Supporting Information

Self-assembled peptide mimetic of a tubular host and supramolecular polymer

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Table 1. Selected backbone torsion angles (deg) for peptide **1**

	ϕ_1/°	ψ_1/°	ϕ_2/°	ψ_2/°	ϕ_3/°	ψ_3/°
Peptide **1**	51.73(5)	37.20(4)	53.99(4)	34.05(5))	-123.61(4)	150.14(3)

Table 2. Hydrogen bonding parameters of peptide **1**[a]

D-H….A	D..H(Å)	H..A(Å)	D..A(Å)	D-H..A (°)
N1-H1….O5 [a]	0.88	2.19	3.057(5)	167
N2-H2….O4[a]	0.88	2.07	2.891(5)	154
N3-H3…O2	0.88	2.17	2.896(5)	140
O5-H5…O3	0.84	2.05	2.817(4)	151

[a]Symmetry equivalent *a*: *y*, 1-*x*+*y*,1/6+*z*.

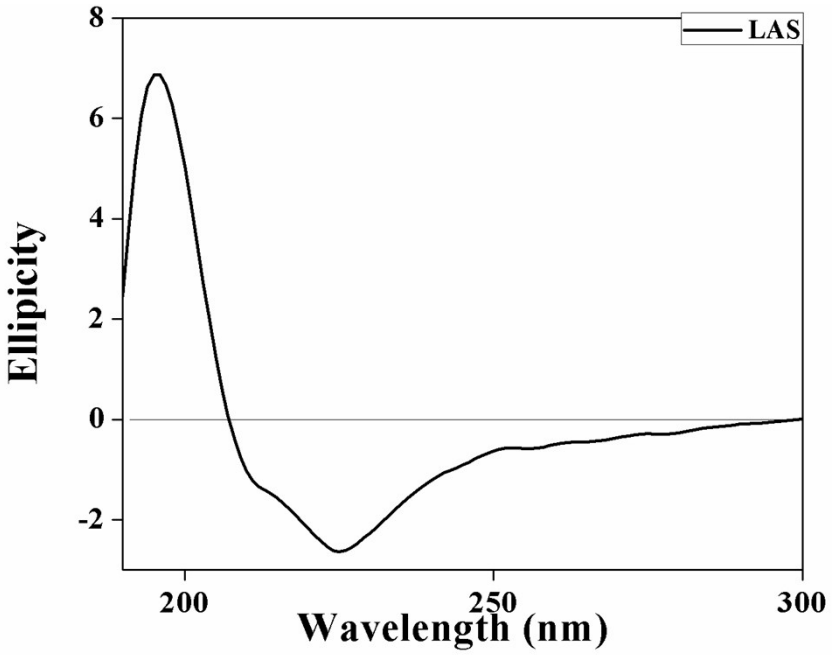


Figure S1. The CD spectra of peptide **1.** In MeOH solution peptide **1** self-assembled to form β-turn like conformation. The Peptide concentration was $1.025X10^{-6}$ (M).

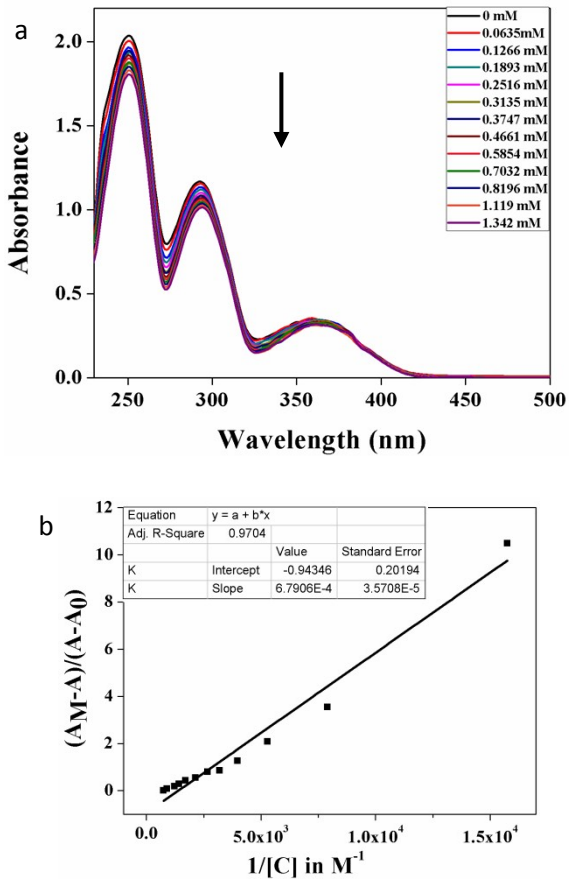


Figure S2: (a) UV-vis study of Coumarin derivative **2** with gradual addition of peptide **1.** (b) Bensi-Hildebrand plot.

The binding constant of peptide 1 and coumarin derivative **2** has calculated using the Bensi-Hildebrand equation where the conc of coumarin derivative **2** keep fixed i.e 1.065×10^{-5} M and peptide **1** added gradually to it. The reverse cannot be done as our peptide is not uv active. The absorbance gradually decreases by adding peptide. Here is the equation witten below.

$$1/(A-A_0)=1/(A_M-A_0)+1/(A_M-A_0).1/[C].1/K$$

where A_0= absorbance of coumarin derivative **2** in absence peptide, A = absorbance of coumarin derivative **2** in presence peptide, A_M = maximum absorbance in presence of peptide **1**, [C] = concentration of peptide **1**, K = binding constant. Plot of $(A_M-A)/(A-A_0)$ vs 1/[C] gives a straight with slope $6.7906x10^{\wedge-4}$ i.e. 1/K. So the binding const is $0.1473x10^4$ M^{-1}.

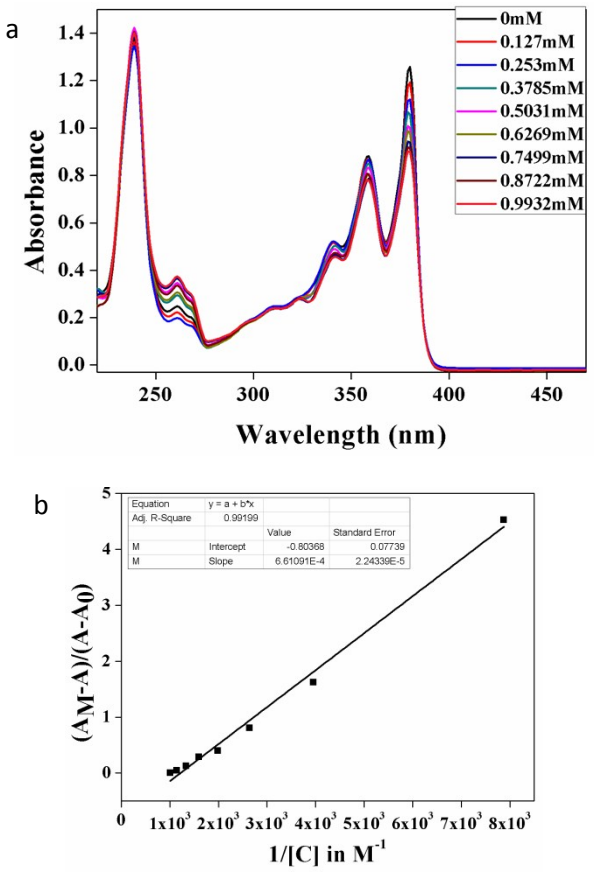


Figure S3: (a) UV-vis study of naphthaline diimide **3** with gradual addition of Peptide **1**. (b) Bensi-Hildebrand Plot.

For Bensi-Hildebrand plot, the concentration of NDI derivative **3** keep fixed i.e 2.41×10^{-5} M and peptide **1** added gradually to it. Plot of $(A_M\text{-}A)/(A\text{-}A_0)$ vs 1/[C] gives a straight line with slope 6.6109x10^-4 i.e. 1/K. So the binding const is $0.1512\text{x}10^4$ M^{-1}.

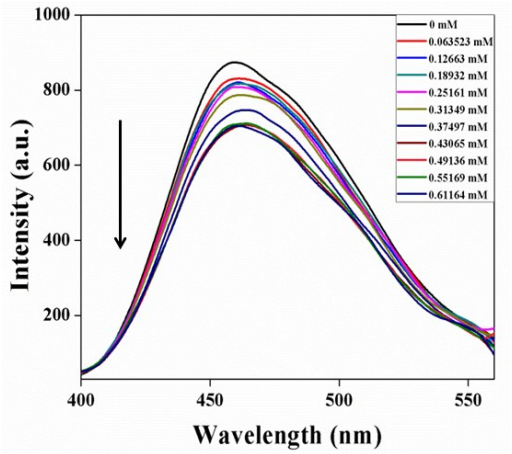


Figure S4: Fluorescence spectra of Coumarin derivative **2** with gradual addition of peptide **1**. Excitation at 290 nm.

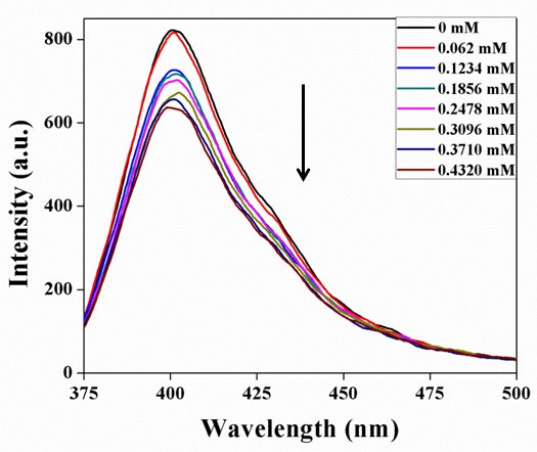


Figure S5: Fluorescence spectra of naphthaline diimide **3** with gradual addition of Peptide **1**. Excitation at 360 nm.

Table 3: Proton shift table of all NH protons in solvent.

