Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

The Helical Supramolecular Assembly of Oligopyridylamide Foldamers in Aqueous Media can be Guided by Adenosine Diphosphates

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Materials. All chemicals were purchased from commercial suppliers and used without further purification. Silica plates (with UV_{254}, aluminum backed, 200 µm) and silica gel (standard grade, particle size = 40−63 µm, 230−400 mesh) for flash column chromatography were purchased from Sorbent Technologies (Norcross, GA). Dry solvents were purchased from Sigma-Aldrich (St. Louis, MO). All other chemicals were purchased from Sigma-Aldrich (St. Louis, MO) and used for synthesis without further purification.

NMR Measurements. NMR spectra were obtained with a Bruker Avance III HD 400 NMR Spectrometer with chemical shifts reported in parts per million (ppm) with respect to TMS.

Optical Measurements. Electronic absorption spectra were recorded on a Cary 100 UV-Visible Spectrophotometer and emission spectra were recorded on Horiba PTI QuantaMaster 400 Fluorometer. UV-Vis and emission spectra were recorded in 10 mm path length cuvettes. Fluorescence spectra of solutions were recorded with 340 nm excitation wavelength. Jasco J-1500 Circular Dichroism was used for CD measurement.

Dynamic light scattering Experiments (DLS). The measurements were carried out using a Malvern Zetasizer Nano Series.

Transmission Electron Microscopy (TEM) Analysis. 5 µl of sample was added onto glow discharged carbon coated 400 mesh Cu/Rh grid (Ted Pella Inc., Redding, CA) l and stain with 1% uranyl acetate (Polysciences, Inc, Warrington, PA)v in ddH_2O. Stained grids were examined under Thermo Fisher Talos 120C transmission electron microscope and photographed with a Gatan OneView digital camera. Water was used as sample solvent instead of HEPES to avoid masking of nanostructures due to HEPES deposition upon drying.

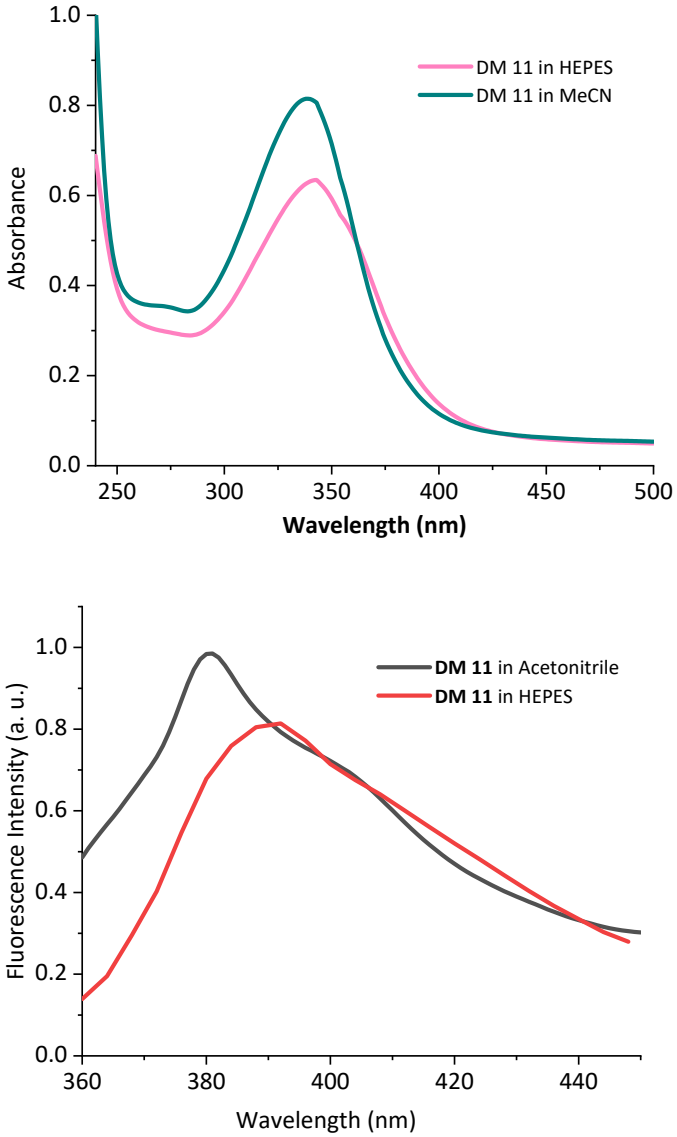


Fig. S1 UV-Vis (top) and fluorescence (bottom) spectra of **DM 11** (20 µM) in different solvents.

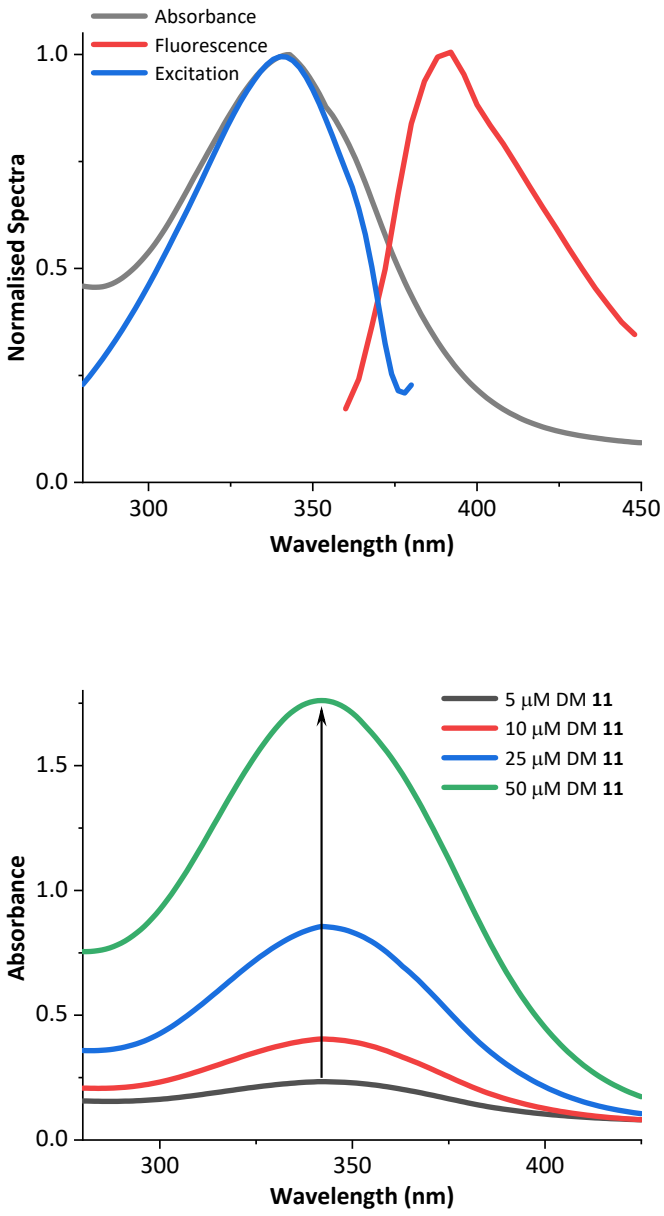


Fig. S2 Top: Normalised absorption, emission and excitation spectra of **DM 11** (20 μM) in HEPES buffer. Red-shifted excitation spectra compared to the absorption maxima was not observed. Bottom: UV-Vis spectra of **DM 11** with increasing concentrations in HEPES buffer. It shows linear increase in absorbance at 342 nm (without any major shift) with increasing concentration of DM 11. These studies explain that the small redshift in HEPES (absorption (4 nm) and emission (10 nm)) compared with the monomeric state in acetonitrile is likely due to solvatochromism.

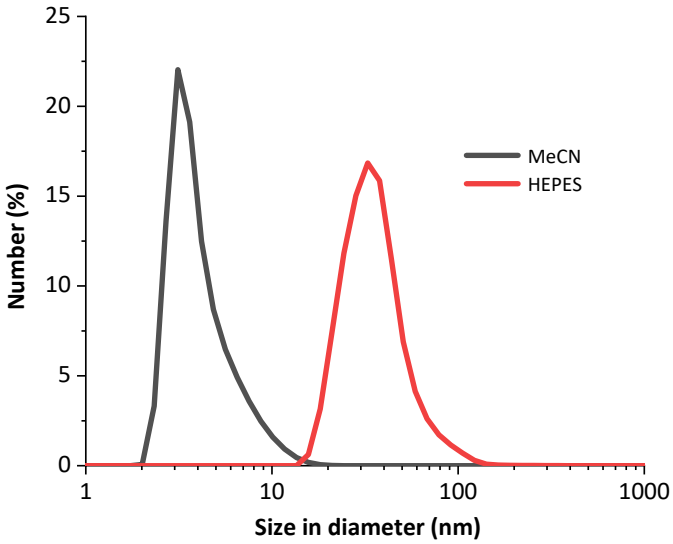


Fig. S3 Size distribution of **DM 11** (20 µM) from DLS measurements in different solvents.

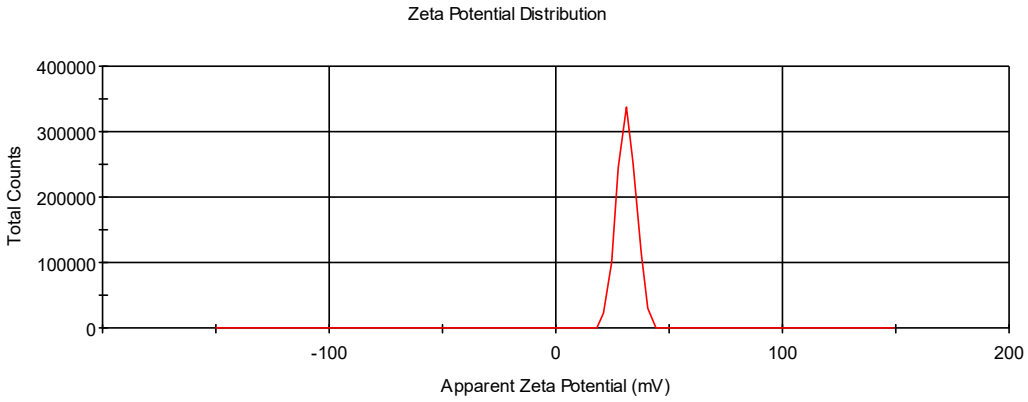


Fig. S4 Zeta-potential measurement of DM 11 in HEPES buffer.

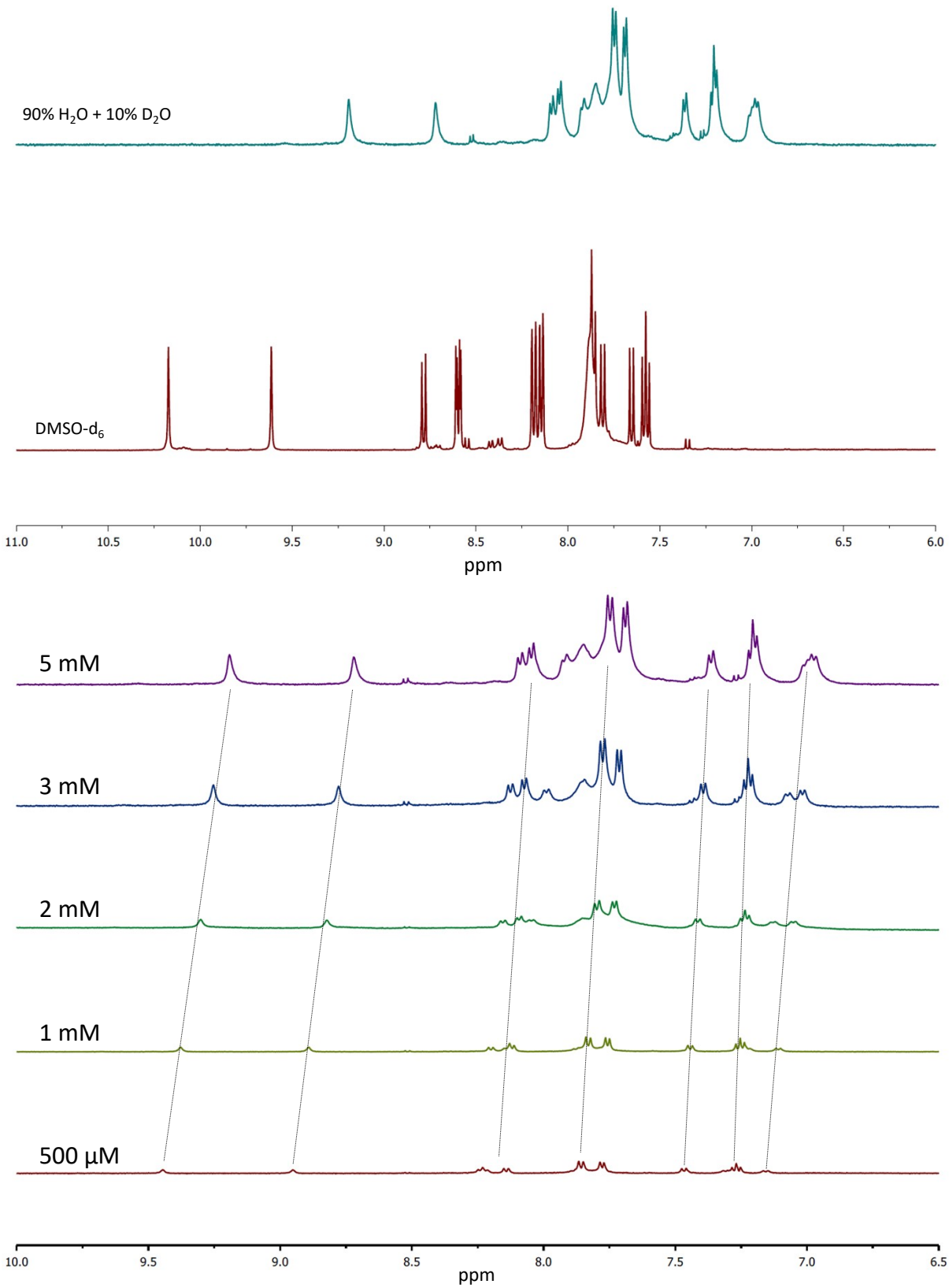


Fig. S5 Top: ^{1}H NMR spectra of **DM 11** (5 mM) in different solvents at 25°C. Bottom: Concentration dependent ^{1}H NMR spectra of DM 11 in 90% H_2O + 10% D_2O at 25°C.

