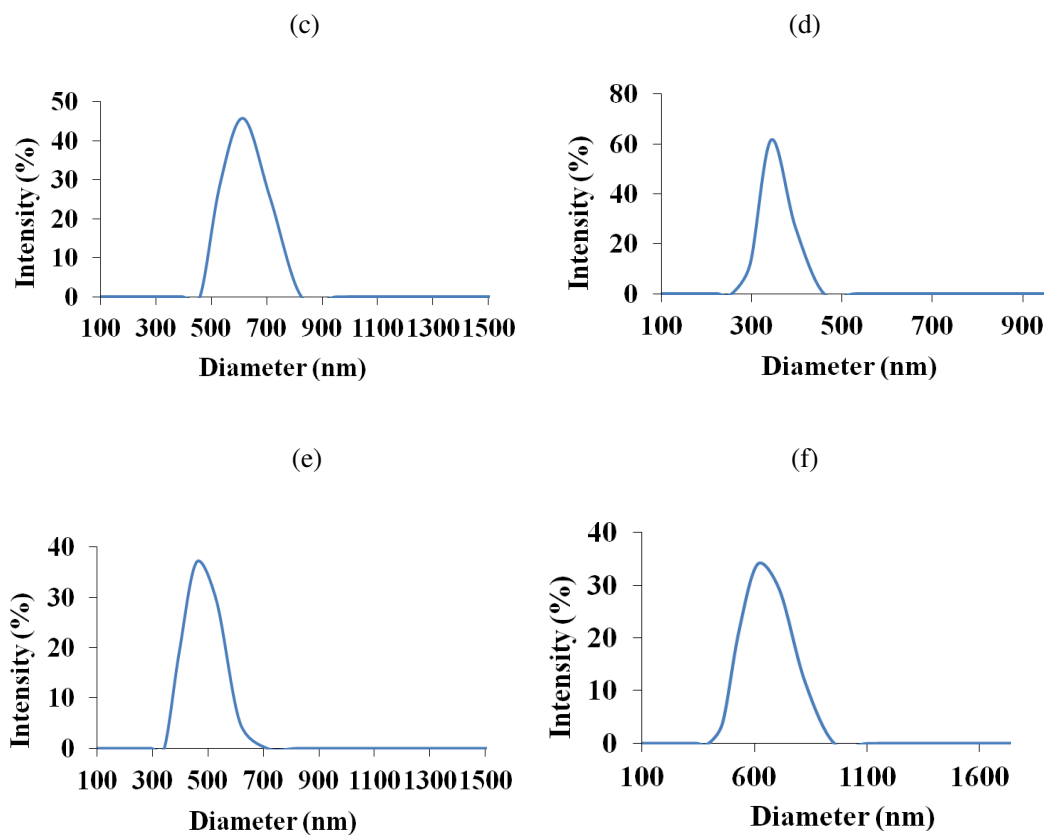


**Figure S5.** SEM images of (a) **1** (3.9 mM) (b) **3** (3.8 mM) (c) **5** (3.6 mM) (d) **8** (2.8 mM) (e) **9** (3.2 mM) in 1:1 CH<sub>3</sub>OH/CHCl<sub>3</sub> respectively.



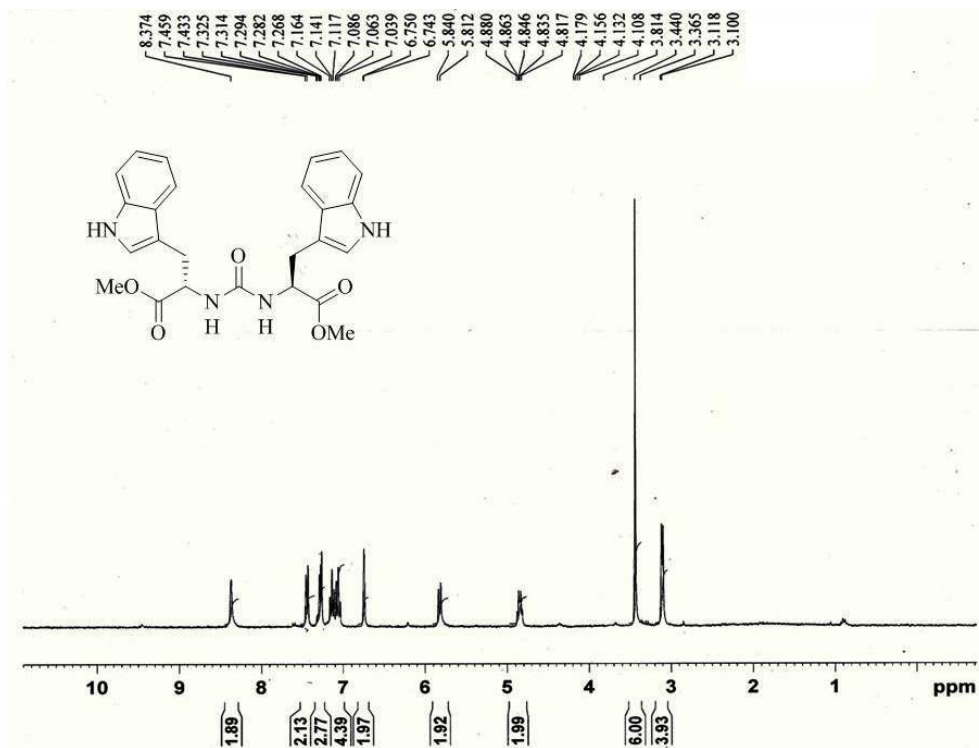
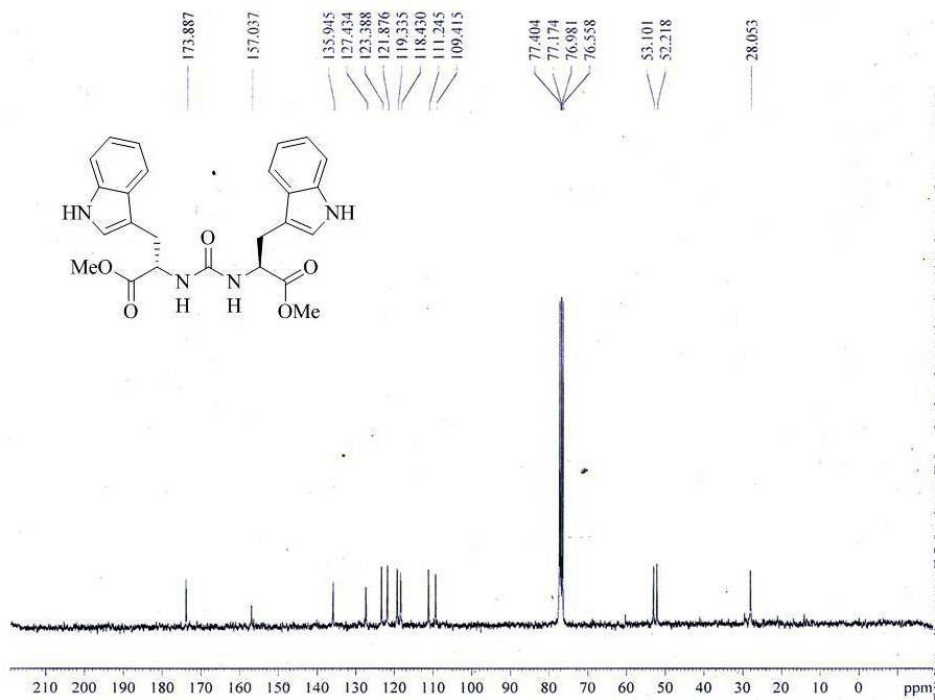
**Figure S6.** Histogram showing average size distribution of vesicles from SEM images of (a) 2 (b) 4 (c) 6 (d) 10.

