

## Supplementary Information

### **Fabrication of self-assembled nanostructures for intracellular drug delivery from diphenylalanine analogues with rigid or flexible chemical linkers**

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## Experimental section

**Peptide synthesis:** The designed Peptides were synthesized by conventional solution-phase methods. Peptide coupling was mediated by dicyclohexylcarbodiimide/1-hydroxybenzotriazole (DCC/HOBt). The products were purified by column chromatography using silica gel (100–200 mesh) as the stationary phase and an n-hexane–ethyl acetate mixture as an eluent. The final compounds were fully characterized by Bruker 500 MHz <sup>1</sup>H-NMR spectroscopy, and mass spectroscopy (Shimadzu, Japan, LCMS-2020 Spectrometer).

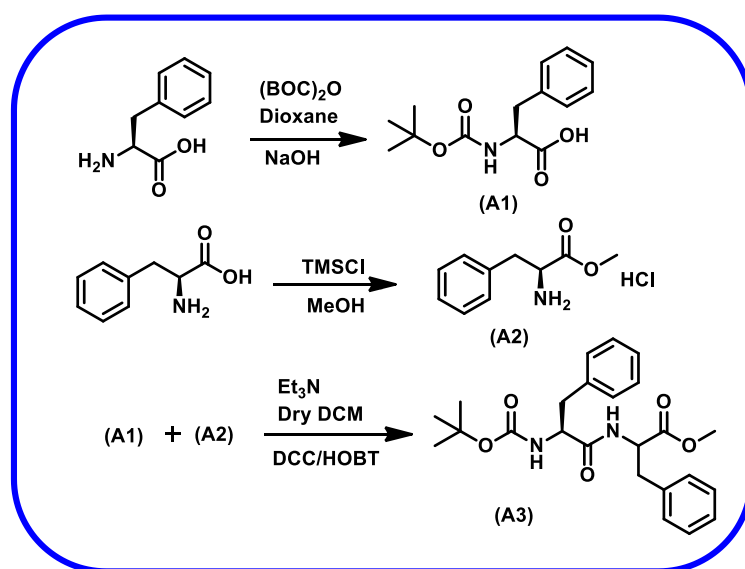
### A. Synthesis of PA1

**Synthesis of BOC-NH-Phe-OH (A1):** A solution of L-phenylalanine (5g, 30.26 mmol) in a mixture of dioxane (50 mL), water (30 mL), and 1 M NaOH (30 mL) was stirred and cooled in an ice-water bath. 7.92 g (36.31 mmol) of Di-tert-butyl dicarbonate was added and stirred continuously at room temperature (RT) for 6 hours. Then, the solution was concentrated using rotary evaporator to about 10–15 mL, cooled in an ice-water bath, covered with a layer of ethyl acetate (about 50 mL), and acidified with a dilute solution of KHSO<sub>4</sub> to pH 2–3 (determined by congo red). The aqueous phase was extracted with ethyl acetate and this operation was performed repeatedly 3 times. The ethyl acetate extracts were collected, pooled and washed with water, dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and evaporated under vacuum. The pure material was obtained as a waxy solid. Yield: 7.25 g (27.32 mmol, 90%) (Scheme S1).<sup>1, 2</sup>

**Synthesis of NH<sub>2</sub>-Phe-OMe Hydrochloride (A2):** L-Phenylalanine 6g (36.32 mmol) was taken in a round bottom flask and dissolved in 80 mL MeOH. Then, 7.83 mL (72.64 mmol) of Trimethyl chlorosilane (TMSCl) was added slowly to the resulting solution in a drop wise manner and stirred for 8 hours at room temperature. After the completion of reaction (as monitored by TLC), the excess solvent was evaporated on a rotary evaporator to get the solid

desired product L-Phenylalanine methyl ester hydrochloride. Yield: 7.56 g (35 mmol, 96.5%) (Scheme S1).<sup>1,3</sup>

**Synthesis of BOC-Phe-Phe-OMe (A3):** 7.25 g (27.32 mmol) of Boc-Phe-OH were dissolved in 50 mL dry DCM in an ice-water bath. NH<sub>2</sub>-Phe-OMe.HCl 6.48 g (30.05mmol) and Et<sub>3</sub>N 4ml, 30 mmol) were then added to the reaction mixture, followed immediately by the addition of 6.76 g (32.78 mmol) dicyclohexylcarbodiimide (DCC) and 5.02 g (32.78 mmol) of HOBT. The reaction mixture was allowed to warm-up to RT and stirred for 48 hours. DCM was evaporated and the residue was dissolved in ethyl acetate (45 mL). The dicyclohexylurea (DCU) was filtered off. The organic layer was washed with 2M HCl (3 X 50 mL), brine (2 X 50 mL) followed by 1 M sodium carbonate (3 X 50 mL) and brine (2 X 50 mL), and finally dried over anhydrous sodium sulfate. It was then evaporated under vacuum to yield Boc-Phe-Phe-OMe as a white solid. The product was purified by silica gel (100–200 mesh) using n-hexane–ethyl acetate (3:1) as eluent. Yield: 10.25 g (24mmol, 87%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz, δppm): 7.22-6.90 (m, 10H, ArH of Phe), 6.23 (s, 1H, NH), 4.88-4.71 (t, 2H, CαH, Phe), 4.27(s, 1H, NH), 3.59(s, 3H, OMe), 3.01- 2.94(m, 4H, CβH, Phe), 1.32 (s, 9H, Boc) (Scheme S1).<sup>1</sup>

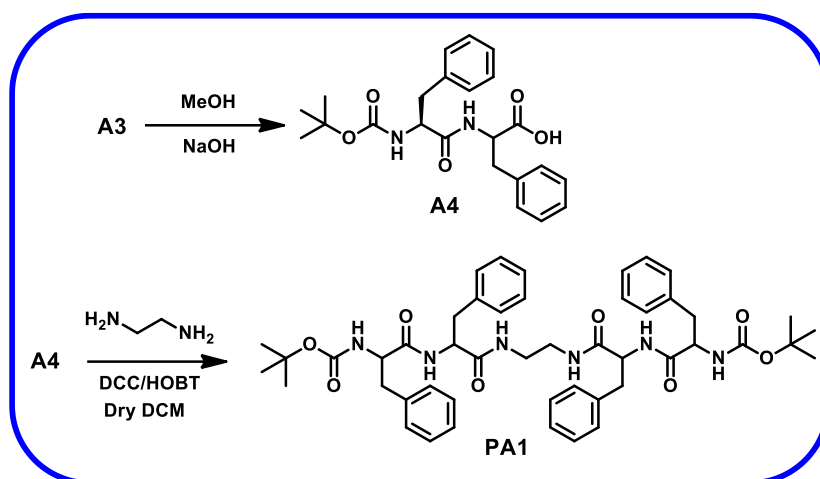


**Scheme S1:** Synthetic methodologies adopted for the synthesis of A1, A2 and A3.

**Synthesis of BOC-NH-Phe-Phe-OH (A4):** In a 250 mL round bottle flask 3 g (7.03 mmol) of Boc-Phe-Phe-OMe, 40 mL MeOH and 2M 12 mL NaOH were added and the progress of saponification was monitored by thin layer chromatography (TLC). The reaction mixture was stirred. After 10 hours, the methanol was removed under vacuum using rotary evaporator; the remaining residue was dissolved in 50 mL of water, and washed with diethyl ether (2 X 50 mL). Then, the pH of the aqueous layer was adjusted to 2 using 1M HCl and extracted with ethyl acetate (3 X 50 mL). The combine extracts were pooled, dried over anhydrous sodium sulfate, and evaporated under vacuum to obtain the compound as a waxy solid. Yield: 2.79 g (6.76 mmol, 96%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz, δppm): 7.21-7.04 (m, 10H, ArH of Phe), 6.75 (s, 1H, NH), 5.25(s, 1H, NH), 4.84-4.45 (m, 2H, CαH, Phe), 3.14- 2.95(m, 4H, CβH, Phe), 1.38 (s, 9H, Boc) (Scheme S2).<sup>1</sup>

**Synthesis of BOC-Phe-Phe-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CO-Phe-Phe-BOC (PA1):** 2.5 g (5.86 mmol) of Boc-Phe-Phe-OH were dissolved in 40 mL dry DCM in an ice-water bath. Ethylene diamine (NH<sub>2</sub>-CH<sub>2</sub>-CH<sub>2</sub>-NH<sub>2</sub>) 176 mg (2.93 mmol) then added to the reaction mixture, followed immediately by the addition of 1.45 g (7.03 mmol) dicyclohexylcarbodiimide (DCC) and 1.07 g (7.03 mmol) of HOBt. The reaction mixture was allowed to warm-up to RT and was stirred for 48 hours. DCM was evaporated and the residue was dissolved in ethyl acetate (45 mL). The dicyclohexylurea (DCU) was filtered off. The organic layer was washed with 2M HCl (3 X 50 mL), followed by brine (2 X 50 mL) then with 1 M sodium carbonate (3 X 50 mL) followed by brine (2 X 50 mL), and finally dried over anhydrous sodium sulfate. It was then evaporated using vacuum to get the **PA1** as a crude product. Then it was purified by column chromatography by silica gel (100–200 mesh) using n-hexane–ethyl acetate as eluent. Yield 1.55 g (1.82 mmol, 62%). (<sup>1</sup>H NMR, DMSO d<sub>6</sub>, 500 MHz, δppm): 8.32-8.30 (d, 1H, NH), 8.04-7.99 (d, 1H, NH), 7.27-7.16 (m, 20H, ArH of Phe), 7.11-7.10 (d, 1H, NH) 6.93-6.92 (d, 1H, NH), 6.77-6.76 (d, 1H, NH Ethylene diamine), 5.59-5.57 (d, 1H, NH Ethylene diamine), 4.50-

4.44 (dd, 2H, C $\alpha$ H, Phe), 4.17-4.10 (m, 2H, C $\alpha$ H, Phe), 3.03-2.95 (m, 4H, CH<sub>2</sub> Ethylene diamine), 2.87-2.82 (d, 2H, C $\beta$ H, Phe), 2.68-2.63 (d, 2H, C $\beta$ H, Phe), 1.76-1.70 (d, 2H, C $\beta$ H, Phe), 1.63-1.59 (d, 2H, C $\beta$ H, Phe), 1.31-1.23 (m, 18H, Boc). <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>,  $\delta$ ppm): 171.88, 171.77, 171.48, 157.10, 156.72, 156.58, 138.52, 129.77, 129.67, 128.52, 128.45, 126.78, 126.61, 126.55, 78.62, 56.38, 56.09, 50.89, 47.98, 33.84, 32.78, 28.58. FTIR (CaF<sub>2</sub>,  $\nu_{\max}$ , cm<sup>-1</sup>): 644 (Amide, N-H out of plane bend), 1163 (Ester (BOC), C-O str), 1243, 1310 (C-N str), 1529-1570 (Amide, N-H inplane bend), 1621, 1650, 1685 (Amide, C=O str), 3320 (Amide, N-H str). ESI-MS (m/z): [M]=848.45 (calculated); 848.50 (observed) (Scheme S2). Elemental analysis calcd (%): (C<sub>48</sub>H<sub>60</sub>N<sub>6</sub>O<sub>8</sub>): C 67.90, H 7.12, N 9.90, O 15.08; found: C 66.82, H 6.93, N 10.15.



**Scheme S2:** Synthetic methodologies adopted for the synthesis of **A4** and **PA1**.

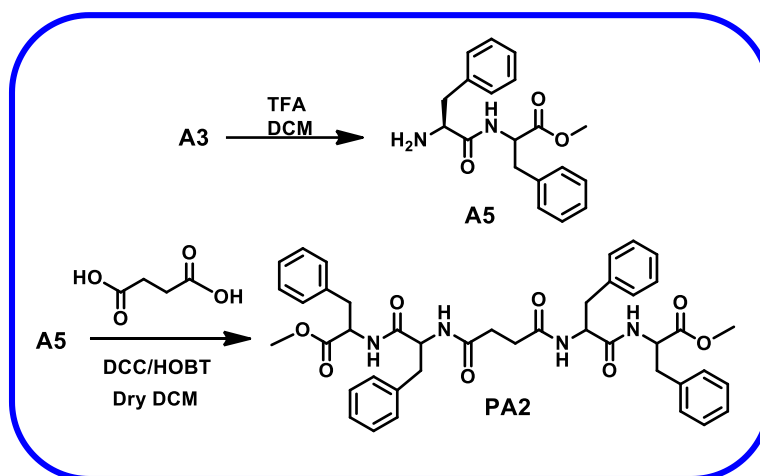
## B. Synthesis of PA2

**Synthesis of NH<sub>2</sub>-Phe-Phe-OMe (A5):** 5 g (11.73 mmol) of Boc-NH-Phe-Phe-OMe was dissolved in 40 mL of DCM in an ice bath. Then, 20 mL of Trifluoroacetic acid (TFA) was added and stirred for 2h. The progress of the reaction was monitored by TLC. After the completion of the reaction solvents were evaporated under vacuum. Then the residual product was dissolved in water and neutralized with NaHCO<sub>3</sub> solution, After neutralization this aqueous layer was extracted with ethyl acetate, and the combined ethylacetate layer was dried over anhydrous sodium sulfate and evaporated under vacuum to obtain an oily product, which was

immediately used for the next reaction. Yield: 3.75 g (11.5 mmol, 97%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz, δppm): 7.57-7.01 (m, 10H, ArH of Phe), 6.85-6.83 (d, 2H, NH<sub>2</sub>) 4.72-3.95 (m, 2H, CαH, Phe), 2.98-2.86 (m, 4H, CβH, Phe) (SchemeS3).