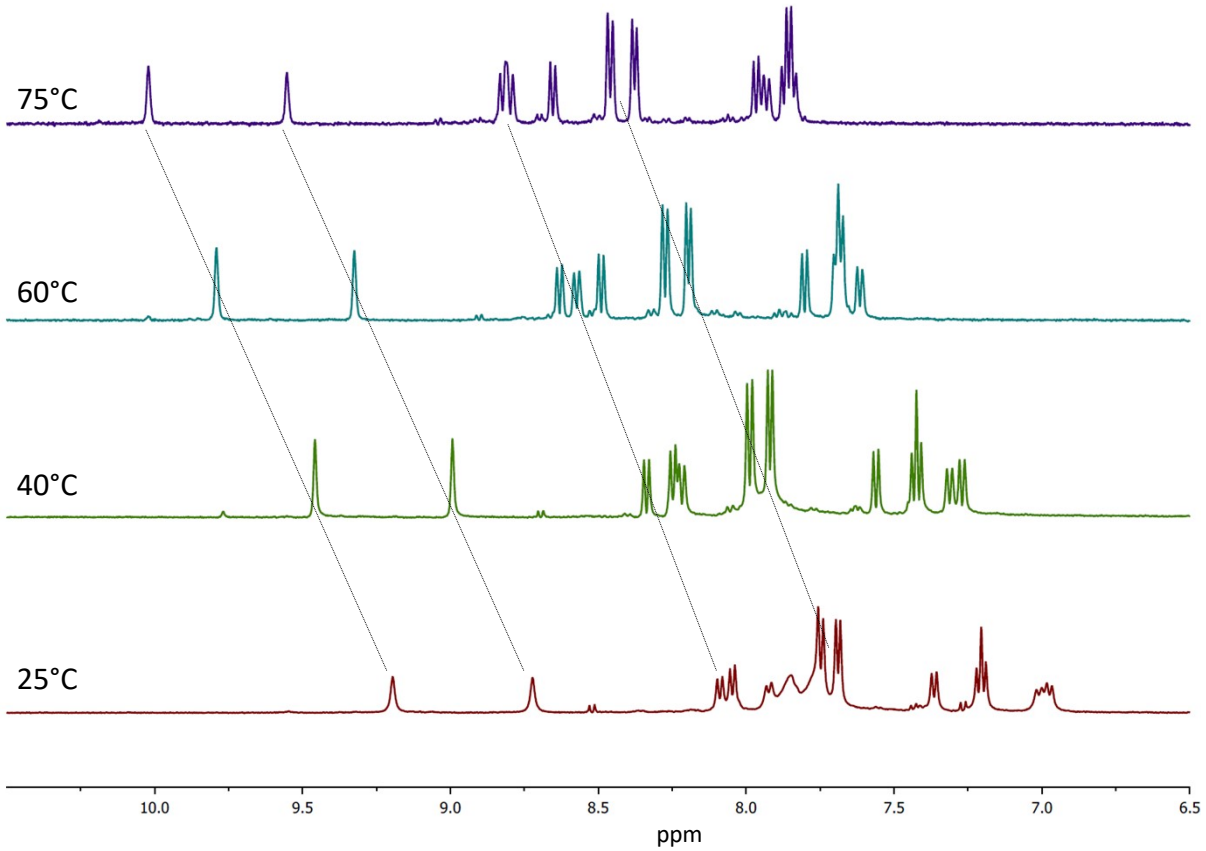


Fig. S6 Temperature dependent ^{1}H NMR spectra of **DM 11** (5 mM) in 90% H_2O + 10% D_2O.

Self-assembly of **DM 11** in solution was investigated by ^{1}H-NMR spectroscopy. In DMSO-d_6, **DM 11** exists as solvated single molecules with the ^{1}H-NMR spectra featuring the sharp signals of the monomeric species (Fig. S5, top). When dissolved in H_2O (10% D_2O), two amide and aromatic protons were upfield-shifted compared to monomeric form. Broadening of these peaks was also observed (Fig. S5, top). We performed concentration dependent ^{1}H NMR of **DM 11** (0.5 - 5 mM) in H_2O (10% D_2O). This also resulted in upfield-shifting of amide and aromatic protons with increasing concentrations (Fig. S5, bottom).

We have measured temperature dependent ^{1}H NMR spectra of **DM 11** (5 mM) in H_2O (10% D_2O) (Fig. S6). Upon increasing temperature from 25°C to 75°C, all amide and aromatic protons are downfield shifted. At 75°C, all peaks are well resolved, and the ammonium protons exchange rapidly with the water hydrogens at this temperature, and therefore their signal is not visible.

All these NMR studies indicate that **DM 11** aggregates in water via stacking of the hydrophobic aromatic units, without significant intermolecular hydrogen bonding.

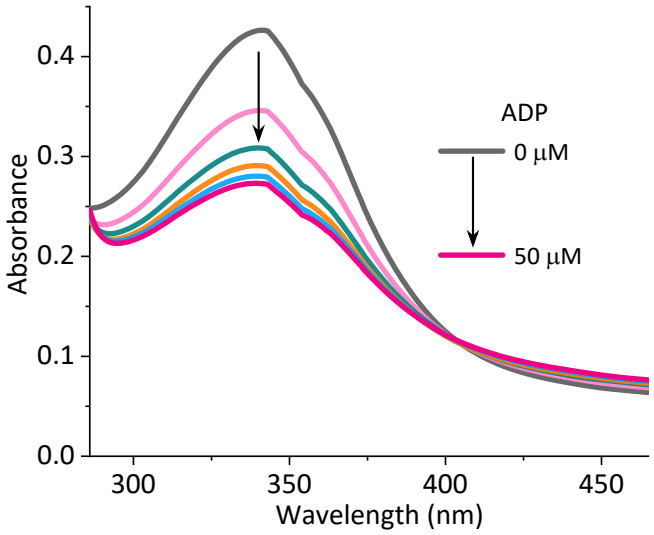


Fig. S7 Absorption spectra of **DM 11** with increasing concentration of ADP. **DM 11** = 20 µM in 10 mM HEPES in all cases.

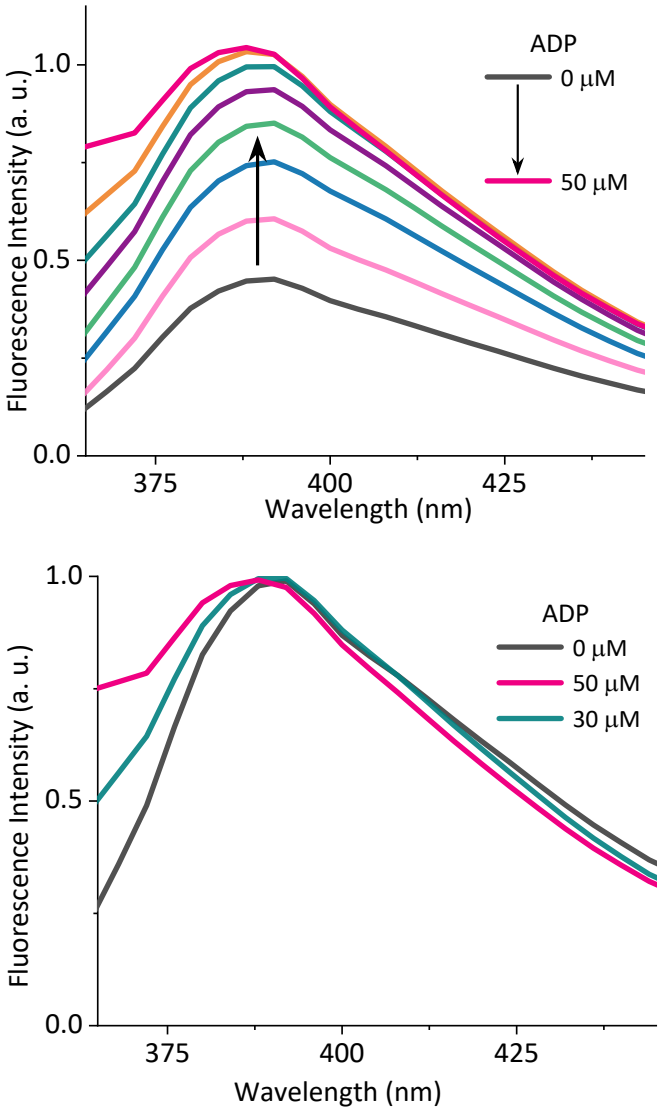
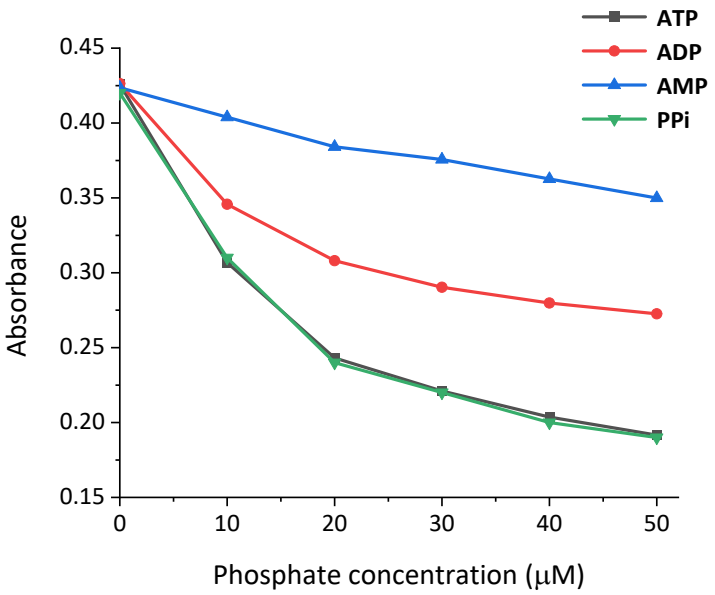


Fig. S8 Top: Fluorescecne spectra of **DM 11** with increasing concentration of ADP. **DM 11** = 20 μM in 10 mM HEPES in all cases. Bottom: Normalised fluorescence spectra at three different concentrations of ADP.



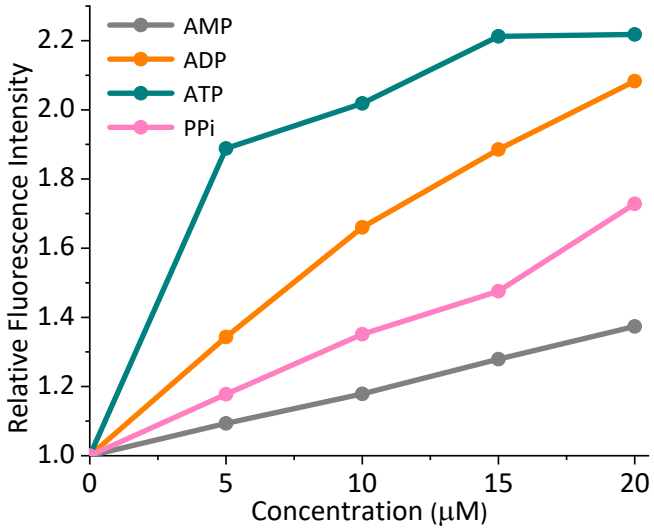


Fig. S9 Top: changes in absorbance of **DM 11** with different adenosine phosphates and PPi. Bottom: Comparative fluorescence of **DM 11** with different adenosine phosphates and PPi. (**DM 11** = 20 μM in 10 mM HEPES in all cases).

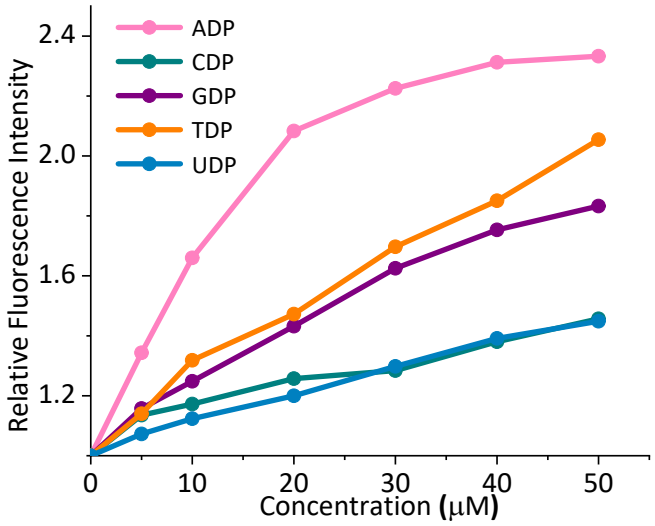


Fig. S10 Comparative fluorescence of **DM 11** with different nucleoside diphosphates. (**DM 11** = 20 μM in 10 mM HEPES in all cases).

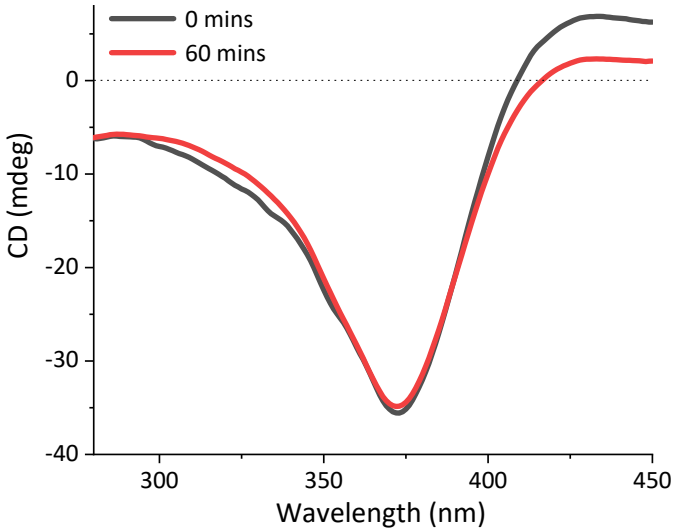


Fig. S11 CD spectra of **DM 11** (100 μM) with 25 μM of ADP at different time in 10 mM HEPES.

