Supplementary Material

Urea-cored peptides for anion binding and vesicle formation

Ishanki Bhardwaj[a], Rachit Sapra[a] and V. Haridas[a]*

[a]*Department of Chemistry, Indian Institute of Technology Delhi (IITD), New Delhi-110016, India.*
E-mail: haridasv@chemistry.iitd.ac.in Tel: +91 01126591380.

Contents

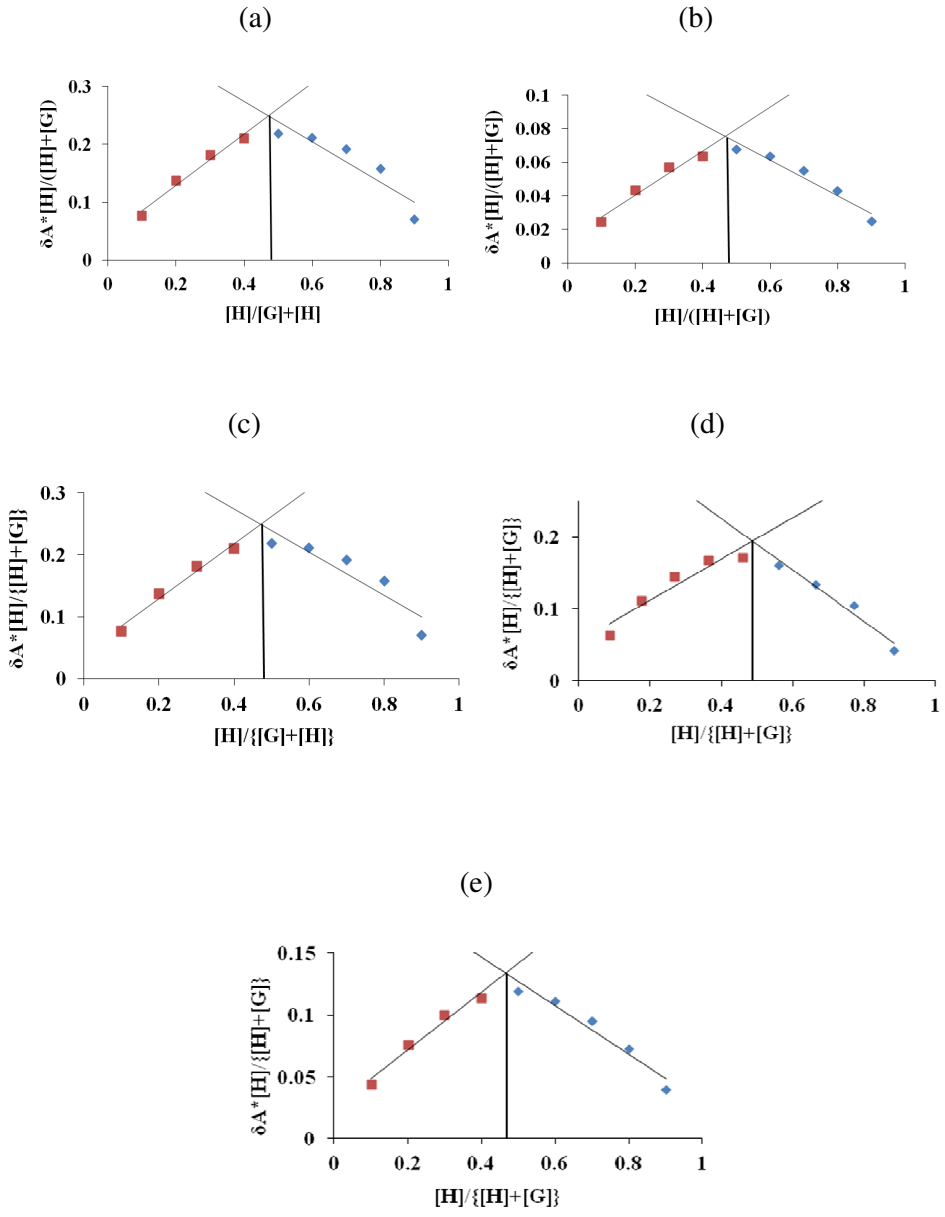
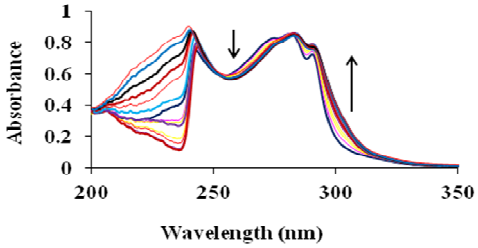
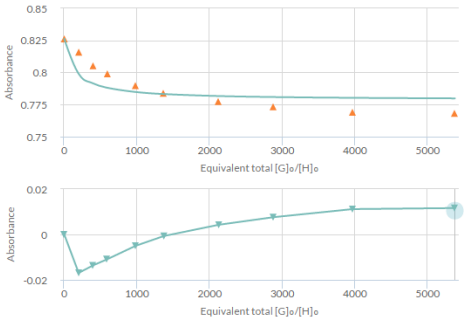


Figure S1. Job plot of (a) **2** (6.4×10^{-5} M)-$H_2PO_4^-$(6.4×10^{-5} M) in $CHCl_3$ (b) **4** (2.1×10^{-5} M)-CH_3COO^- (2.1×10^{-5} M) in $CHCl_3$ (c) **10** (4.3×10^{-5} M)-F^-(4.3×10^{-5} M) (d) **10** (4.3×10^{-5} M)-$H_2PO_4^-$(4.3×10^{-5} M) (e) **10** (4.3×10^{-5} M)-HSO_4^- (4.3×10^{-5} M) in acetone respectively.

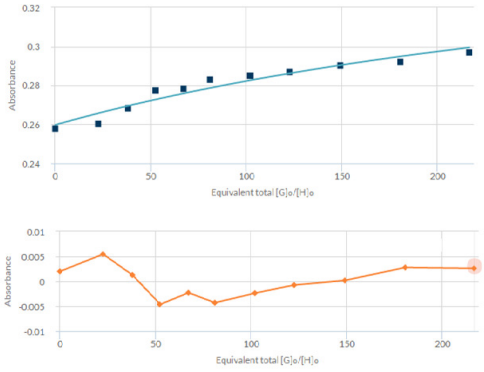
(a)



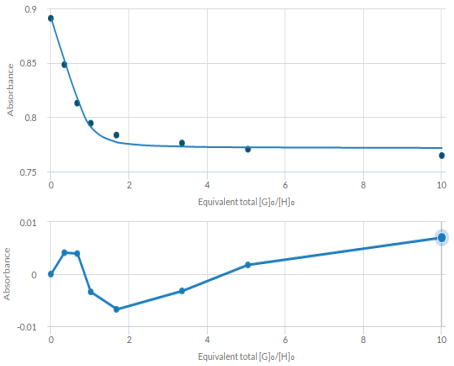
(b)



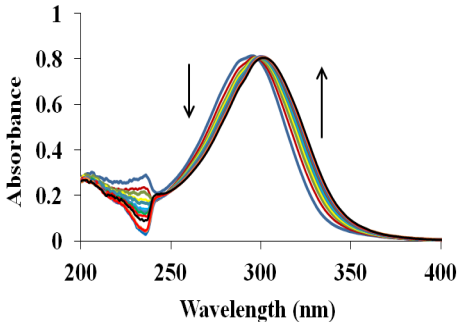
(c)



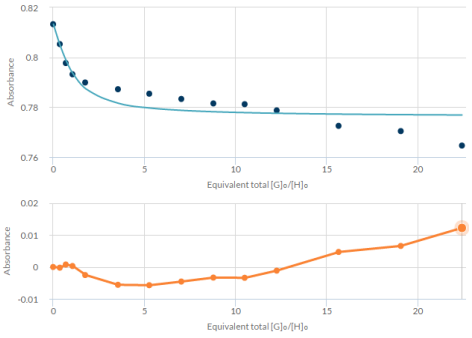
(d)



(e)



(f)



(g) (h)

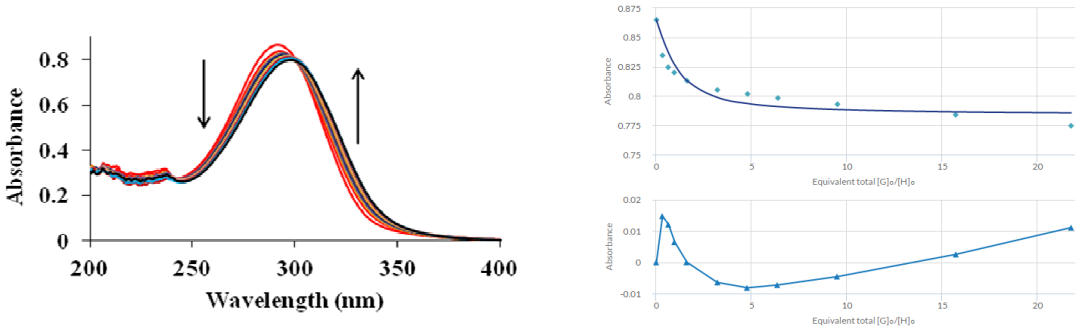


Figure S2. (a) UV-vis. titration profile for **2** (6.4×10^{-5} M) with $H_2PO_4^-$ (5.1×10^{-2} M) (0.0-123.0 equiv) (b) Screenshot showing the fitting and residual plot for UV-vis titration of **2** with $H_2PO_4^-$ (c) Screenshot showing the fitting and residual plot for UV-vis titration of **4** with CH_3COO^- (d) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with $H_2PO_4^-$ (e) UV-vis. titration profile for **10** (4.35×10^{-5} M) with F^- (3.1×10^{-2} M) (0.0-22.5 equiv) in acetone (f) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with F^- (g) UV-vis. titration profile for **10** (4.35×10^{-5} M) with HSO_4^- (2.8×10^{-2} M) (0.0-22.0 equiv) in acetone (h) Screenshot showing the fitting and residual plot for UV-vis titration of **10** with HSO_4^- (Temperature 296-298 K).