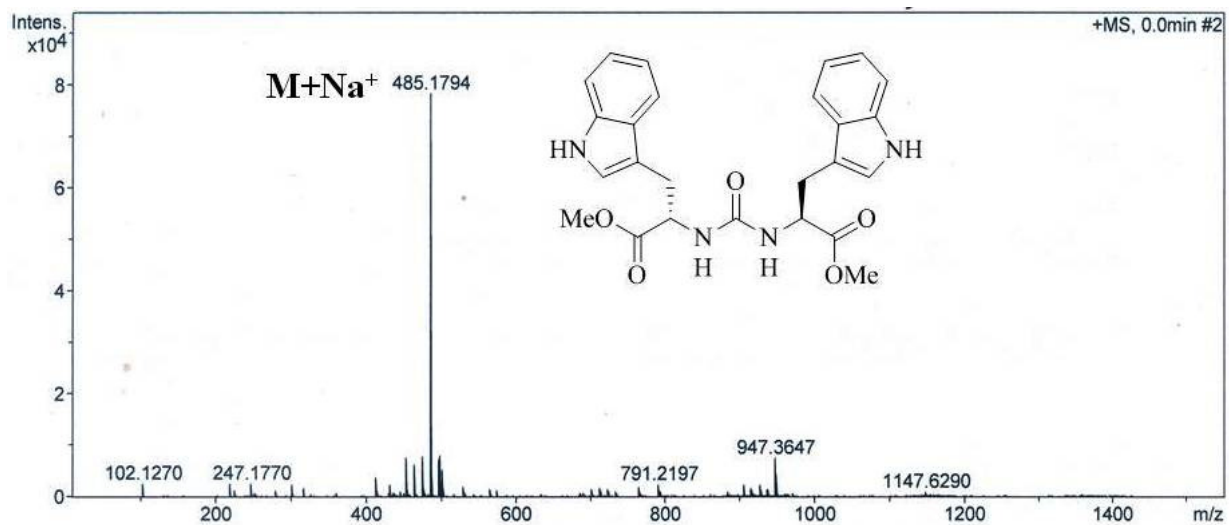




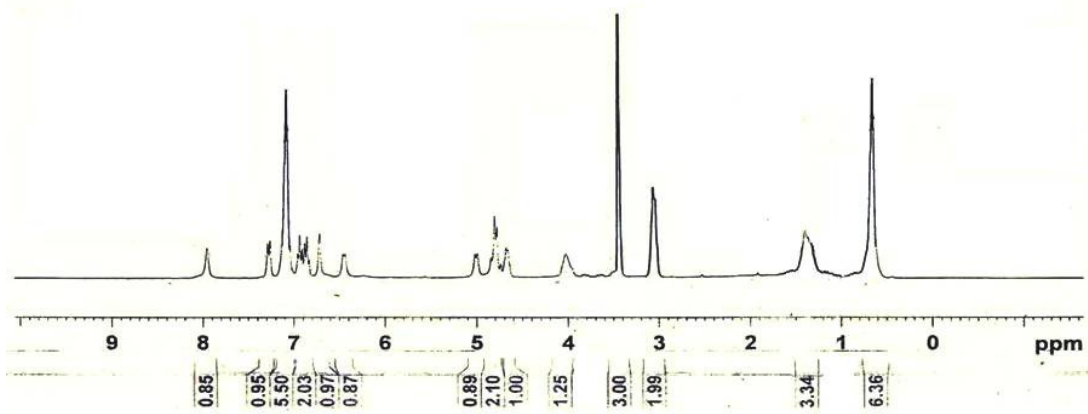
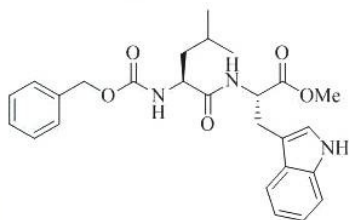
**Figure S7.** Dynamic light scattering graph showing average size distribution of (a) **2** (b) **4** (c) **6** (d) **10** (e) **10** + 5.0 equiv.  $\text{H}_2\text{PO}_4^-$  (f) **10** + 5.0 equiv.  $\text{HSO}_4^-$  in methanol respectively.