**Synthesis of OMe-Phe-Phe-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-Phe-Phe-OMe (PA2):** 2g (6.12 mmol) was dissolved in 40 mL dry DCM in an ice water bath. 360mg (3.06 mmol) of Succinic acid (COOH-CH<sub>2</sub>-CH<sub>2</sub>-COOH) was then added to the reaction mixture, followed by immediate addition of 1.51 g (7.34 mmol) dicyclohexylcarbodiimide (DCC) and 1.12 g (7.34 mmol) of HOBt. The reaction mixture was allowed to warm-up at RT and stirred for 48 hours. After the completion of reaction (monitored by TLC) DCM was evaporated and the residue was dissolved in ethyl acetate (45 mL). The dicyclohexylurea (DCU) was filtered off. The organic layer was washed with 2M HCl (3 X 50 mL), followed by brine (2 X 50 mL) then with 1 M sodium carbonate (3 X 50 mL) followed by brine (2 X 50 mL), and finally dried over anhydrous sodium sulfate. After that this was evaporated under vacuum to yield **PA2** as a crude product (white solid). Then the crude product was purified by column chromatography by silica gel (100–200 mesh) using n-hexane–ethyl acetate as eluent. Yield 1.56 g (2.12 mmol, 69.6%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz, δppm): 7.25-7.21 (m, 5H, ArH of Phe), 7.18-7.16 (m, 5H, ArH of Phe), 7.13-7.11 (m, 4H, ArH of Phe), 7.08 (d, *J*=7Hz, 2H, ArH of Phe), 6.89-6.87 (m, 4H, ArH of Phe), 5.74 (d, *J*= 7.5Hz, 2H, NH), 4.67-4.63 (m, 2H, CαH), 4.51-4.48 (m, 2H, CαH), 3.65(s, 6H, OMe), 3.08-3.00 (m, 4H, CβH), 2.97-2.93 (m, 2H, CβH), 2.90-2.86 (m, 2H, CβH), 2.10 (s, 4H, CH<sub>2</sub>-CH<sub>2</sub>). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>, δppm): 171.16, 168.79, 156.84, 135.21, 129.35, 129.12, 128.84, 128.74, 127.51, 127.38, 54.66, 53.65, 52.56, 49.27, 38.29, 37.79, 33.95, 25.63, 24.98. FTIR (CaF<sub>2</sub>, ν<sub>max</sub>, cm<sup>-1</sup>): 695, 748 (Amide, N-H out of plane bend), 1163, 1182 (Ester, C-O str), 1266, 1283 (C-N str), 1547 (Amide, N-H inplane bend), 1660, 1695 (Amide, C=O str), 1733 (Ester, C=O str), 3320 (Amide, N-H str). ESI-MS (m/z): [M-H]<sup>+</sup>=733.33

(calculated); 733.35 (observed) (SchemeS3). Elemental analysis calcd (%): (C<sub>42</sub>H<sub>46</sub>N<sub>4</sub>O<sub>8</sub>): C 68.65, H 6.31, N 7.62, O 17.92; found: C 67.54, H 7.03, N 6.98.

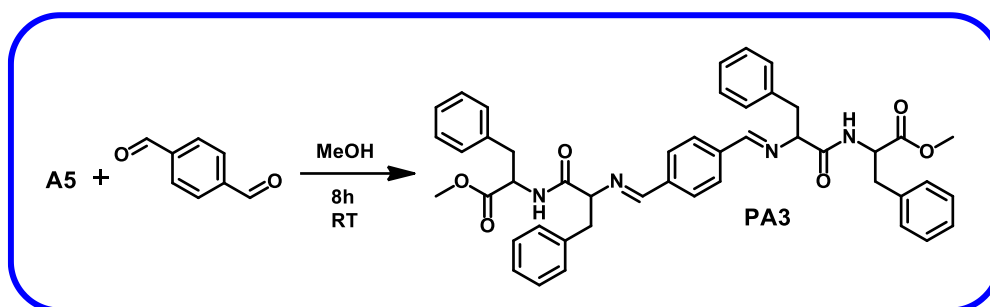


**Scheme S3:** Synthetic methodologies adopted for the synthesis of **A5** and **PA2**.

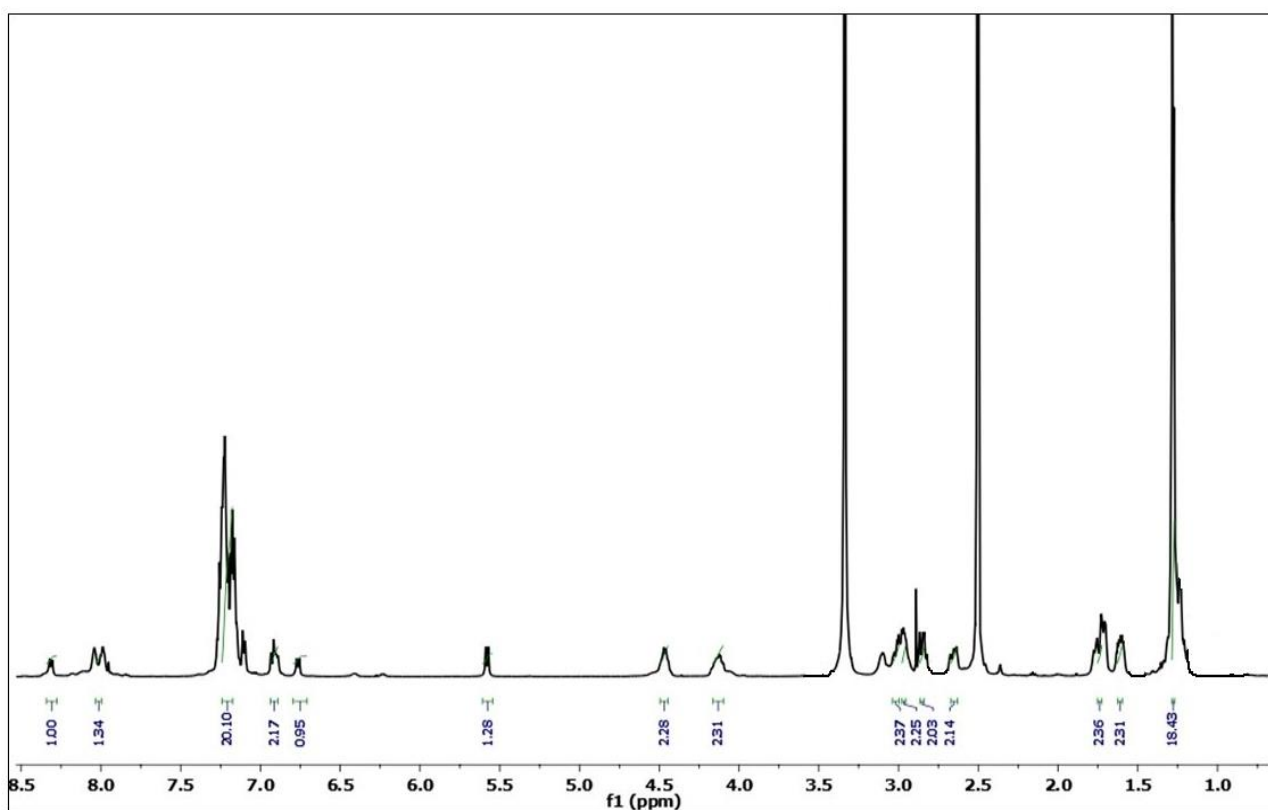
### C. Synthesis of OMe-Phe-Phe-N=CH-C<sub>6</sub>H<sub>4</sub>-CH=N-Phe-Phe-OMe (**PA3**):

1.0 gm (3.06 mmol) of NH<sub>2</sub>-Phe-Phe-OMe was dissolved in 40 ml of methanol. Then Terephthalaldehyde (205 mg, 1.53 mmol) added to the methanolic solution of A5. The resulting mixture was stirred for 8h. After the reaction was completed (confirmed by TLC) white solid precipitate appeared. This precipitate was filtered off and washed with n-hexane and cold methanol and dried in desiccator to afford OMe-Phe-Phe-N=CH-C<sub>6</sub>H<sub>4</sub>-CH=N-Phe-Phe-OMe (**PA3**) as a white colour pure product. Yield: 970 mg (1.29 mmol, 84.5%). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz, δppm): 7.93 (s, 1H, N=CH), 7.3-7.27 (m, 5H, ArH of Phe), 7.22-7.19 (m, 2H, ArH of Phe), 7.04-7.03 (5H, ArH of Phe), 3.97 (m, broad signal 2H, CaH), 3.37 (s, 3H, OMe), 2.59-2.55 (m, 2H, CβH), 2.25-2.20 (m, 2H, CβH). <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>, δppm): 170.21, 164.75, 159.85, 143.53, 139.58, 130.48, 130.33, 128.24, 128.02, 126.15, 57.11, 40.50, 40.41, 40.33, 39.57, 39.41. FTIR (CaF<sub>2</sub>, ν<sub>max</sub>, cm<sup>-1</sup>): 697, 757 (Amide, N-H out of plane bend), 1192, 1210 (Ester, C-O str), 1268 (C-N str), 1458 (Imine, C-H str), 1502 (Amide, N-H inplane bend), 1659, 1676 (Amide, C=O str/Imine C=N str), 1737 (Ester, C=O), 3198 (Amide, N-H str). (ESI-MS (m/z): [M+H]<sup>+</sup> =751.34 (calculated); 751.50 (observed) (SchemeS4). Elemental

analysis calcd (%): (C<sub>46</sub>H<sub>46</sub>N<sub>4</sub>O<sub>6</sub>): C 73.58, H 6.17, N 7.46, O 12.78; found: C 72.43, H 5.64, N 8.13.