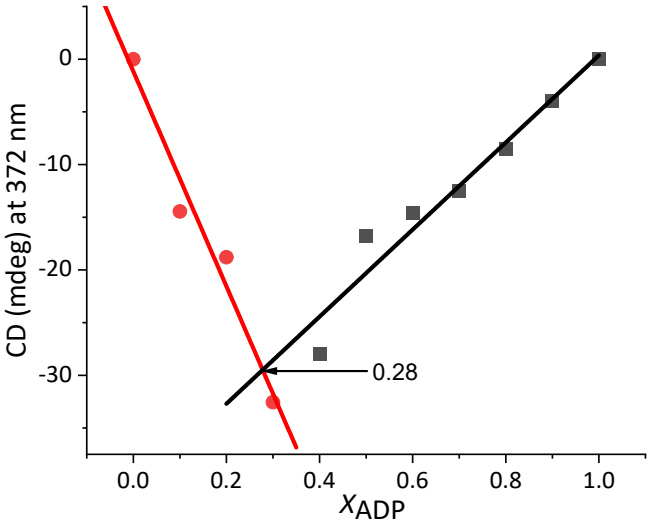


Fig. S12 Job plot of **DM 11** upon titration with ADP (Total concentration = 100 µM in 10 mM HEPES).

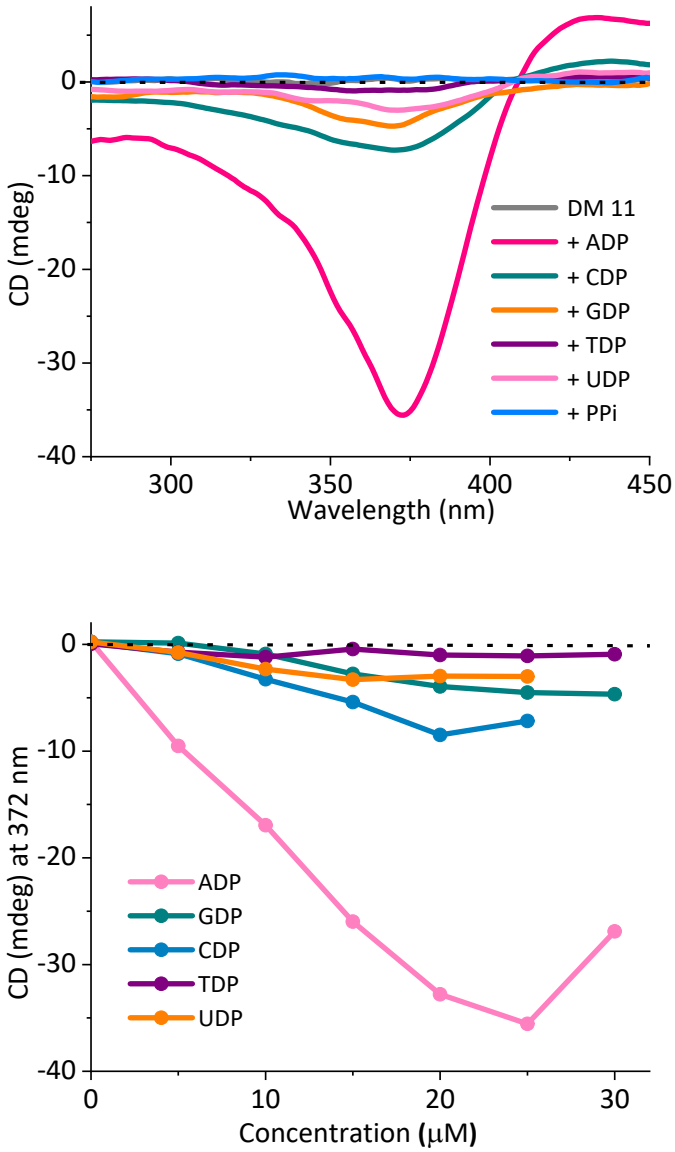


Fig. S13 Top: Changes in CD spectra of **DM 11** with 25 μM of different nucleoside diphosphates. Bottom: Plot of CD intensity at 372 nm upon titration of different nucleoside diphosphates. (**DM 11** = 100 μM in 10 mM HEPES in all cases).

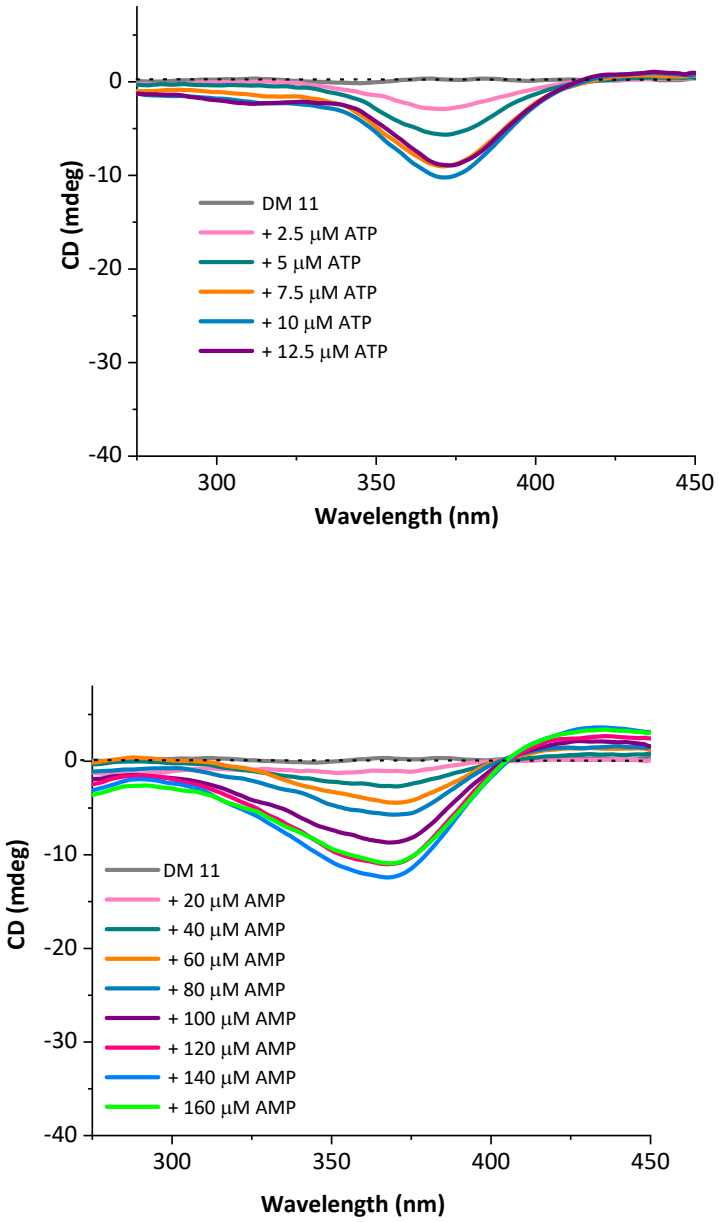
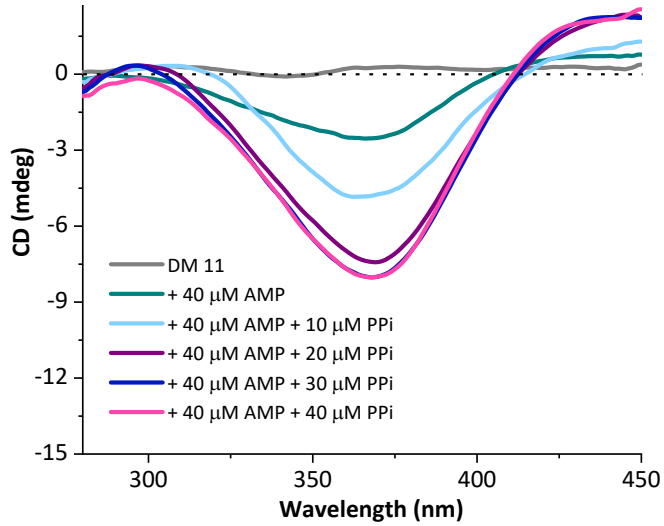


Fig. S14 Changes in CD spectra of **DM 11** with increasing concentration of ATP (top) and AMP (bottom). (**DM 11** = 100 µM in 10 mM HEPES).



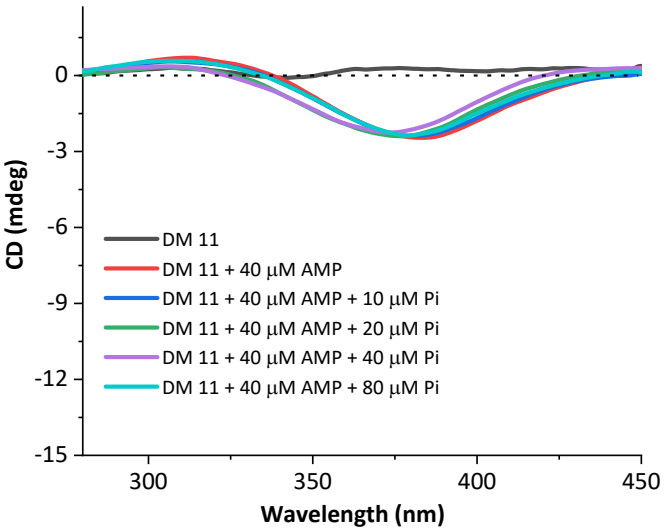


Fig. S15 Changes in CD spectra of AMP (0.4 equivalent)-**DM 11** assembly with increasing concentration of PPi (top) and Pi (bottom). (**DM 11** = 100 μM in 10 mM HEPES).

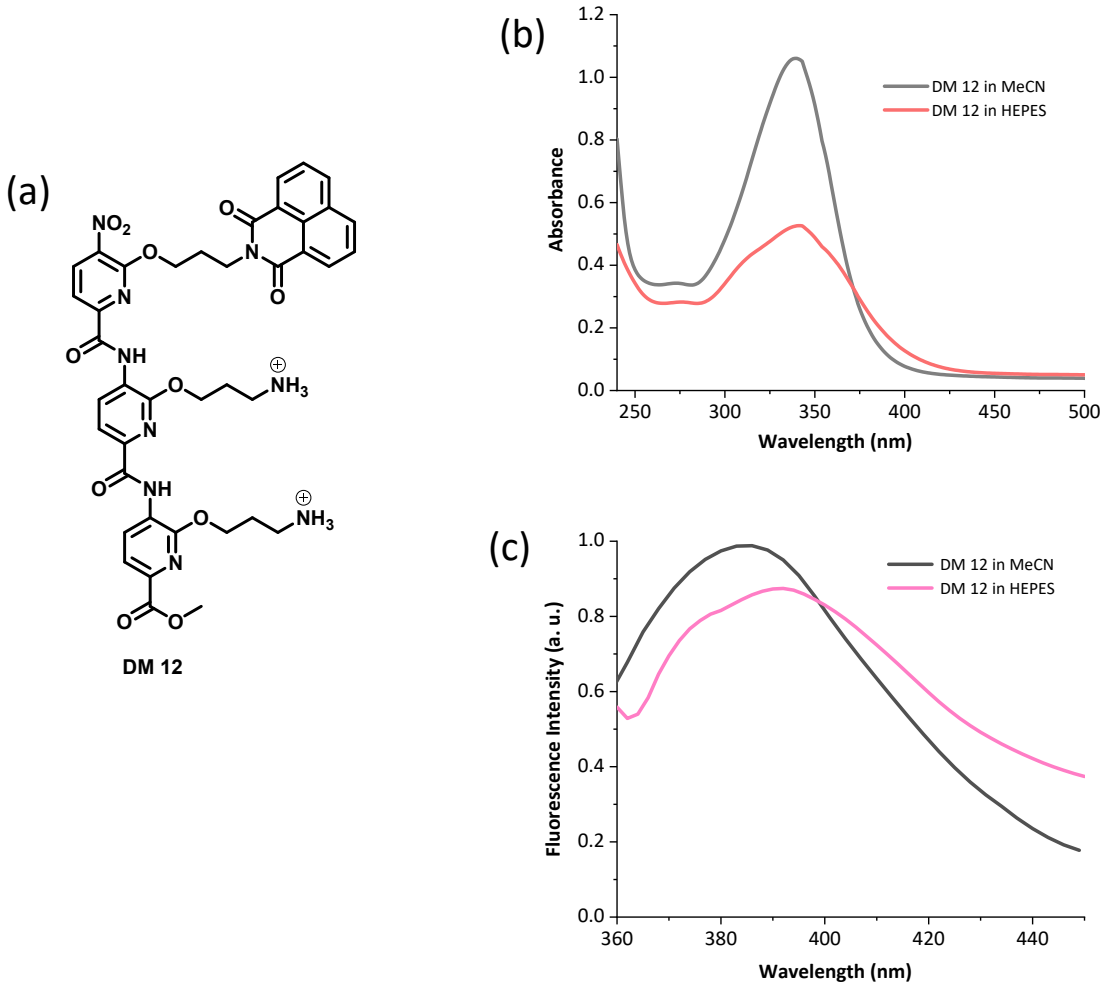


Fig. S16 (a) Chemical structure of **DM 12**; (b) UV-Vis and (c) fluorescence spectra of **DM 12** (20 μM) in different solvents.

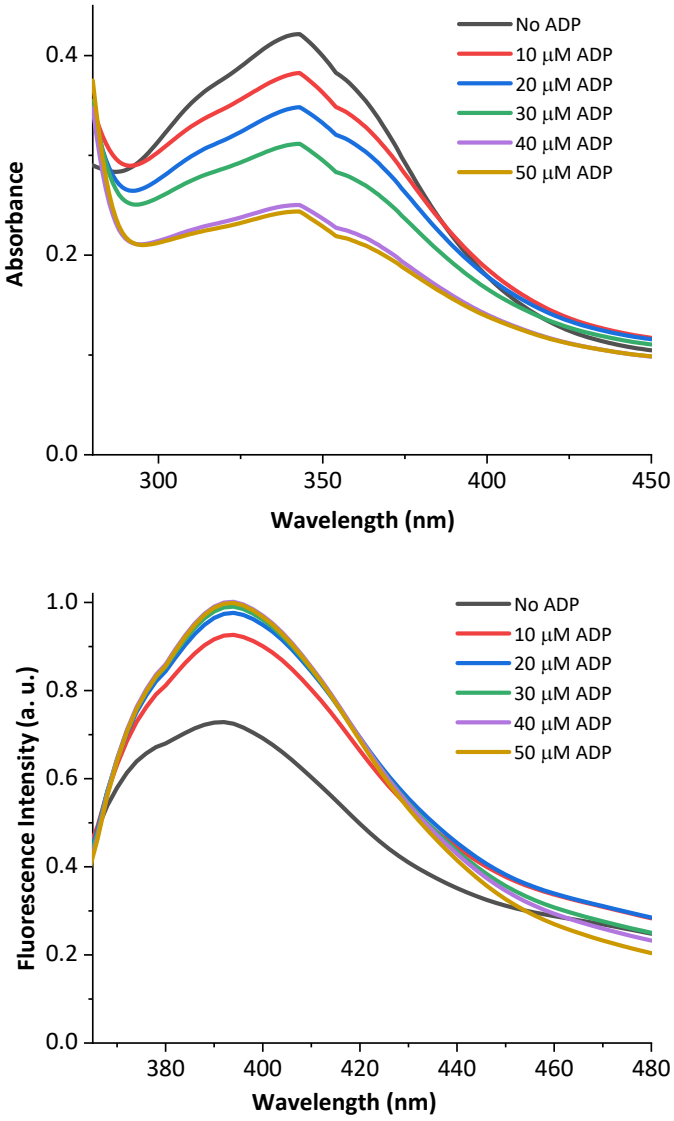


Fig. S17 Absorption (top) and fluorescence (bottom) spectra of **DM 12** with increasing concentration of ADP. (**DM 12** = 20 µM in 10 mM HEPES in all cases).