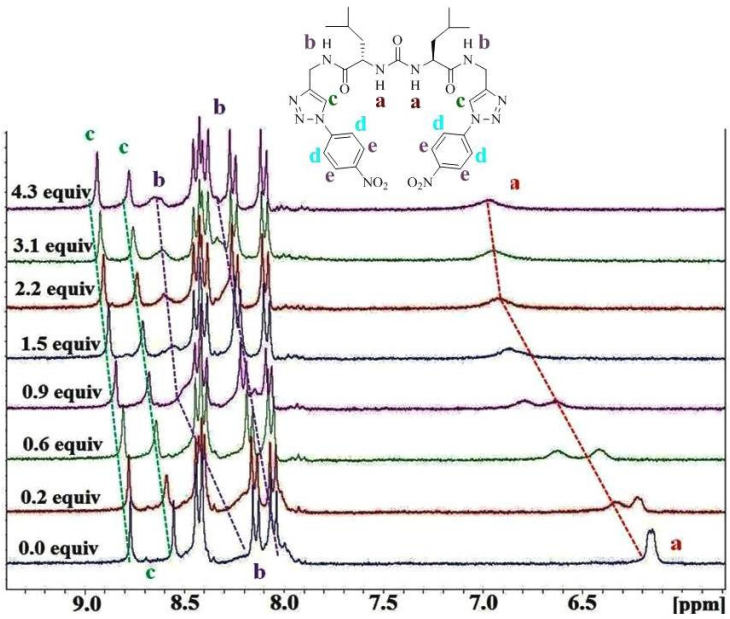


Figure S3. Partial ^{1}H NMR titration profile **10** (4.34 x 10^{-3} M) with HSO_4^- (4.1 x 10^{-1} M) (0.0-4.3 equiv) in acetone-d_6.

Compound	Urea NH	Peptide NH	Triazole CH	Indole NH
4 + CH_3COO^-	2.40	~ 0.0	NA	1.78
10 + $H_2PO_4^-$	2.00	1.0	0.80	NA
10 + 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}H NMR titration experiments for **4** and **10** (NA= not applicable).

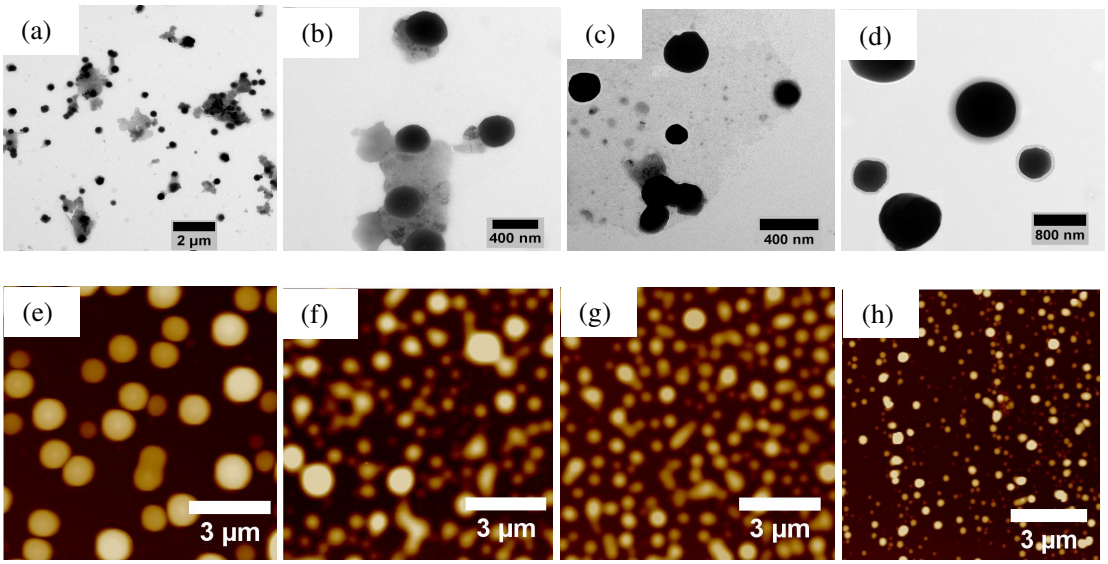


Figure S4. TEM images (stained with 0.2 % phosphotungstic acid) of (a) **2** (3.2 mM) (b) **4** (2.9 mM) (c) **6** (2.8 mM) (d) **10** (2.8 mM). AFM images (tapping mode) of (e) **2** (3.2 mM) (f) **4** (2.9 mM) (g) **6** (2.8 mM) (h) **10** (2.8 mM) in 1:1 $CH_3OH/CHCl_3$ respectively.

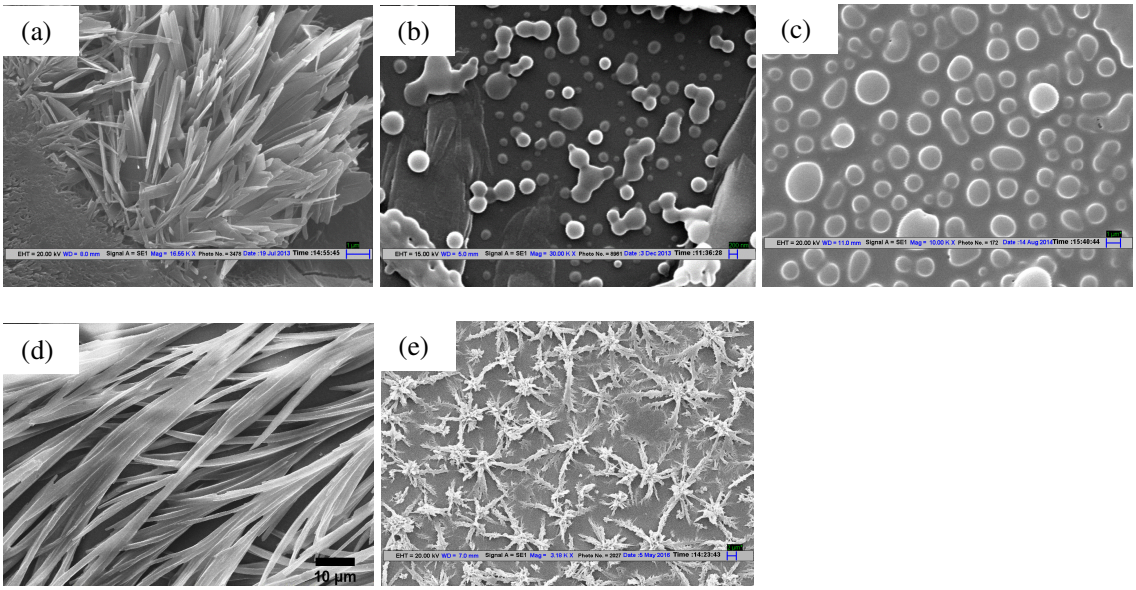


Figure S5. SEM images of (a) **1** (3.9 mM) (b) **3** (3.8 mM) (c) **5** (3.6 mM) (d) **8** (2.8 mM) (e) **9** (3.2 mM) in 1:1 $CH_3OH/CHCl_3$ respectively.