DMSO-d_6 Volume added (µl)	Ser- NH	Aib-NH	Leu-NH	OH
0	7.0615	6.7218	5.0262	4.573
5	7.0768	6.8192	5.0902	4.5711
10	7.10065	6.9852	5.2008	4.5628
15	7.1102	7.1779	5.3287	4.5396
20	7.11115	7.2314	5.3740	4.5315
25	7.10735	7.2944	5.4337	4.5138
30	7.1045	7.3211	5.4690	4.5014
35	7.094	7.3363	5.4909	4.4795
40	7.0844	7.3535	5.5138	4.4623

Proton	Δδ
Ser NH	0.0229
Aib NH	0.6317
Leu NH	0.4876
OH	0.1107

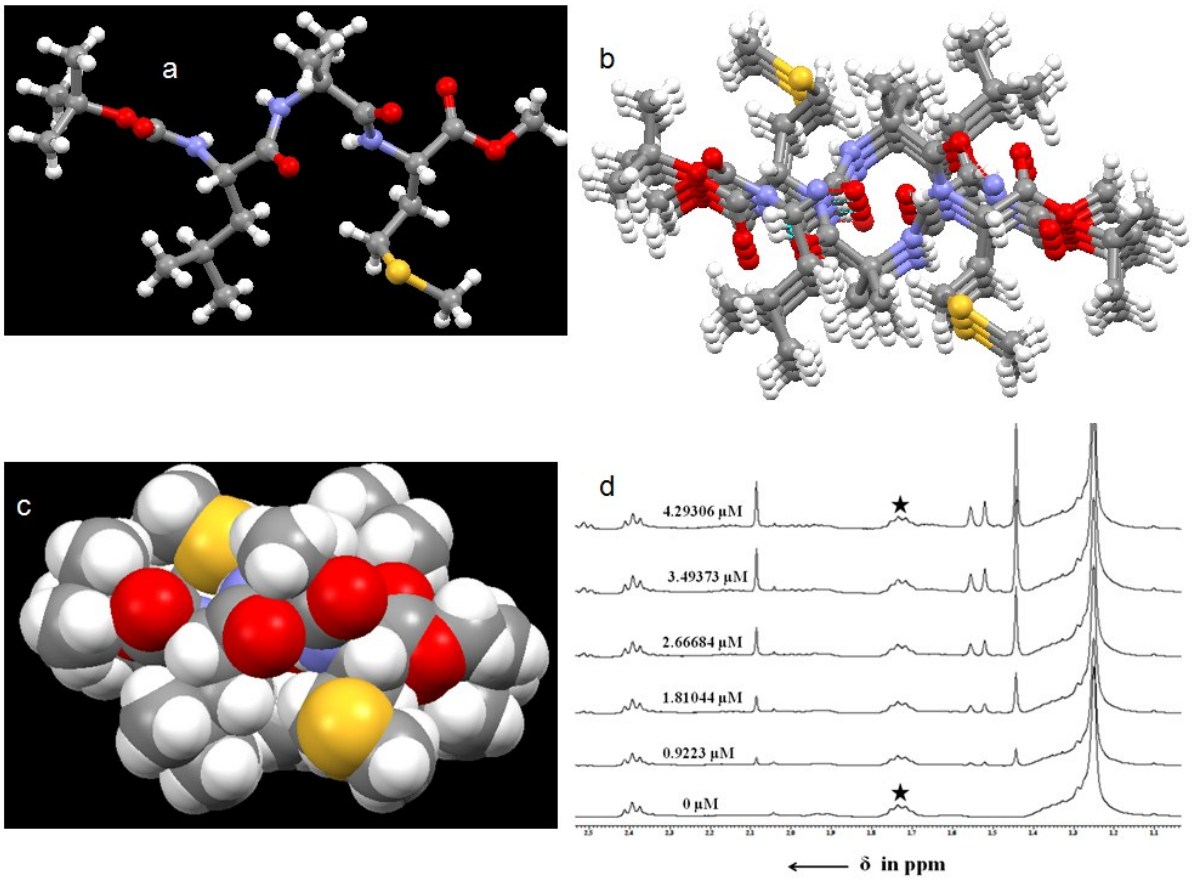


Figure S6: (a) the solid state conformation of Boc-Leu-Aib-Met-OMe showing non beta turn structure (CCDC number 1453988). (b) The ball and stick model showing higher order self-assembly of Boc-Leu-Aib-Met-OMe. (c) The space fill model showing non tubular assembly in higher order. (d) Part of ^{1}H NMR spectra of coumarin derivative **2** with increasing amount of peptide Boc-Leu-Aib-Met-OMe in $CDCl_3$.

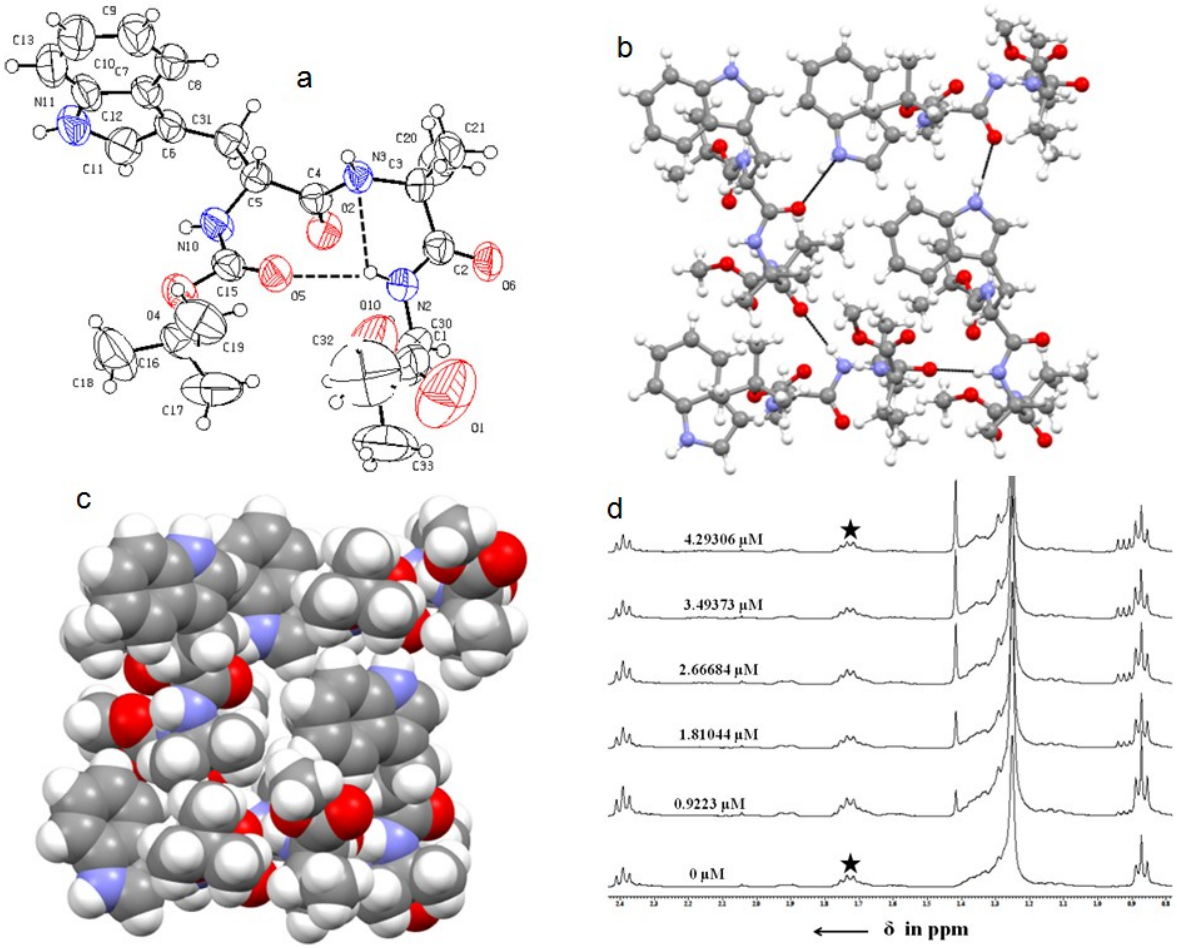


Figure S7: (a) the solid state conformation of Boc-Trp-Aib-Val-OMe showing beta turn structure (CCDC number 1426948). (b) The ball and stick model showing higher order cage like assembly of Boc-Trp-Aib-Val-OMe. (c) The space fill model showing cage like assembly in higher order. (d) Part of ^{1}H NMR spectra of coumarin derivative **2** with increasing amount of peptide Boc-Trp-Aib-Val-OMe in $CDCl_3$.