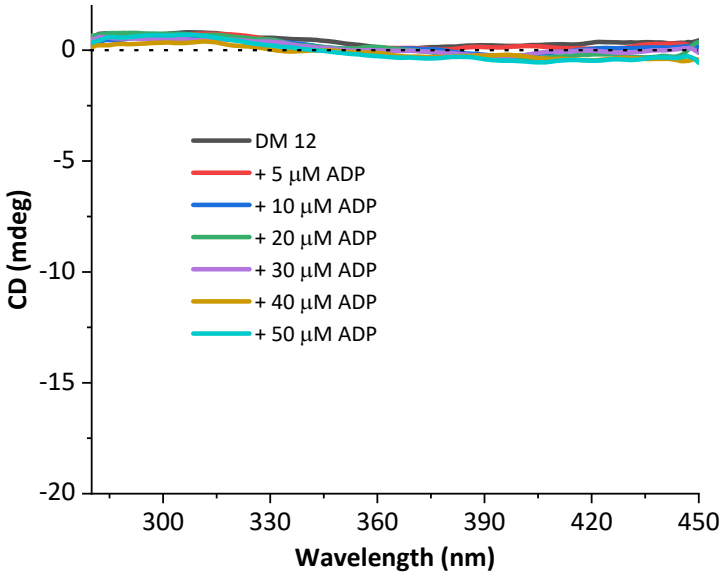


Fig. S18 Changes in CD spectra of **DM 12** with increasing concentration of ADP. (**DM 12** = 100 µM in 10 mM HEPES in all cases) .

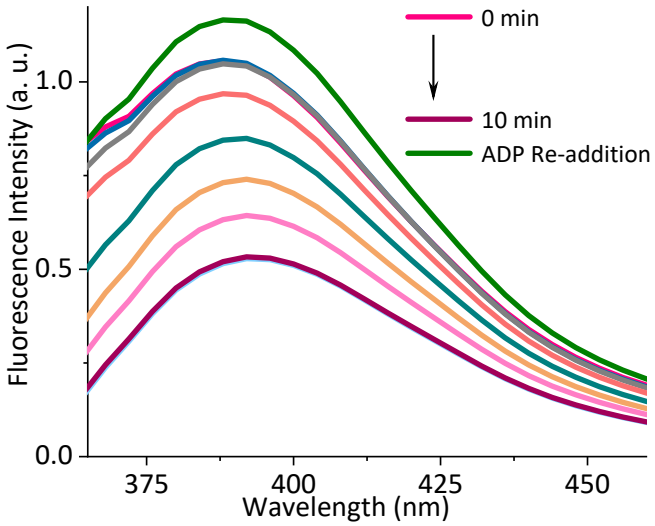


Fig. S19 Changes in fluorescence spectra over time upon ALP enzyme treatment and subsequent addition of similar amount of fresh ADP to the ADP-**DM 11** assembly. (**DM 11** = 20 µM, ADP = 50 µM, ALP = 1 U/mL)

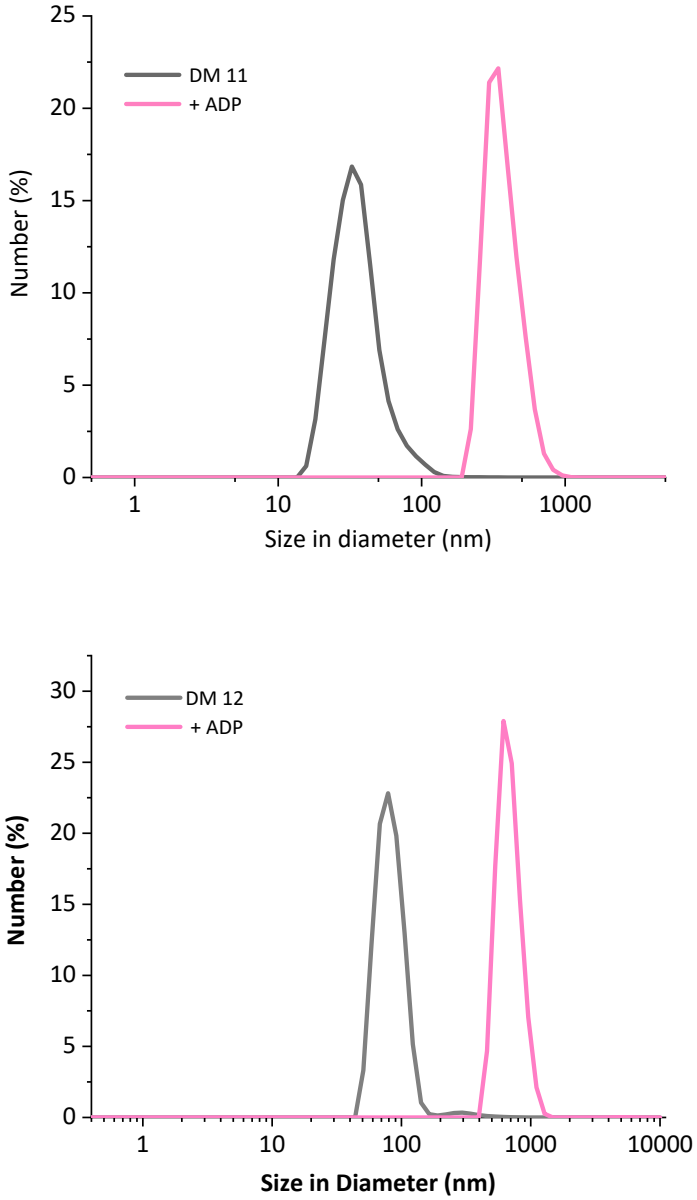


Fig. S20 Size distribution of (top) **DM 11** (20 µM) and (bottom) **DM 12** (20 µM) with ADP (20 µM) from DLS measurements in HEPES buffer.

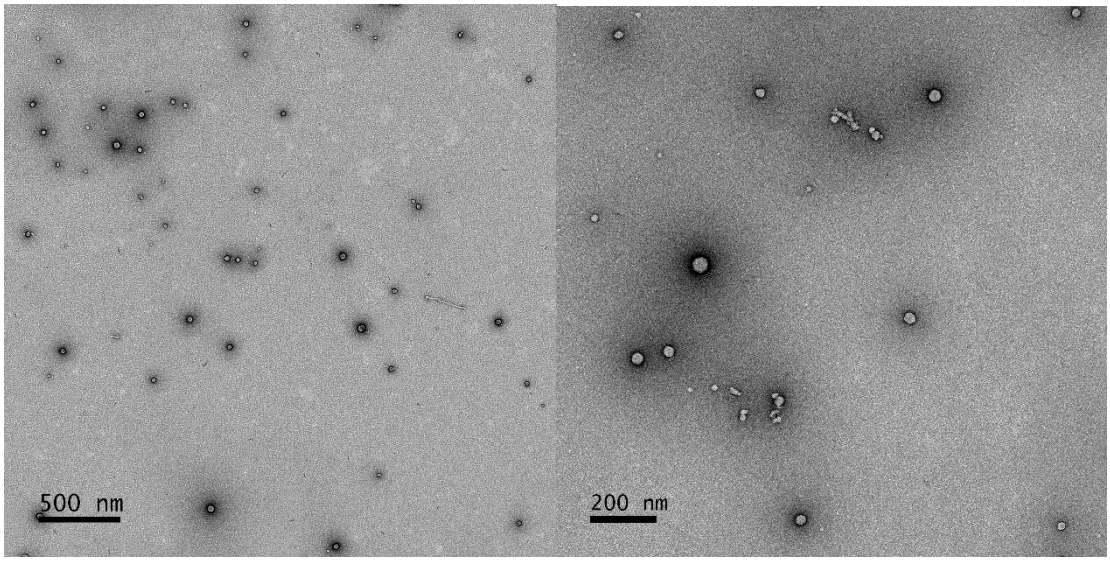


Fig. S21 TEM images of **DM 11** showed formation of spherical vesicle-like structures.

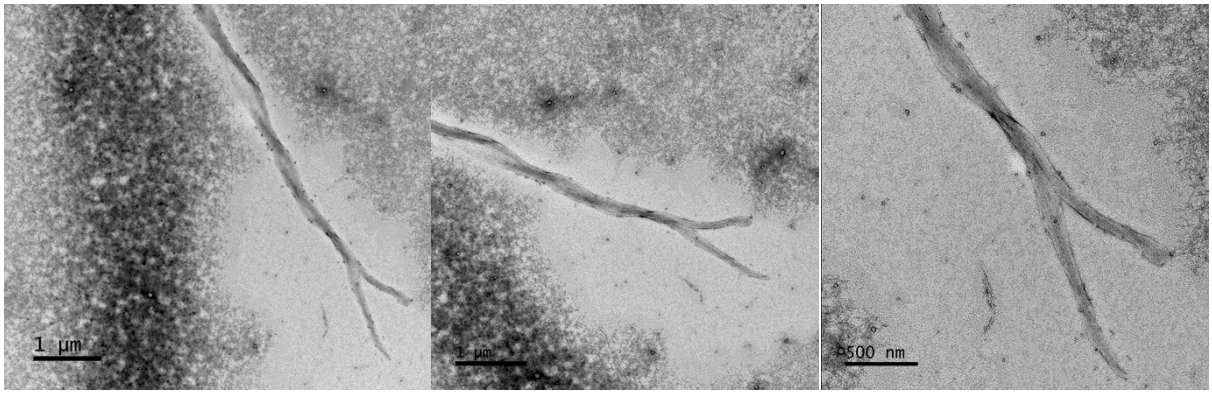


Fig. S22 TEM images of ADP-**DM 11** assembly showed formation of left-handed double helix. (**DM 11** = 100 µM, ADP = 25 µM).

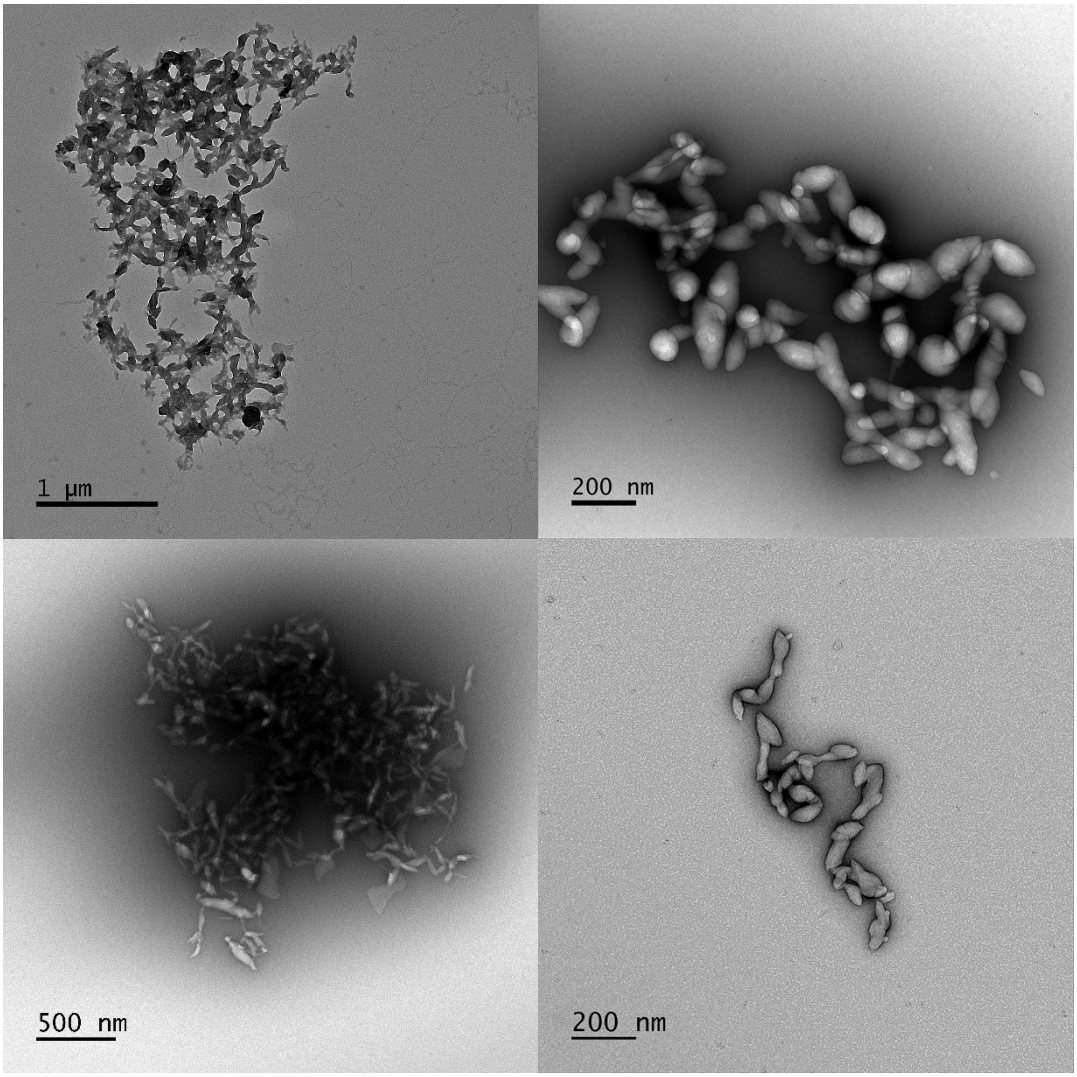


Fig. S23 TEM images of ATP-**DM 11** (top panel) and AMP-**DM 11** (bottom panel) assembly. (**DM 11** = 100 µM, ATP = 10 µM and AMP = 140 µM).