## Spectral Data

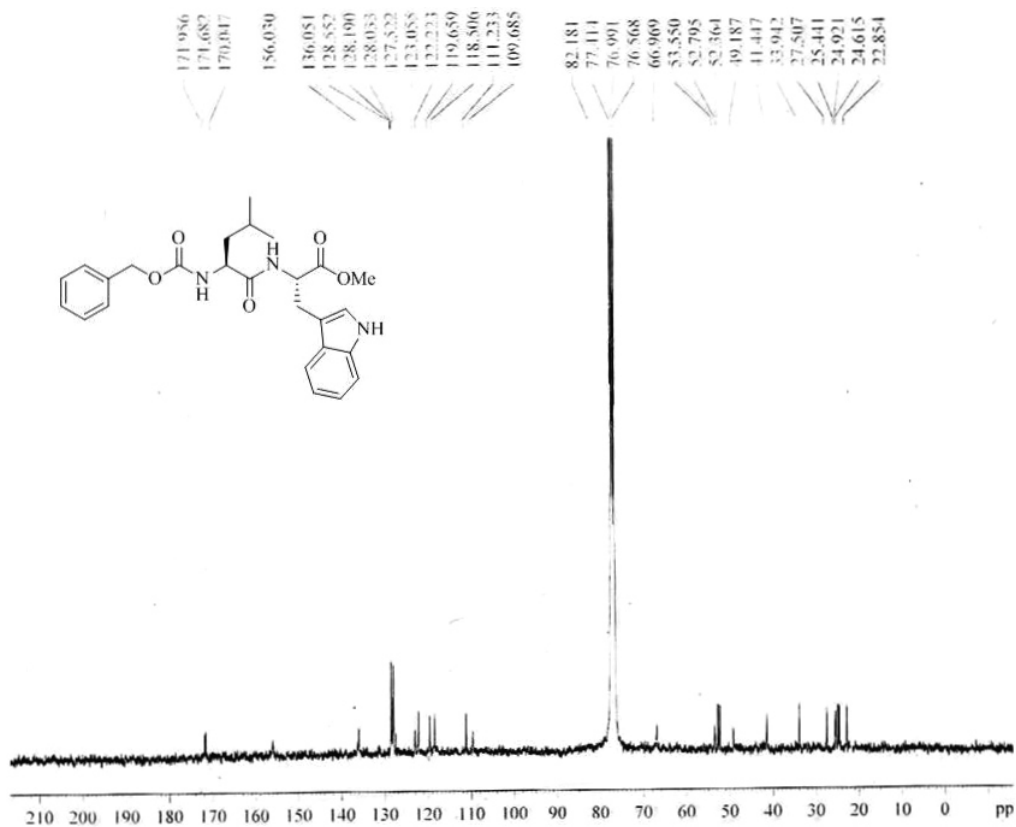
<sup>1</sup>H NMR of **2** (CDCl<sub>3</sub>, 300 MHz)<sup>13</sup>C NMR of **2** (CDCl<sub>3</sub>, 75 MHz)



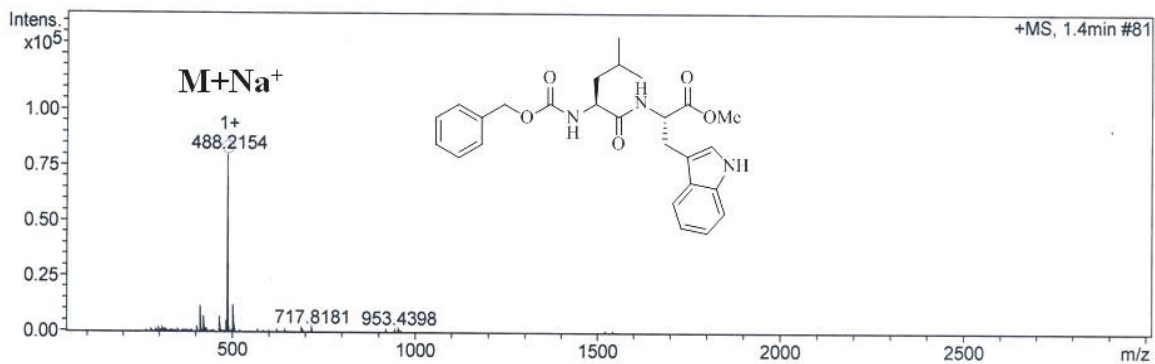
HRMS of 2

<sup>1</sup>H NMR of 3 (CDCl<sub>3</sub>, 300 MHz)