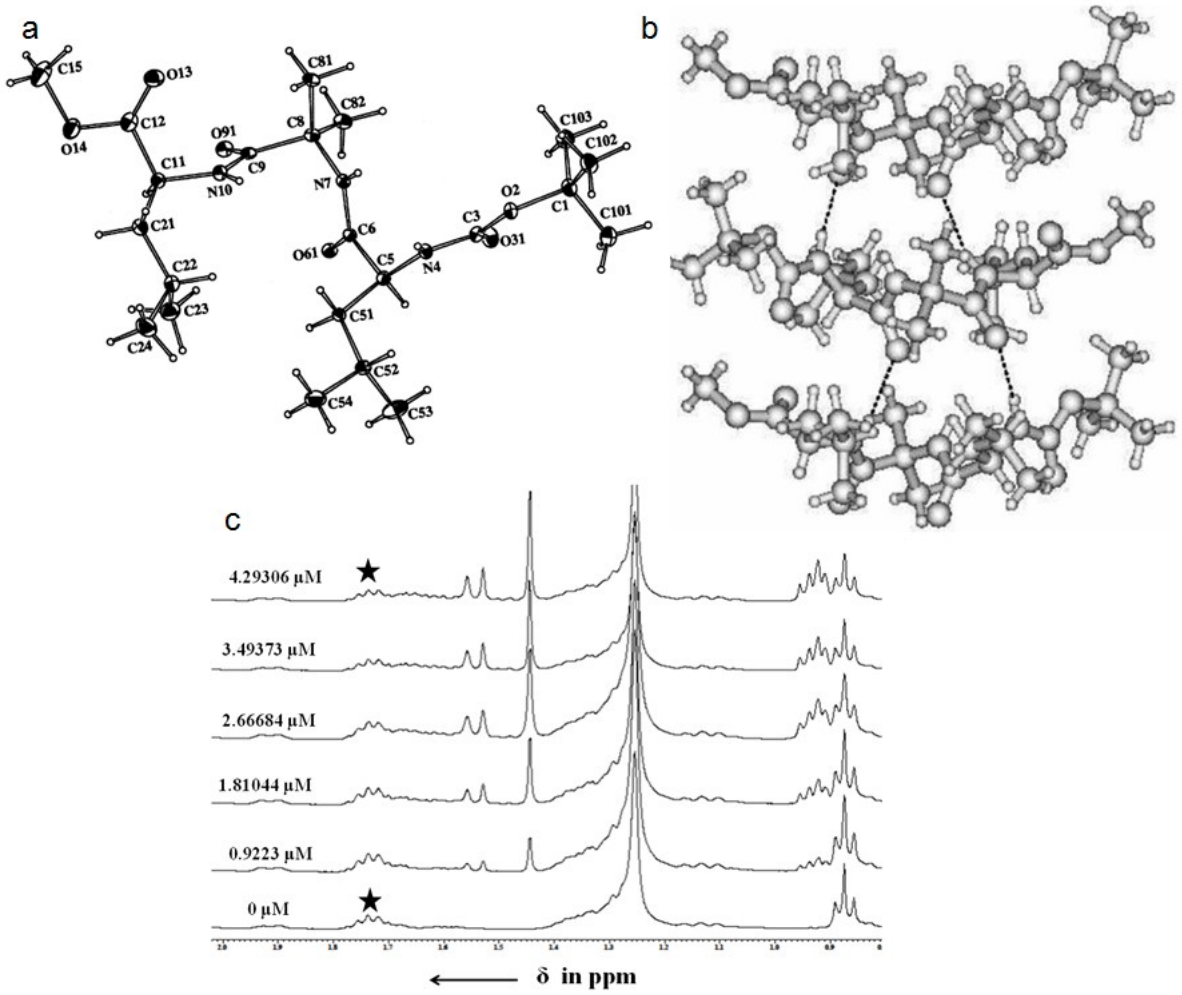


Figure S8: (a) the solid state conformation of Boc-Leu-Aib-Leu-OMe showing non beta turn structure (CCDC number 208708). (b) The ball and stick model showing higher order self-assembly of Boc-Leu-Aib-Leu-OMe. (c) Part of ^{1}H NMR spectra of coumarin derivative **2** with increasing amount of peptide Boc-Leu-Aib-Leu-OMe in $CDCl_3$.

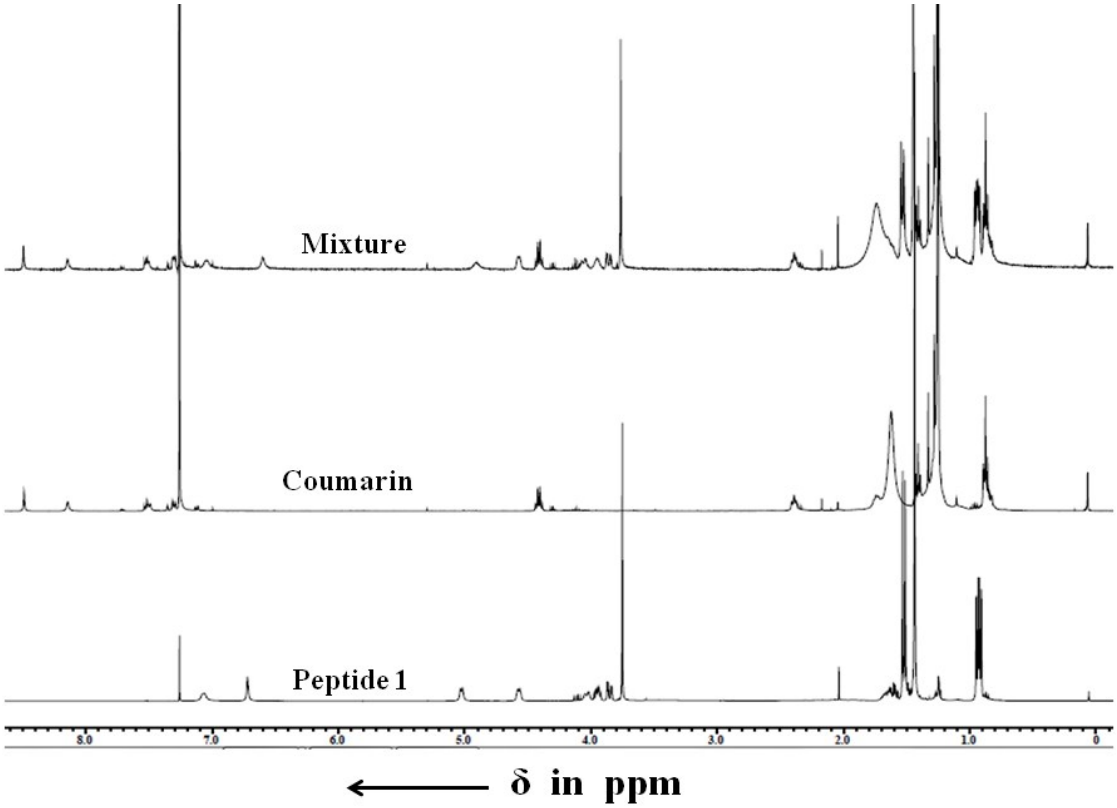


Figure S9: ^{1}H NMR spectra of mixed crystals obtained from peptide **1** and coumarin derivative **2** showing the existence of both the components.

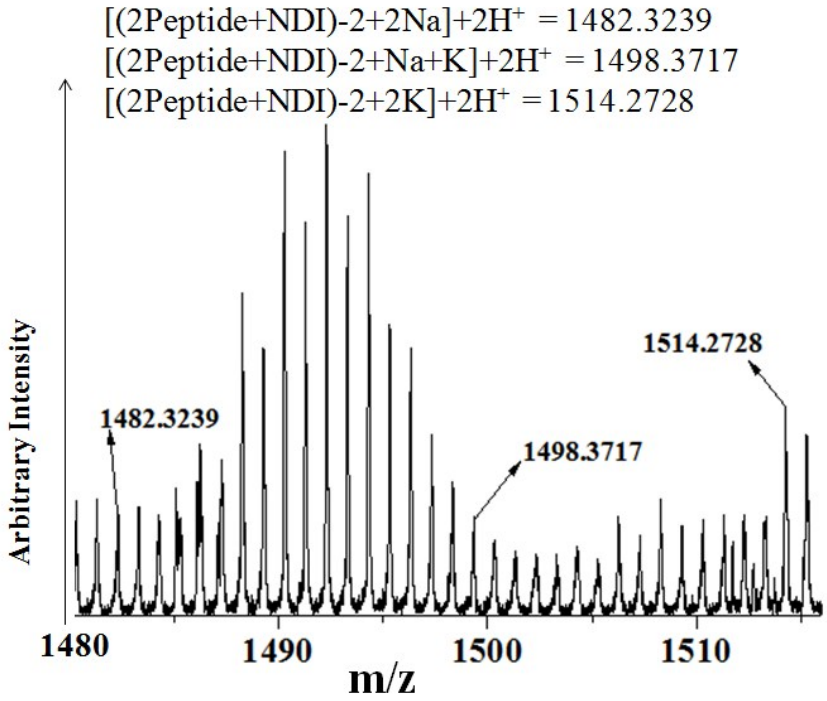
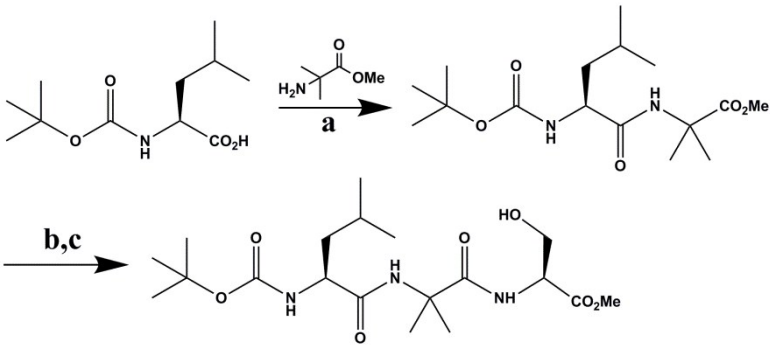


Figure S10: Mass spectrum of the fiber obtained from peptide **1** and diimide **3.**



Reagents and conditions: (a) Dry DCM, H-Aib-OMe, DCC, HOBt, 0°C, 77.8% yield; (b) MeOH, 2M NaOH, 86.8% yield; (c) Dry DCM, H-Ser-OMe, DCC, HOBt, 0°C, 78.89% yield.