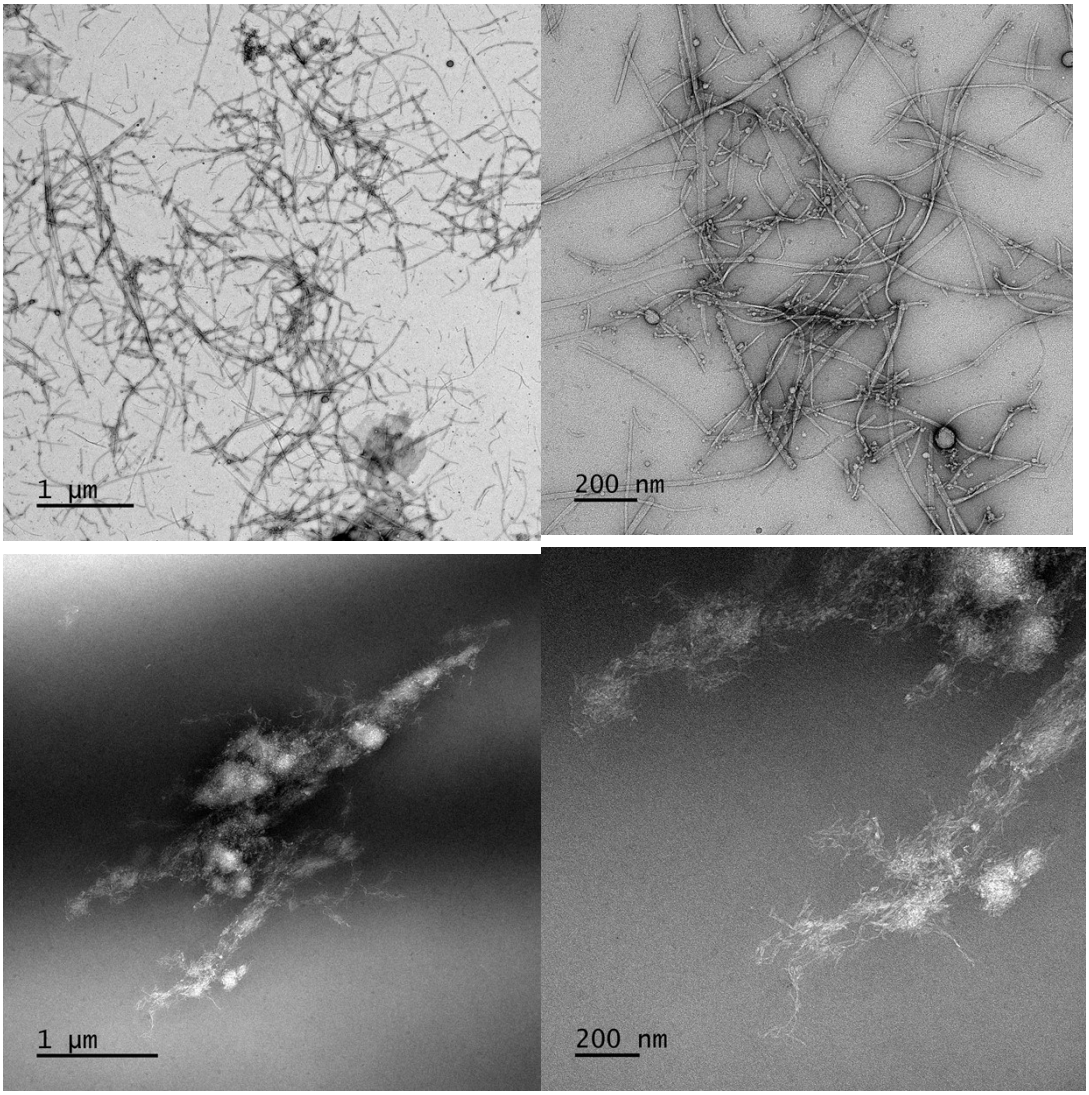
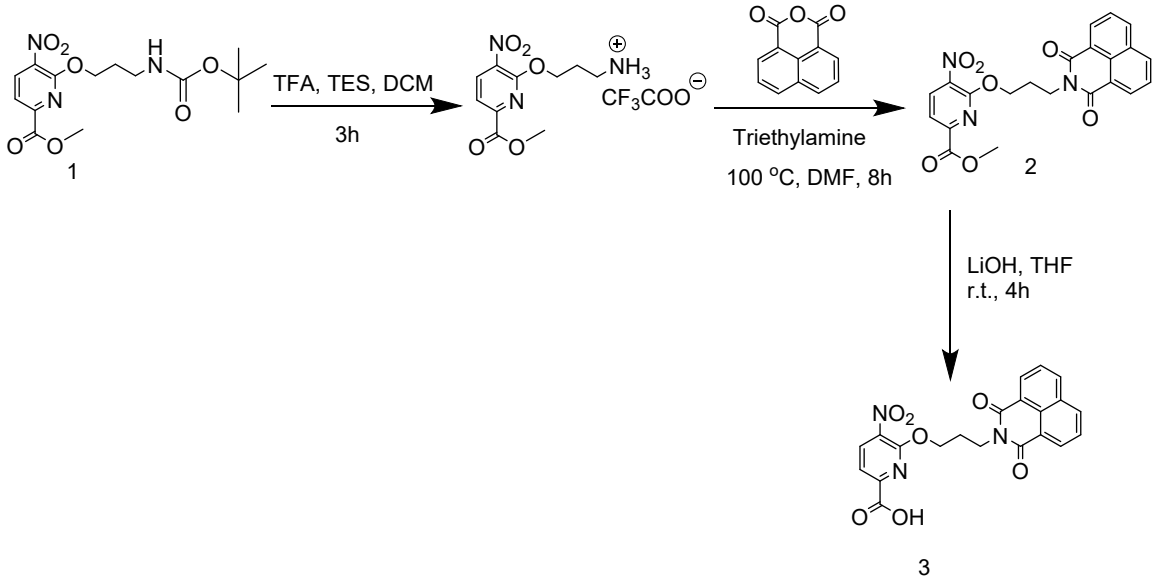


Fig. S24 TEM images of **DM 12** (Top panel) showed formation of 1-D nanoribbons. TEM images of ADP-**DM 12** assembly (bottom panel) showed formation of undefined aggegates. (**DM 12** = 100 µM, ADP = 25 µM).

Synthetic details

Synthesis of compound 3

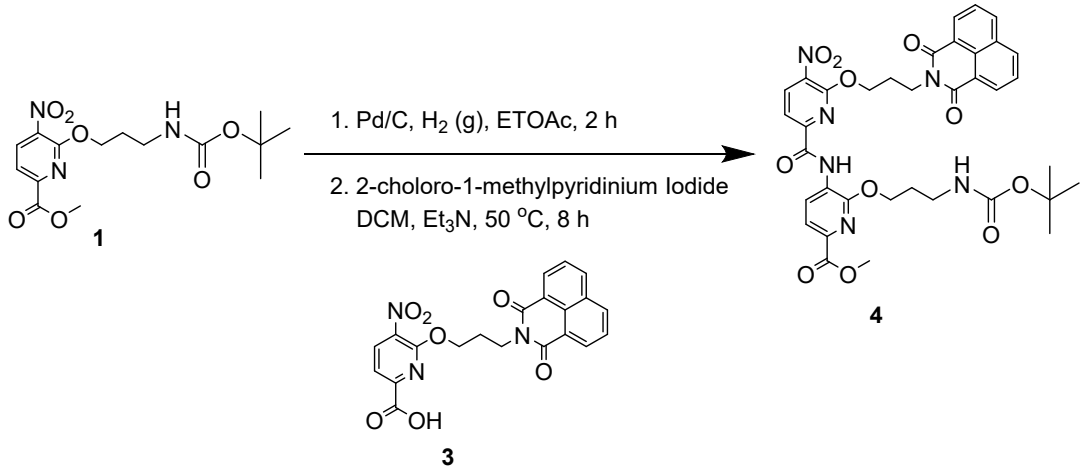


Compound 1 was synthesized according to previous protocol.[1] Compound 1 (100 mg, 0.28 mmol) was deprotected in a mixture of 5 mL dichloromethane (DCM), 250 µL triethylsilane (TES) and 500 µL trifluoroacetic acid (TFA). The reaction mixture was stirred constantly for 3 h. The reaction mixture was dried under rotovap which resulted in a thick oil. The compound was washed with cold diethyl ether (3 × 5 mL) to afford the product as a yellow solid. This product was used for next step without further purification. Deprotected product was mixed with 1,8-naphthalic anhydride (50 mg, 0.25 mmol) in 5 mL dimethylformamide (DMF) solvent. Triethylamine (87 µL, 0.63 mmol) was added to the mixture and heated for overnight at 100 ºC. Then DMF was evaporated under rotovap which resulted yellow oil. It was dissolved in 5 mL DCM and washed with brine solution (3 × 20 mL). The organic layer was dried over Na_2SO_4, filtered, and concentrated. Flash column chromatography (50 to 70% Ethylacetate in hexane, v/v) afforded the desired product 2 as yellow coloured solid (116 mg, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) 8.43-8.50 (m, 5H), 7.85 (t, *J* = 7.6 Hz, 2H), 7.76 (d, *J* = 8.0 Hz, 1H), 4.58-4.62 (t, *J* = 5.8 Hz, 2H), 4.24-4.27 (t, *J* = 6.6 Hz, 2H), 3.83 (s, 3H), 2.18-2.21 (t, *J* = 6.2 Hz, 2H) ppm. MS-ESI (*m/z*): calculated for $C_{22}H_{18}N_3O_7$ (M+H): 436.1, found 436.1.

To a solution of compound 2 (110 mg, 0.25 mmol) in 15 mL tetrahydrofuran (THF), 10 mL of 0.2 N Lithium hydroxide (LiOH) was added, and the reaction was stirred for 4 h at room temperature. The pH of the reaction solution was adjusted to 4 by adding 0.1 M HCl. The

aqueous layer was extracted with EtOAc (2×30 mL). The organic layers were combined, dried over Na_2SO_4, and concentrated on rotovap to afford the desired product 3 as yellow solid (99 mg, 94%). ^{1}H NMR (400 MHz, DMSO-d_6) 13.69 (br, 1H), 8.43-8.47 (m, 5H), 7.85 (t, *J* = 7.6 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 1H), 4.61 (t, *J* = 5.9 Hz, 2H), 4.26 (t, *J* = 6.7 Hz, 2H), 2.18 (t, *J* = 6.2 Hz, 2H) ppm. MS-ESI (*m/z*): calculated for $C_{21}H_{16}N_3O_7$ (M+H): 422.0, found 422.1.

Synthesis of compound 4

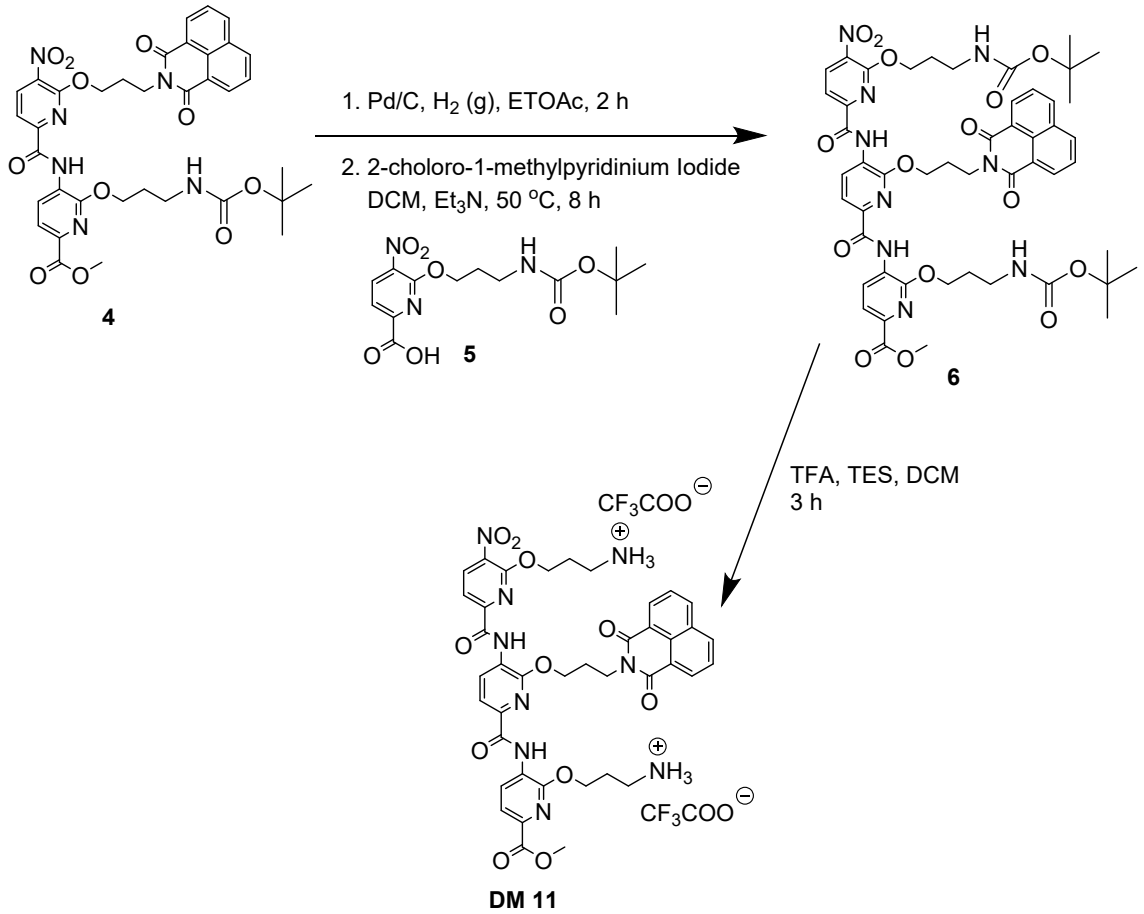


To a solution of compound 1 (100 mg, 0.32 mmol) in EtOAc (10 mL), Pd/C (10% by wt.) was added, and the reaction mixture was stirred in the atmosphere of H_2 (g) at room temperature for 2h. The progress of the reaction was monitored using TLC. The disappearance of the starting material confirms the completion of the reaction. The reaction mixture was filtered, and the filtrate was dried over rotovap to afford the desired product as a yellow solid, which is used in next step without further characterization.