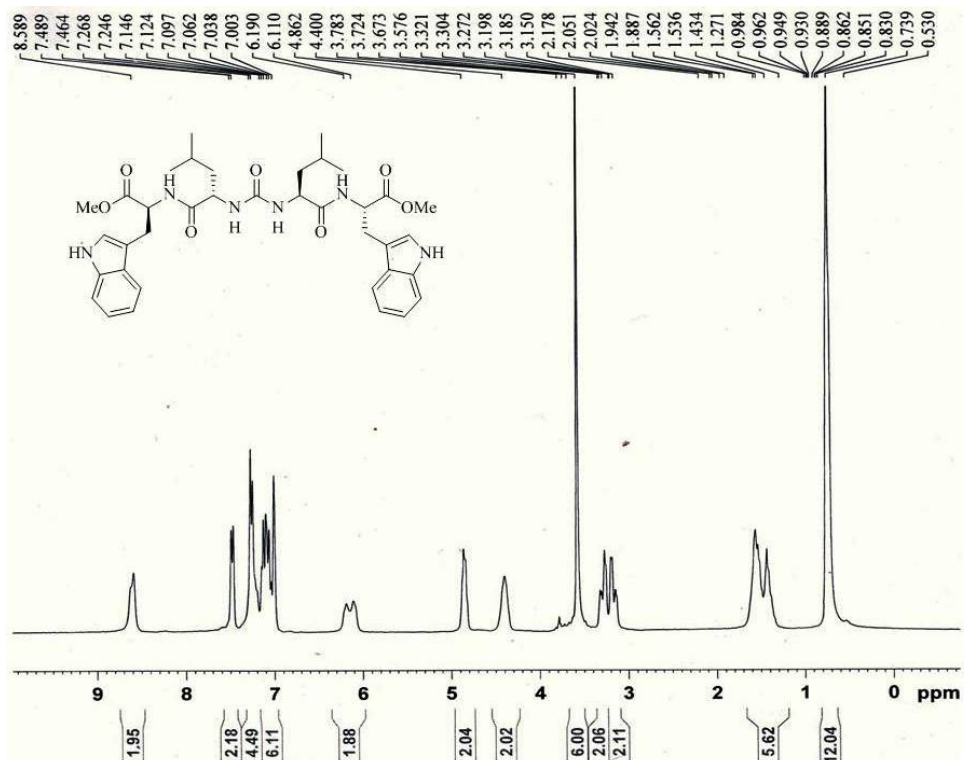




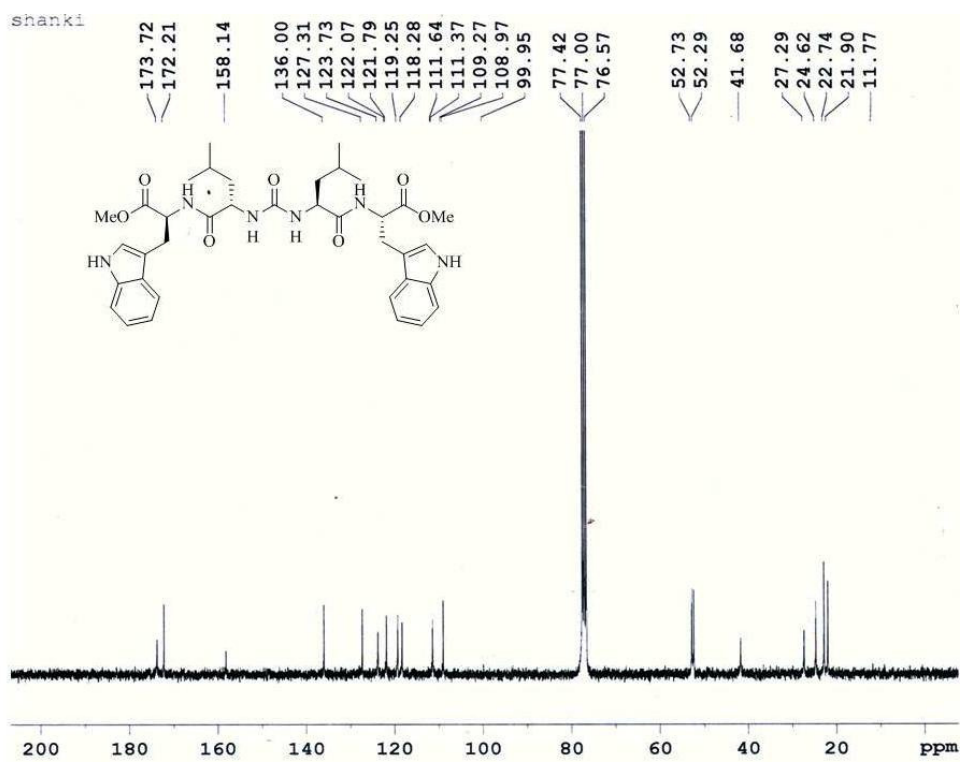
<sup>13</sup>C NMR of **3** (CDCl<sub>3</sub>, 75 MHz)



HRMS of **3**

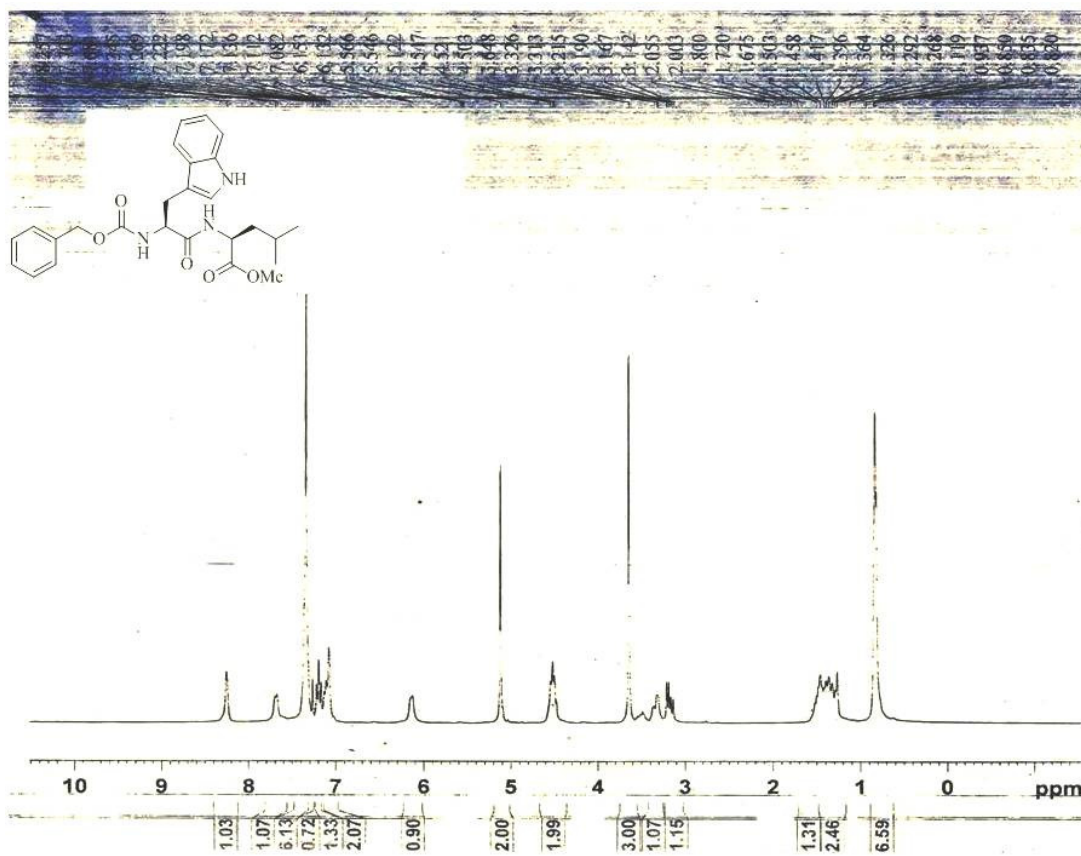
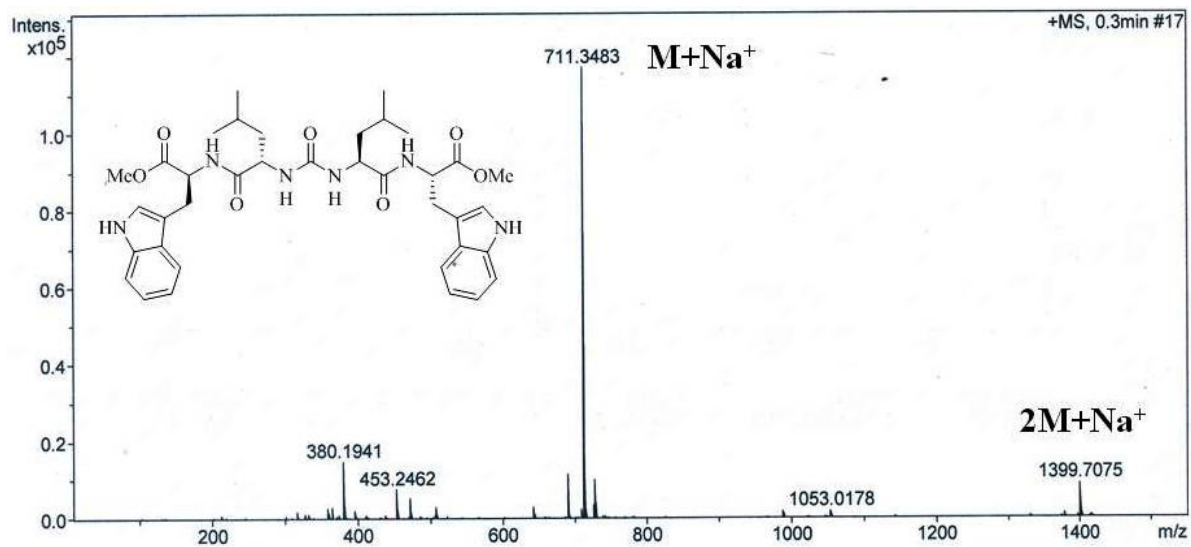