Figure S11: Schematic presentation of synthesis of tripeptide **1**

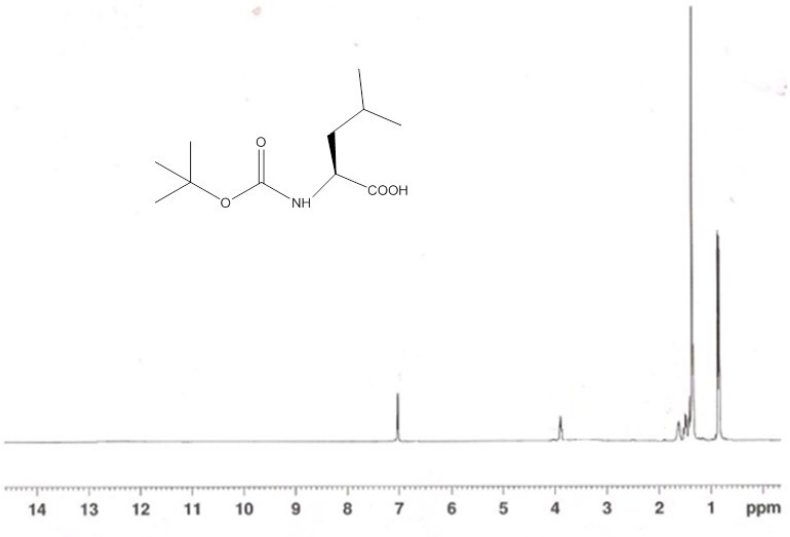


Figure S12: ^{1}H NMR (DMSO-d_6, 500 MHz, δ in ppm) spectra of Boc-Leu-OH

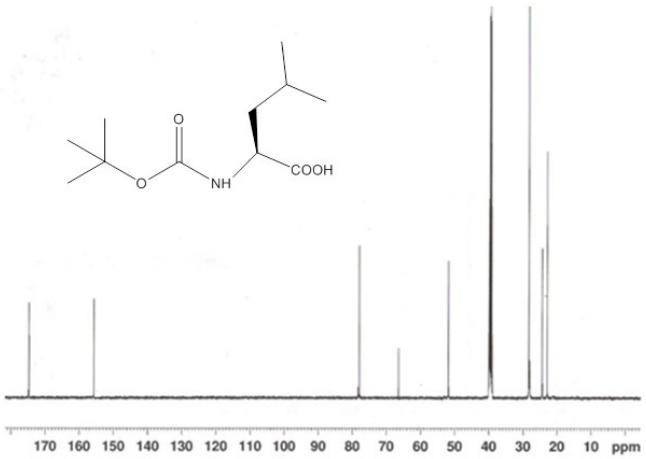


Figure S13: ^{13}C NMR (DMSO-d_6, 125 MHz, δ in ppm) spectra of Boc-Leu-OH.

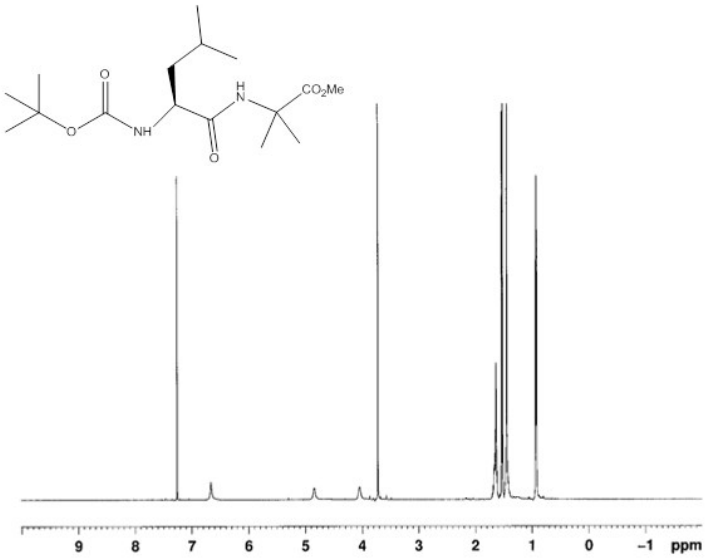


Figure S14: ^{1}H NMR ($CDCl_3$, 500 MHz, δ in ppm) spectra of Boc-Leu-Aib-OMe

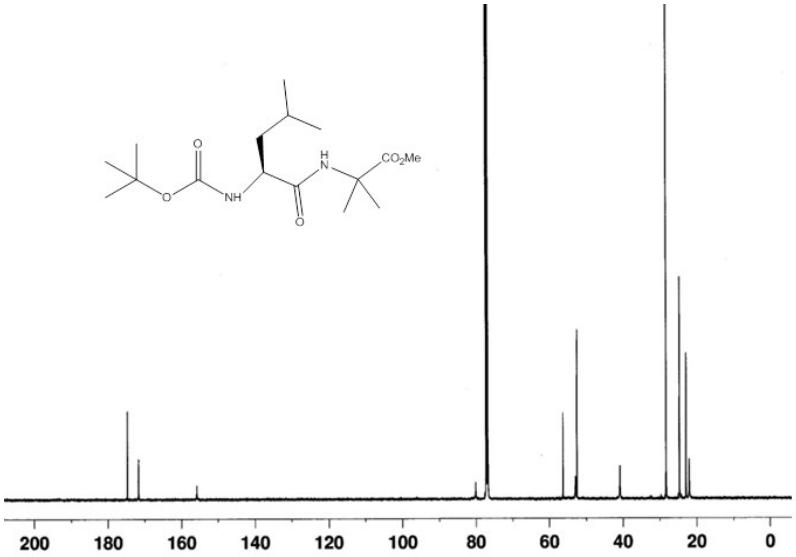


Figure S15: ^{13}C NMR ($CDCl_3$, 125 MHz, δ in ppm) spectra of Boc-Leu-Aib-OMe

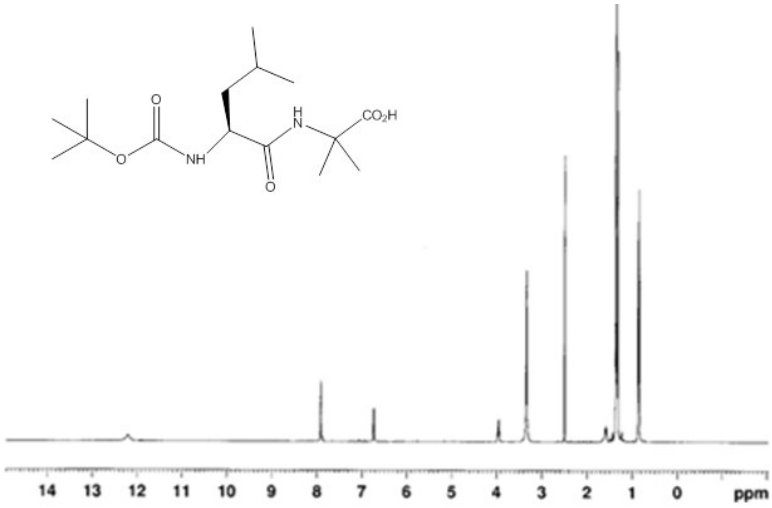


Figure S16: ^{1}H NMR (DMSO-d_6, 500 MHz, δ in ppm) spectra of Boc-Leu-Aib-OH

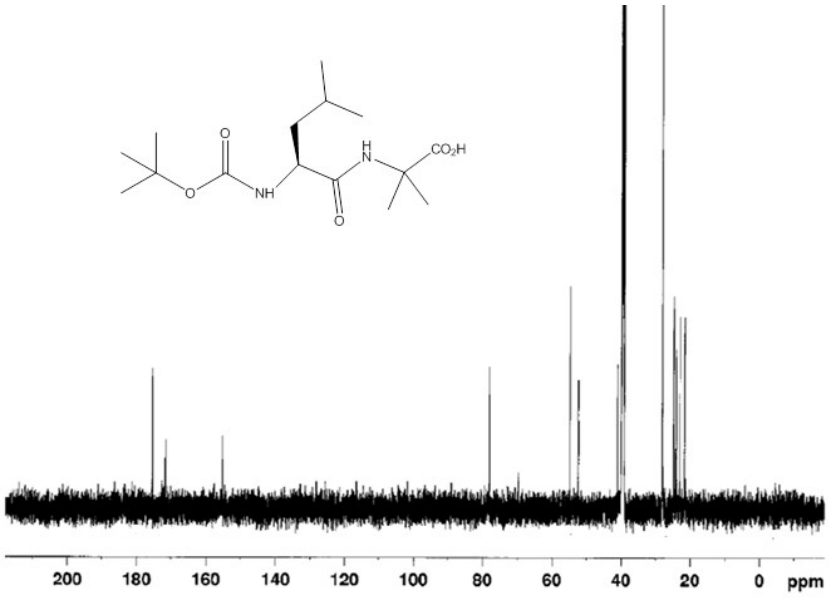


Figure S17: ^{13}C NMR (DMSO-d_6, 125 MHz, δ in ppm) spectra of Boc-Leu-Aib-OH

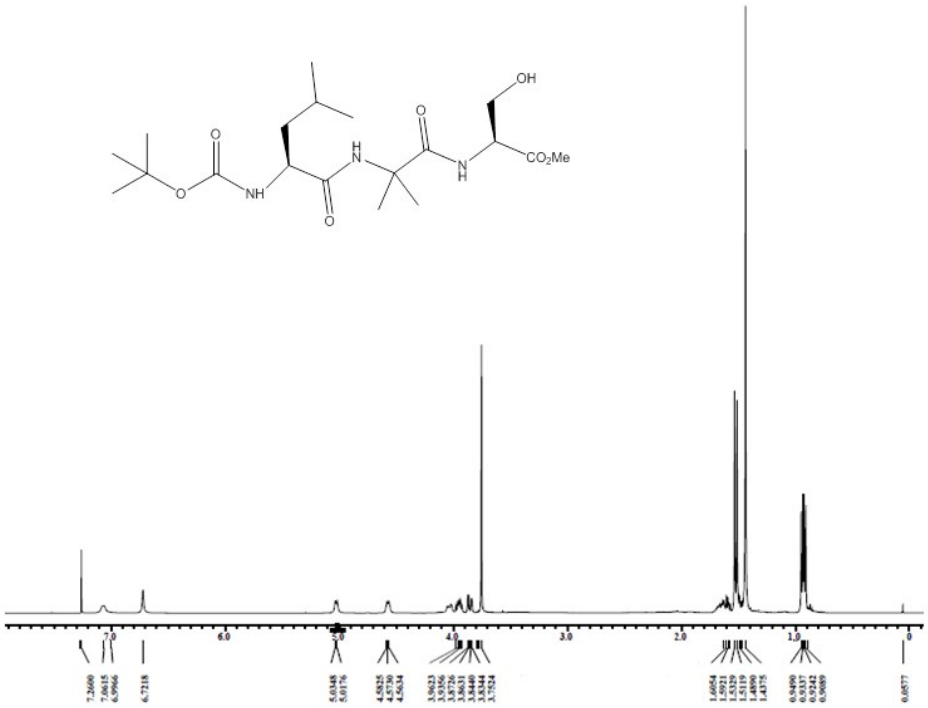


Figure S18: ^{1}H NMR ($CDCl_3$, 500 MHz, δ in ppm) spectra of Boc-Leu-Aib-Ser-OMe