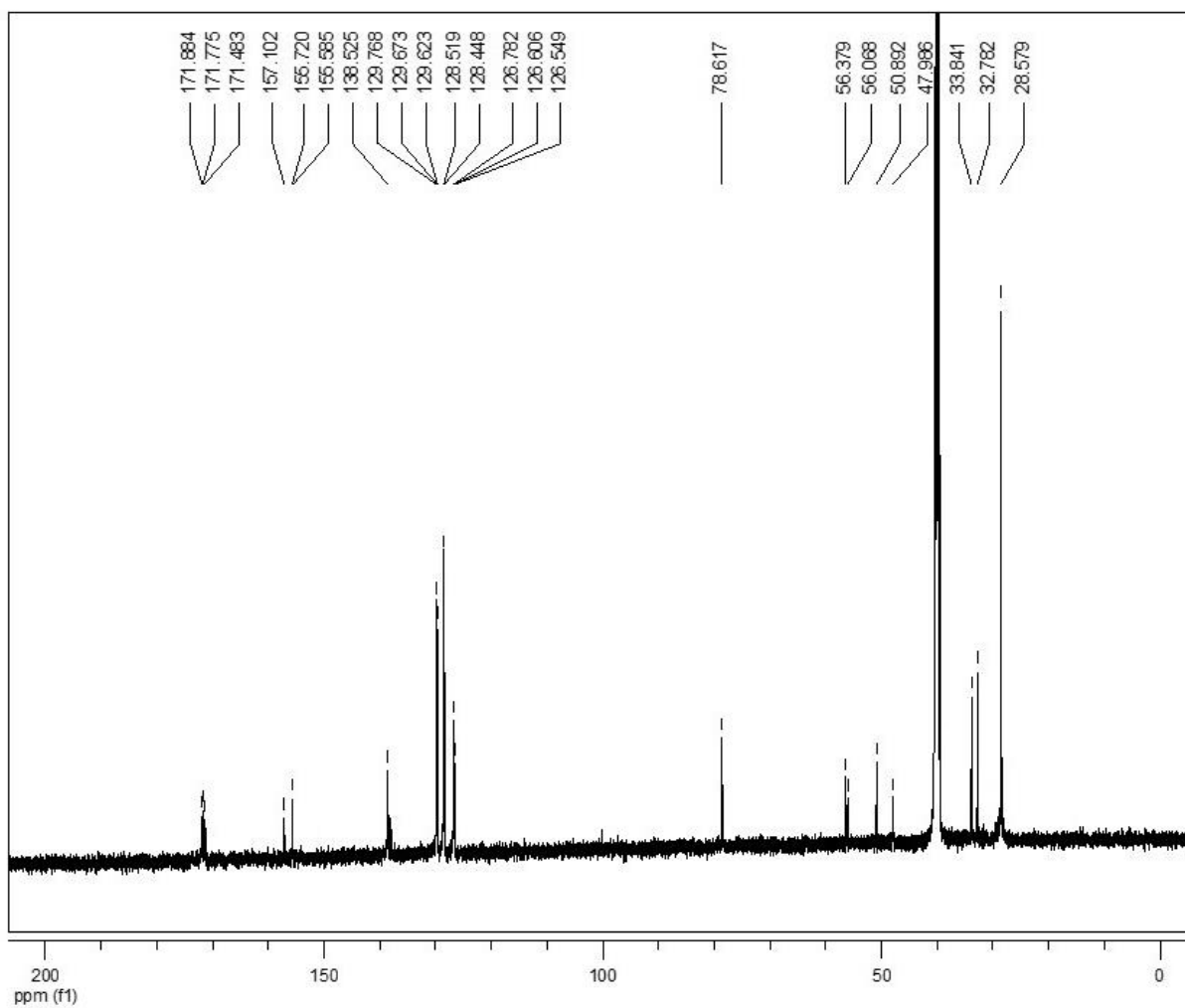


**Scheme S4:** Synthetic methodologies adopted for the synthesis of **PA3**.

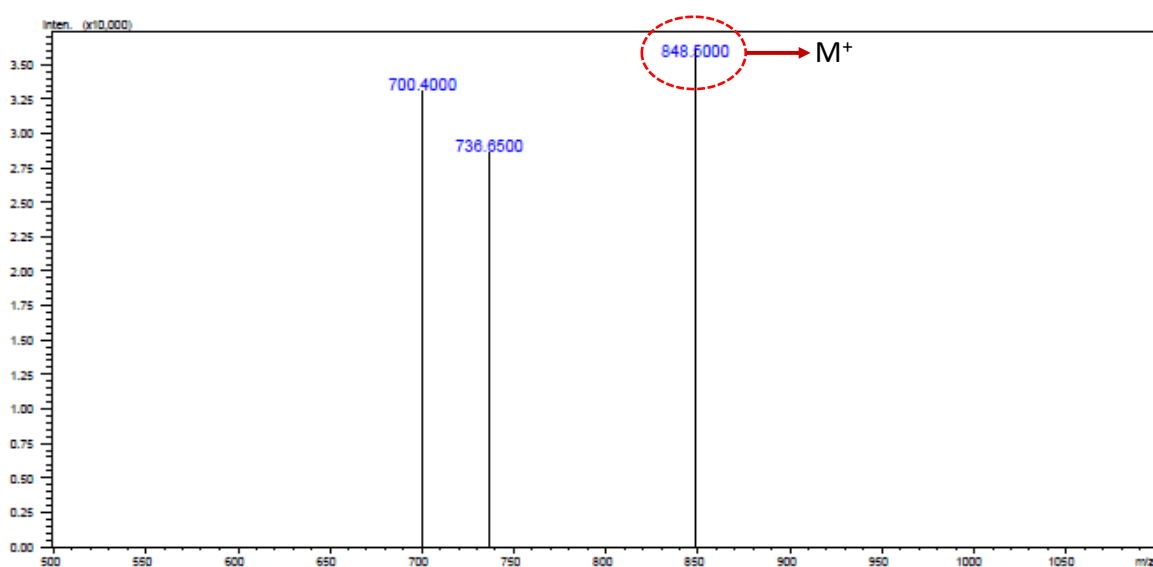


**Figure S1.** <sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 500 MHz, δppm) of BOC-Phe-Phe-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CO-Phe-Phe-BOC (**PA1**).

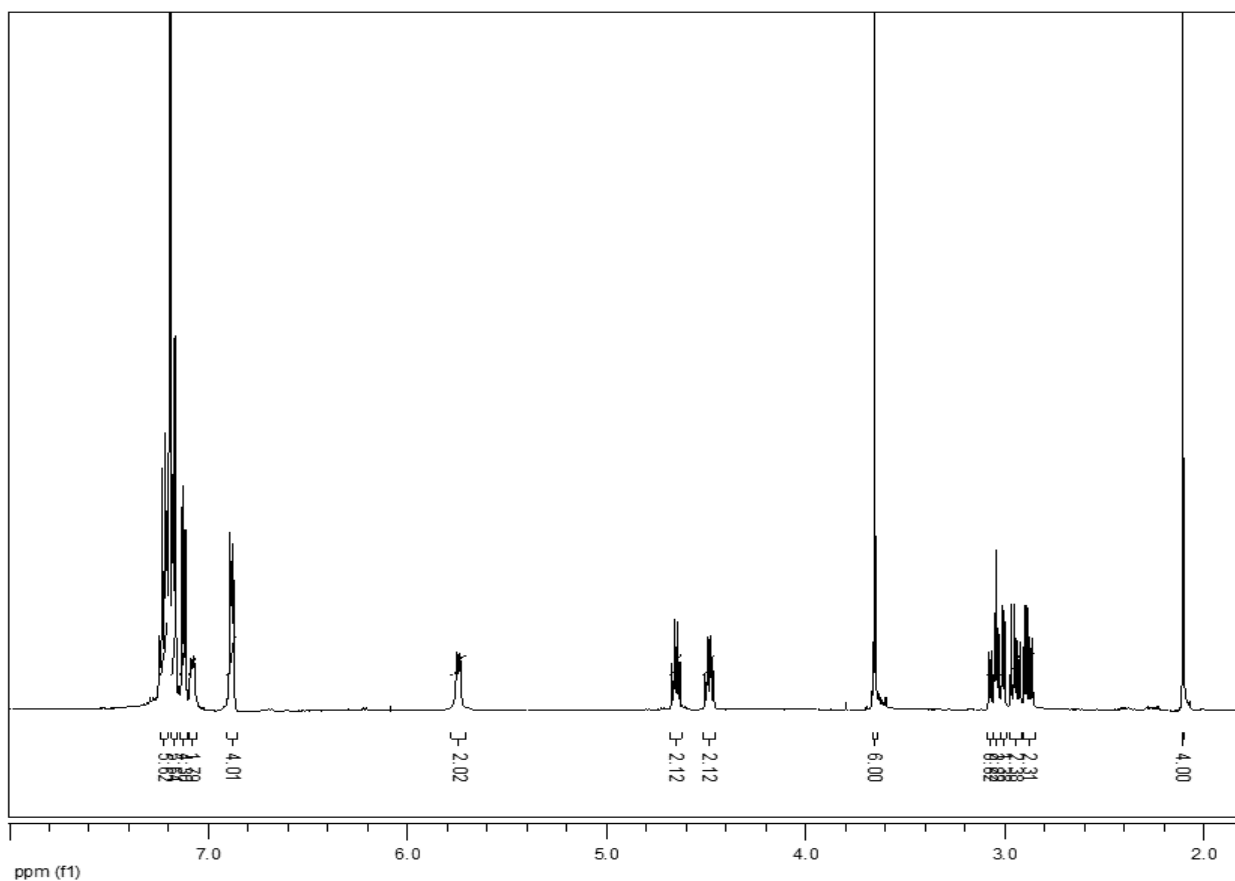




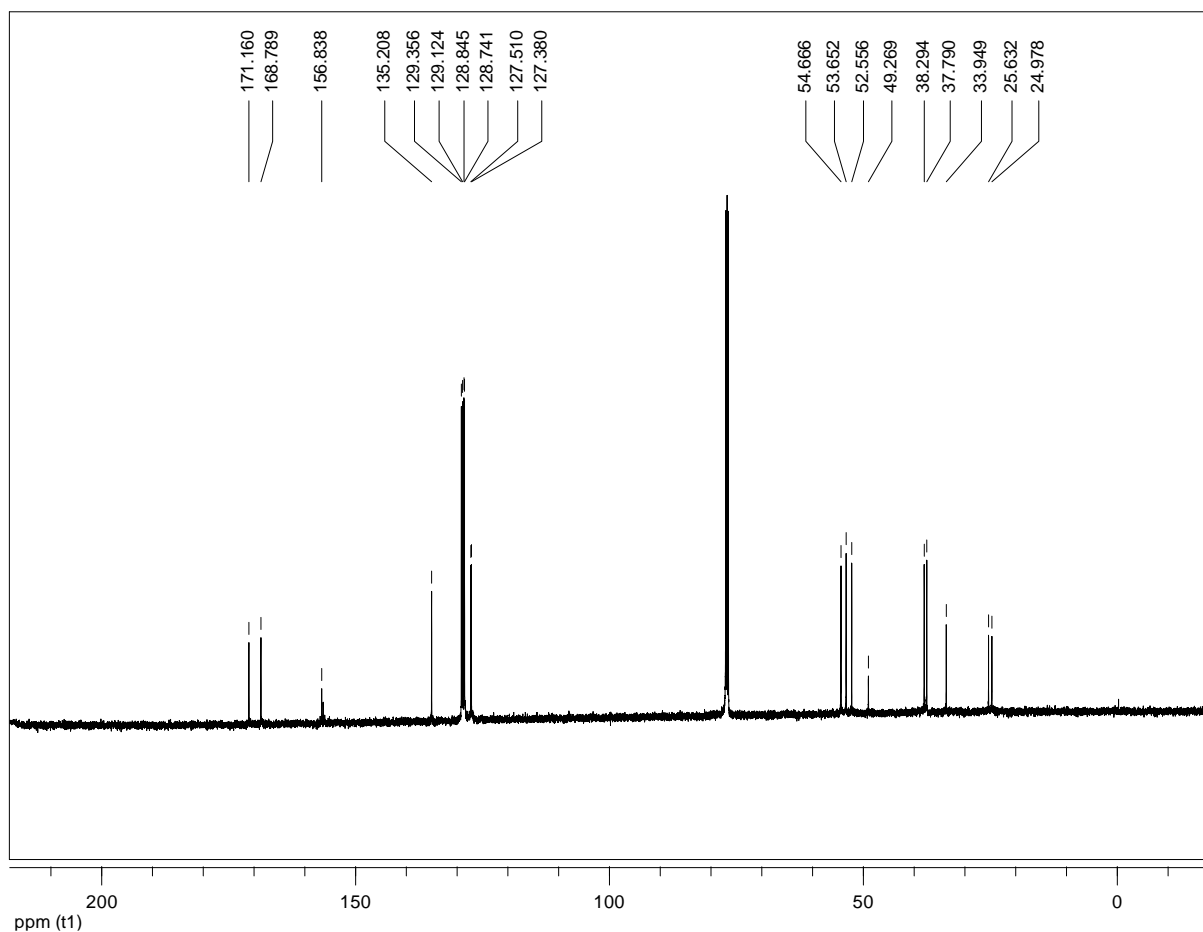
**Figure S2.**  $^{13}\text{C}$  NMR (DMSO- $d_6$ , 125 MHz,  $\delta\text{ppm}$ ) of BOC-Phe-Phe-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CO-Phe-Phe-BOC (**PA1**).



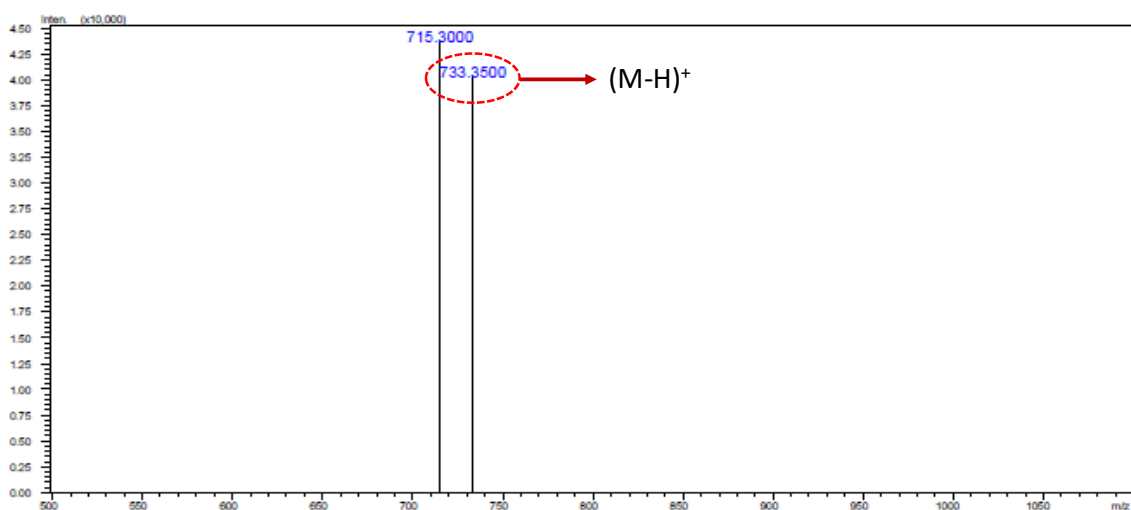
**Figure S3.** ESI Mass spectra of BOC-Phe-Phe-CO-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CO-Phe-Phe-BOC (**PA1**).