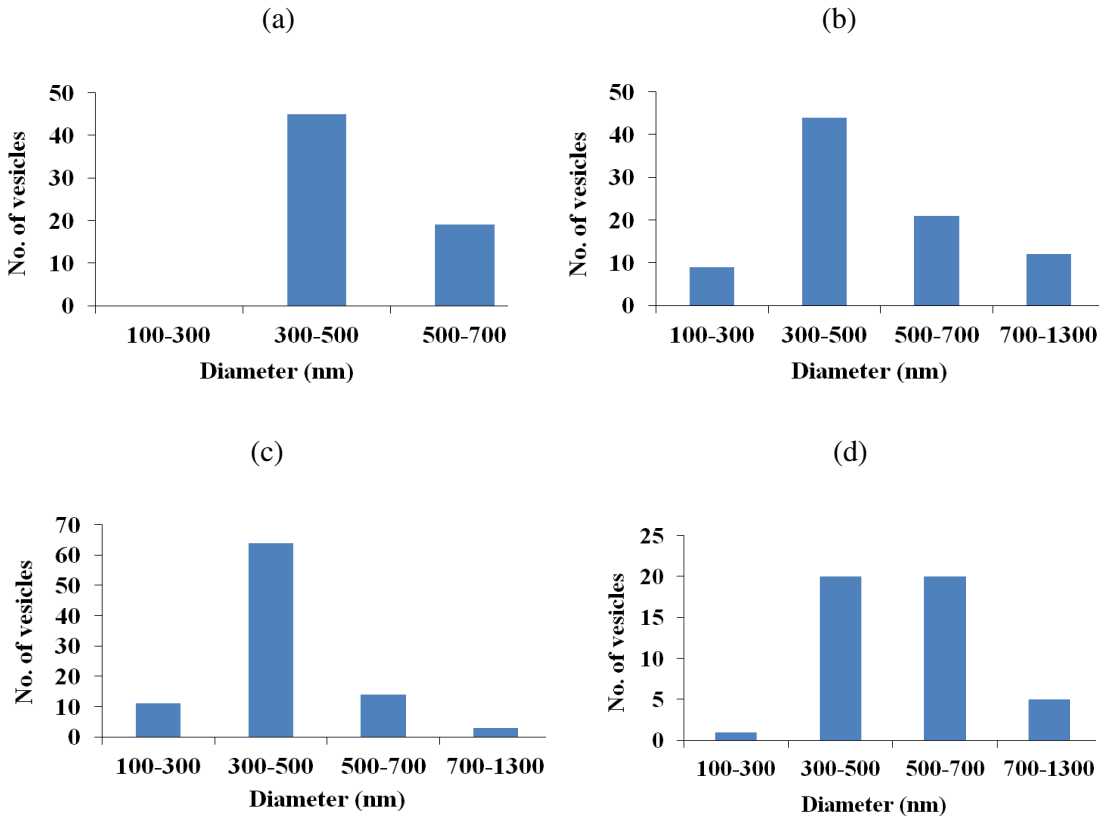
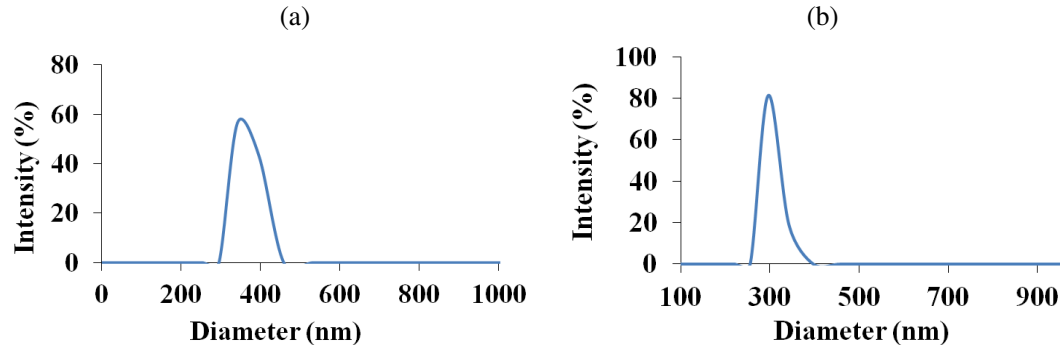


Figure S6. Histogram showing average size distribution of vesicles from SEM images of (a) **2** (b) **4** (c) **6** (d) **10**.



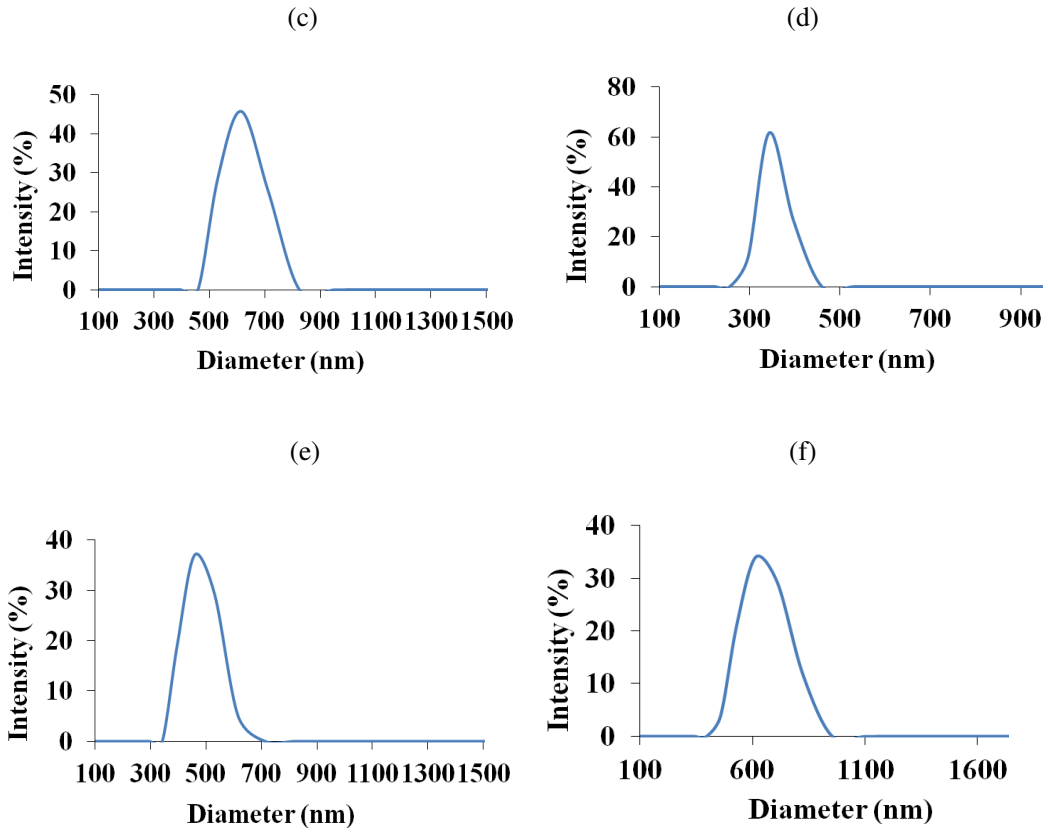
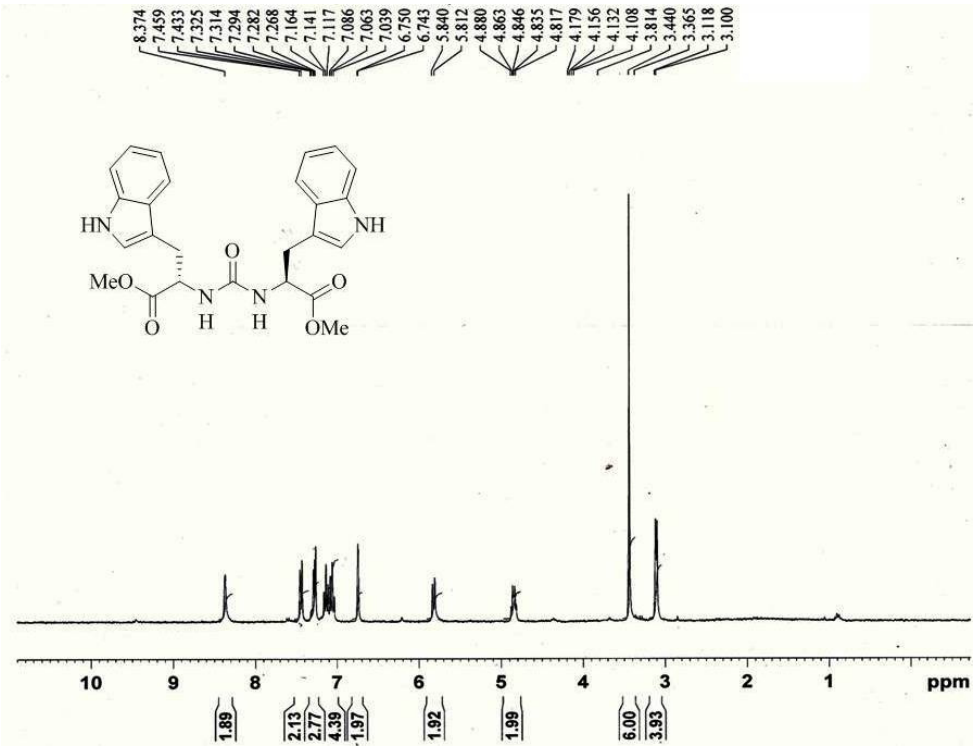
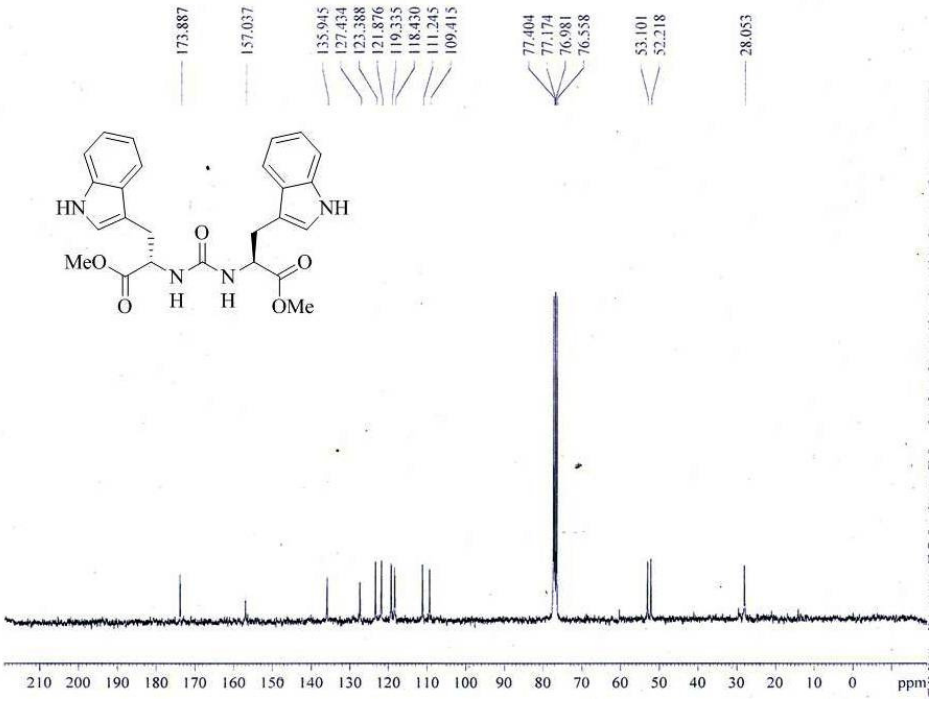


Figure S7. Dynamic light scattering graph showing average size distribution of (a) **2** (b) **4** (c) **6** (d) **10** (e) **10** + 5.0 equiv. $H_2PO_4^-$ (f) **10** + 5.0 equiv. HSO_4^- in methanol respectively.