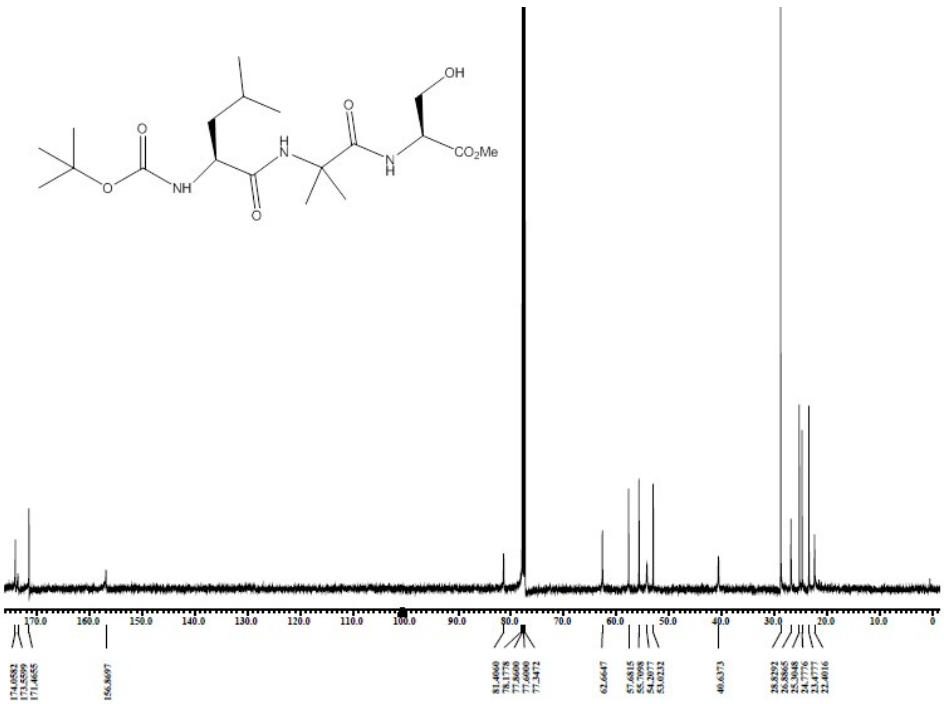


Figure S19: ^{13}C NMR ($CDCl_3$, 125 MHz, δ in ppm) spectra of Boc-Leu-Aib-Ser-OMe

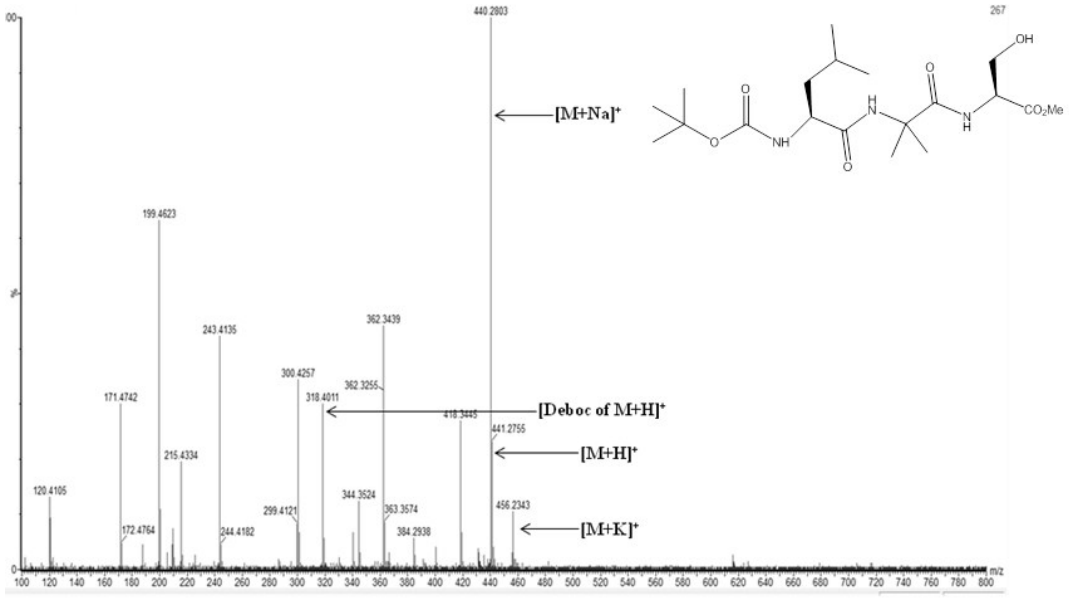


Figure S20: Mass specta of Boc-Leu-Aib-Ser-OMe

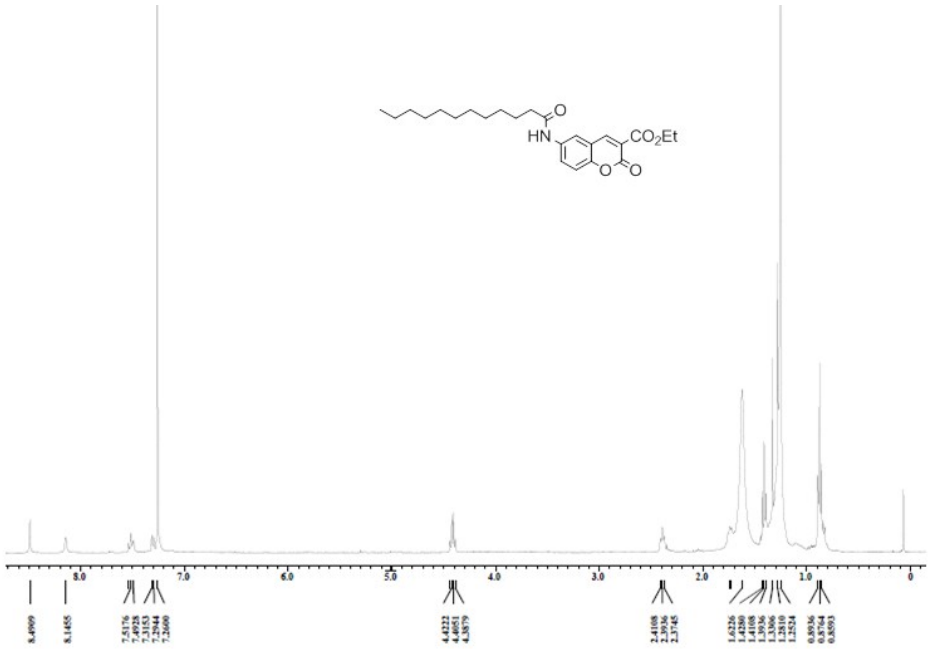


Figure S21: ^{1}H NMR ($CDCl_3$, 500 MHz, δ in ppm) spectra of Coumarin Derivative

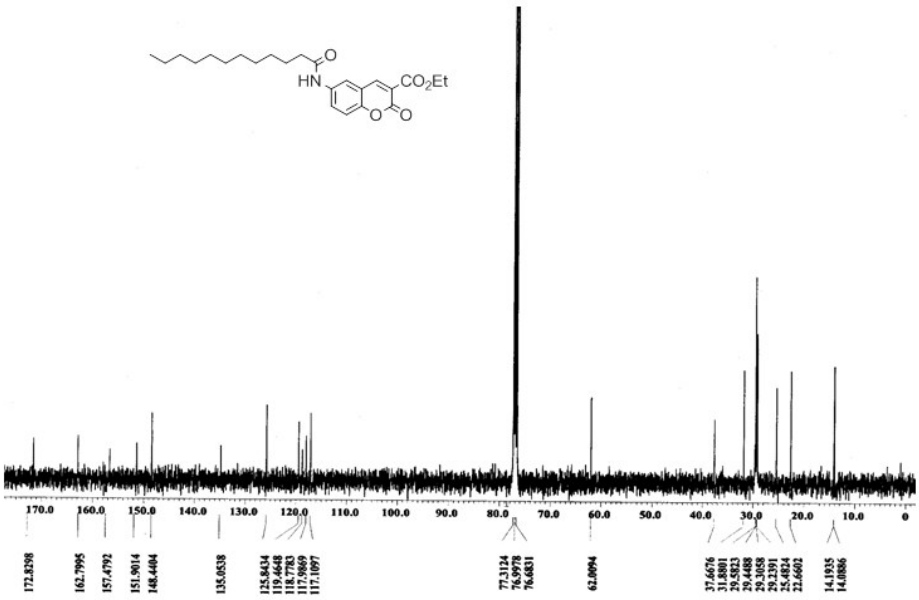


Figure S22: ^{13}C NMR ($CDCl_3$, 125 MHz, δ in ppm) spectra of Coumarin Derivative

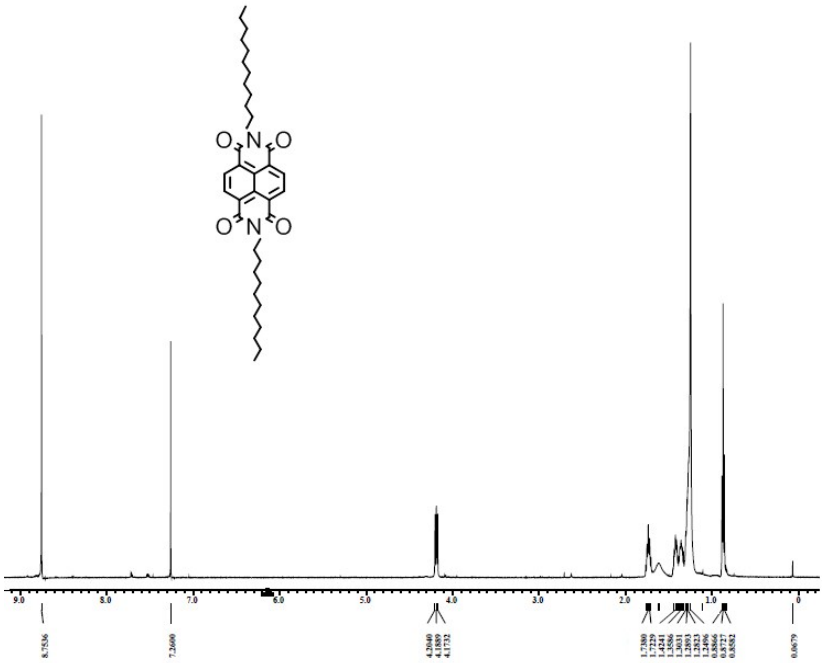


Figure S23: ^{1}H NMR ($CDCl_3$, 500 MHz, δ in ppm) spectra of naphthaline diimide **3**.