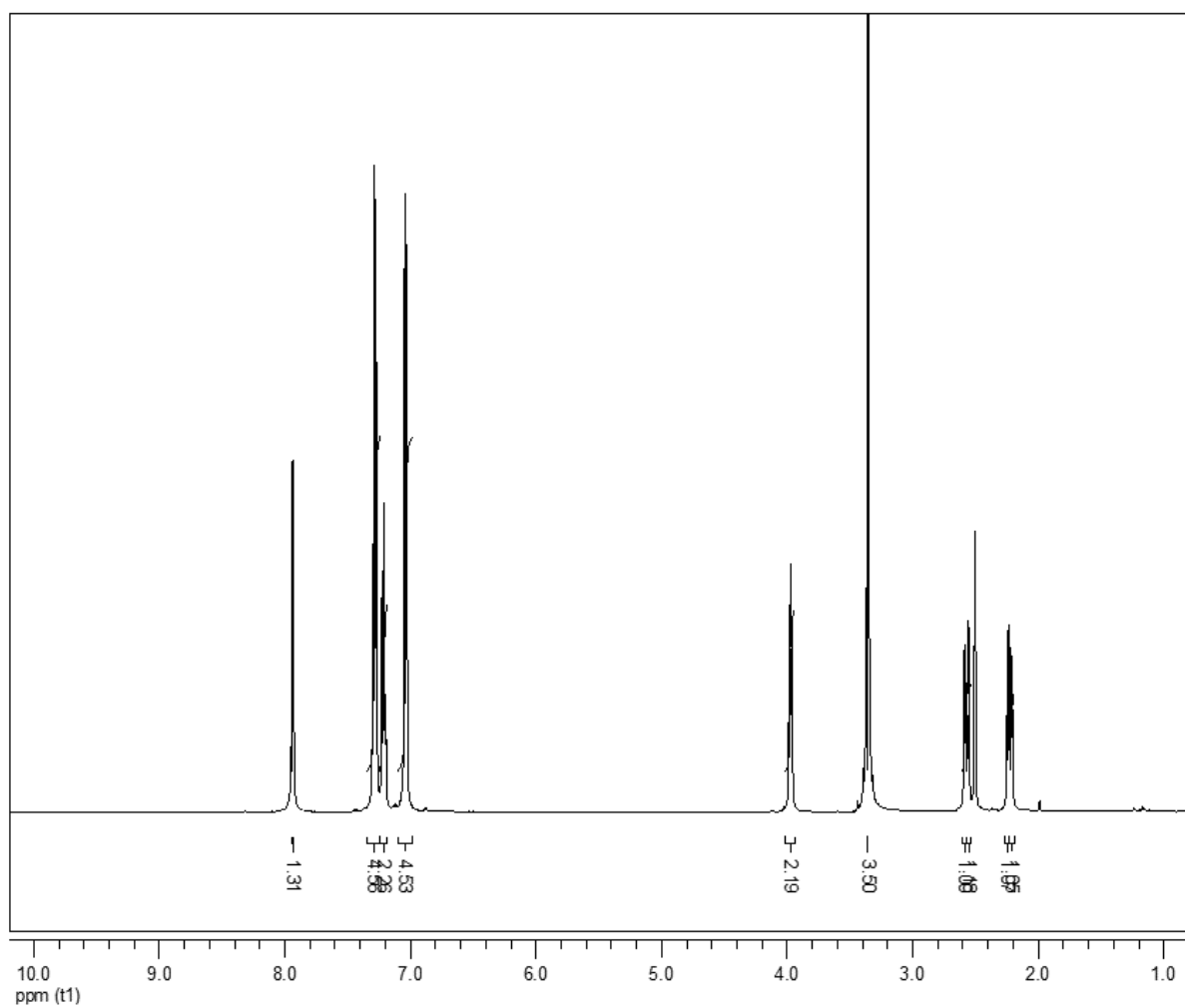
**Figure S4.**  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 500 MHz,  $\delta$ ppm) of OMe-Phe-Phe-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-Phe-Phe-OMe (**PA2**).



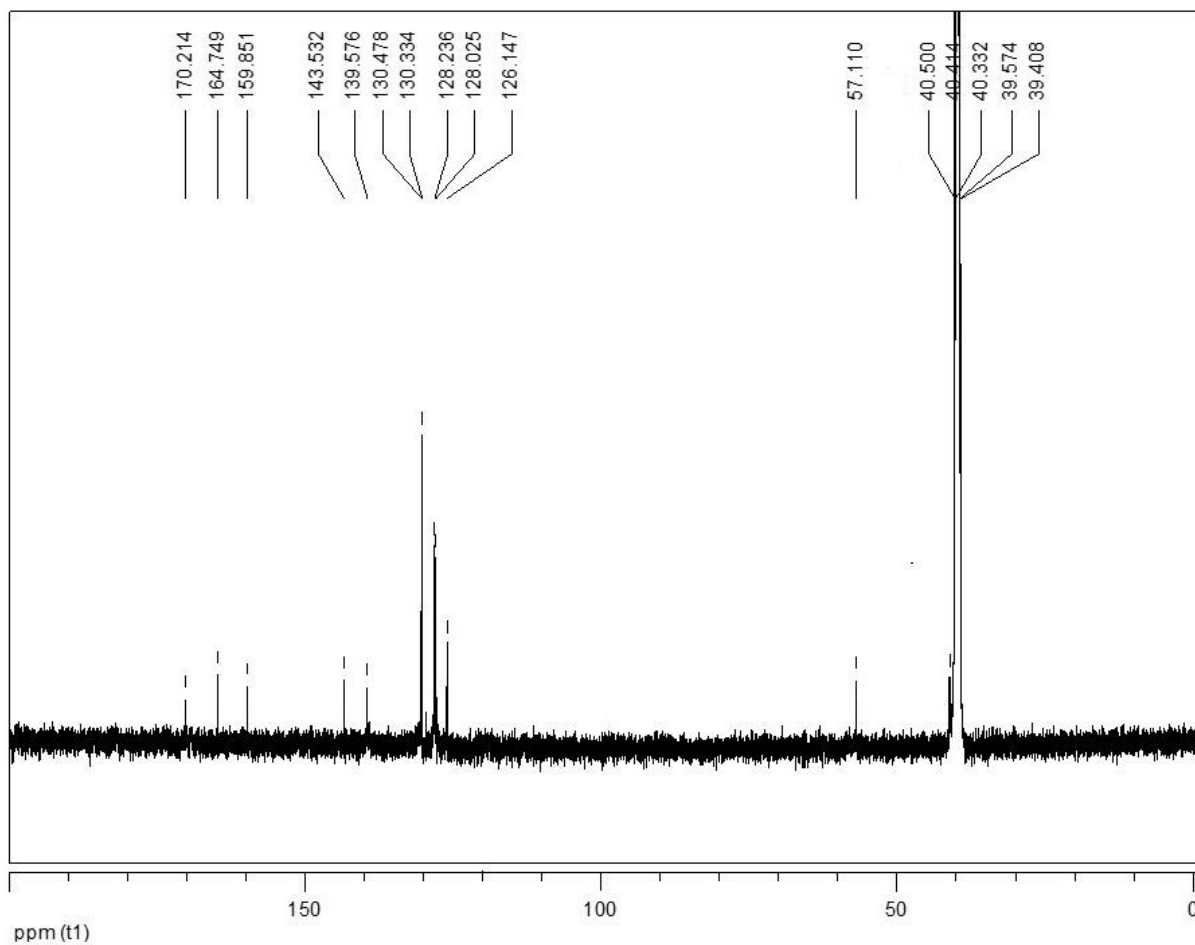
**Figure S5.**  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 125 MHz,  $\delta\text{ppm}$ ) of OMe-Phe-Phe-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-Phe-Phe-OMe (**PA2**).



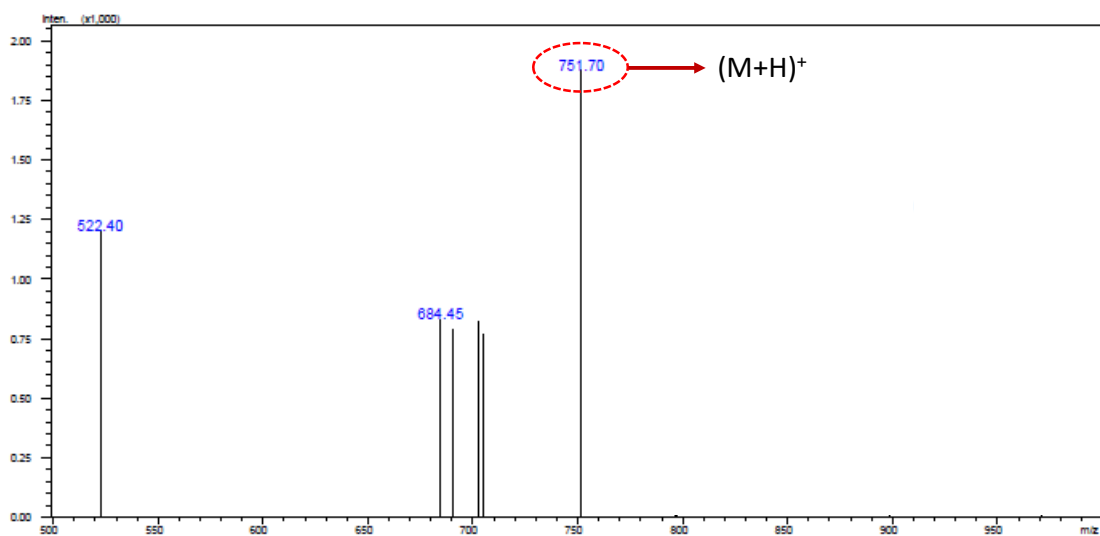
**Figure S6.** ESI Mass spectra of OMe-Phe-Phe-NH-CO-CH<sub>2</sub>-CH<sub>2</sub>-CO-NH-Phe-Phe-OMe (**PA2**).



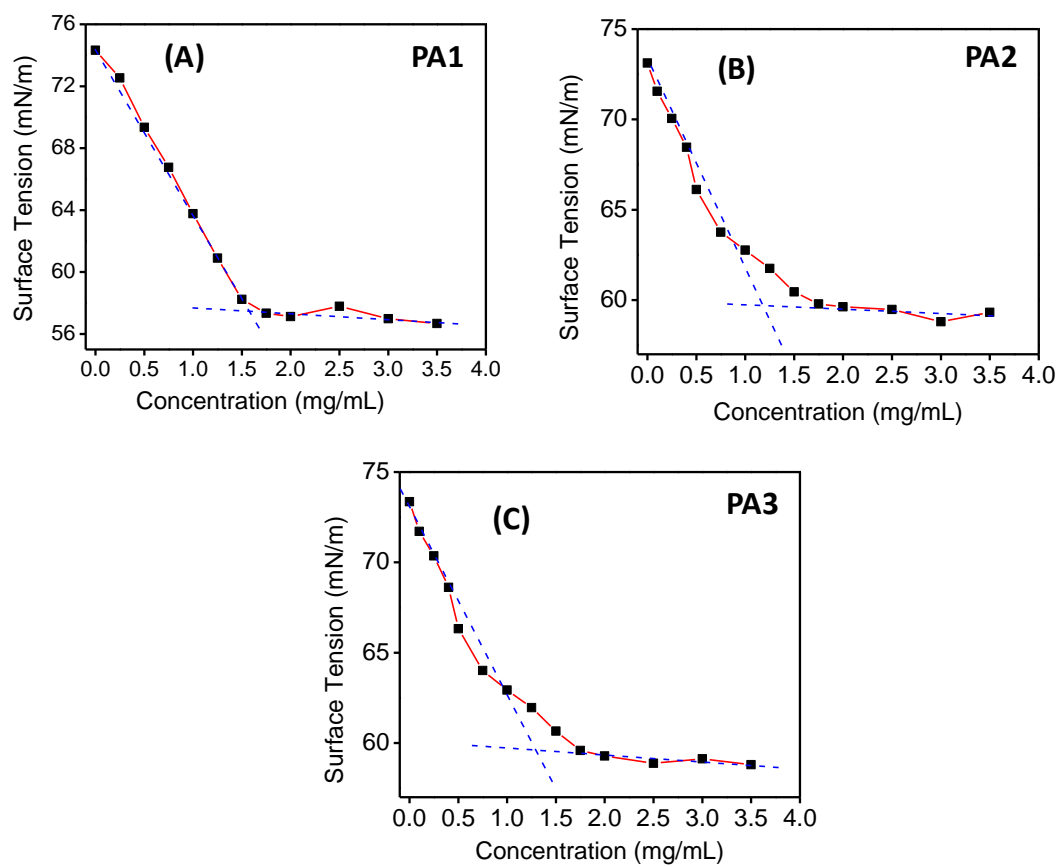
**Figure S7.** <sup>1</sup>H NMR (DMSO d<sub>6</sub>, 500 MHz, δppm) of OMe-Phe-Phe-N=CH-C<sub>6</sub>H<sub>4</sub>-CH=N-Phe-Phe-OMe (**PA3**).