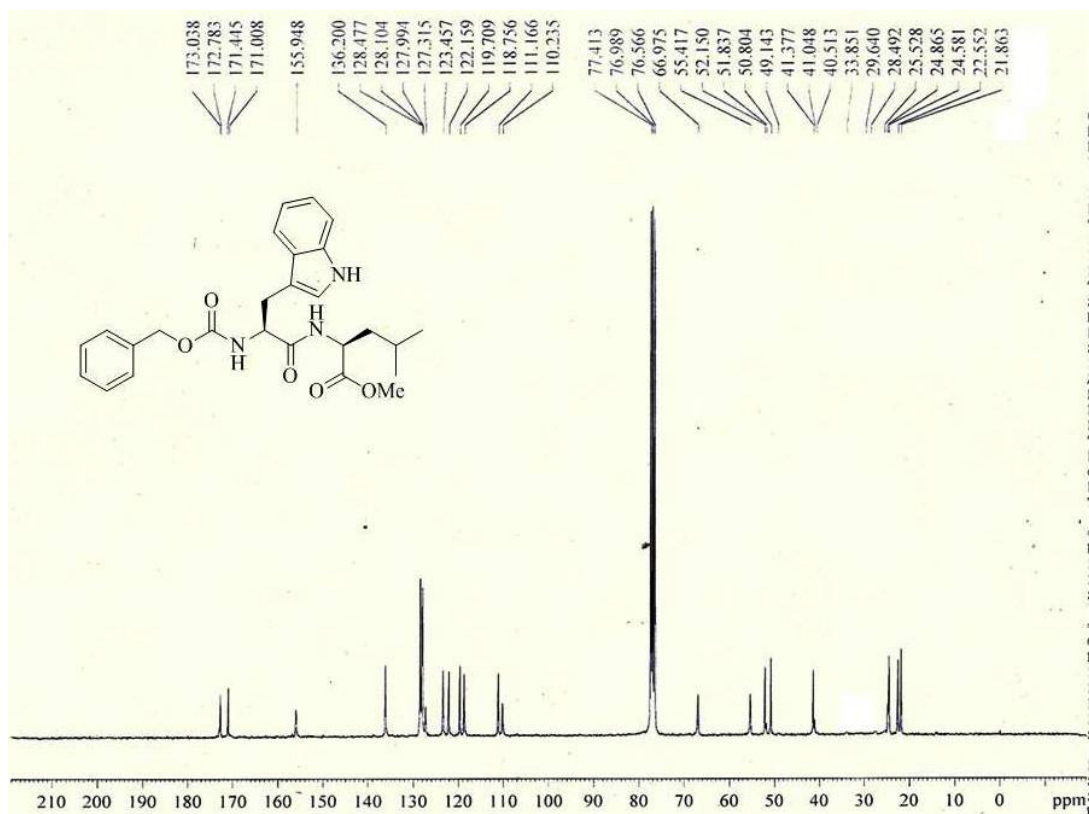
<sup>1</sup>H NMR of 4 (CDCl<sub>3</sub>, 300 MHz)



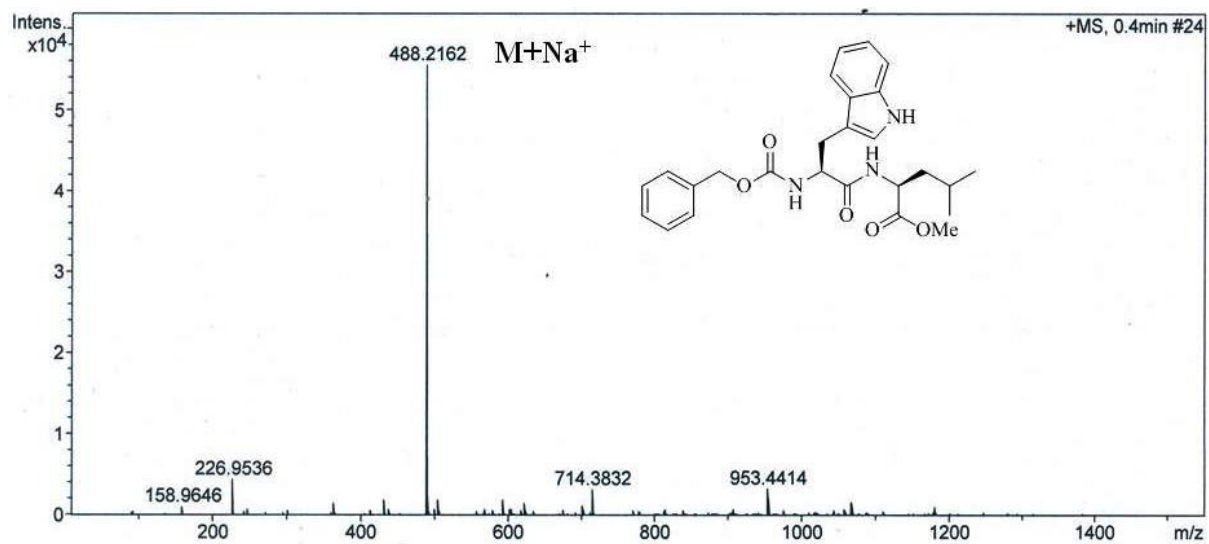
<sup>13</sup>C NMR of 4 (CDCl<sub>3</sub>, 75 MHz)