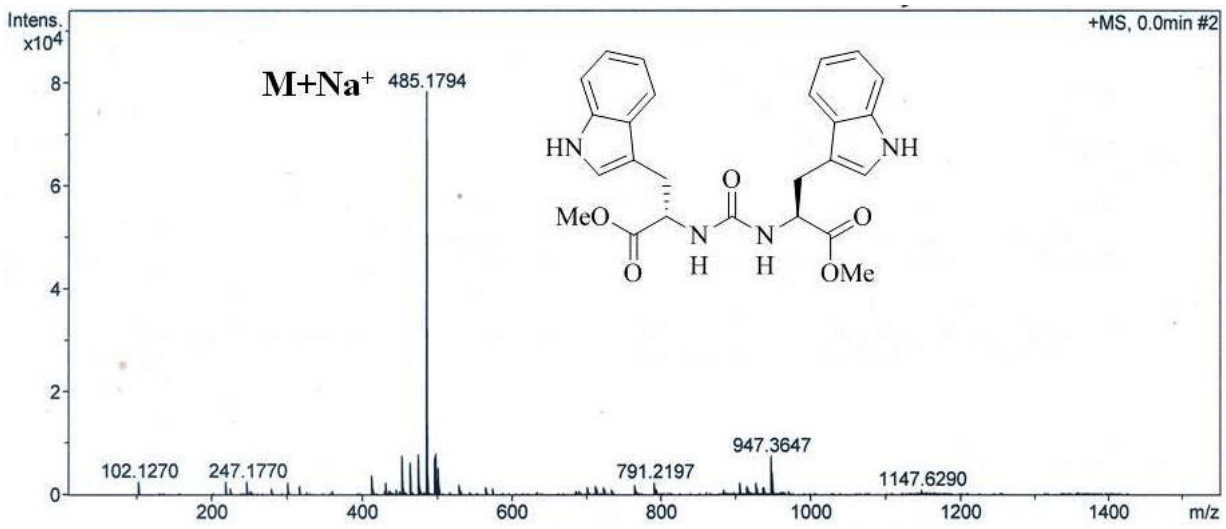
Spectral Data



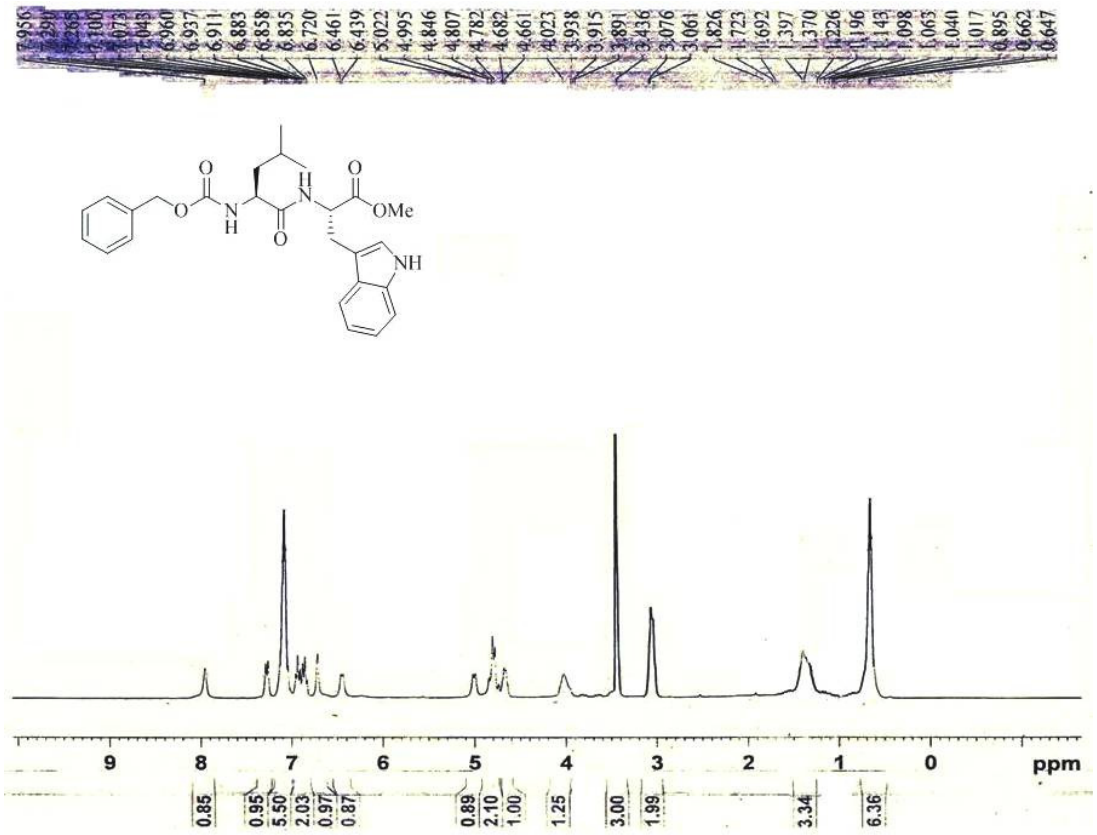
^{1}H NMR of **2** ($CDCl_3$, 300 MHz)



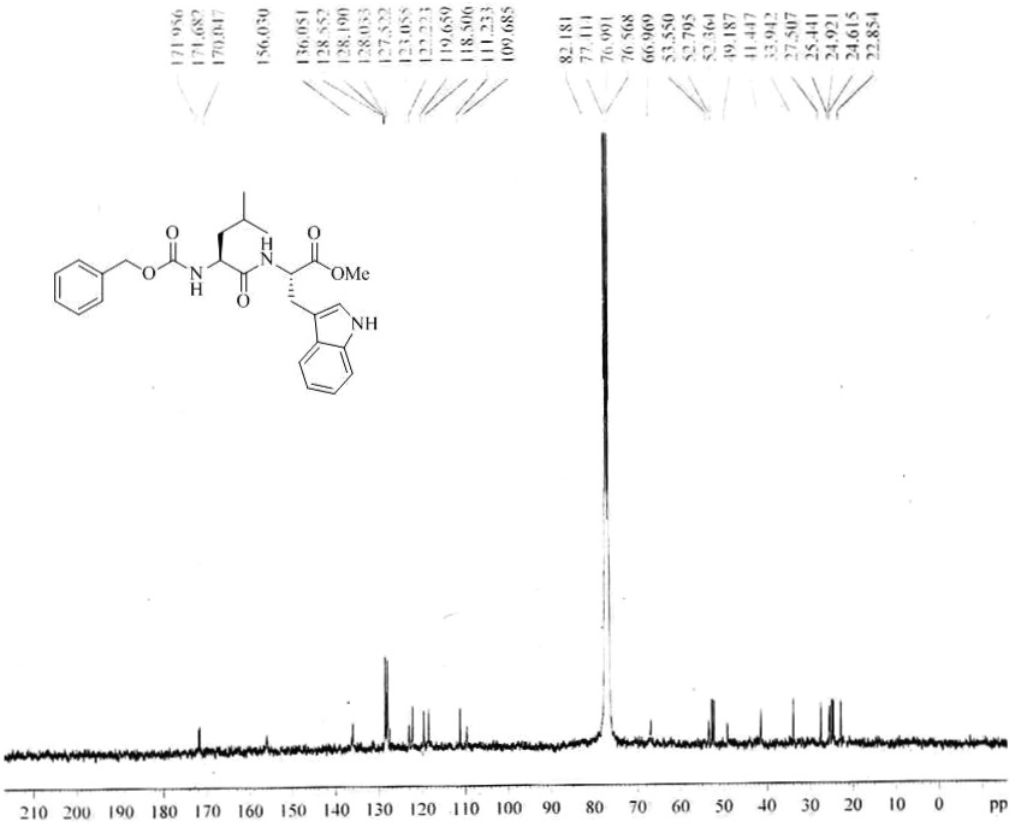
^{13}C NMR of **2** ($CDCl_3$, 75 MHz)