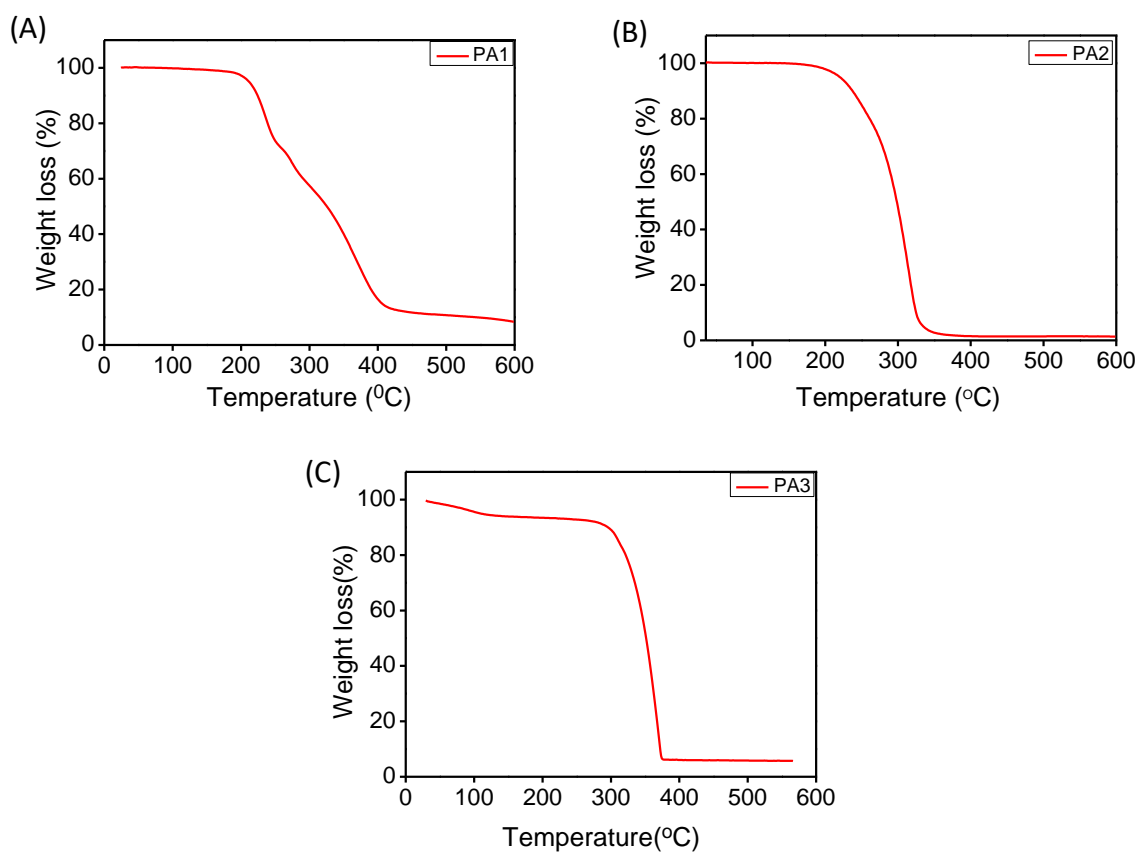
**Figure S8.**  $^{13}\text{C}$  NMR (DMSO  $d_6$ , 500 MHz,  $\delta$ ppm) of OMe-Phe-Phe-N=CH-C<sub>6</sub>H<sub>4</sub>-CH=N-Phe-Phe-OMe (**PA3**).



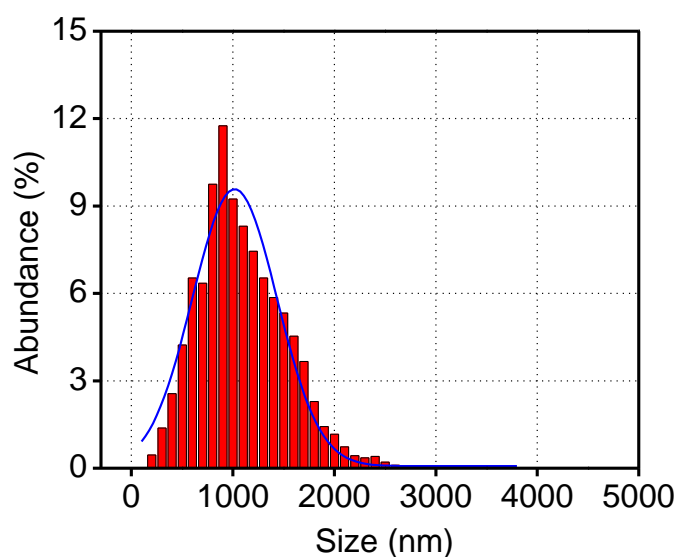
**Figure S9.** ESI Mass spectra of OMe-Phe-Phe-N=CH-C<sub>6</sub>H<sub>4</sub>-CH=N-Phe-Phe-OMe (**PA3**).



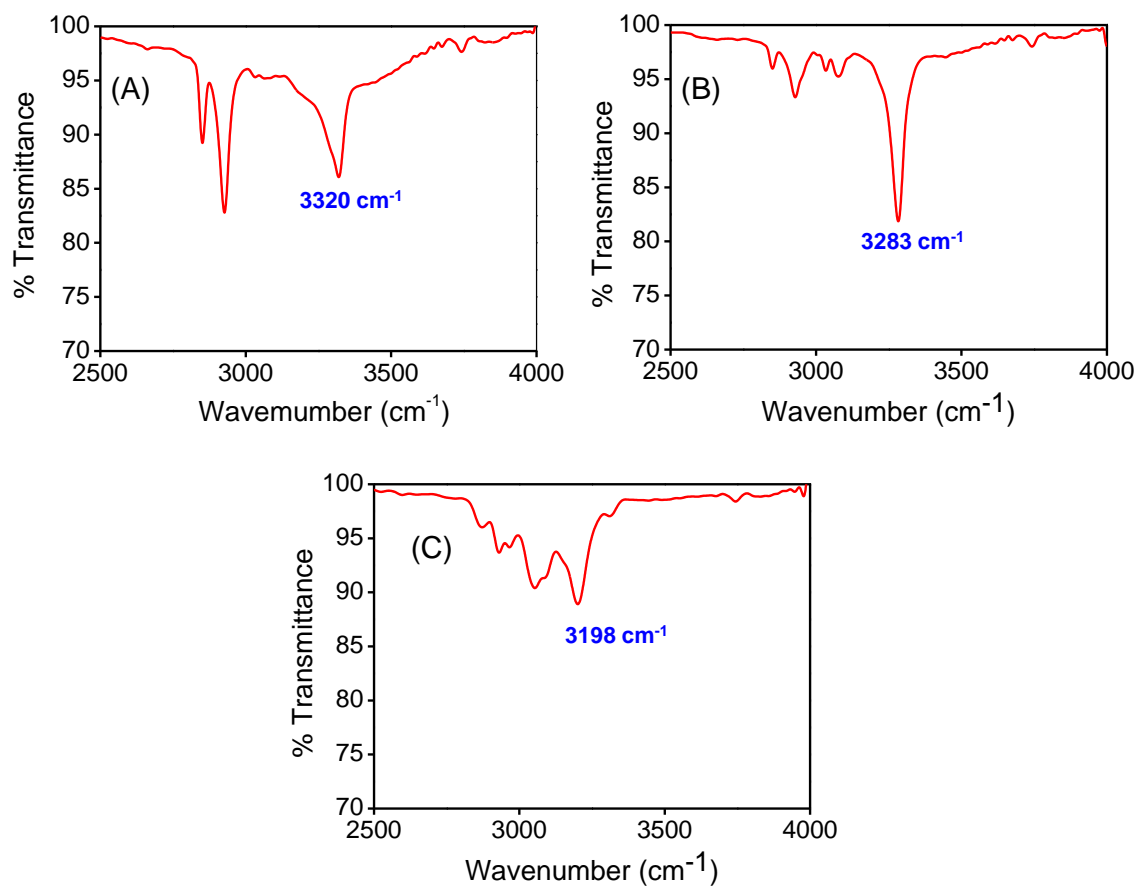
**Figure S10.** Critical aggregation concentration (CAC) for the self-assembly of (A) **PA1**, (B) **PA2** and (C) **PA3**.



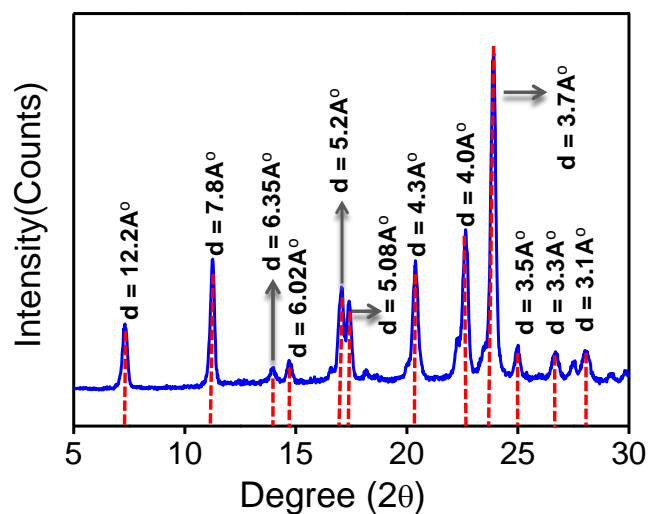
**Figure S11.** Weight-loss profile for PA1, PA2 and PA3 obtained using thermogravimetric analysis (TGA).



**Figure S12.** Size distribution obtained from Dynamic lighting scattering measurements for the spherical nanostructures formed by self-assembly of PA1 in 50% aqueous ethanol medium. The average hydrodynamic diameter of the spherical structures is  $969.65 \pm 17.66$  nm.

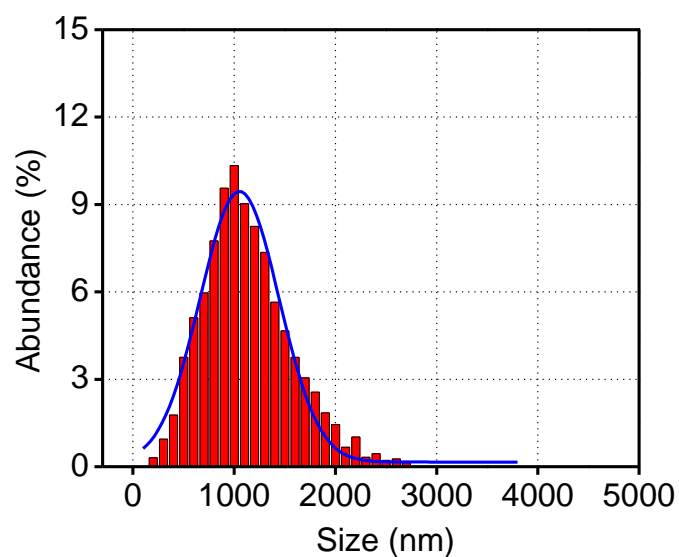


**Figure S13.** FTIR spectra of the PA1 (A), PA2 (B) and PA3 (C) in the self-assembled state.

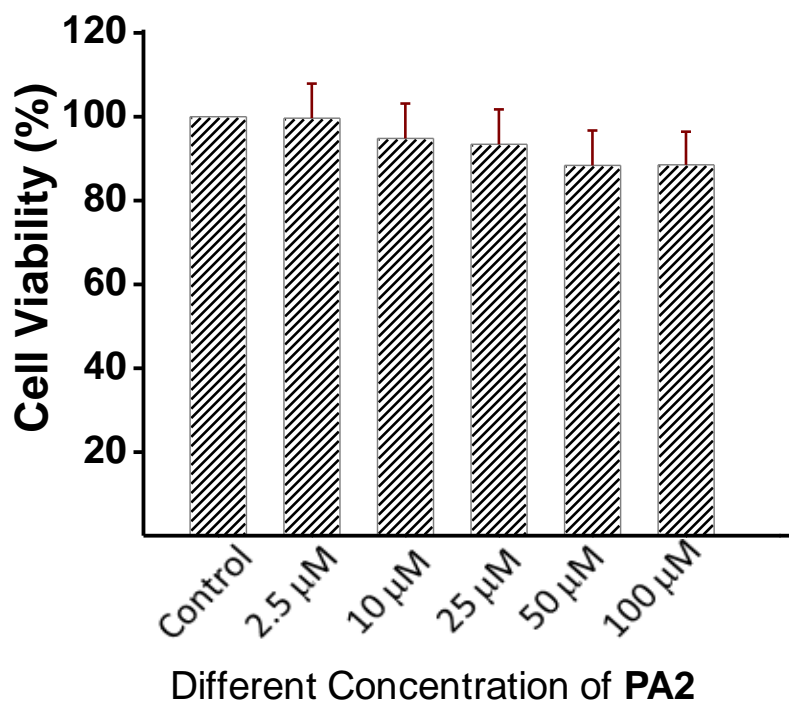


**Figure S14.** Powder X-ray diffraction pattern of the self-assembled structure formed by PA3 in 100 % aqueous medium.





**Figure S15.** Size distribution obtained from Dynamic lighting scattering measurements for the spherical nanostructures formed by self-assembly of **PA1** in 50% aqueous ethanol medium after DOX encapsulation. The average hydrodynamic diameter of the spherical structures is  $1033.23 \pm 32.81$  nm.