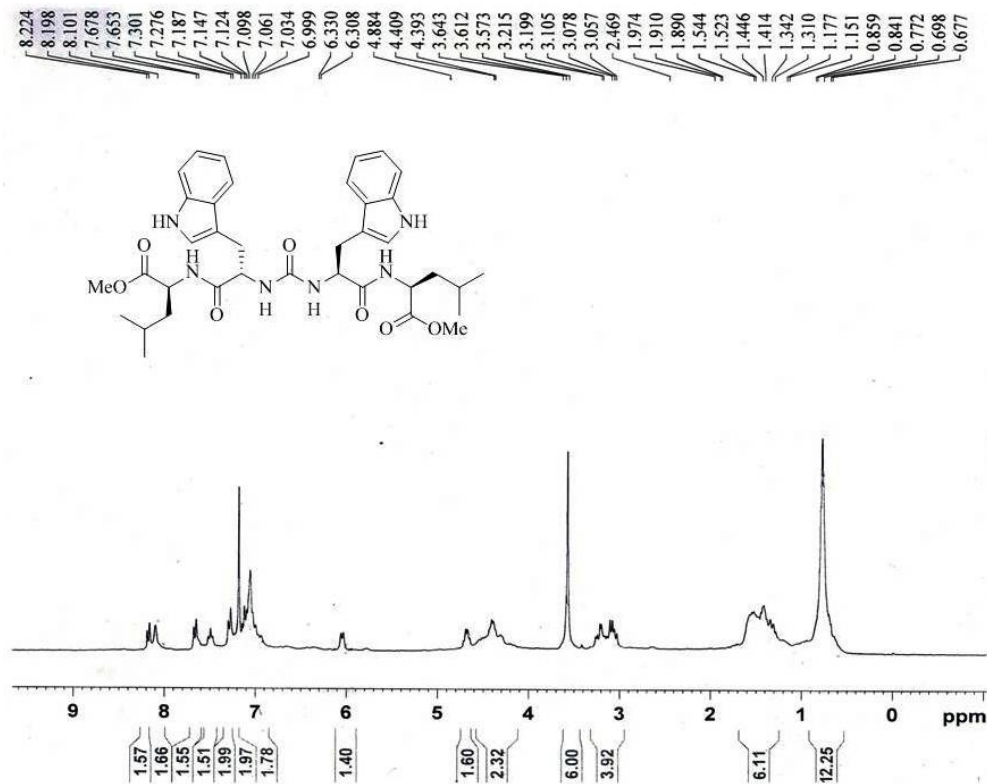
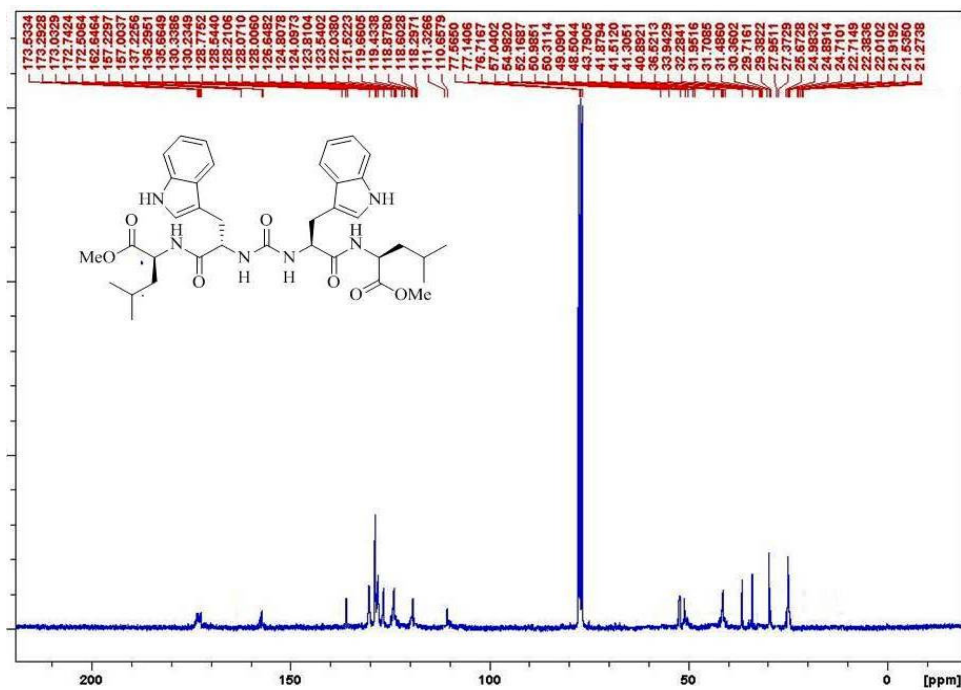


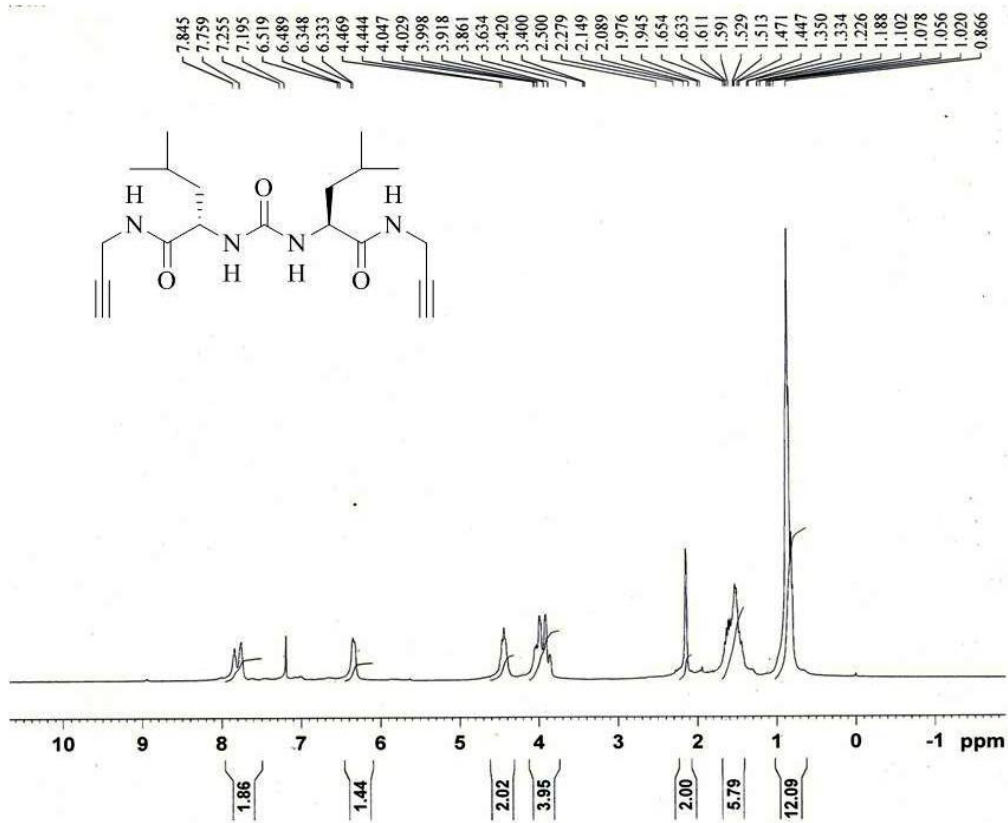
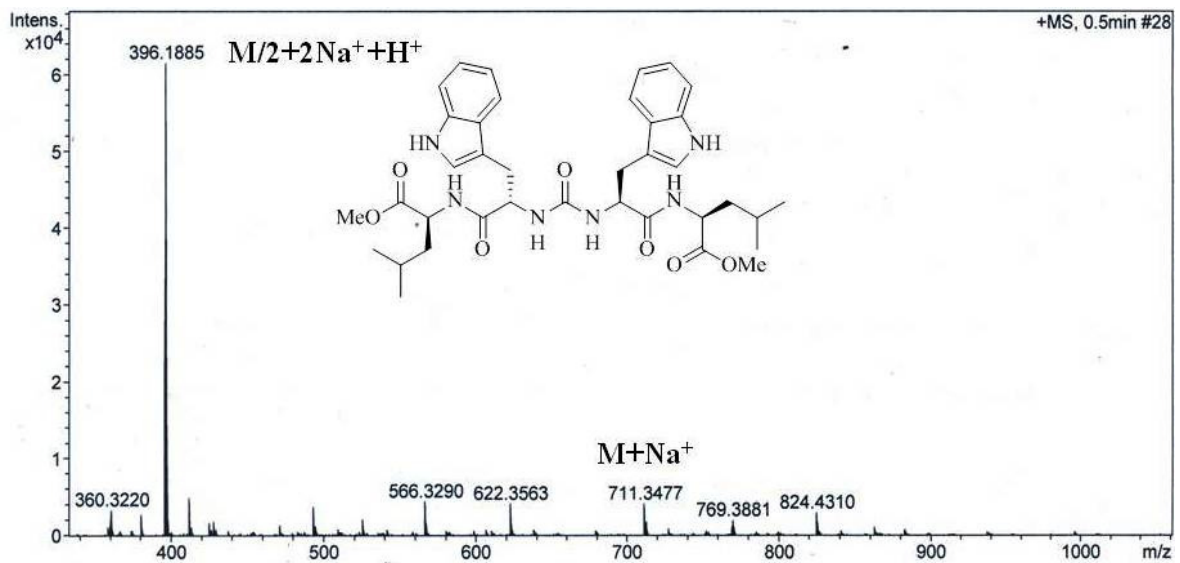