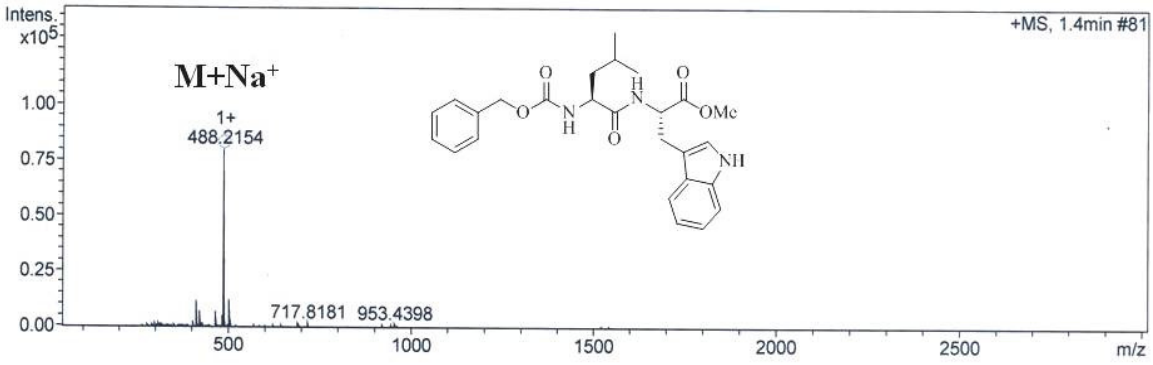
HRMS of **2**



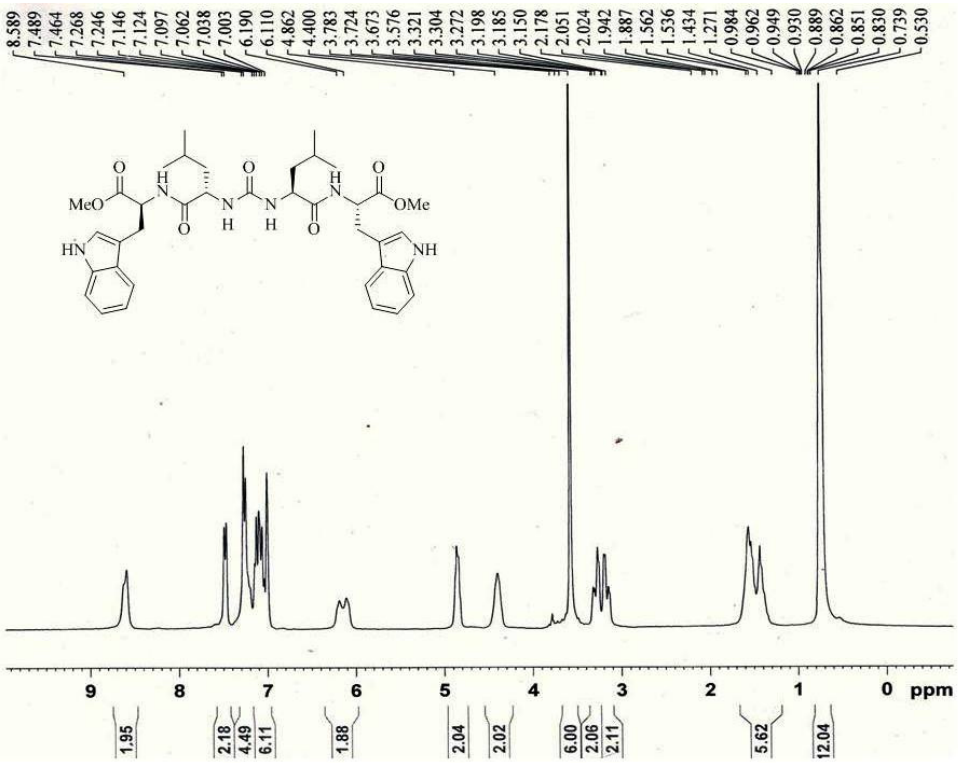
^{1}H NMR of **3** ($CDCl_3$, 300 MHz)



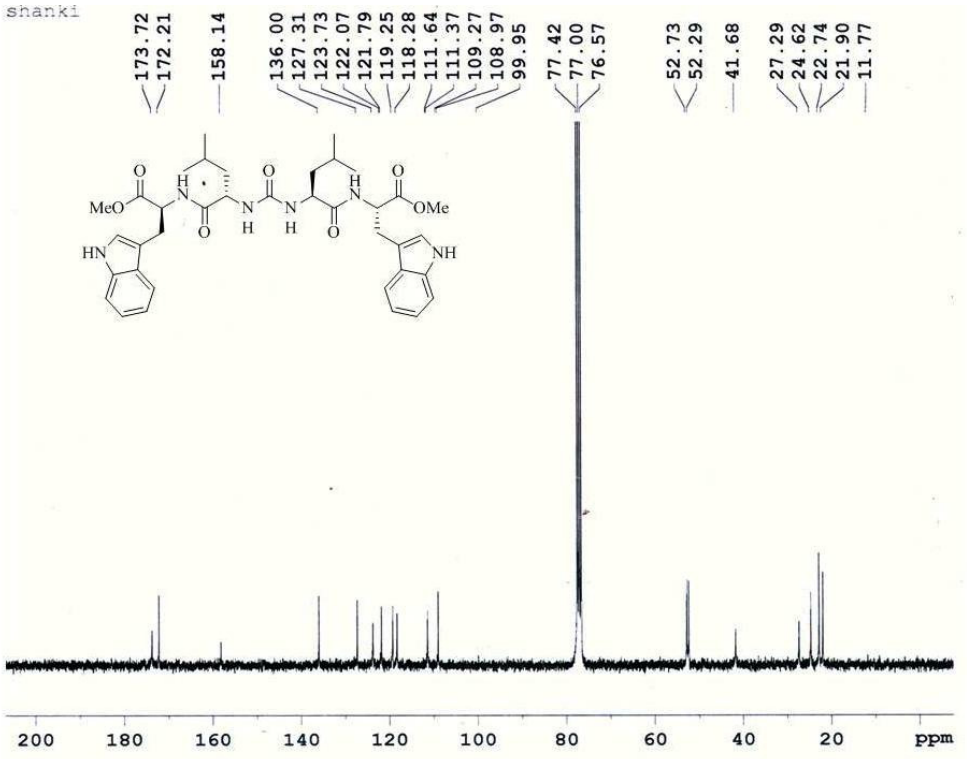
^{13}C NMR of **3** ($CDCl_3$, 75 MHz)