**Figure S16.** Cell viability was estimated by MTT assay. HEK293 cells were cultured in the presence of 0–100 μM of **PA2** at 37°C for 24 h and after that the viability was assessed with standard protocol.

## Theoretical Calculation Data

For PA1 (with ethylenediamine)

C	-4.643752000	-2.187996000	-0.462388000
C	-4.523353000	-0.769531000	0.112767000
C	-4.569174000	-0.738409000	1.642751000
O	-4.423028000	-3.188012000	0.205632000
N	-4.931373000	-2.194479000	-1.792701000
C	-4.208203000	0.633982000	2.163247000
C	-2.966535000	0.857530000	2.759054000
C	-2.583205000	2.138202000	3.145133000
C	-3.436442000	3.216507000	2.937464000
C	-4.683294000	3.003404000	2.353803000
C	-5.064938000	1.721168000	1.972782000
C	-3.175995000	0.564816000	-1.448121000
C	-1.860943000	1.338609000	-1.563626000
C	-1.486228000	1.619897000	-3.025944000
O	-4.084551000	0.681411000	-2.270189000
N	-3.258055000	-0.220491000	-0.356869000
C	-0.209470000	2.419449000	-3.122377000
C	1.020740000	1.819130000	-2.846508000
C	2.196287000	2.560692000	-2.852382000
C	2.159028000	3.920219000	-3.154873000
C	0.941085000	4.528122000	-3.444943000
C	-0.235388000	3.782477000	-3.419305000
N	-1.984686000	2.544388000	-0.770767000
C	-0.955887000	2.978460000	0.010204000
O	0.029969000	2.308416000	0.264441000
O	-1.205357000	4.218601000	0.449013000
C	-0.158832000	5.010053000	1.087137000
C	-0.872170000	6.328709000	1.373043000
C	0.312489000	4.367756000	2.390200000
C	0.989325000	5.221288000	0.103008000
C	-4.613333000	-3.342414000	-2.619868000
C	-3.207797000	-3.214372000	-3.228269000
N	-2.193616000	-3.000273000	-2.212970000
C	-1.819131000	-4.018602000	-1.389303000
C	-1.104038000	-3.571694000	-0.109076000
C	-0.461424000	-4.767577000	0.617265000
O	-2.051615000	-5.191729000	-1.625273000
C	0.416355000	-4.318889000	1.762145000
C	1.805015000	-4.452196000	1.689729000
C	2.628681000	-3.972918000	2.707631000
C	2.068313000	-3.349074000	3.819273000
C	0.683805000	-3.216334000	3.906645000
C	-0.132128000	-3.697950000	2.888047000
C	-0.035307000	-1.429641000	0.433952000
C	1.302517000	-0.691803000	0.391984000
C	1.574884000	-0.006304000	1.741111000
O	-0.963973000	-1.024128000	1.131040000
N	-0.128340000	-2.522631000	-0.360640000
C	2.911816000	0.695225000	1.738548000
C	3.127697000	1.808784000	0.919096000
C	4.364016000	2.443015000	0.899479000
C	5.407777000	1.974573000	1.695990000
C	5.207727000	0.859486000	2.503795000
C	3.967766000	0.223124000	2.518278000
N	2.377524000	-1.587574000	0.005050000
C	3.329605000	-1.178464000	-0.898194000
O	3.154486000	-0.309148000	-1.729396000

O	4.431903000	-1.920692000	-0.739687000
C	5.637122000	-1.647035000	-1.516030000
C	6.622369000	-2.676961000	-0.970327000
C	5.375401000	-1.883387000	-3.002074000
C	6.126554000	-0.229884000	-1.225911000
H	-5.315977000	-0.139266000	-0.305194000
H	-5.573058000	-1.038996000	1.961339000
H	-3.876428000	-1.492789000	2.027271000
H	-4.951837000	-1.281948000	-2.242127000
H	-2.277965000	0.028475000	2.889193000
H	-1.608593000	2.287654000	3.599525000
H	-3.134340000	4.218458000	3.228575000
H	-5.359601000	3.838297000	2.193901000
H	-6.037948000	1.563947000	1.511775000
H	-1.062144000	0.763121000	-1.088417000
H	-1.379695000	0.657487000	-3.542083000
H	-2.319476000	2.142010000	-3.507333000
H	-2.461273000	-0.287348000	0.275902000
H	1.075961000	0.759100000	-2.613954000
H	3.130984000	2.062530000	-2.616106000
H	3.075325000	4.503640000	-3.165786000
H	0.903428000	5.586883000	-3.686202000
H	-1.185738000	4.265119000	-3.635837000
H	-2.701703000	3.213810000	-1.007541000
H	-1.725565000	6.165758000	2.038678000
H	-0.183890000	7.030793000	1.853547000
H	-1.237678000	6.777750000	0.444636000
H	1.014559000	5.044369000	2.888756000
H	-0.537215000	4.206150000	3.059821000
H	0.812795000	3.416149000	2.207787000
H	1.478857000	4.278607000	-0.147189000
H	1.731192000	5.894961000	0.544436000
H	0.618133000	5.669307000	-0.823365000
H	-4.658770000	-4.229469000	-1.985638000
H	-5.358778000	-3.443583000	-3.415133000
H	-2.959738000	-4.125456000	-3.778046000
H	-3.168287000	-2.370147000	-3.924406000
H	-2.093157000	-2.063737000	-1.846540000
H	-1.877241000	-3.124359000	0.525793000
H	-1.266808000	-5.422564000	0.961683000
H	0.121716000	-5.352494000	-0.102075000
H	2.249964000	-4.933271000	0.821561000
H	3.706109000	-4.090885000	2.630973000
H	2.704700000	-2.974686000	4.615780000
H	0.237341000	-2.731495000	4.769538000
H	-1.209537000	-3.573392000	2.957962000
H	1.230829000	0.081225000	-0.380995000
H	0.759343000	0.698261000	1.917095000
H	1.541661000	-0.760745000	2.536186000
H	0.746704000	-2.798807000	-0.791394000
H	2.314904000	2.170030000	0.296401000
H	4.512007000	3.307594000	0.258227000
H	6.372860000	2.472925000	1.682067000
H	6.016027000	0.483157000	3.124603000
H	3.814096000	-0.650490000	3.148623000
H	2.727581000	-2.189378000	0.742005000
H	6.247688000	-3.692478000	-1.131892000
H	7.586721000	-2.577274000	-1.477750000
H	6.775947000	-2.527992000	0.102814000
H	6.317131000	-1.799466000	-3.554487000
H	4.974640000	-2.889928000	-3.161284000
H	4.668512000	-1.152724000	-3.397306000

H	5.433935000	0.516802000	-1.616791000
H	7.106618000	-0.081294000	-1.691477000
H	6.224860000	-0.077683000	-0.146726000

**For PA2 (with Succinic acid)**

C	-6.619945000	0.325327000	1.799516000
C	-5.710666000	-0.698951000	1.109659000
C	-6.399314000	-1.430867000	-0.064696000
O	-6.239710000	1.339025000	2.327114000
O	-7.896402000	-0.083528000	1.797052000
C	-5.427290000	-2.281476000	-0.846236000
C	-5.016572000	-1.893860000	-2.123169000
C	-4.133407000	-2.681584000	-2.857384000
C	-3.626962000	-3.859322000	-2.312990000
C	-4.009591000	-4.242277000	-1.029359000
C	-4.907025000	-3.461181000	-0.307836000
C	-4.406583000	0.910497000	-0.179096000
C	-3.005357000	1.491233000	-0.430793000
C	-2.472965000	2.209368000	0.824524000
O	-5.387345000	1.349185000	-0.765016000
N	-4.465766000	-0.072529000	0.747042000
C	-1.366125000	3.188816000	0.523239000
C	-0.031397000	2.857126000	0.753457000
C	0.984943000	3.778619000	0.513579000
C	0.675124000	5.045727000	0.028103000
C	-0.653346000	5.383406000	-0.223655000
C	-1.665125000	4.459942000	0.022002000
N	-2.095122000	0.497394000	-1.002689000
C	-8.815969000	0.796530000	2.443810000
C	-0.964175000	-1.603412000	-1.361039000
C	-0.391760000	-2.840870000	-0.660821000
C	1.793857000	1.560088000	-1.990367000
C	3.084625000	0.987468000	-1.405842000
C	3.978450000	0.504106000	-2.569402000
O	0.764275000	0.938264000	-2.134178000
O	1.959492000	2.819022000	-2.388610000
C	5.258334000	-0.125981000	-2.077105000
C	5.368351000	-1.512988000	-1.954719000
C	6.533366000	-2.091052000	-1.458062000
C	7.604806000	-1.287951000	-1.078032000
C	7.504291000	0.096068000	-1.196066000
C	6.337368000	0.671242000	-1.690327000
C	2.553723000	0.099935000	0.808365000
C	2.194858000	-1.172332000	1.597679000
C	3.403511000	-2.113525000	1.782176000
O	2.600481000	1.194496000	1.350415000
N	2.811461000	-0.098051000	-0.507795000
C	4.534367000	-1.431146000	2.513959000
C	4.618361000	-1.480054000	3.906573000
C	5.645476000	-0.827354000	4.581216000
C	6.604500000	-0.113539000	3.867440000
C	6.527727000	-0.057044000	2.478819000
C	5.499733000	-0.710601000	1.808306000
N	1.024977000	-1.844673000	1.032327000
C	0.802146000	3.440588000	-2.954952000
C	-1.622090000	-0.616873000	-0.409221000
O	-1.771132000	-0.862261000	0.796127000
C	0.995428000	-2.518644000	-0.142119000
O	1.996477000	-2.780846000	-0.813922000
H	-5.464574000	-1.441528000	1.878472000
H	-7.205634000	-2.047032000	0.344001000

H	-6.854126000	-0.686894000	-0.720699000
H	-5.397916000	-0.965944000	-2.541019000
H	-3.840618000	-2.374737000	-3.857904000
H	-2.938852000	-4.475515000	-2.884683000
H	-3.619319000	-5.158495000	-0.595716000
H	-5.215964000	-3.778447000	0.686085000
H	-3.161311000	2.234526000	-1.215048000
H	-3.323695000	2.734490000	1.274329000
H	-2.137732000	1.464654000	1.549685000
H	-3.595129000	-0.422076000	1.133446000
H	0.225711000	1.879351000	1.148502000
H	2.009872000	3.487196000	0.716859000
H	1.465437000	5.768855000	-0.152417000
H	-0.904201000	6.371738000	-0.598946000
H	-2.703240000	4.734630000	-0.154901000
H	-1.800500000	0.649287000	-1.955722000
H	-9.793209000	0.325041000	2.344622000
H	-8.552974000	0.919338000	3.497314000
H	-8.809572000	1.775067000	1.958377000
H	-1.747598000	-1.917491000	-2.058824000
H	-0.190493000	-1.088105000	-1.939257000
H	-1.069868000	-3.161641000	0.134486000
H	-0.283007000	-3.650482000	-1.384482000
H	3.592007000	1.779254000	-0.848498000
H	3.409295000	-0.220175000	-3.165248000
H	4.190500000	1.361565000	-3.216293000
H	4.530608000	-2.146694000	-2.236560000
H	6.599859000	-3.170483000	-1.362172000
H	8.511628000	-1.737482000	-0.685508000
H	8.336233000	0.729804000	-0.902770000
H	6.262261000	1.752880000	-1.776783000
H	1.893101000	-0.807850000	2.582169000
H	3.052655000	-2.985895000	2.344523000
H	3.737750000	-2.472270000	0.806572000
H	2.714682000	-1.041256000	-0.877184000
H	3.873024000	-2.039511000	4.468136000
H	5.698275000	-0.878180000	5.664992000
H	7.407788000	0.395375000	4.392324000
H	7.269665000	0.494782000	1.908886000
H	5.444971000	-0.659384000	0.725076000
H	0.116999000	-1.548513000	1.379372000
H	1.081840000	4.478607000	-3.126554000
H	0.535002000	2.951755000	-3.895718000
H	-0.033655000	3.386840000	-2.254209000

**For PA3 (with Terephthalaldehyde)**

C	6.238114000	-1.795459000	0.489291000
C	6.709916000	-0.361071000	0.631743000
C	7.678516000	-0.019794000	-0.531594000
O	5.313474000	-2.130108000	-0.218115000
O	6.996676000	-2.637423000	1.187666000
C	8.874814000	-0.935054000	-0.591060000
C	9.968433000	-0.728271000	0.251792000
C	11.046431000	-1.607419000	0.244397000
C	11.044834000	-2.708455000	-0.608312000
C	9.960768000	-2.922381000	-1.455016000
C	8.884404000	-2.040031000	-1.445070000
C	5.581522000	1.756791000	1.084305000
C	4.283434000	2.547164000	0.899062000
C	4.553936000	3.702455000	-0.100781000
O	6.565172000	2.268677000	1.603167000