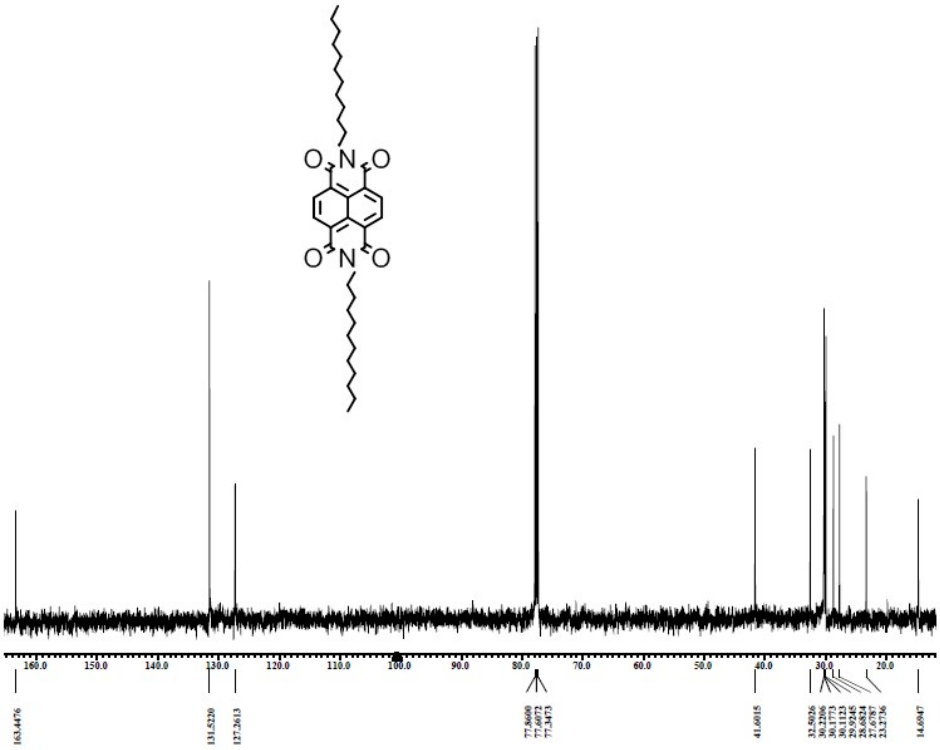


Figure S24: ^{13}C NMR ($CDCl_3$, 125 MHz, δ in ppm) spectra of naphthaline diimide **3**

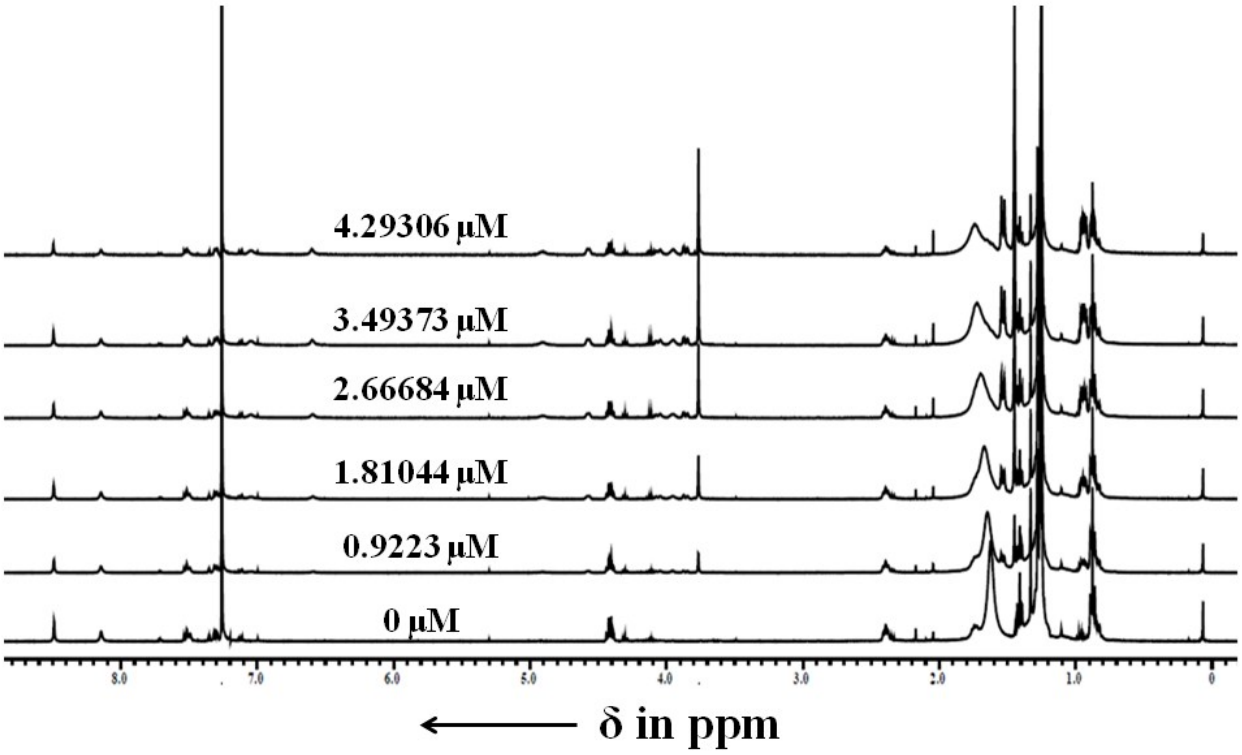


Figure S25: Plot of ^{1}H NMR spectra of coumarin derivative **2** with increasing amount of peptide **1** in $CDCl_3$.

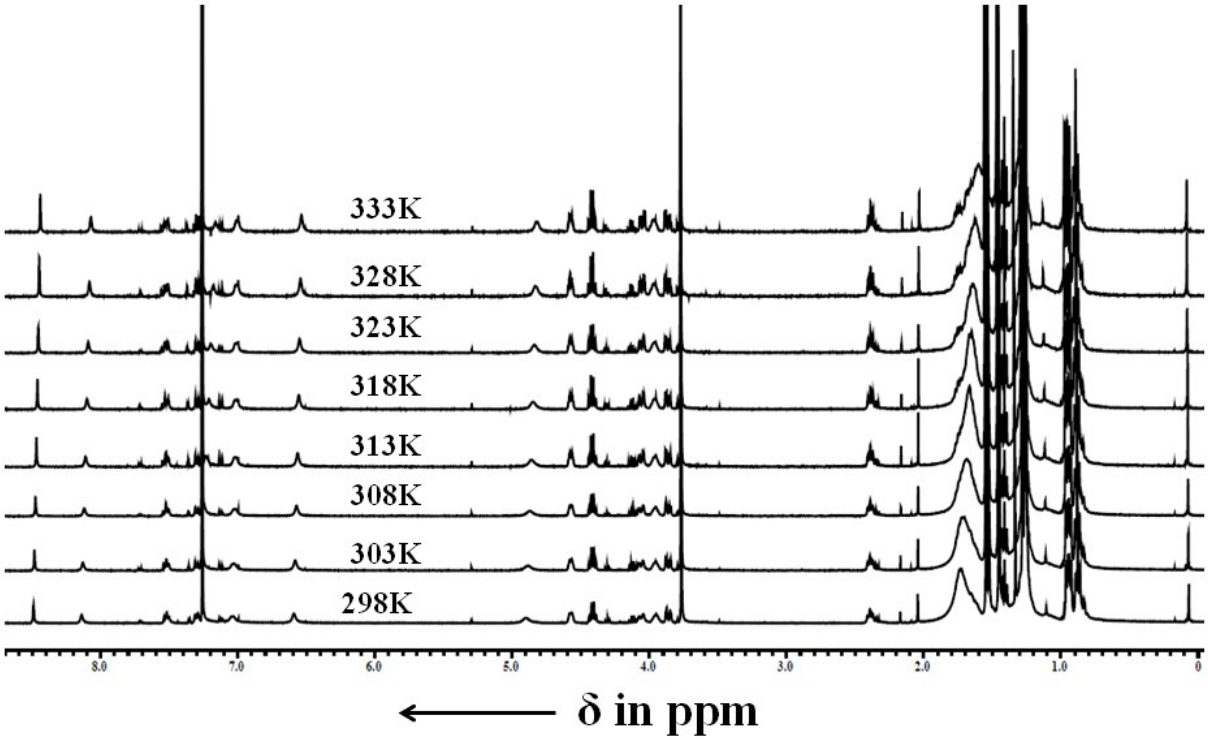


Figure S26: Plot of the variable temperature ^{1}H NMR spectra of coumarin derivative **2** and peptide **1**(4.29 μM) in $CDCl_3$.

