

Supplementary Information

Orange Red Emitting Naphthalene Diimide Derivative Containing Dendritic Wedges: Aggregation

Induced Emission (AIE) and Detection of Picric acid (PA) in Aqueous Medium

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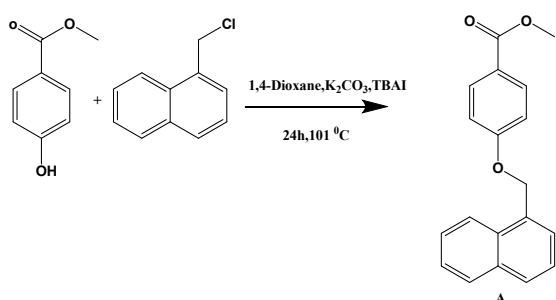
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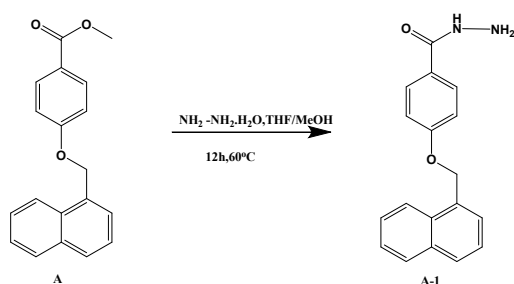
Synthesis of compound **A**



Scheme. S1 Synthetic scheme for compound **A**.

Methyl-4-dihydroxybenzoate (2 g, 0.014 mole), potassium carbonate (3.86 g, 0.027 mole) and 40 mL 1,4-dioxane were taken in a 250 mL round bottom flask. 1-chloro methyl naphthalene (3.7 g, 0.02 mole) was added followed by the addition of a catalytic amount of tertiary butyl ammonium iodide (0.48 g, 0.0013 mole). The solution mixture was refluxed for 24 hours. Solvent was evaporated and extracted with ethyl acetate water mixture. The organic layer was dried over anhydrous Na_2SO_4 . The solid was then crystallized from methanol to get compound **A** (3.9 g, 91 %); ^1H NMR (500 MHz, CDCl_3) δ : 3.9 (s, 3H), 5.55 (s, 2H), 7.06 (t, 2H), 7.44-7.6 (m, 4H), 7.62 (m, 2H), 8.02 (d, 3H). ^{13}C NMR (100 MHz, CDCl_3): δ 52.07, 68.9, 114.7, 123.16, 125.4, 126.21, 126.80, 126.78, 126.88, 128.97, 129.46, 131.85, 133.99, 162.74, 167.01. IR (KBr) ν = 1925, 1874, 1787, 1701, 1650, 1629, 1535, 1513, 1477, 1383, and 1318 cm^{-1} .

Synthesis of compound **A-1**

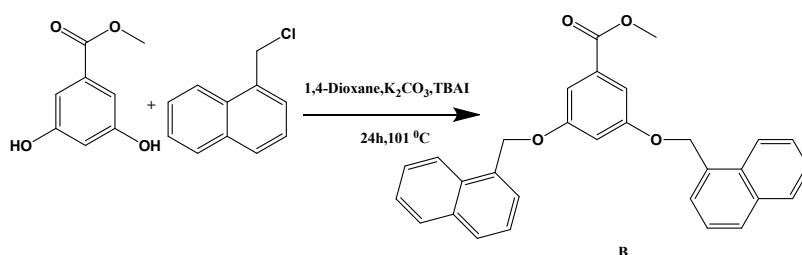


Scheme .S2 Synthetic scheme for compound **A-1**.

Compound **A** (2.5g, 0.008 mole) and hydrazine monohydrate (19.40 mL, 0.4 mole) were dissolved in MeOH (30 mL) and THF (15 mL). The reaction mixture was stirred at 60 °C for 12 hours. After the reaction mixture was cooled to room

temperature, solvent was evaporated by applying vacuum. The residue was dissolved in DCM and washed many times with water to remove excess of hydrazine mono hydrate. The organic layer was then dried over anhydrous Na_2SO_4 . Crude product was purified by column chromatography ethyl acetate /Hexane (3:7)mixture as eluent. (2.2 g, 88%); $^1\text{H NMR}$ (500 MHz, CDCl_3) : δ 3.37 (s,2H), 5.49(s,2H),7.03(s,2H),7.43-7.59(m,4H) ,7.73(d,2H), 7.87(m,2H), 7.89(d,1H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3) : δ 68.80, 114.91, 123.51, 125.31, 126.04, 126.61, 126.70, 128.77, 129.29, 131.43, 131.58, 133.81, 161.73, 168.30.IR(KBr) ν =3209, 3050, 2920, 2476,1790, 1761, 1718, 1682, 1610, 1581, 1538,1509,1451,1386 and 1314 cm^{-1} . ESI-MS : m/z Calcd for $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2$:292.33, found: 293[M+H] $^+$.

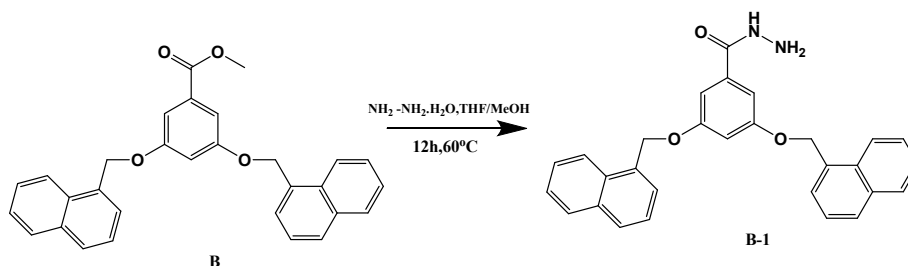
Synthesis of compound B



Scheme.S2 Synthetic scheme for compound B.