N	5.549414000	0.492958000	0.610918000
C	3.379183000	4.641088000	-0.190946000
C	2.392912000	4.469363000	-1.164848000
C	1.258093000	5.275933000	-1.181097000
C	1.095301000	6.269994000	-0.220817000
C	2.075547000	6.455545000	0.751701000
C	3.206509000	5.645764000	0.765080000
N	3.219319000	1.702567000	0.403838000
C	6.750184000	-4.025473000	0.961188000
C	-7.240400000	2.568999000	-0.561685000
C	-7.410203000	1.073101000	-0.362857000
C	-7.892878000	0.822038000	1.092373000
O	-6.183598000	3.152458000	-0.515655000
O	-8.424848000	3.170694000	-0.724656000
C	-7.782095000	-0.628278000	1.501911000
C	-6.934862000	-1.002048000	2.546086000
C	-6.807481000	-2.337152000	2.922771000
C	-7.524892000	-3.320597000	2.249338000
C	-8.369464000	-2.959103000	1.202227000
C	-8.498550000	-1.624557000	0.833808000
C	-6.132407000	-0.724421000	-1.403512000
C	-4.791913000	-1.455882000	-1.369007000
C	-4.973965000	-2.678611000	-0.425167000
O	-7.087567000	-1.188228000	-2.010348000
N	-6.176424000	0.398602000	-0.648460000
C	-3.747539000	-3.550631000	-0.406225000
C	-2.760738000	-3.378021000	0.567046000
C	-1.577518000	-4.110428000	0.522422000
C	-1.365795000	-5.031378000	-0.499494000
C	-2.346431000	-5.219377000	-1.471296000
C	-3.525938000	-4.483310000	-1.423210000
N	-3.735870000	-0.601776000	-0.872059000
C	-8.378973000	4.593865000	-0.840151000
C	-1.538966000	1.079761000	-0.008181000
C	-0.421005000	1.740474000	0.477387000
C	0.863288000	1.245608000	0.226496000
C	1.015615000	0.074126000	-0.521453000
C	-0.102318000	-0.585421000	-1.008268000
C	-1.386733000	-0.091725000	-0.755093000
C	-2.550199000	-0.835391000	-1.265650000
C	2.026873000	1.985422000	0.741229000
H	7.234828000	-0.233387000	1.581626000
H	7.106847000	-0.070147000	-1.464801000
H	7.985637000	1.019439000	-0.379893000
H	9.971322000	0.130034000	0.919684000
H	11.890784000	-1.431646000	0.904551000
H	11.887309000	-3.393696000	-0.616163000
H	9.954793000	-3.774682000	-2.128524000
H	8.036634000	-2.210970000	-2.105179000
H	4.046230000	2.994698000	1.875860000
H	5.450708000	4.223239000	0.247989000
H	4.777568000	3.263768000	-1.079615000
H	4.707307000	0.176605000	0.144816000
H	2.508562000	3.683180000	-1.906279000
H	0.498915000	5.122882000	-1.942388000
H	0.210492000	6.899522000	-0.231121000
H	1.958903000	7.233117000	1.501060000
H	3.966539000	5.789404000	1.530003000
H	7.437275000	-4.554768000	1.619654000
H	5.713979000	-4.276363000	1.198411000
H	6.955592000	-4.275385000	-0.082746000
H	-8.152263000	0.691274000	-1.067803000

H	-7.287256000	1.433622000	1.772312000
H	-8.925786000	1.178311000	1.176218000
H	-6.365344000	-0.238687000	3.070975000
H	-6.143410000	-2.607233000	3.738742000
H	-7.423185000	-4.363388000	2.534443000
H	-8.927089000	-3.720126000	0.664671000
H	-9.140536000	-1.359801000	-0.001168000
H	-4.594568000	-1.827502000	-2.384317000
H	-5.206317000	-2.305574000	0.577688000
H	-5.849185000	-3.230465000	-0.780451000
H	-5.310345000	0.710569000	-0.228361000
H	-2.916687000	-2.646446000	1.355496000
H	-0.818423000	-3.955924000	1.283617000
H	-0.442773000	-5.602318000	-0.537834000
H	-2.191468000	-5.940603000	-2.268610000
H	-4.285713000	-4.626672000	-2.188444000
H	-9.414199000	4.912497000	-0.955840000
H	-7.937858000	5.036814000	0.056102000
H	-7.787715000	4.886745000	-1.710826000
H	-2.537136000	1.462663000	0.176948000
H	-0.537889000	2.659385000	1.046636000
H	2.013420000	-0.308225000	-0.710414000
H	0.014151000	-1.503650000	-1.578578000
H	-2.327105000	-1.631356000	-1.989894000
H	1.800747000	2.819718000	1.420441000

**PA1 -Dimer**

C	3.127847000	-4.383846000	-2.805312000
C	4.591302000	-4.098871000	-2.413120000
C	5.411051000	-3.538268000	-3.577043000
O	2.586476000	-3.854314000	-3.761946000
N	2.498001000	-5.202420000	-1.915336000
C	6.754630000	-3.022861000	-3.115482000
C	6.983176000	-1.649586000	-3.016157000
C	8.185364000	-1.160087000	-2.513464000
C	9.182914000	-2.042694000	-2.111623000
C	8.970386000	-3.415762000	-2.216736000
C	7.764862000	-3.900058000	-2.713949000
C	4.418782000	-3.489702000	-0.026125000
C	4.418509000	-2.320947000	0.965372000
C	3.314925000	-2.519573000	2.007043000
O	4.301046000	-4.654398000	0.355555000
N	4.538948000	-3.134007000	-1.318374000
C	3.283161000	-1.482506000	3.108414000
C	3.648003000	-0.151133000	2.891229000
C	3.577259000	0.787594000	3.916638000
C	3.130482000	0.413307000	5.180800000
C	2.766239000	-0.910598000	5.413004000
C	2.853240000	-1.847766000	4.387348000
N	5.725683000	-2.197248000	1.569511000
C	6.517656000	-1.117709000	1.332821000
O	6.279709000	-0.276395000	0.479232000
O	7.564188000	-1.131996000	2.164774000
C	8.449314000	0.022849000	2.271512000
C	9.410685000	-0.394833000	3.381310000
C	9.209909000	0.226109000	0.962508000
C	7.644701000	1.250266000	2.701755000
C	1.059119000	-5.138406000	-1.732429000
C	0.698366000	-4.134325000	-0.632474000
N	1.131965000	-2.787026000	-0.956332000
C	0.384648000	-1.995321000	-1.758399000

C	1.075224000	-0.734196000	-2.289178000
C	0.010692000	0.283727000	-2.725623000
O	-0.762036000	-2.267683000	-2.088879000
C	0.553495000	1.643290000	-3.091245000
C	-0.070144000	2.786815000	-2.585906000
C	0.436770000	4.057494000	-2.844929000
C	1.575699000	4.204927000	-3.632663000
C	2.187319000	3.073677000	-4.171733000
C	1.680910000	1.804114000	-3.903022000
C	3.314445000	0.095711000	-1.777490000
C	4.062155000	1.276651000	-1.156889000
C	5.148439000	1.754718000	-2.141487000
O	3.862492000	-0.627796000	-2.606631000
N	2.034788000	-0.125260000	-1.368263000
C	5.864104000	2.991214000	-1.661840000
C	6.807920000	2.896498000	-0.637072000
C	7.482104000	4.024113000	-0.185898000
C	7.222848000	5.268484000	-0.757718000
C	6.273919000	5.376408000	-1.769907000
C	5.594431000	4.243451000	-2.213198000
N	3.153502000	2.333192000	-0.762628000
C	3.413945000	3.059390000	0.381081000
O	4.080326000	2.648261000	1.312545000
O	2.781138000	4.230825000	0.303103000
C	2.888417000	5.235748000	1.357092000
C	2.048434000	6.379609000	0.796655000
C	2.285985000	4.723771000	2.662874000
C	4.347699000	5.654413000	1.515696000
H	5.055427000	-5.007036000	-2.014275000
H	5.525644000	-4.334261000	-4.320759000
H	4.830160000	-2.742013000	-4.050328000
H	3.041609000	-5.443785000	-1.090329000
H	6.195975000	-0.964907000	-3.317742000
H	8.340054000	-0.087236000	-2.435223000
H	10.123838000	-1.663799000	-1.723149000
H	9.746157000	-4.111442000	-1.909800000
H	7.604424000	-4.973693000	-2.787325000
H	4.250512000	-1.390841000	0.418438000
H	2.352577000	-2.519614000	1.476984000
H	3.419731000	-3.523842000	2.432837000
H	4.612053000	-2.154426000	-1.578645000
H	4.006296000	0.185995000	1.923232000
H	3.872636000	1.809708000	3.703700000
H	3.073007000	1.145643000	5.980757000
H	2.426882000	-1.219968000	6.397539000
H	2.593816000	-2.884717000	4.588040000
H	5.964642000	-2.794154000	2.346791000
H	9.948753000	-1.305546000	3.101476000
H	10.141045000	0.400332000	3.560059000
H	8.866203000	-0.583455000	4.311361000
H	9.934936000	1.038063000	1.082311000
H	9.752787000	-0.687795000	0.701261000
H	8.536601000	0.469818000	0.141053000
H	6.907513000	1.546567000	1.954198000
H	8.326591000	2.089773000	2.874229000
H	7.116665000	1.040617000	3.637876000
H	0.611506000	-4.836519000	-2.681240000
H	0.677754000	-6.129999000	-1.467524000
H	-0.381635000	-4.108711000	-0.478348000
H	1.165955000	-4.422991000	0.313751000
H	2.116490000	-2.569517000	-0.895085000
H	1.667137000	-1.079412000	-3.145872000



H	-0.543248000	-0.148307000	-3.563029000
H	-0.718317000	0.396037000	-1.915255000
H	-0.955768000	2.670604000	-1.964907000
H	-0.055455000	4.930286000	-2.426499000
H	1.979038000	5.192960000	-3.832610000
H	3.064637000	3.178508000	-4.804306000
H	2.182735000	0.932562000	-4.315810000
H	4.563613000	0.923424000	-0.249200000
H	5.856613000	0.932857000	-2.266331000
H	4.689110000	1.937828000	-3.118779000
H	1.662107000	0.591700000	-0.756831000
H	6.991633000	1.924219000	-0.190873000
H	8.212885000	3.930649000	0.612601000
H	7.753171000	6.150677000	-0.411191000
H	6.061403000	6.343473000	-2.216908000
H	4.850663000	4.331502000	-3.002192000
H	2.762496000	2.886821000	-1.518552000
H	1.019291000	6.046014000	0.630261000
H	2.034825000	7.216061000	1.502093000
H	2.461615000	6.729681000	-0.154321000
H	2.351332000	5.514718000	3.417724000
H	1.232906000	4.462852000	2.528409000
H	2.822653000	3.847041000	3.027231000
H	4.953066000	4.835217000	1.907397000
H	4.409366000	6.503454000	2.204706000
H	4.761333000	5.957658000	0.549656000
C	-5.687937000	4.272344000	-1.791419000
C	-5.481901000	3.015469000	-2.650278000
C	-4.117393000	2.968483000	-3.342091000
O	-4.756841000	4.953088000	-1.384243000
N	-6.994973000	4.473945000	-1.468153000
C	-3.928360000	1.663417000	-4.081278000
C	-3.295603000	0.584732000	-3.461032000
C	-3.178977000	-0.645840000	-4.099793000
C	-3.704248000	-0.815290000	-5.377291000
C	-4.337613000	0.252849000	-6.008850000
C	-4.446662000	1.482527000	-5.365069000
C	-6.787386000	1.226552000	-1.568188000
C	-6.649414000	-0.113238000	-0.843903000
C	-7.873946000	-0.418998000	0.030343000
O	-7.872677000	1.653461000	-1.961725000
N	-5.621288000	1.874189000	-1.754389000
C	-7.774085000	-1.788260000	0.658358000
C	-6.841198000	-2.037768000	1.667215000
C	-6.692844000	-3.310907000	2.204820000
C	-7.491556000	-4.356394000	1.747043000
C	-8.429556000	-4.120350000	0.746176000
C	-8.562313000	-2.845099000	0.201511000
N	-6.401170000	-1.133831000	-1.839098000
C	-5.433605000	-2.077098000	-1.649108000
O	-4.574483000	-1.997356000	-0.786804000
O	-5.574924000	-3.056708000	-2.546782000
C	-4.857648000	-4.322408000	-2.405945000
C	-5.400048000	-5.137469000	-3.577055000
C	-3.352528000	-4.121846000	-2.549746000
C	-5.242481000	-4.975125000	-1.079533000
C	-7.372815000	5.236074000	-0.293460000
C	-7.519880000	4.319601000	0.931533000
N	-6.302541000	3.574848000	1.199108000
C	-5.214955000	4.214135000	1.711686000
C	-3.882604000	3.489127000	1.501400000
C	-2.774321000	4.092339000	2.384186000