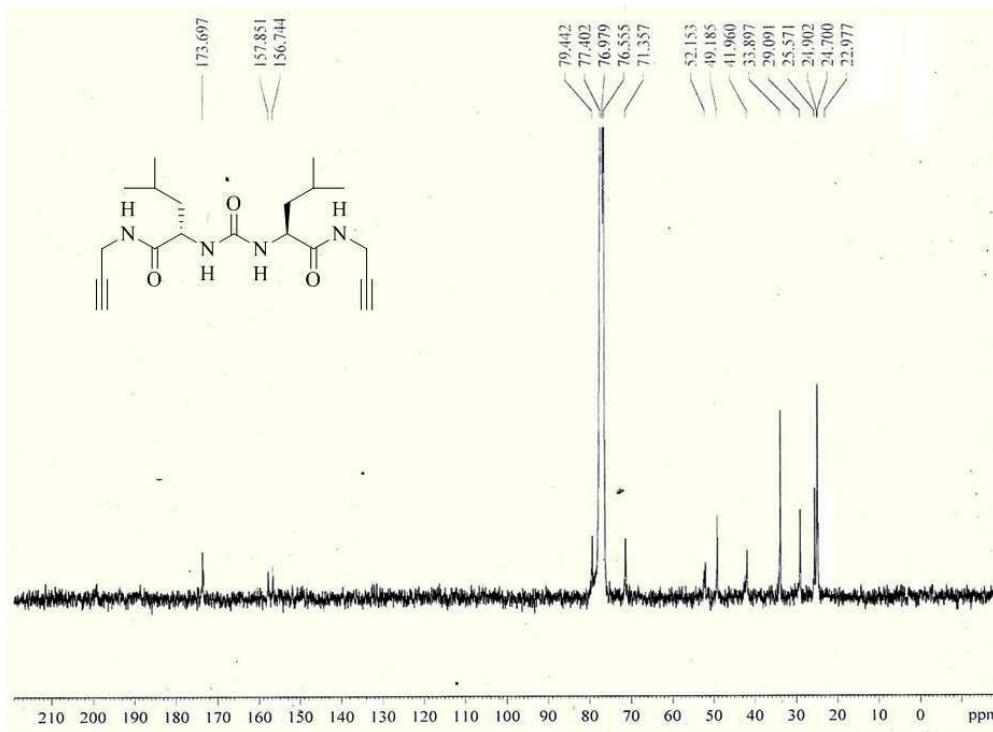
<sup>13</sup>C NMR of **5** (CDCl<sub>3</sub>, 75 MHz)



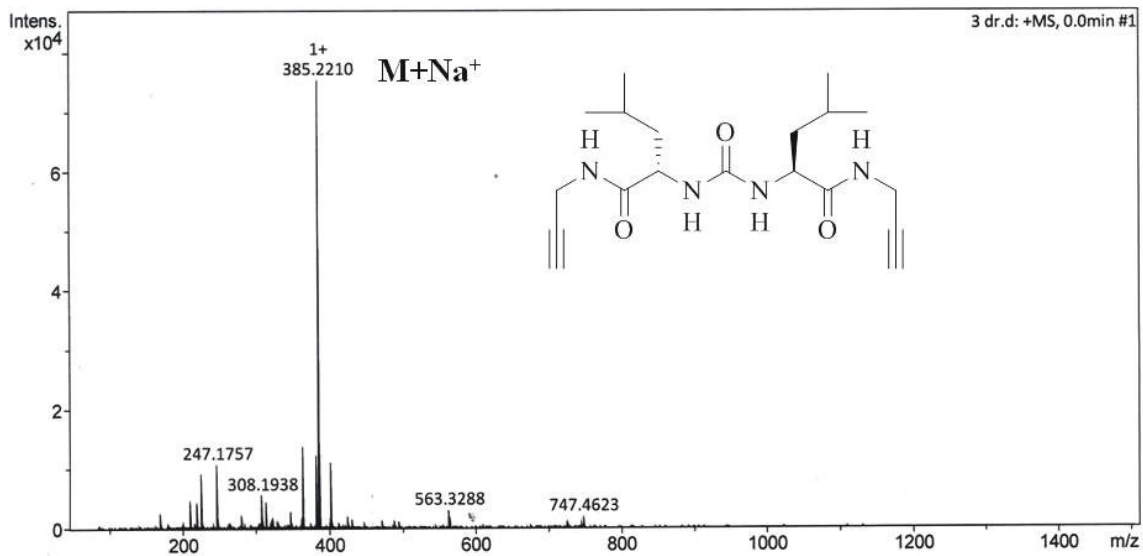
HRMS of **5**

 $^1\text{H}$  NMR of 6 (CDCl<sub>3</sub>, 300 MHz) $^{13}\text{C}$  NMR of 6 (CDCl<sub>3</sub>, 75 MHz)