In dichloromethane (10 mL, anhydrous), compound 3 (160 mg, 0.38 mmol), triethylamine (89 µL, 0.64 mmol) and 2-chloro-1-methylpyridinium iodide (97 mg, 0.38 mmol) were added and the reaction stirred for 20 min. at 60 °C. Then above reduced product in dichloromethane (10 mL, anhydrous) was added and the reaction mixture was stirred at 60 °C for 8 h in the atm. of argon. The volatiles were removed on rotovap. Column chromatography (40 to 60% ethyl acetate in hexane, v/v) afforded the desired product 4 as yellow solid (186 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) 10.13 (s, 1H), 8.76 (d, *J* = 8.0 Hz, 1H), 8.45 (dd, *J* = 6.5 Hz, 0.68 Hz, 2H), 8.31 (d, *J* = 8.0 Hz, 1H), 8.12 (d, *J* = 7.7 Hz, 2H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.65 (t, *J* = 7.6 Hz, 2H), 5.72 (t, *J* = 5.8 Hz, 1H), 4.72 (t, *J* = 5.8 Hz, 2H), 4.54 (t, *J* = 6.0 Hz, 2H), 4.40

(t, *J* = 6.7 Hz, 2H), 3.92 (s, 3H), 3.13 (br, 2H), 2.36 (t, *J* = 6.2 Hz, 2H), 1.91 (t, *J* = 5.6 Hz, 2H), 1.34 (s, 9H) ppm. MS-ESI (*m/z*): calculated for $C_{36}H_{37}N_6O_{11}$ (M+H): 729.2, found 729.3.

Synthesis of DM 11

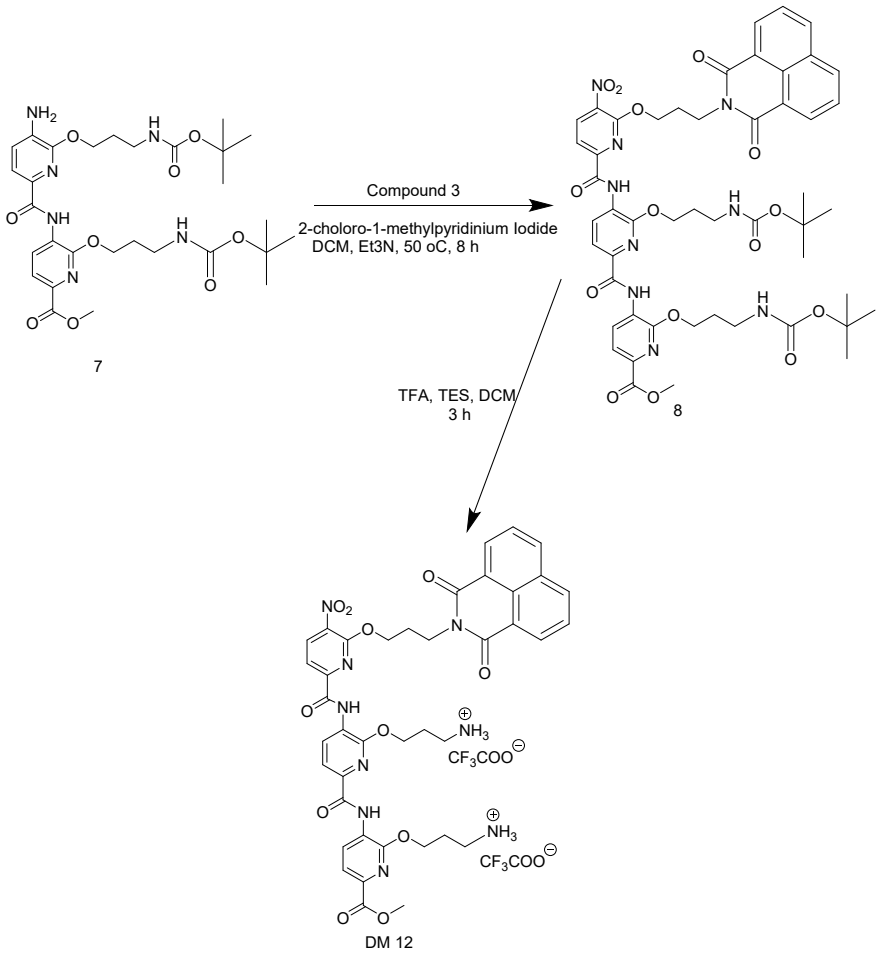


To a solution of compound 4 (100 mg, 0.14 mmol) in EtOAc (10 mL), Pd/C (10% by wt.) was added, and the reaction started with constant stirring in the atmosphere of H_2 (g) at room temperature for 2h. The progress of the reaction was monitored using TLC. The disappearance of the starting material confirms the completion of the reaction. The reaction mixture was filtered, and the filtrate was dried over rotovap to afford the desired product as a yellow solid, which is used in next step without further characterization.

Compound 5 was synthesized according to previous protocol.[1] In dichloromethane (10 mL, anhydrous), compound 5 (56 mg, 0.16 mmol), triethylamine (30 µL, 0.21 mmol) and 2-chloro-1-methylpyridinium iodide (41 mg, 0.16 mmol) were added and the reaction stirred for 20 min. at 60 °C. Then above reduced product in dichloromethane (10 mL, anhydrous) was added and the reaction mixture was stirred at 60 °C for 8 h in the atm. of argon. The volatiles were

removed on rotovap. Column chromatography (60 to 80% ethyl acetate in hexane, v/v) afforded the desired product 6 as yellow solid (100 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) 10.21 (s, 1H), 9.82 (s, 1H), 8.83 (d, *J* = 8.0 Hz, 1H), 8.68 (d, *J* = 8.0 Hz, 1H), 8.31 (t, *J* = 8.2 Hz, 3H), 8.01 (d, *J* = 7.6 Hz, 2H), 7.80 (t, *J* = 7.7 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 2H), 5.81 (s, 1H), 5.38 (s, 1H), 4.75 (t, *J* = 5.7 Hz, 2H), 4.68 (t, *J* = 5.9 Hz, 2H), 4.61 (t, *J* = 5.7 Hz, 2H), 4.41 (t, *J* = 6.3 Hz, 2H), 3.93 (s, 3H), 3.38 (m, 2H), 3.22 (m, 2H), 2.37 (t, *J* = 6.0 Hz, 2H), 2.01-2.09 (m, 4H), 1.36 (s, 9H), 1.33 (s, 9H) ppm. MS-ESI (*m/z*): calculated for $C_{50}H_{56}N_9O_{15}$ (M+H): 1022.3, found 1022.4.

Then the product 6 was subjected to deprotection by stirring in 10 mL of DCM:TFA:TES (80:15:5, v/v) cocktail for 3h. The reaction mixture was dried under rotovap which resulted in oily product. The compound was washed with cold diethyl ether (3 × 5 mL) to afford the pure product DM 11 as yellow solid (101 mg, 99%). HRMS (m/z): calculated for $C_{40}H_{40}N_9O_{11}$ $(M + H)^+$: 822.2842, found 822.2826. ^{1}H NMR (400 MHz, DMSO-d_6) 10.17 (s, 1H), 9.61 (s, 1H), 8.78 (d, *J* = 8.0 Hz, 1H), 8.59 (dd, *J* = 5.2 Hz, 2.8 Hz, 2H), 8.18 (d, *J* = 8.0 Hz, 2H), 8.14 (d, *J* = 7.1 Hz, 2H), 7.80-7.87 (m, 8H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 2H), 4.77 (t, *J* = 4.8 Hz, 2H), 4.53-4.58 (dd, *J* = 7.3 Hz, 6.5 Hz, 4H), 4.37 (t, *J* = 5.4 Hz, 2H), 3.89 (s, 3H), 3.10 (m, 4H), 2.38 (t, *J* = 5.2 Hz, 2H), 2.17-2.20 (m, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) 164.8, 164.1, 162.0, 159.6, 154.1, 152.4, 151.7, 148. 2, 139.5, 138.0, 137.9, 136.4, 134.8, 131.2, 130.7, 127.3, 127.2, 126.3, 126.0, 125.5, 125.4, 122.0, 120.8, 117.3, 116.1, 66.7, 65.4, 64.1, 52.7, 38.7, 36.9, 36.2, 27.4, 27.2, 26.7 ppm.

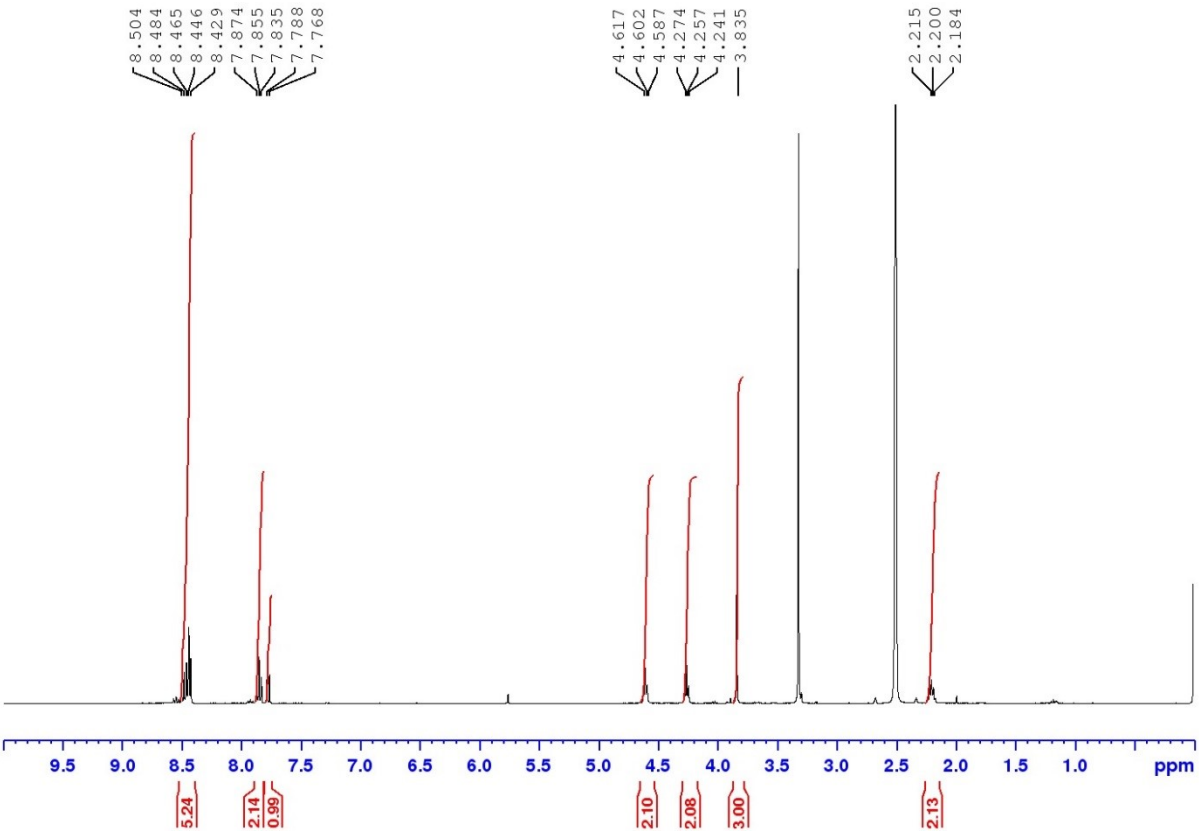


Synthesis of compound 12

In dichloromethane (10 mL, anhydrous), compound 3 (50 mg, 0.12 mmol), triethylamine (28 µL, 0.2 mmol) and 2-chloro-1-methylpyridinium iodide (31 mg, 0.12 mmol) were added and the reaction stirred for 20 min. at 60 °C. Then compound 7[1] (62 mg, 0.10 mmol) in dichloromethane (10 mL, anhydrous) was added and the reaction mixture was stirred at 60 °C for 8 h in the atm. of argon. The volatiles were removed on rotovap. Column chromatography (60 to 80% ethyl acetate in hexane, v/v) afforded the desired product 8 as yellow solid (75 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) 10.27 (s, 1H), 10.16 (s, 1H), 8.90-8.95 (dd, *J* = 8.1 Hz, 5.7 Hz, 2H), 8.54 (d, *J* = 7.1 Hz, 2H), 8.38 (t, *J* = 7.9 Hz, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.97 (t, *J* = 7.5 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 2H), 5.76 (s, 1H), 5.50 (s, 1H), 4.81 (m, 2H), 4.69 (m, 2H), 4.47-4.55 (m, 4H), 3.98 (s, 3H), 3.38 (m, 2H), 3.27 (m, 2H), 2.45 (t, *J* = 5.7 Hz, 2H), 2.06-2.16 (m, 4H), 1.45 (s, 9H), 1.32 (s, 9H) ppm. MS-ESI (*m/z*): calculated for $C_{50}H_{56}N_9O_{15}$ (M+H): 1022.3, found 1022.3.

Then the product 8 was subjected to deprotection by stirring in 10 mL of DCM:TFA:TES (80:15:5, v/v) cocktail for 3h. The reaction mixture was dried under rotovap which resulted in oily product. The compound was washed with cold diethyl ether (3 × 5 mL) to afford the pure product DM 12 as yellow solid (76 mg, 99%). HRMS (m/z): calculated for $C_{40}H_{40}N_9O_{11}$ $(M + H)^+$: 822.2842, found 822.2853. ^{1}H NMR (400 MHz, DMSO-d_6) 10.15 (s, 1H), 10.03 (s, 1H), 8.79 (d, *J* = 7.8 Hz, 1H), 8.74 (d, *J* = 7.9 Hz, 1H), 8.57 (d, *J* = 7.6 Hz, 1H), 8.38 (t, *J* = 7.1 Hz, 4H), 7.94 (br, 6H), 7.78-7.87 (m, 5H), 4.78 (m, 2H), 4.49-4.59 (m, 4H), 4.33 (m, 2H), 3.86 (s, 3H), 3.07 (m, 4H), 2.35 (m, 2H), 2.15-2.17 (m, 4H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) 164.8, 164.1, 162.1, 160.6, 154.7, 152.6, 151.9, 148.9, 139.9, 138.1, 138.0, 136.4, 134.7, 131.7, 131.0, 127.8, 127.5, 126.1, 125.9, 125.7, 122.4, 120.8, 117.7, 116.2, 66.2, 64.1, 64.0, 52.8, 37.7, 36.3, 36.2, 27.2, 26.9 ppm.