O	-5.273708000	5.301826000	2.260161000
C	-1.488740000	3.315027000	2.236006000
C	-0.951849000	2.577216000	3.295250000
C	0.167573000	1.763869000	3.112887000
C	0.764741000	1.679071000	1.857994000
C	0.250781000	2.428341000	0.804086000
C	-0.857362000	3.242293000	0.992980000
C	-3.396541000	1.166358000	0.852975000
C	-3.081651000	-0.207014000	1.450454000
C	-1.920792000	-0.874818000	0.693273000
O	-3.152676000	1.429569000	-0.324326000
N	-3.980509000	2.049732000	1.701345000
C	-1.547135000	-2.185098000	1.339972000
C	-2.387503000	-3.293849000	1.202800000
C	-2.078268000	-4.500428000	1.819929000
C	-0.922120000	-4.616921000	2.589171000
C	-0.088614000	-3.513428000	2.744929000
C	-0.401994000	-2.304015000	2.127871000
N	-2.809606000	-0.080819000	2.870302000
C	-3.284566000	-1.003905000	3.769876000
O	-4.264624000	-1.699251000	3.590096000
O	-2.524199000	-0.959214000	4.871565000
C	-2.775732000	-1.843184000	6.002707000
C	-1.648575000	-1.472460000	6.963316000
C	-4.139703000	-1.534159000	6.616228000
C	-2.650114000	-3.301021000	5.567141000
H	-6.283876000	2.940241000	-3.392907000
H	-4.049999000	3.823192000	-4.022866000
H	-3.340986000	3.105596000	-2.583391000
H	-7.633933000	3.739421000	-1.764734000
H	-2.897781000	0.700556000	-2.457708000
H	-2.662339000	-1.454265000	-3.590330000
H	-3.617255000	-1.773783000	-5.881156000
H	-4.745451000	0.130339000	-7.008306000
H	-4.941318000	2.312202000	-5.866208000
H	-5.753232000	-0.096440000	-0.218180000
H	-7.945133000	0.358321000	0.802175000
H	-8.774389000	-0.331591000	-0.586443000
H	-4.759722000	1.480095000	-1.383859000
H	-6.209359000	-1.237695000	2.043244000
H	-5.946728000	-3.470018000	2.976147000
H	-7.381541000	-5.352339000	2.166551000
H	-9.057498000	-4.929671000	0.384060000
H	-9.291527000	-2.667478000	-0.585773000
H	-7.133905000	-1.355263000	-2.496949000
H	-5.180931000	-4.635706000	-4.524503000
H	-4.932408000	-6.126862000	-3.590770000
H	-6.483710000	-5.263963000	-3.491803000
H	-2.853648000	-5.096214000	-2.500997000
H	-3.118805000	-3.674598000	-3.520373000
H	-2.939807000	-3.481579000	-1.771371000
H	-4.912051000	-4.381694000	-0.225658000
H	-4.785087000	-5.968085000	-1.015208000
H	-6.328885000	-5.086476000	-1.011429000
H	-6.591914000	5.975994000	-0.109158000
H	-8.313702000	5.762880000	-0.482242000
H	-7.759348000	4.916664000	1.814512000
H	-8.327240000	3.597557000	0.771932000
H	-6.116493000	2.766546000	0.621237000
H	-3.637538000	3.634635000	0.442598000
H	-2.649436000	5.140012000	2.096393000
H	-3.104892000	4.097028000	3.428838000

H	-1.427636000	2.623916000	4.272371000
H	0.576942000	1.198336000	3.945647000
H	1.643633000	1.057485000	1.718587000
H	0.722257000	2.405666000	-0.170497000
H	-1.252987000	3.811425000	0.155416000
H	-3.971569000	-0.837318000	1.339434000
H	-2.229834000	-1.032960000	-0.342125000
H	-1.060253000	-0.194529000	0.686287000
H	-4.011288000	1.729735000	2.663099000
H	-3.286891000	-3.190124000	0.604281000
H	-2.742793000	-5.351326000	1.698419000
H	-0.676899000	-5.558768000	3.071645000
H	0.808669000	-3.588835000	3.351405000
H	0.254108000	-1.445295000	2.260694000
H	-1.896545000	0.294147000	3.101659000
H	-1.718127000	-0.418900000	7.251570000
H	-1.709061000	-2.085830000	7.867591000
H	-0.676105000	-1.639419000	6.489251000
H	-4.265141000	-2.112127000	7.537744000
H	-4.210971000	-0.470672000	6.867309000
H	-4.945865000	-1.791468000	5.927372000
H	-3.437440000	-3.573329000	4.862962000
H	-2.720013000	-3.949691000	6.446833000
H	-1.682809000	-3.467842000	5.084839000

**PA2 -Dimer**

C	1.769684000	-0.108589000	5.650021000
C	3.152742000	-0.341001000	5.034037000
C	3.568400000	-1.827292000	5.117666000
O	1.215009000	-0.874839000	6.401687000
O	1.291302000	1.084312000	5.294982000
C	4.821571000	-2.080699000	4.314614000
C	4.737580000	-2.527216000	2.992671000
C	5.879686000	-2.660964000	2.209289000
C	7.129935000	-2.361511000	2.743768000
C	7.229608000	-1.929857000	4.064134000
C	6.082378000	-1.789631000	4.839875000
C	2.450701000	-0.303557000	2.712622000
C	2.692409000	0.267399000	1.312282000
C	2.259811000	1.738051000	1.159636000
O	1.600816000	-1.175364000	2.900532000
N	3.215849000	0.196394000	3.693814000
C	0.945373000	2.124987000	1.798751000
C	0.782394000	3.441871000	2.233813000
C	-0.429312000	3.881922000	2.756910000
C	-1.499026000	2.998698000	2.876039000
C	-1.339478000	1.679690000	2.462575000
C	-0.134034000	1.246651000	1.917765000
N	4.061320000	0.057584000	0.846532000
C	0.021056000	1.446338000	5.831543000
C	6.452336000	0.420700000	0.542906000
C	6.909753000	1.667623000	-0.251304000
C	3.908667000	-2.654827000	-1.893363000
C	4.385543000	-1.871468000	-3.114688000
C	5.708167000	-2.479914000	-3.636924000
O	3.940010000	-2.270621000	-0.743862000

O	3.497952000	-3.865195000	-2.248105000
C	6.831014000	-2.455197000	-2.623188000
C	6.923029000	-3.444962000	-1.639095000
C	7.925675000	-3.401033000	-0.676555000
C	8.855322000	-2.362880000	-0.683797000
C	8.779646000	-1.378866000	-1.663774000
C	7.777712000	-1.429506000	-2.629678000
C	3.490147000	0.351157000	-2.672356000
C	3.776679000	1.840867000	-2.414606000
C	4.002562000	2.604231000	-3.735735000
O	2.334647000	-0.050257000	-2.765322000
N	4.554376000	-0.471472000	-2.819947000
C	4.147317000	4.084164000	-3.480796000
C	3.021777000	4.866707000	-3.212001000
C	3.155790000	6.220376000	-2.921563000
C	4.418383000	6.808076000	-2.896431000
C	5.544774000	6.033818000	-3.160050000
C	5.409180000	4.678336000	-3.447469000
N	4.813743000	2.069419000	-1.415267000
C	3.042480000	-4.714008000	-1.184913000
C	5.155594000	0.715133000	1.277510000
O	5.136302000	1.579959000	2.160879000
C	6.125642000	1.763396000	-1.545587000
O	6.628760000	1.454424000	-2.628676000
H	3.855265000	0.255078000	5.627922000
H	3.713828000	-2.079105000	6.172423000
H	2.743752000	-2.438712000	4.747811000
H	3.762834000	-2.745415000	2.564436000
H	5.787570000	-2.978068000	1.174052000
H	8.020831000	-2.457680000	2.129760000
H	8.201436000	-1.697920000	4.490476000
H	6.166341000	-1.443318000	5.867892000
H	2.075339000	-0.356994000	0.667620000
H	3.047390000	2.374893000	1.569955000
H	2.198667000	1.941095000	0.081385000
H	3.935014000	0.871293000	3.442676000
H	1.614020000	4.137178000	2.146920000
H	-0.539828000	4.916737000	3.067743000
H	-2.458864000	3.335656000	3.249171000
H	-2.157362000	0.972939000	2.545067000
H	-0.055532000	0.216718000	1.585219000
H	4.186691000	-0.700514000	0.179663000
H	-0.750347000	0.752647000	5.491784000
H	0.051703000	1.446525000	6.924172000
H	-0.184158000	2.441509000	5.440492000
H	7.200778000	0.187264000	1.304410000
H	6.367203000	-0.449332000	-0.117186000
H	6.785998000	2.556391000	0.376107000
H	7.961507000	1.572843000	-0.524752000
H	3.615542000	-1.992283000	-3.884274000
H	5.496918000	-3.507116000	-3.947544000
H	5.994523000	-1.921201000	-4.534157000
H	6.207738000	-4.264253000	-1.633302000
H	7.982130000	-4.178625000	0.079725000
H	9.641418000	-2.329795000	0.064984000
H	9.502394000	-0.568864000	-1.685583000
H	7.730081000	-0.650576000	-3.384163000
H	2.848814000	2.221216000	-1.980399000
H	4.887514000	2.209238000	-4.238697000
H	3.131002000	2.406657000	-4.370172000
H	5.483478000	-0.060800000	-2.847723000
H	2.032882000	4.412901000	-3.226733000

H	2.271191000	6.815786000	-2.715228000
H	4.523431000	7.865406000	-2.671637000
H	6.532634000	6.485142000	-3.140534000
H	6.288397000	4.068523000	-3.640217000
H	4.486332000	2.324516000	-0.495572000
H	2.216275000	-4.239089000	-0.653718000
H	2.711499000	-5.630204000	-1.670304000
H	3.862758000	-4.915741000	-0.491047000
C	-4.795195000	5.479097000	-0.137036000
C	-3.931324000	4.554605000	-0.996926000
C	-2.439020000	4.872015000	-0.777592000
O	-4.390135000	6.476350000	0.407615000
O	-6.078918000	5.097287000	-0.137167000
C	-1.543678000	3.984552000	-1.605121000
C	-0.985712000	2.836967000	-1.039429000
C	-0.178245000	1.988918000	-1.791521000
C	0.072159000	2.269349000	-3.133607000
C	-0.485953000	3.408599000	-3.711344000
C	-1.281702000	4.261048000	-2.949256000
C	-4.253246000	2.624567000	0.457773000
C	-4.400362000	1.097161000	0.534862000
C	-5.852987000	0.635104000	0.282471000
O	-4.180794000	3.306288000	1.472666000
N	-4.251575000	3.160504000	-0.783892000
C	-6.799335000	1.085673000	1.366173000
C	-7.403881000	2.342435000	1.314062000
C	-8.254167000	2.756827000	2.334032000
C	-8.510426000	1.918542000	3.415947000
C	-7.910844000	0.663286000	3.473020000
C	-7.059020000	0.248459000	2.453438000
N	-3.431932000	0.368923000	-0.286900000
C	-6.932780000	5.850440000	0.720936000
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**PA3-dimer**

C	-5.694658000	1.929594000	-2.605127000
C	-6.279081000	2.829254000	-1.527207000
C	-7.136746000	2.023461000	-0.511841000
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O	-6.635558000	1.452639000	-3.403806000
C	-8.555876000	1.790253000	-0.967249000
C	-9.484473000	2.829635000	-0.870401000
C	-10.800283000	2.646174000	-1.283464000
C	-11.204999000	1.416643000	-1.797776000
C	-10.284253000	0.377237000	-1.900991000
C	-8.966108000	0.562454000	-1.490085000
C	-5.308962000	4.502425000	-0.018668000
C	-3.992894000	4.978705000	0.593945000

C	-3.783716000	4.179296000	1.913380000
O	-6.386386000	4.966219000	0.331762000
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C	-1.420475000	3.591187000	2.553326000
C	-0.190220000	3.899051000	3.125592000
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C	-1.041276000	6.047851000	3.792469000
C	-2.275501000	5.729691000	3.232136000
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C	-6.213648000	0.470294000	-4.351869000
C	3.964981000	-0.506881000	1.573841000
C	4.505116000	0.912883000	1.701256000
C	3.881410000	1.740039000	2.840817000
O	4.017720000	-1.160789000	0.555848000
O	3.479869000	-0.949370000	2.730677000
C	4.425490000	3.149982000	2.838270000
C	3.614171000	4.231142000	2.494909000
C	4.133860000	5.522288000	2.428410000
C	5.481039000	5.747058000	2.692977000
C	6.301194000	4.673371000	3.037455000
C	5.775304000	3.388270000	3.112883000
C	5.491366000	1.868468000	-0.325461000
C	5.285563000	3.001504000	-1.345866000
C	6.358913000	4.078155000	-1.048199000
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C	5.528103000	6.401395000	-1.559431000
C	5.349567000	7.475825000	-2.425555000
C	5.870830000	7.425882000	-3.715460000
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N	3.981329000	3.578135000	-1.161616000
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