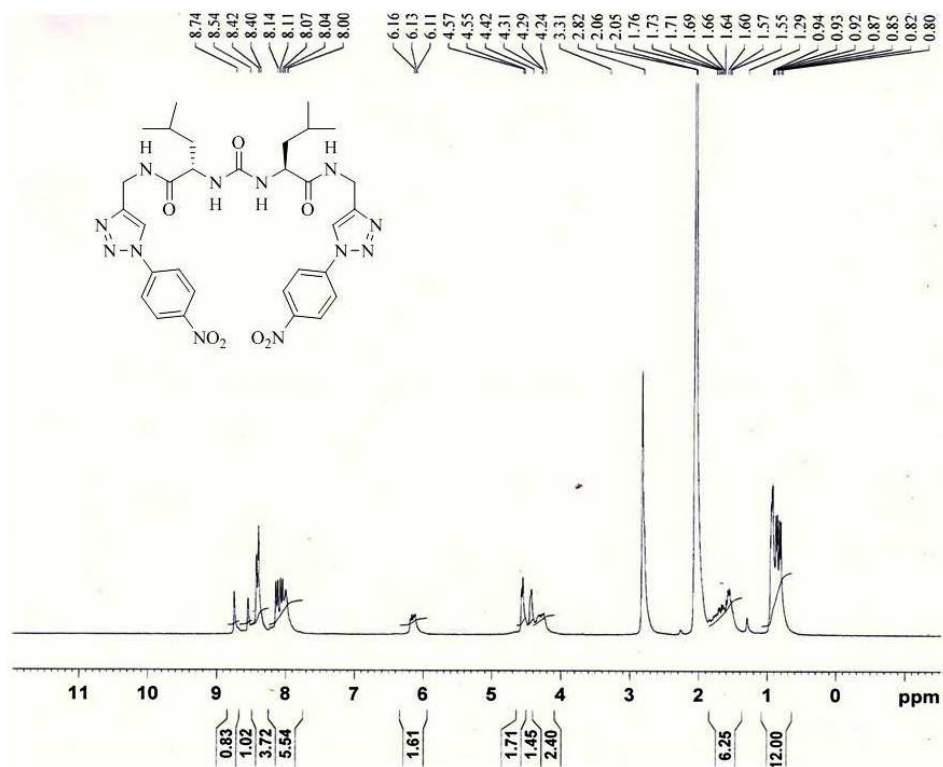




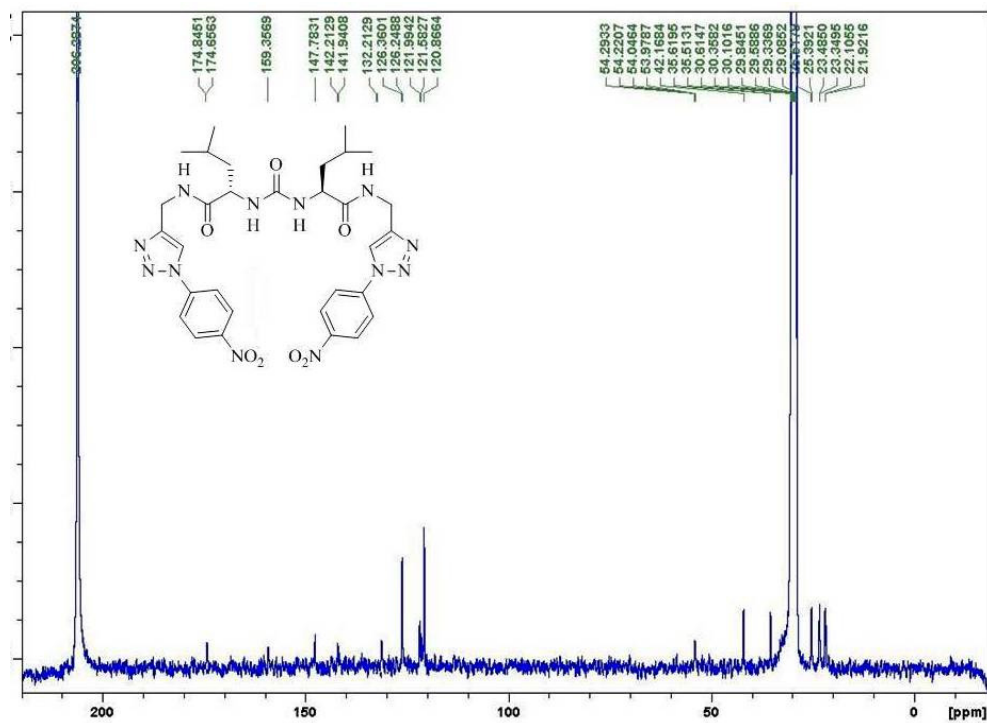
<sup>13</sup>C NMR of **9** (CDCl<sub>3</sub>, 75 MHz)



HRMS of **9**

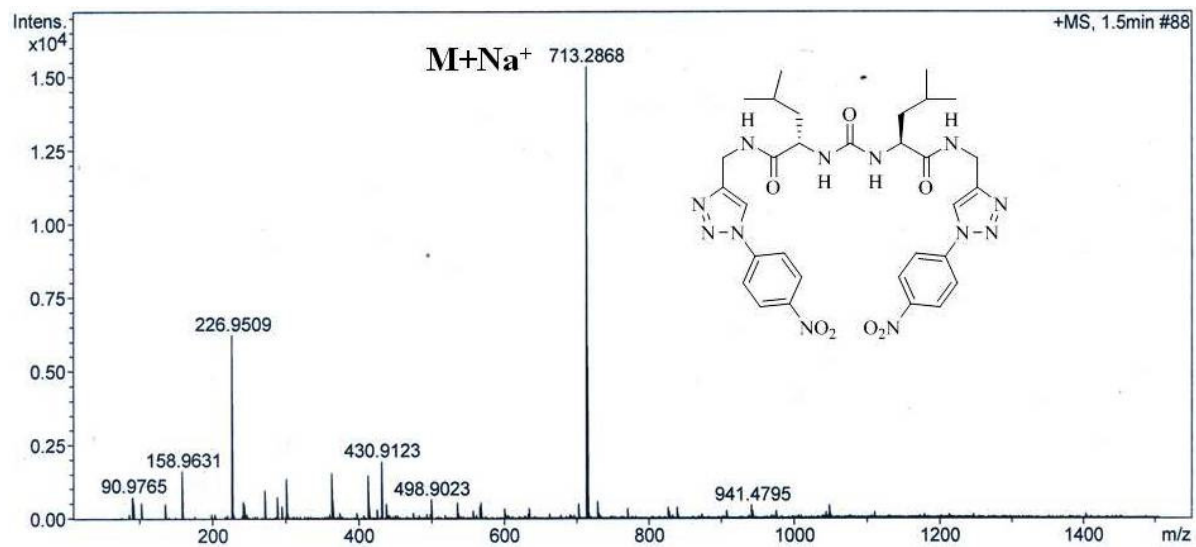


<sup>1</sup>H NMR of **10** (Acetone-*d*<sub>6</sub>, 300 MHz)



<sup>13</sup>C NMR of **10** (Acetone-*d*<sub>6</sub>, 75 MHz)



HRMS of **10**