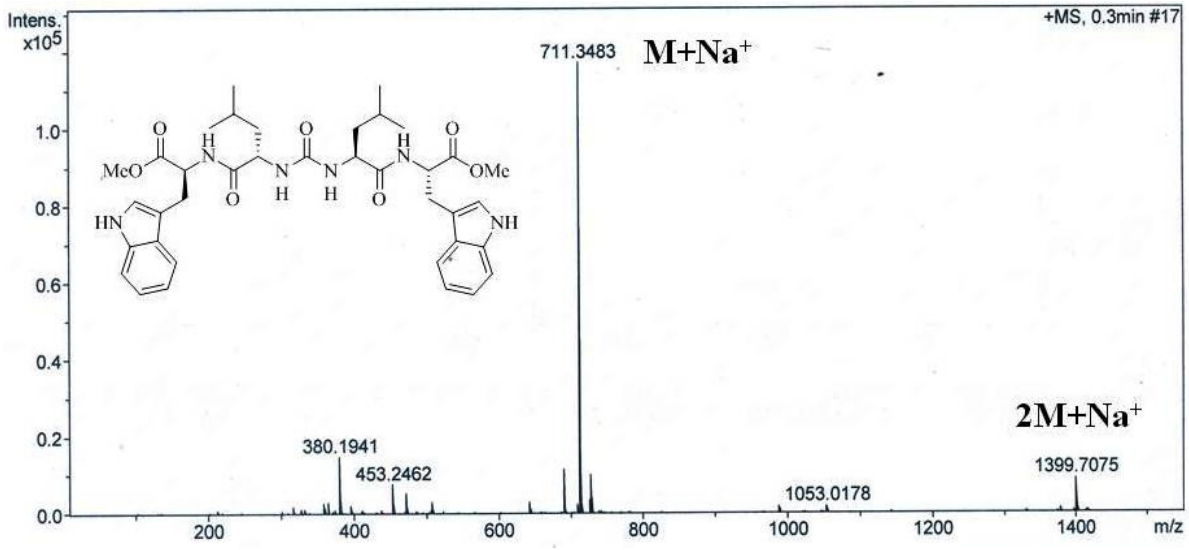
HRMS of **3**



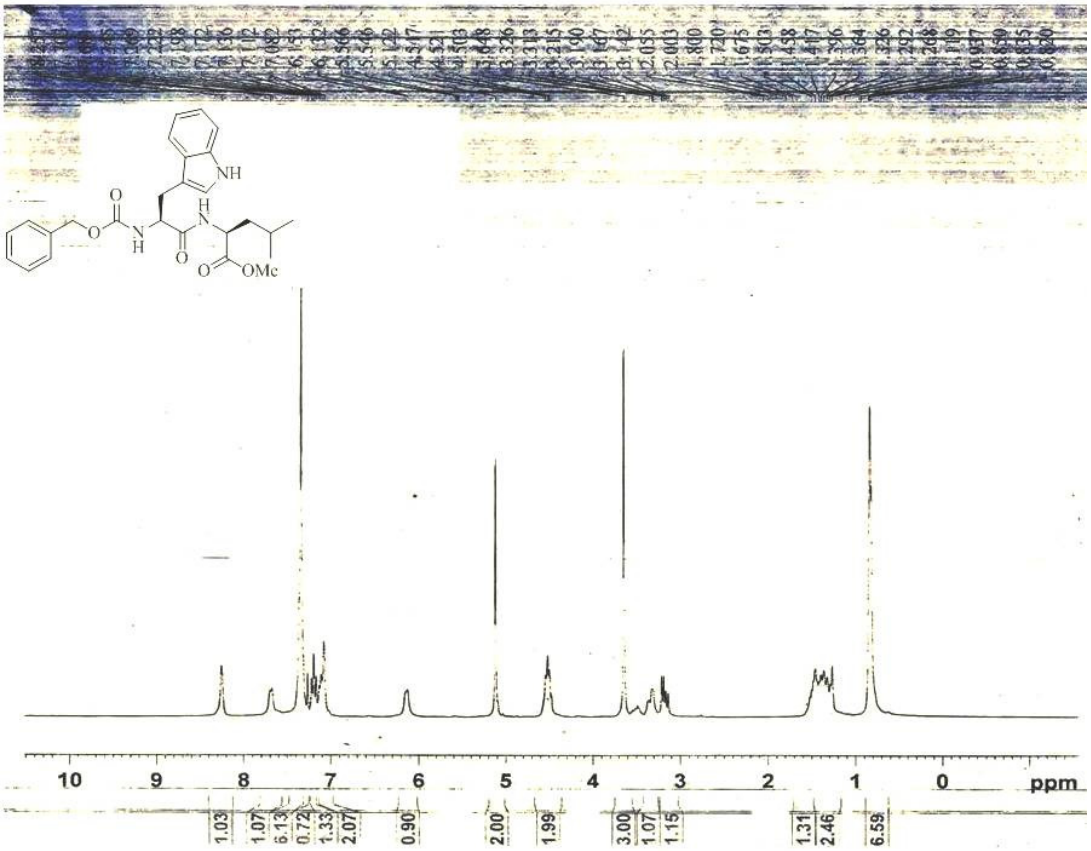
^{1}H NMR of **4** ($CDCl_3$, 300 MHz)



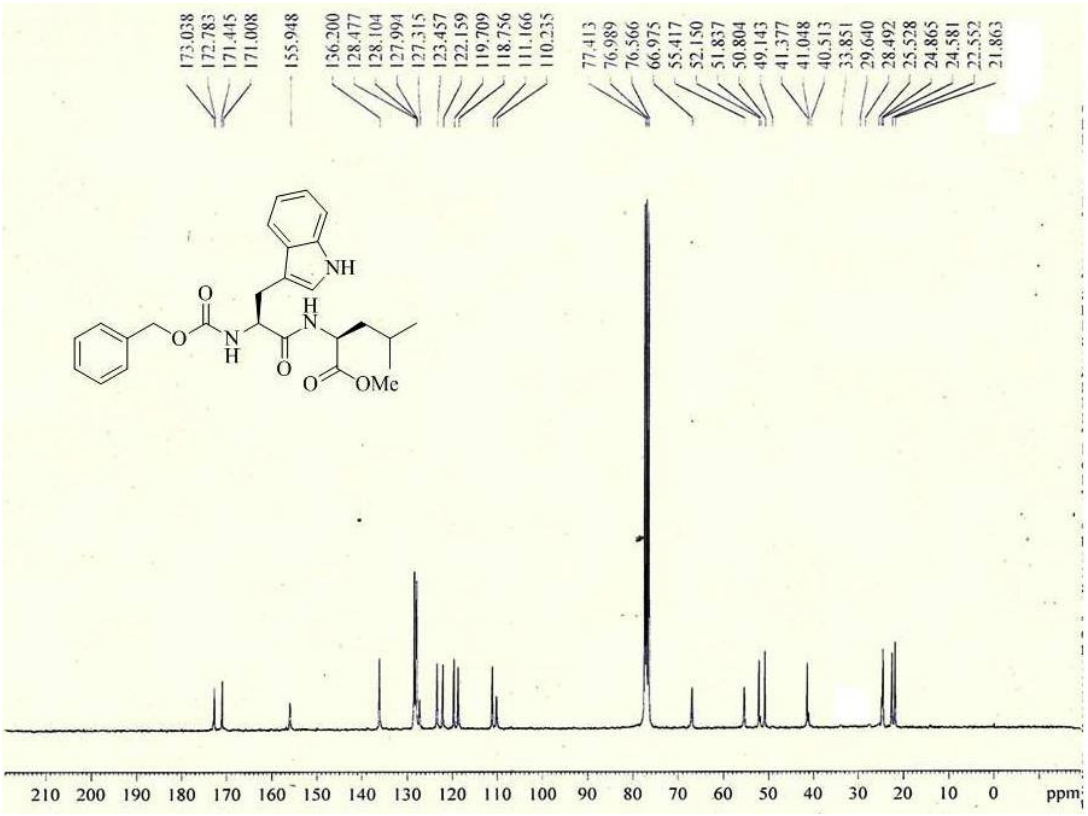
^{13}C NMR of **4** ($CDCl_3$, 75 MHz)



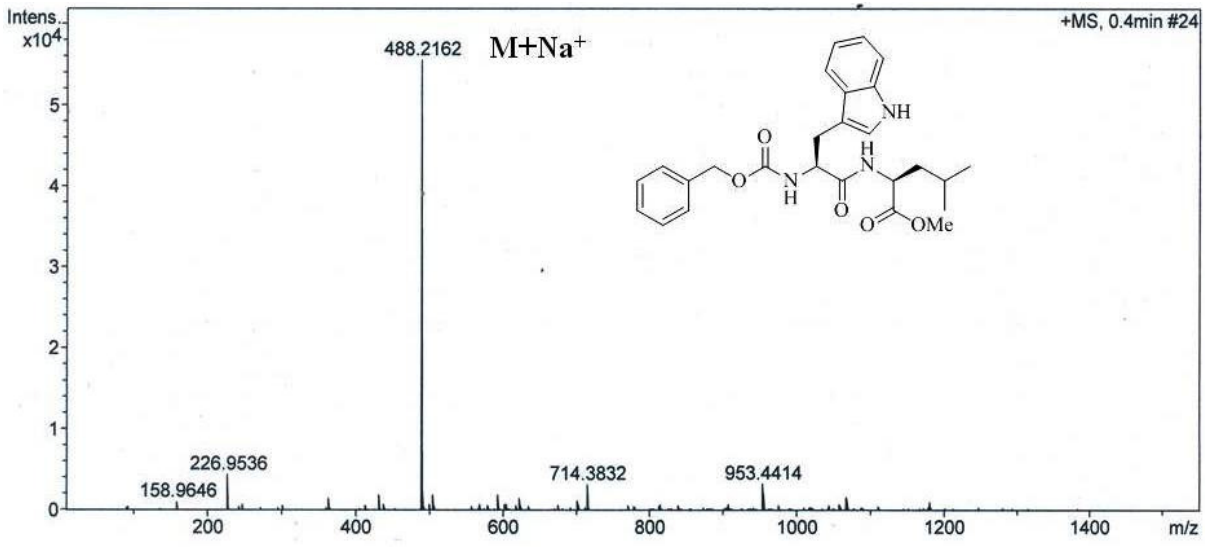
HRMS of **4**



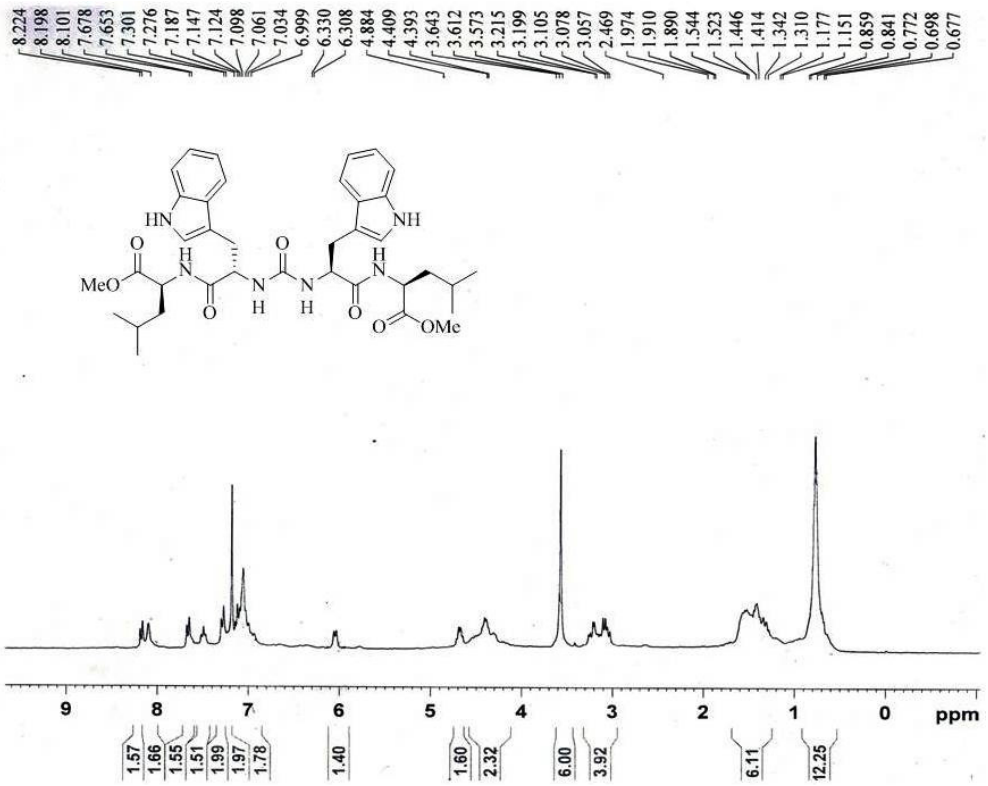
^{1}H NMR of **5** ($CDCl_3$, 300 MHz)