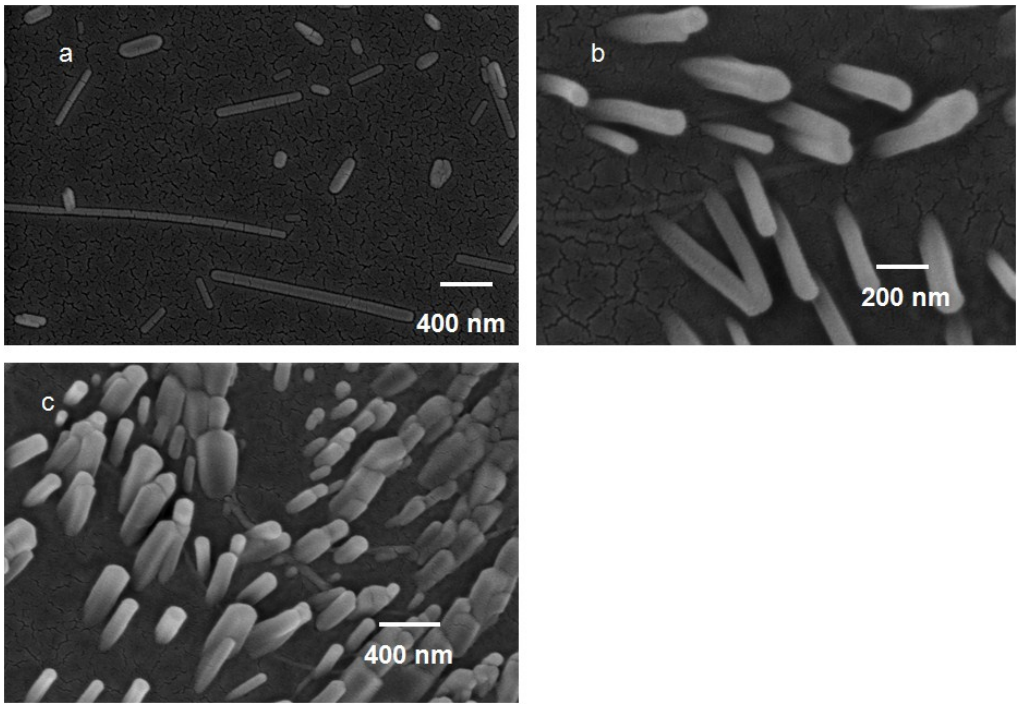


Figure S27: (a) FE-SEM image of peptide **1** showing unbranched polydisperse modular nanotubes morphology. (b) and (c) The unbranched polydisperse columnar morphology of peptide **1** and coumarin derivative **2** mixture.

Sample Name:	LAS 104 1		
SOP Name:	mansettings.nano		
File Name:	LAS 104.dts	**Dispersant Name:**	Dichloromethane
Record Number:	1	**Dispersant RI:**	1.424
Material RI:	1.59	**Viscosity (cP):**	0.4130
Material Absorbtion:	0.010	**Measurement Date and Time:**	16 March 2016 10:36:54

Temperature (°C):	25.0	**Duration Used (s):**	30
Count Rate (kcps):	189.8	**Measurement Position (mm):**	4.65
Cell Description:	Glass cuvette with square aperture	**Attenuator:**	11

			Size (d.nm):	**% Intensity:**	**St Dev (d.nm):**
Z-Average (d.nm):	1448	**Peak 1:**	59.73	100.0	7.538
PdI:	1.000	**Peak 2:**	0.000	0.0	0.000
Intercept:	0.375	**Peak 3:**	0.000	0.0	0.000

Result quality : Refer to quality report

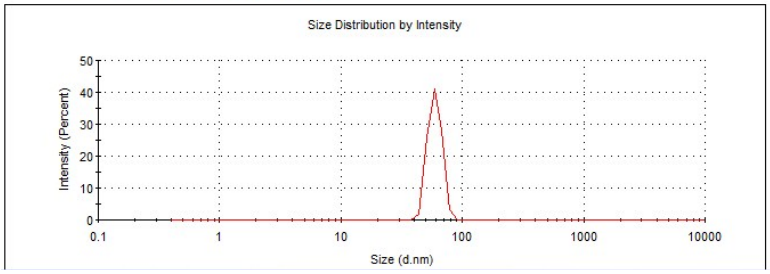


Figure S28: DLS data of peptide 1.

Sample Name:	Cou104 1		
SOP Name:	mansettings.nano		
File Name:	Cou104.dts	**Dispersant Name:**	Dichloromethane
Record Number:	1	**Dispersant RI:**	1.424
Material RI:	1.59	**Viscosity (cP):**	0.4130
Material Absorbtion:	0.010	**Measurement Date and Time:**	16 March 2016 10:45:16

Temperature (°C):	25.0	**Duration Used (s):**	30
Count Rate (kcps):	182.3	**Measurement Position (mm):**	4.65
Cell Description:	Glass cuvette with square aperture	**Attenuator:**	11

			Size (d.nm):	**% Intensity:**	**St Dev (d.nm):**
Z-Average (d.nm):	2296	**Peak 1:**	65.47	100.0	9.785
PdI:	0.998	**Peak 2:**	0.000	0.0	0.000
Intercept:	0.371	**Peak 3:**	0.000	0.0	0.000

Result quality : Refer to quality report

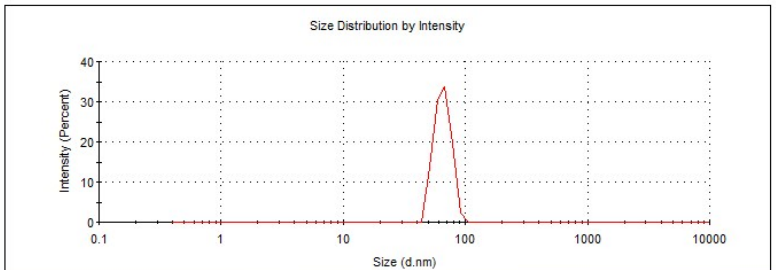


Figure S29: DLS data of coumarin 2.

Sample Name:	NDI 104 1		
SOP Name:	mansettings.nano		
File Name:	NDI 104.dts	**Dispersant Name:**	Dichloromethane
Record Number:	1	**Dispersant RI:**	1.424
Material RI:	1.59	**Viscosity (cP):**	0.4130
Material Absorbtion:	0.010	**Measurement Date and Time:**	16 March 2016 10:53:11

Temperature (°C):	25.0	**Duration Used (s):**	30
Count Rate (kcps):	265.9	**Measurement Position (mm):**	4.65
Cell Description:	Glass cuvette with square aperture	**Attenuator:**	11

			Size (d.nm):	**% Intensity:**	**St Dev (d.nm):**
Z-Average (d.nm):	1435	**Peak 1:**	209.6	100.0	34.89
PdI:	0.632	**Peak 2:**	0.000	0.0	0.000
Intercept:	0.464	**Peak 3:**	0.000	0.0	0.000

Result quality : Refer to quality report

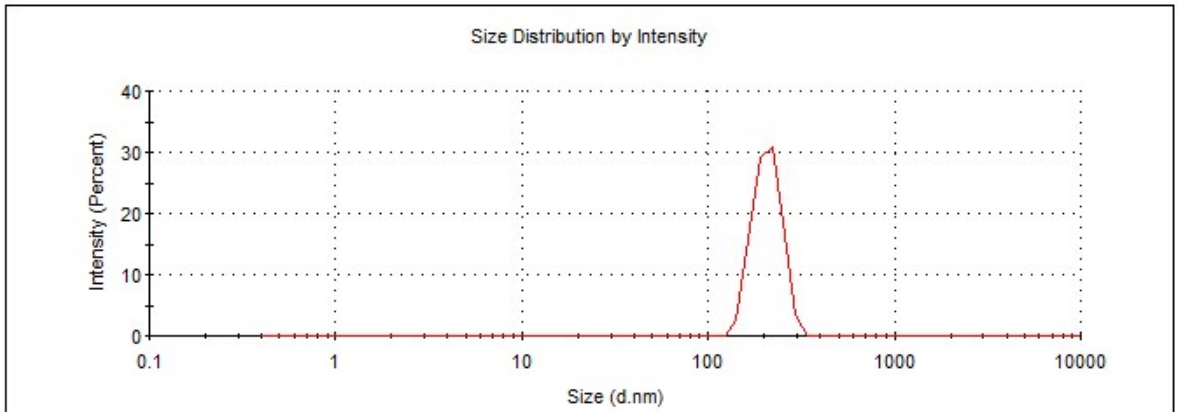


Figure S30: DLS data of diimide 3.