^{1}H NMR spectra compound 2 (top) and compound 3 (bottom).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8.446
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7.835
7.788
7.768
4.617
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4.274
4.257
4.241
3.835
2.215
2.200
2.184
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
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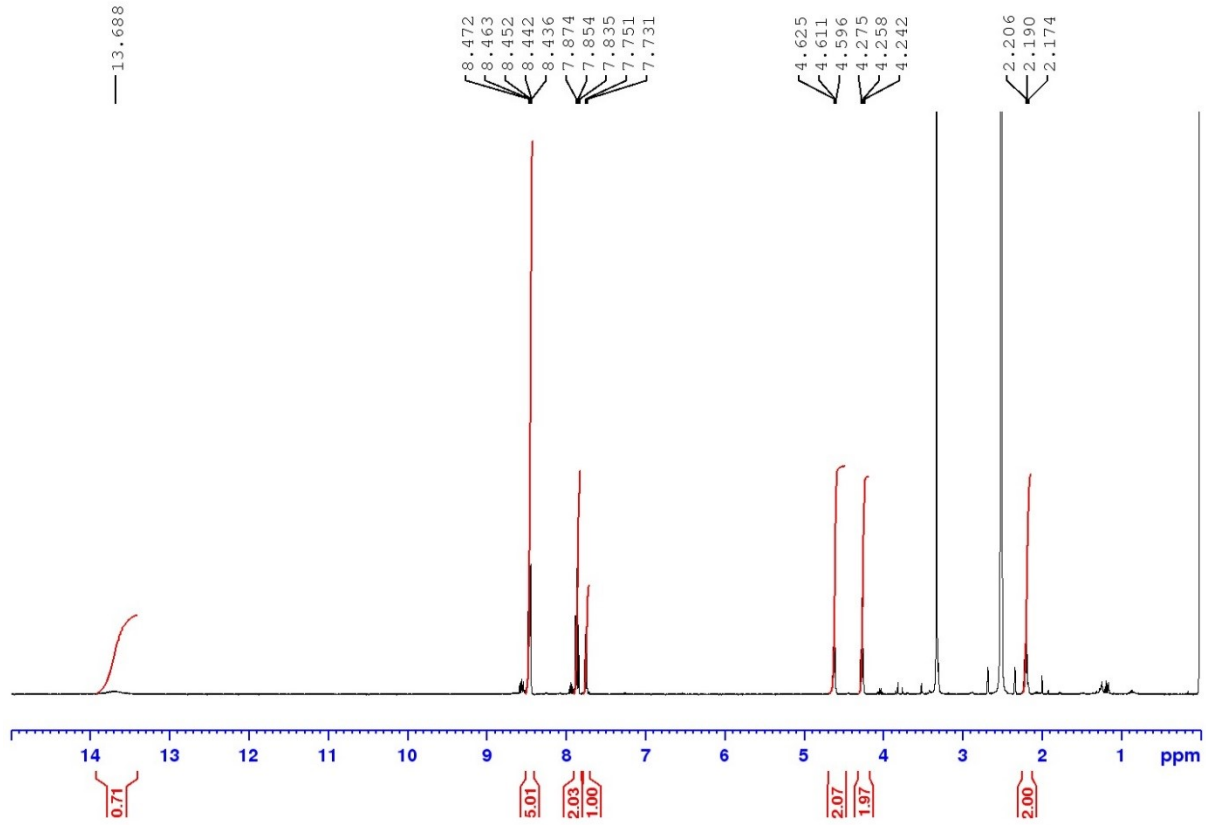
0.99
2.10
2.08
3.00
2.13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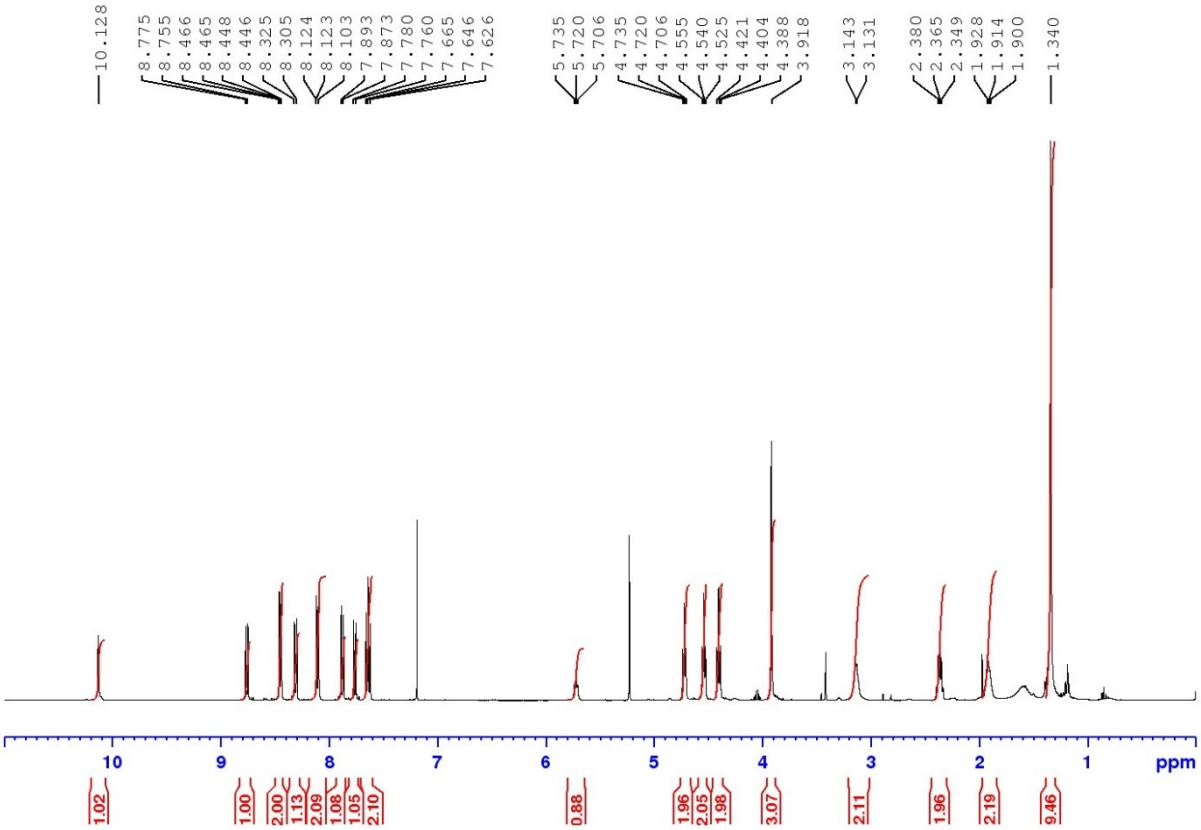
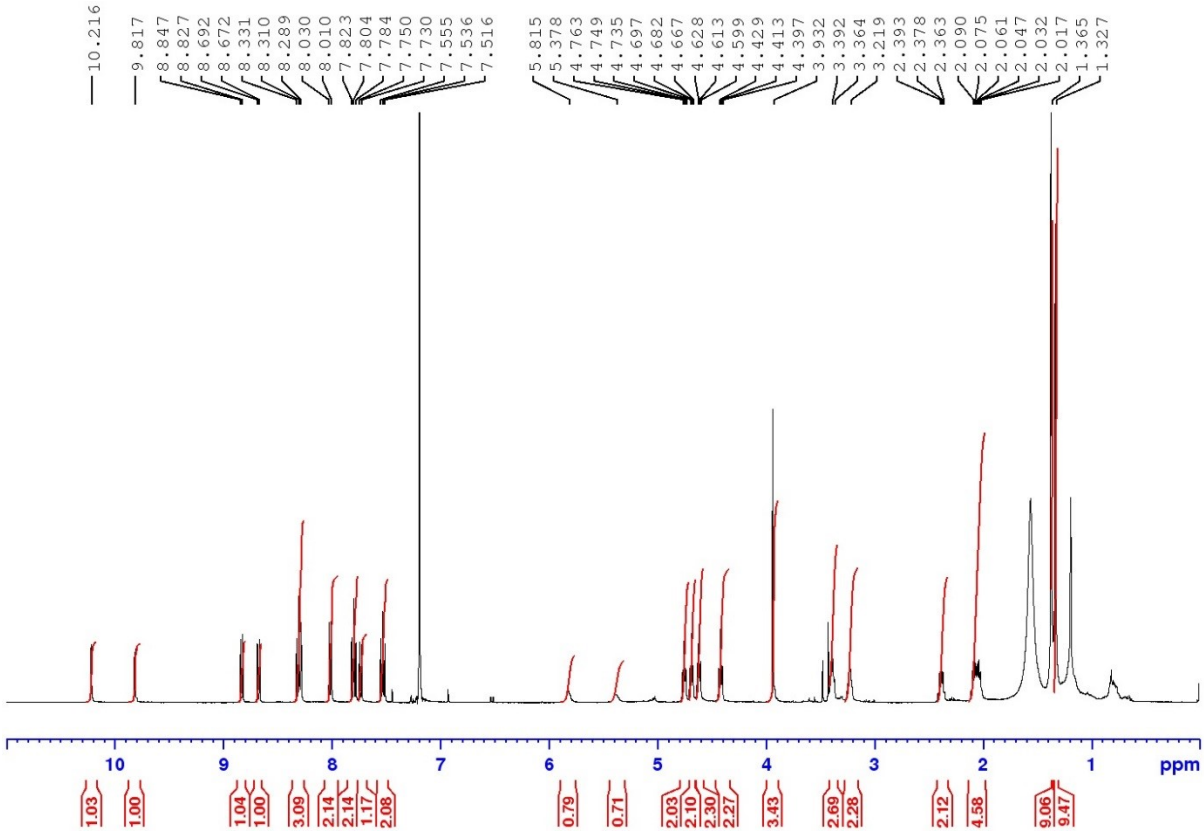
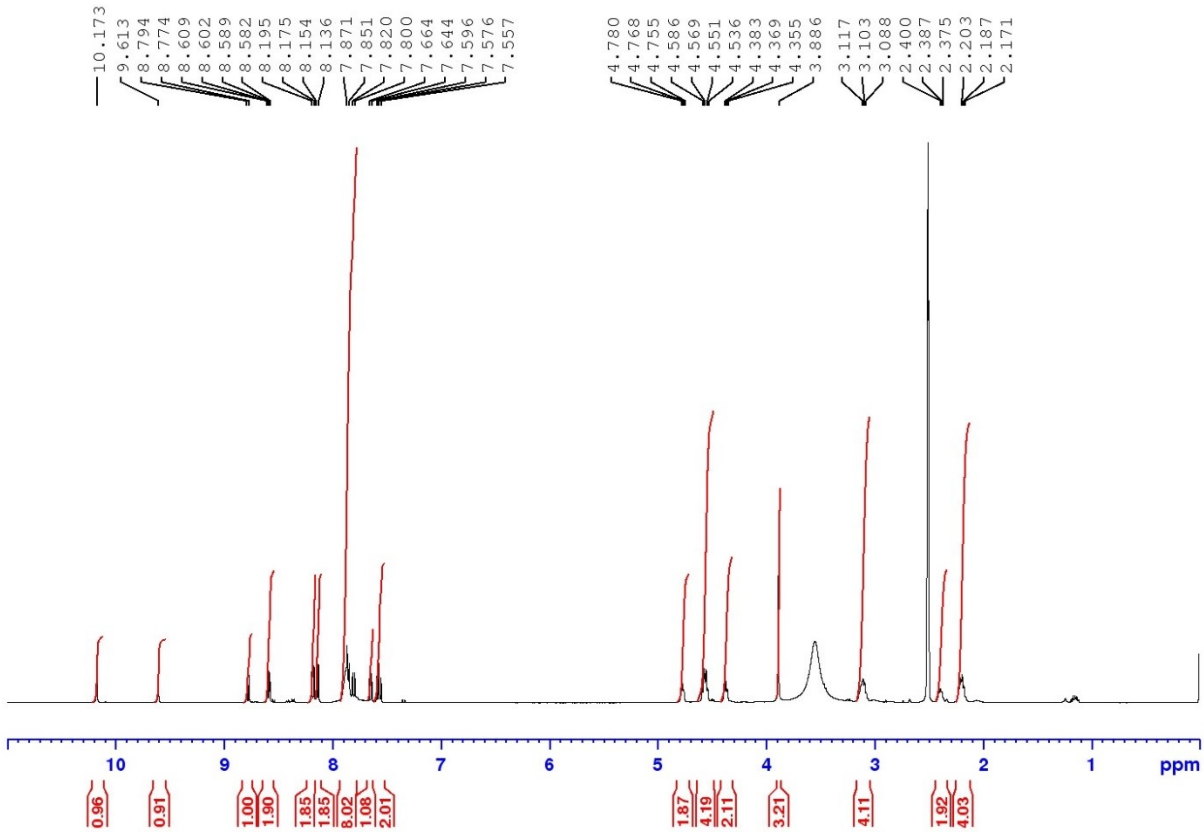
8.452
8.442
8.436
7.874
7.854
7.835
7.751
7.731
4.625
4.611
4.596
4.275
4.258
4.242
2.206
2.190
2.174
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
0.71
5.01
2.03
1.00
2.07
1.97
2.00

^{1}H NMR spectra compound 4 (top) and compound 6 (bottom).