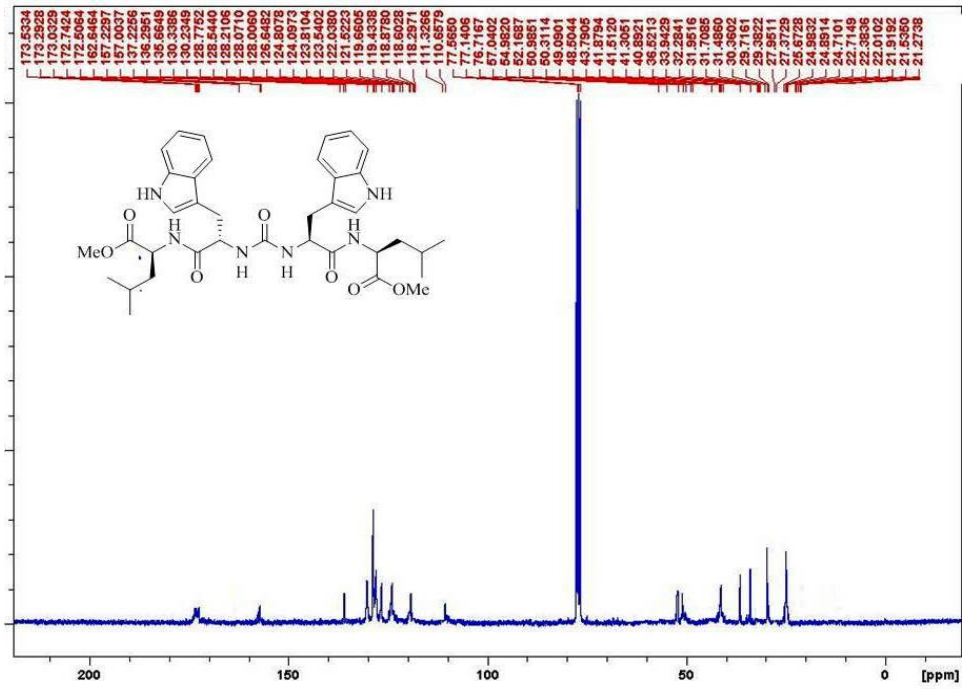
^{13}C NMR of **5** ($CDCl_3$, 75 MHz)



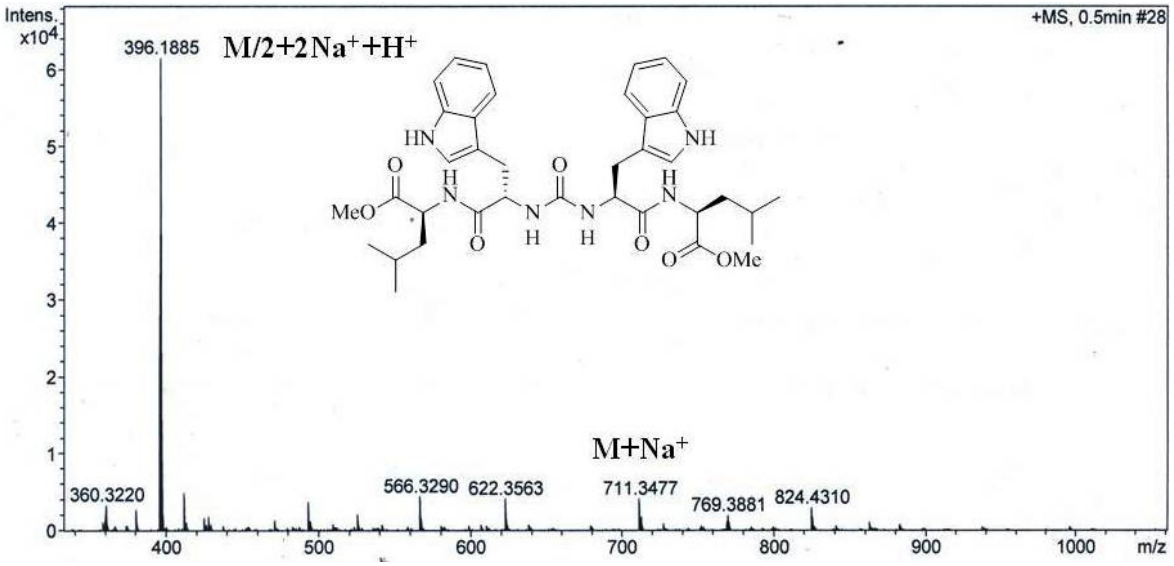
HRMS of **5**



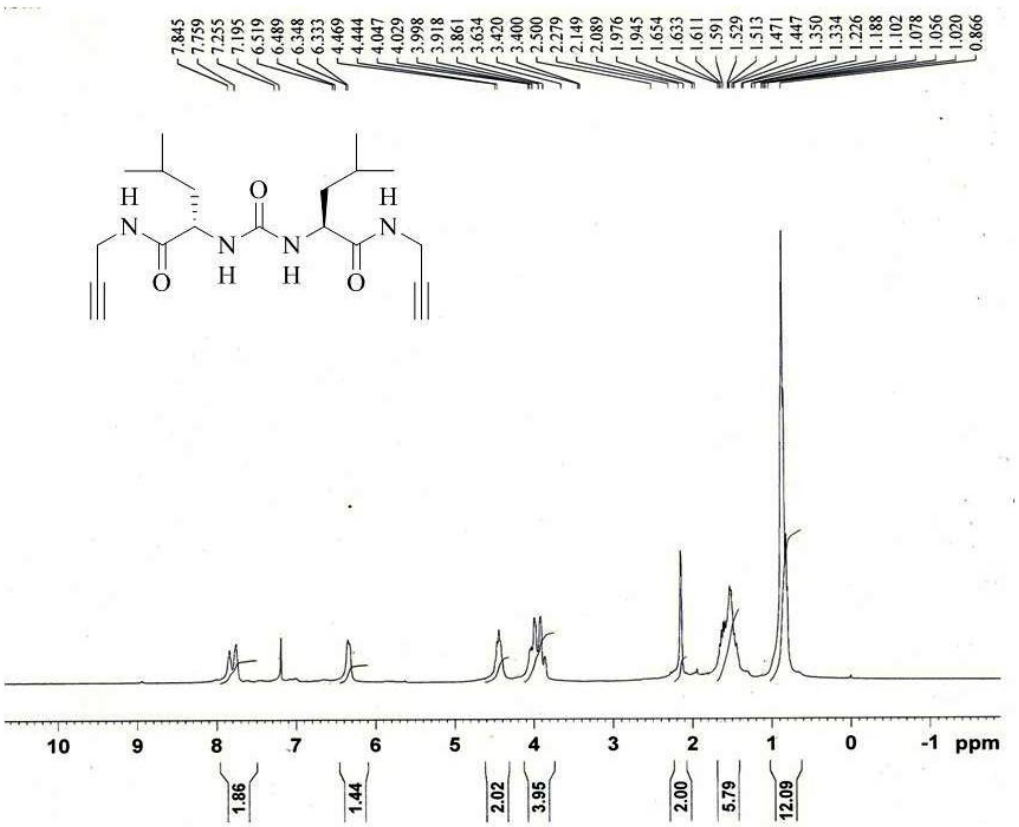
^{1}H NMR of **6** ($CDCl_3$, 300 MHz)



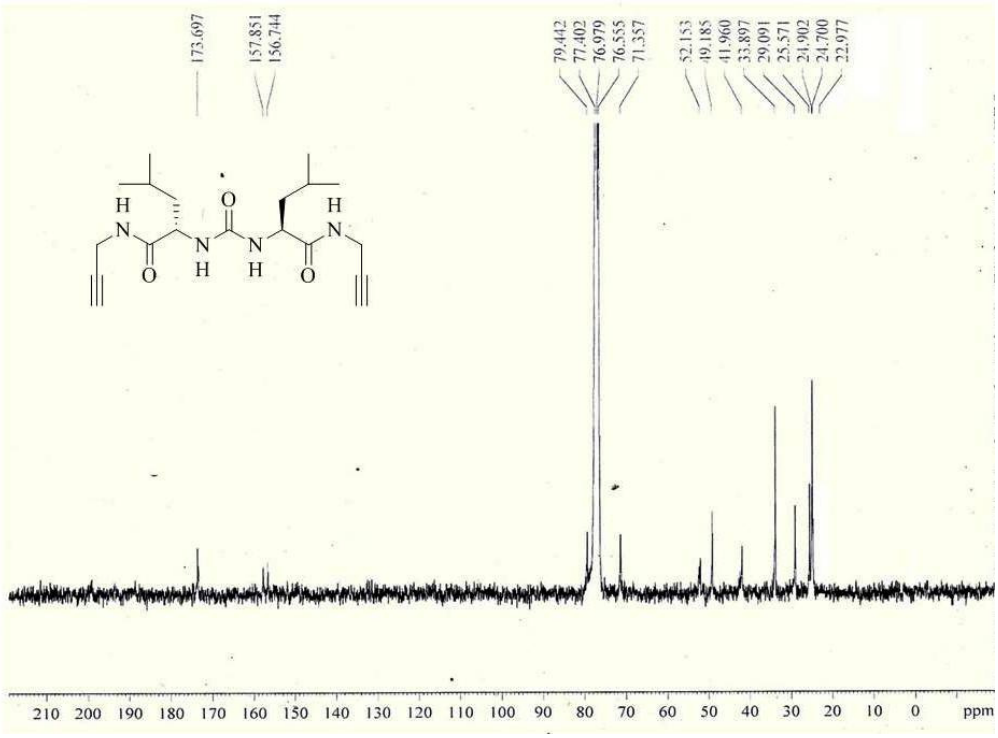
^{13}C NMR of **6** ($CDCl_3$, 75 MHz)