Sample Name:	LAScou4 1		
SOP Name:	mansettings.nano		
File Name:	LAScou4.dts	**Dispersant Name:**	Dichloromethane
Record Number:	1	**Dispersant RI:**	1.424
Material RI:	1.59	**Viscosity (cP):**	0.4130
Material Absorbtion:	0.010	**Measurement Date and Time:**	14 March 2016 20:17:49

Temperature (°C):	25.0	**Duration Used (s):**	30
Count Rate (kcps):	99.2	**Measurement Position (mm):**	4.65
Cell Description:	Glass cuvette with square aperture	**Attenuator:**	10

			Size (d.nm):	**% Intensity:**	**St Dev (d.nm):**
Z-Average (d.nm):	2896	**Peak 1:**	251.2	100.0	26.95
PdI:	0.870	**Peak 2:**	0.000	0.0	0.000
Intercept:	0.580	**Peak 3:**	0.000	0.0	0.000

Result quality : Refer to quality report

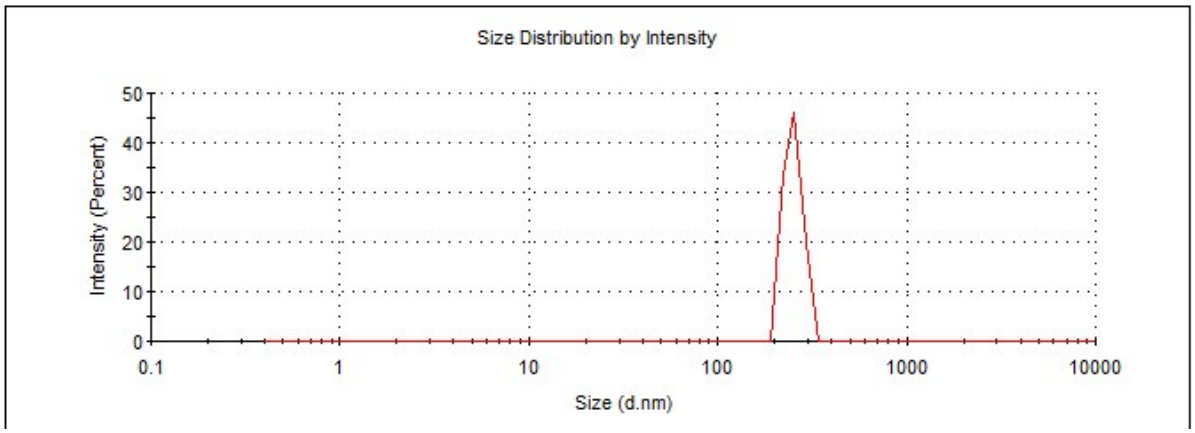
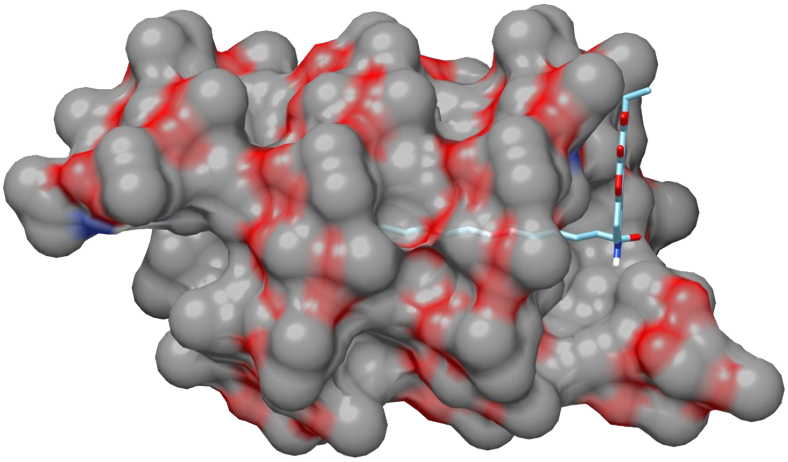


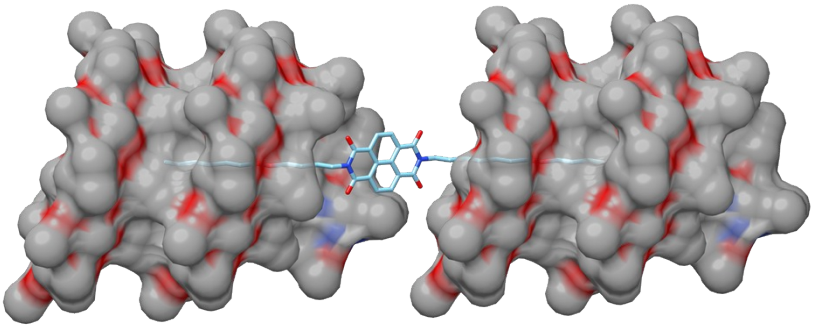
Figure S31: DLS data of mixture of peptide 1 and coumarin 2.



```
Detected 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -764819232
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   3         -9.9      3.586      4.649
```

Figure S32: The docking study of peptide 1 supramolecular tube and coumarin 2.



```
Detected 4 CPUs
Reading input ... done.
Setting up the scoring function ... done.
Analyzing the binding site ... done.
Using random seed: -1192870512
Performing search ... done.
Refining results ... done.

mode |   affinity | dist from best mode
     | (kcal/mol) | rmsd l.b.| rmsd u.b.
-----+------------+----------+----------
   4         -6.9      1.255      1.313
```

Figure S33: The docking study of peptide 1 supramolecular tube and diimide 3.

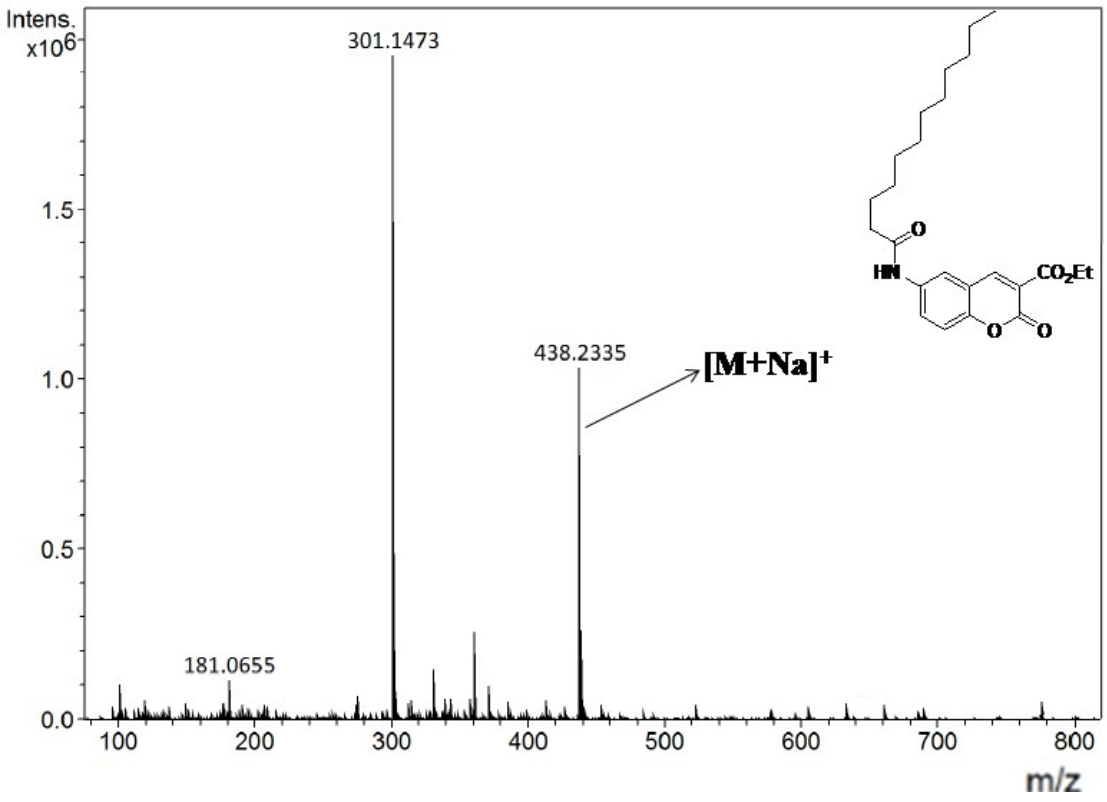


Figure S34: The mass data of coumarin 2.

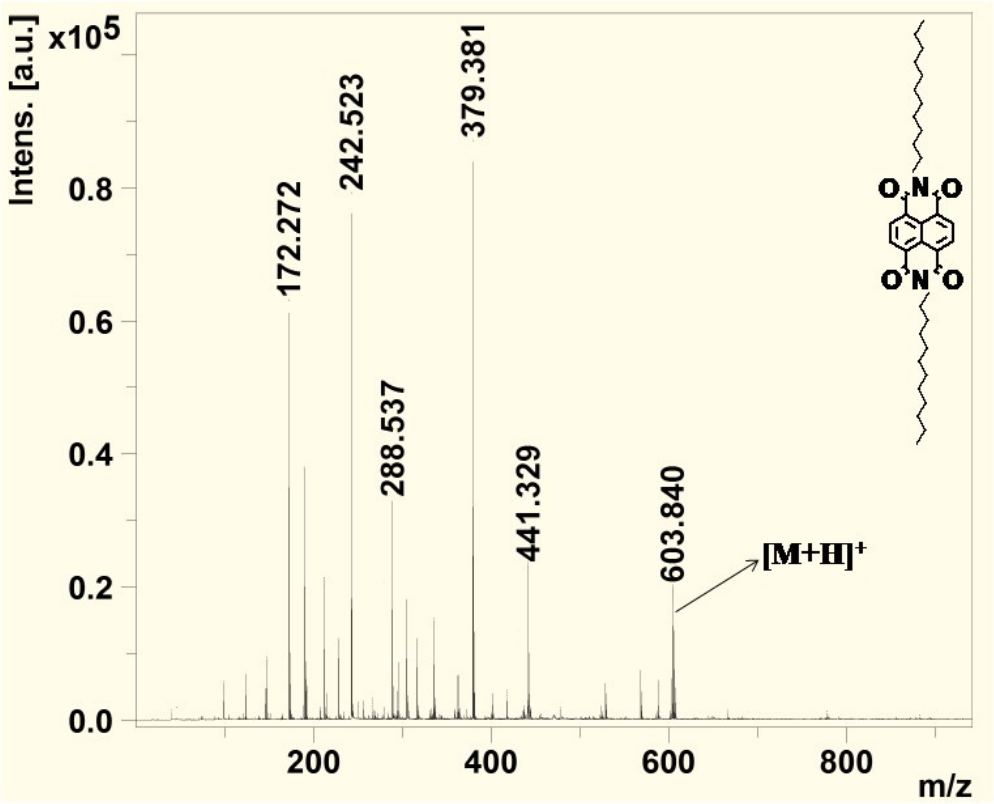


Figure S35: The mass data of diimide 3.