^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of compound DM 11.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8.609
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8.582
8.195
8.175
8.154
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7.851
7.820
7.800
7.664
7.644
7.596
7.576
7.557
4.780
4.768
4.755
4.586
4.569
4.551
4.536
4.383
4.369
4.355
3.886
3.117
3.103
3.088
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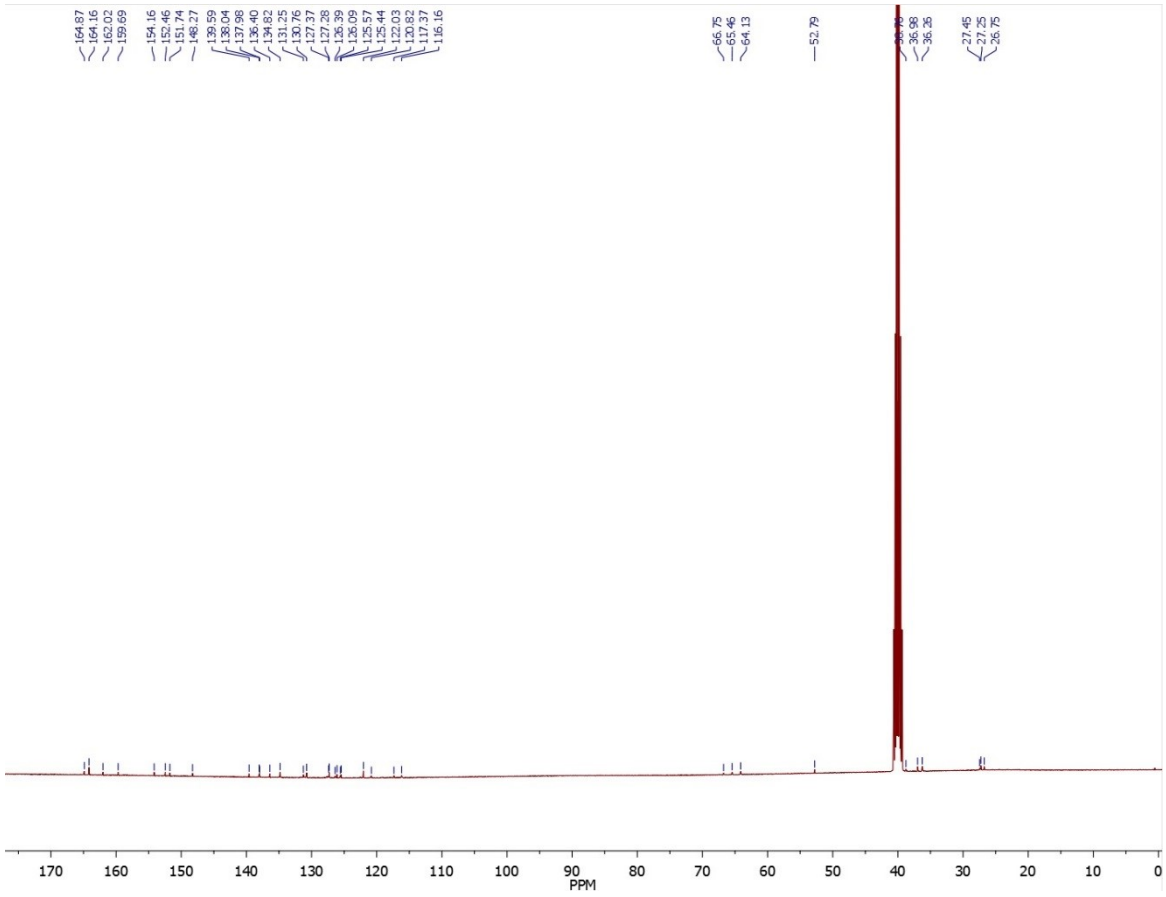
2.375
2.203
2.187
2.171
10
9
8
7
6
5
4
3
2
1
ppm
0.96
0.91
1.00
1.90
1.85
1.85
8.02
1.08
2.01
1.87
4.19
2.11
3.21
4.11
1.92
4.03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164.16
162.02
159.69
154.16
152.46
151.74
148.27
139.59
138.04
137.98
136.40
134.82
131.25
130.76
127.37
127.28
126.39
126.09
125.57
125.44
122.03
120.82
117.37
116.16
66.75
65.46
64.13
52.79
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36.26
27.45
27.25
26.75
170
160
150
140
130
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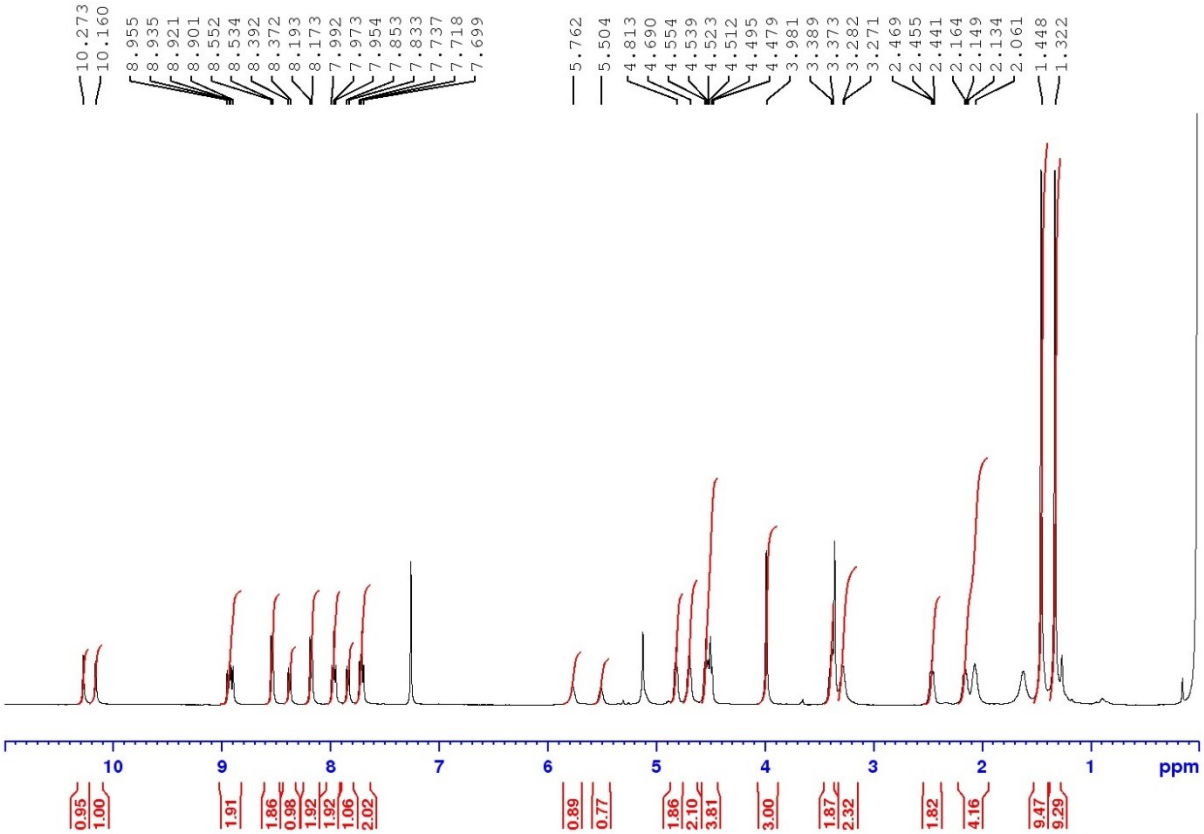
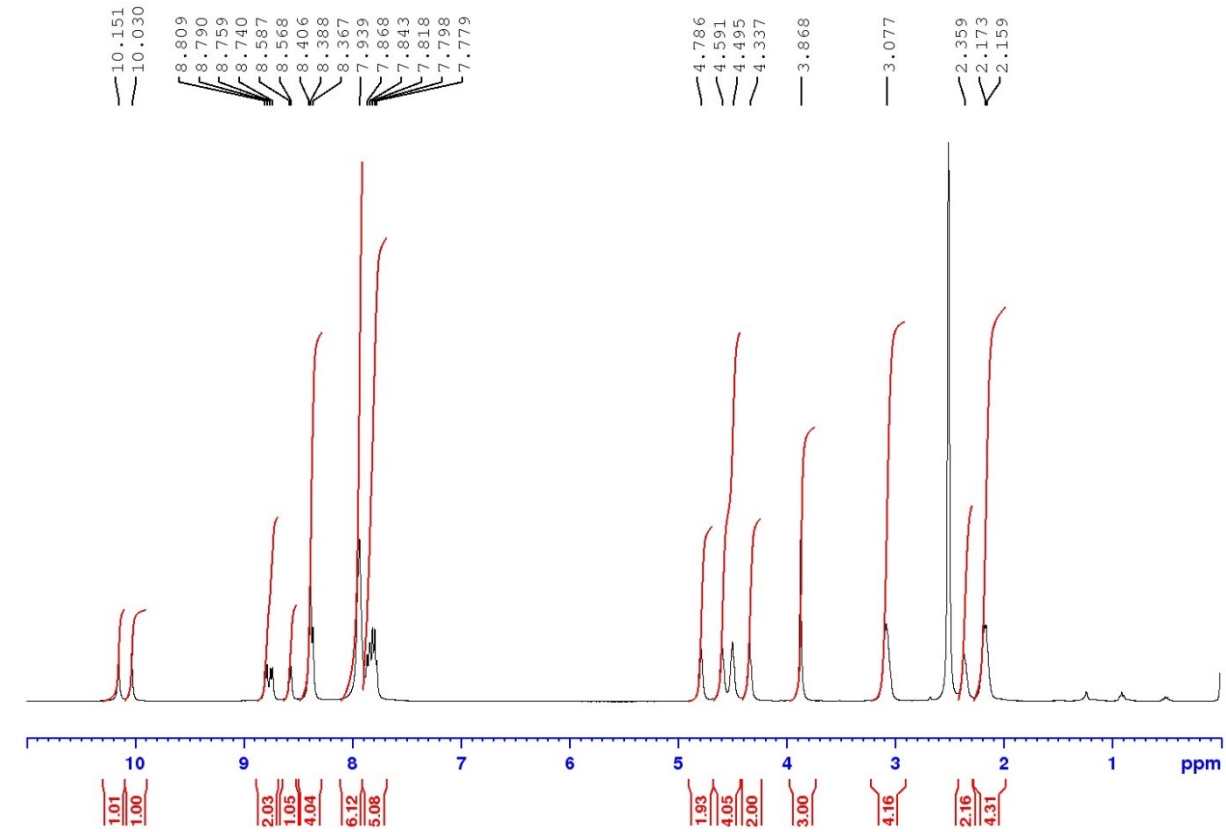
110
100
90
80
70
60
50
40
30
20
10
0
PPM

^{1}H NMR spectra compound 8



^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of compound DM 12.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8.759
8.740
8.587
8.568
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7.843
7.818
7.798
7.779
4.786
4.591
4.495
4.337
3.868
3.077
2.359
2.173
2.159
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.00
2.03
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4.04
6.12
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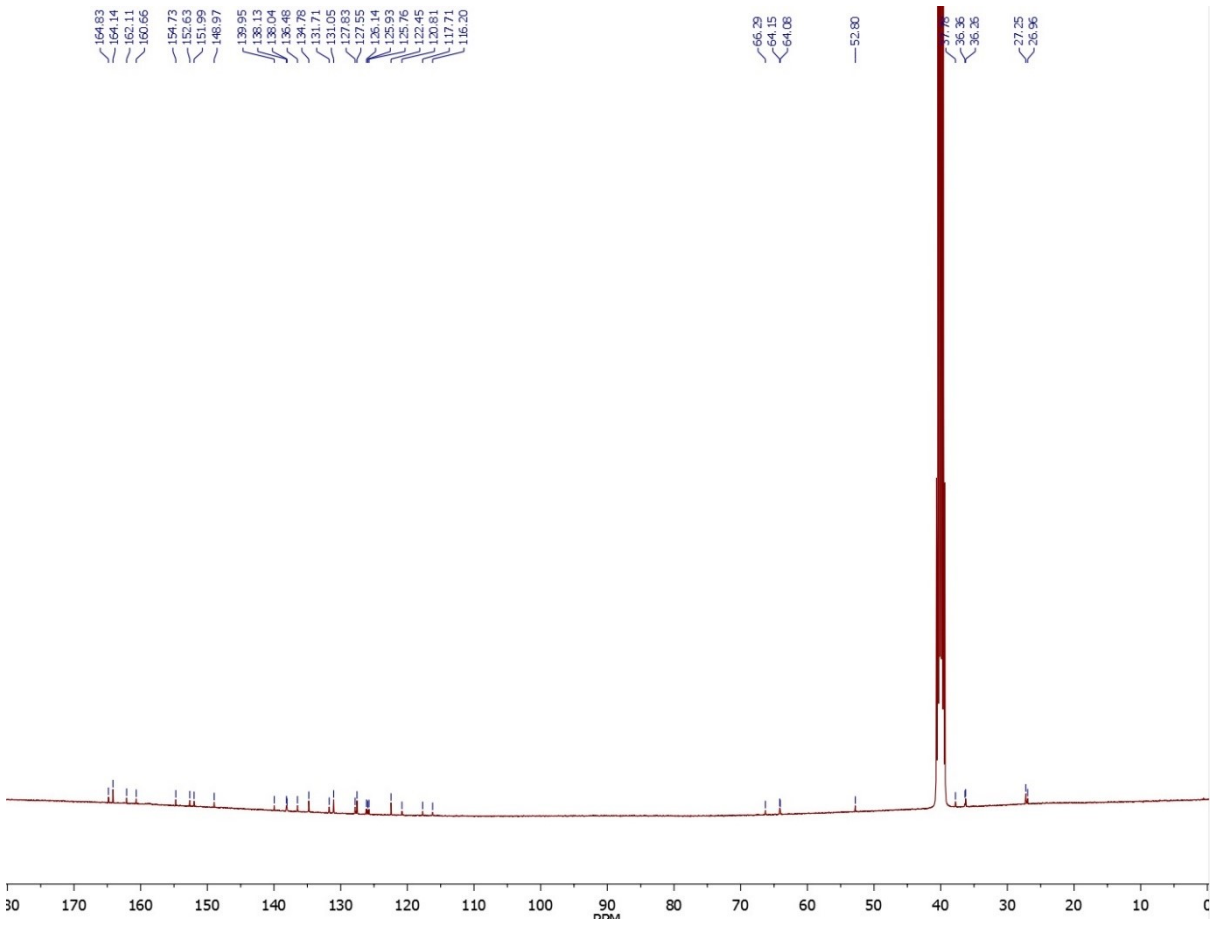
4.05
2.00
3.00
4.16
2.16
4.31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160.66
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152.63
151.99
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139.95
138.13
138.04
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131.71
131.05
127.83
127.55
126.14
125.93
125.76
122.45
120.61
117.71
116.20
66.29
64.15
64.08
52.80
37.78
36.36
36.26
27.25
26.96
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

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1. Kumar, S.; Hamilton, A. D., α-Helix Mimetics as Modulators of Aβ Self-Assembly. *Journal of the American Chemical Society* **2017,** *139* (16), 5744-5755.