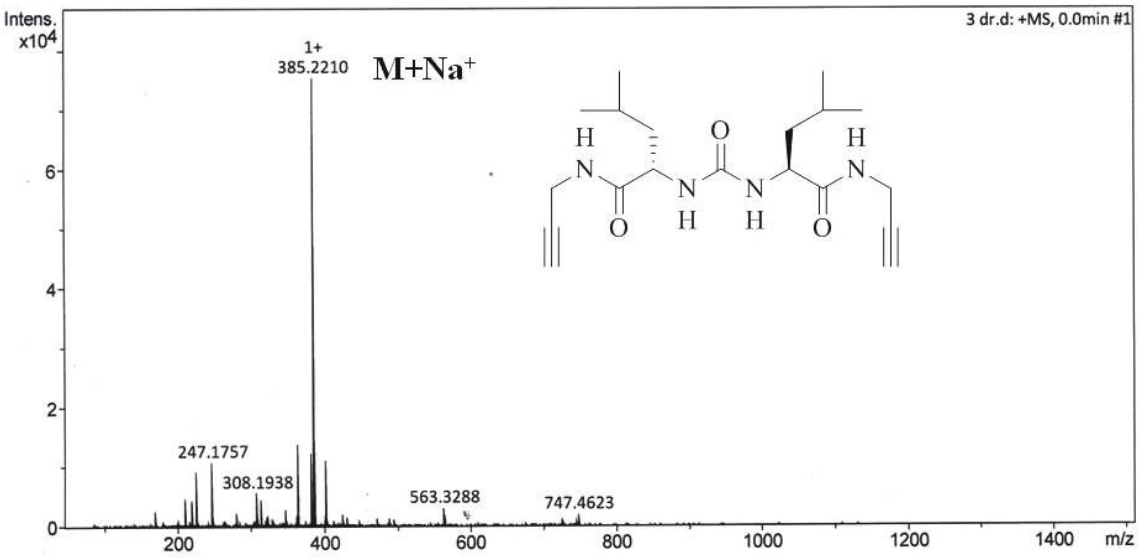
HRMS of **6**



^{1}H NMR of **9** ($CDCl_3$, 300 MHz)



^{13}C NMR of **9** ($CDCl_3$, 75 MHz)



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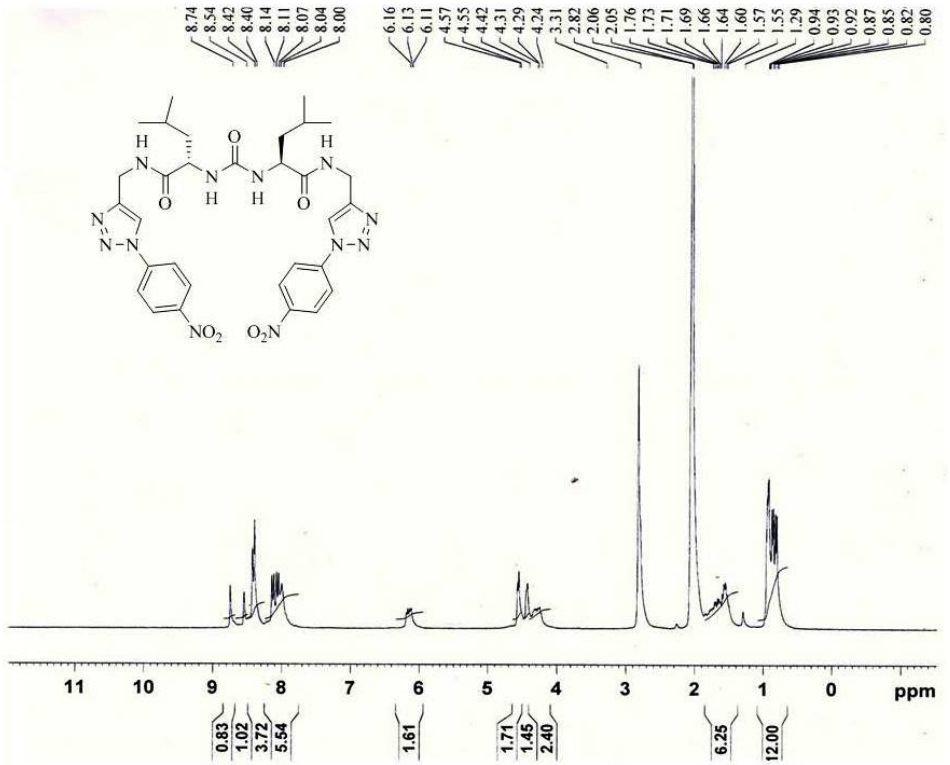
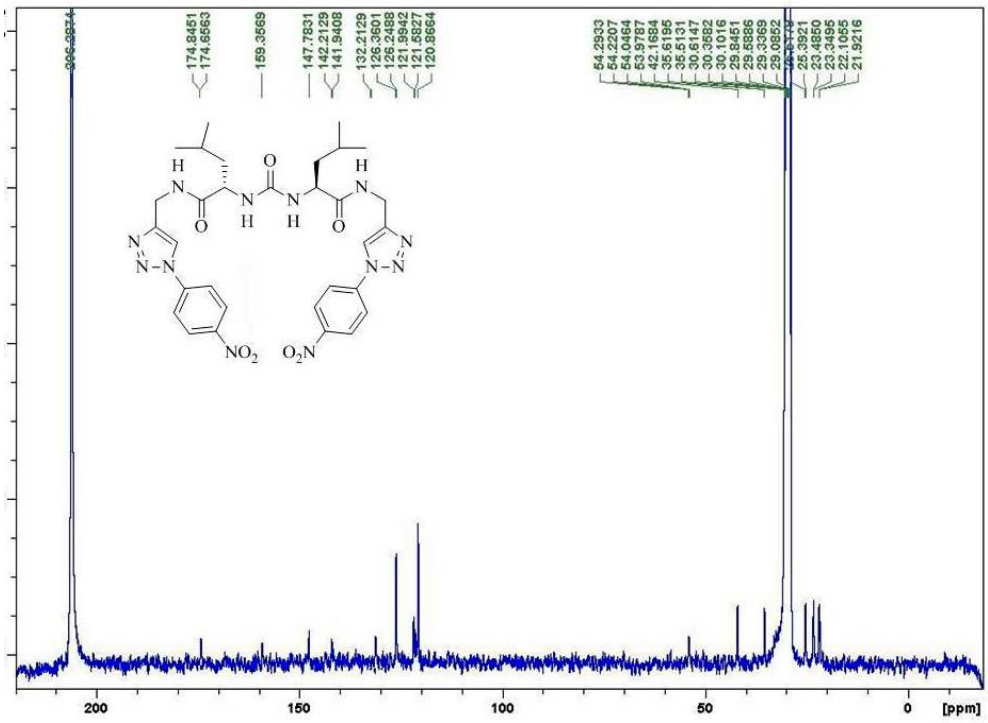
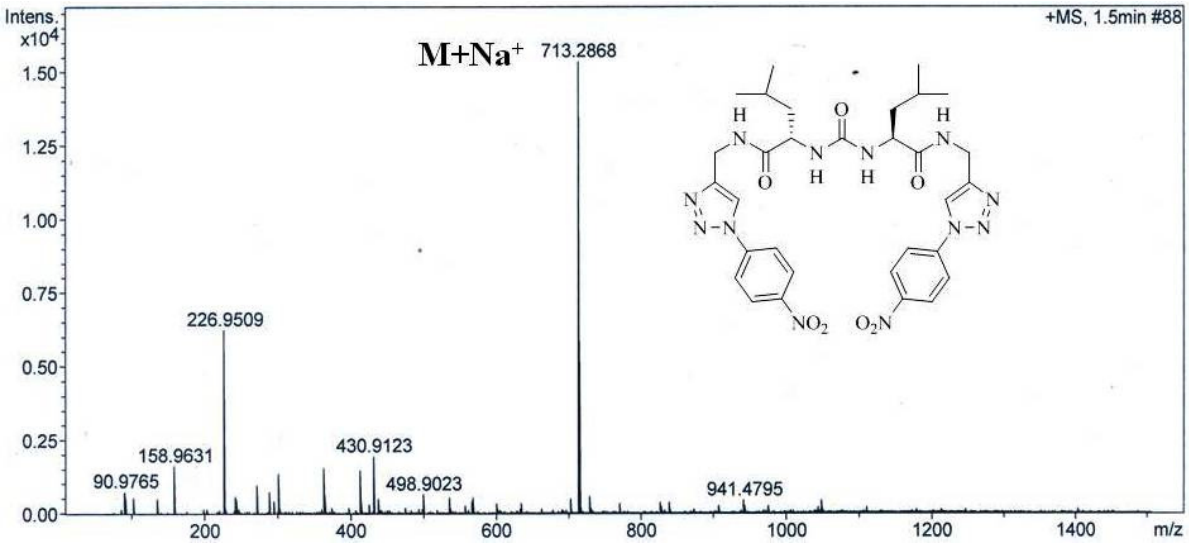


^{1}H NMR of **10** (Acetone-d_6, 300 MHz)



^{13}C NMR of **10** (Acetone-d_6, 75 MHz)



HRMS of **10**