Methyl-3, 5-dihydroxybenzoate (2 g, 0.0118 mole) , potassium carbonate (4.8 g, 0.035 mole) and 40 mL of 1,4-dioxane were taken in 250 mL round bottom flask. 1-chloro methyl naphthalene (5.25 g, 0.0297 mole) was added followed by the addition of a catalytic amount of tertiary butyl ammonium iodide (0.5 g, 0.0013 mole). The solution mixture was refluxed for 24 hours. Solvent was evaporated and extracted with ethyl acetate water mixture . The organic layer was dried over anhydrous Na_2SO_4 . The solid was crystallized from methanol to get **B** (4.8,86 %); $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 3.86 (s, 3H), 5.43 (s, 4H), 7.87 (d, 1H), 7.37-7.54 (m ,10H),7.82 (m,4H),7.97(s,2H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 52.34,69.04,107.43,108.63,123.71,125.35,126.02,126.59,126.80,128.77,129.25,131.59,131.88,132.29,133.85,160.0,166.85.IR(KBr) ν = 3138, 2490, 1719, 1513, 1433, 1367, 1315, 1263, 1155 and 1042 cm^{-1} . ESI-MS: m/z Calcd for $\text{C}_{30}\text{H}_{24}\text{O}_4$:448.51, found: 471[M +Na] $^+$.

Synthesis of compound B-1

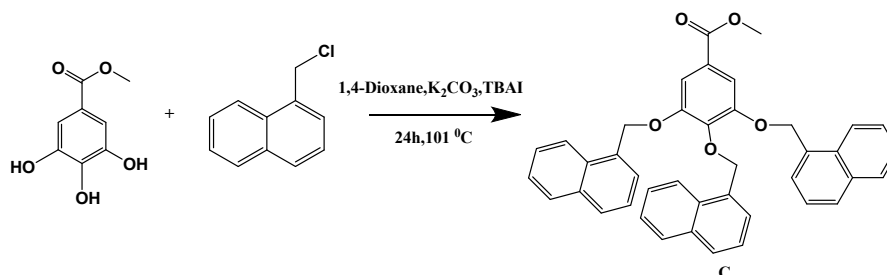


Scheme.S3 Synthetic scheme for compound B-1.

Compound **B** (2 g, 0.0044 mole) and hydrazine monohydrate (10.8 mL, 0.22 mole) were dissolved in MeOH (30 mL) and THF (15 mL). The reaction mixture was stirred at 60°C for 12 hours. After the reaction mixture was cooled to room temperature, solvent was evaporated by applying vacuum. The residue was dissolved in DCM and washed many times with

water to remove excess of hydrazine mono hydrate. The organic layer was then dried over anhydrous Na_2SO_4 . Crude product was purified by column chromatography ethyl acetate /Hexane (3:7) mixture as eluent. (1.8 g, 90%); $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 4.04 (s,2H), 5.34(s,4H), 6.85(t,1H), 7.08(d,2H),7.42(t,2H), 7.49-7.53(m,6H),7.57(s,2H),7.81-7.87 (m,2H), 7.96 (d,2H). $^{13}\text{C NMR}$ (100 MHz, CDCl_3): δ 69.02,105.7, 106.19,123.62, 125.32 ,126.0, 126.6, 126.7, 128.7, 129.2, 131.51, 133.82, 134.9,137.1,160.26,168.42.IR(KBr) ν = 3345, 3131, 2490, 1825, 1767, 1686, 1628, 1554, 1458, 1379 and 1281 cm^{-1} . ESI-MS : m/z Calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{O}_3$:448.51, found: 471[M+Na] $^+$.

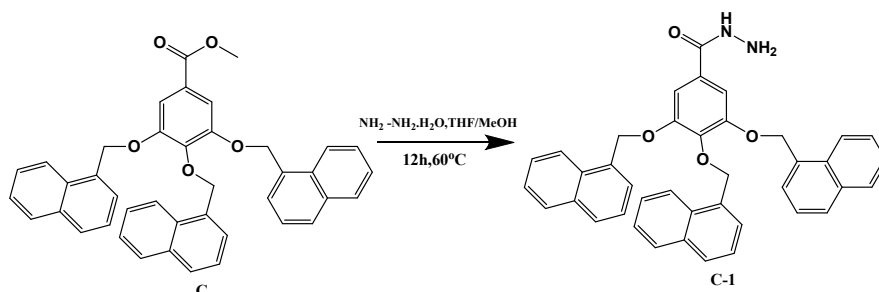
Synthesis of compound C



Scheme. S4 Synthetic scheme for compound C.

Methyl-3,4, 5-dihydroxybenzoate (3 g, 0.016 mole) ,potassium carbonate (13.5g, 0.097mole) and 100 mL of 1,4-dioxane were taken in 250 mL round bottom flask . 1-chloro methyl naphthalene (9.89 g, 0.055 mole) was added followed by the addition of a catalytic amount of tertiary butyl ammonium iodide (0.59 g, 0.0016 mole). The solution mixture was refluxed for 24 hours. . Solvent was evaporated and extracted with ethyl acetate water mixture . The organic layer was dried over anhydrous Na_2SO_4 . The solid was crystallized from methanol to get C (8.4 g,86 %); $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 4.12 (s, 3H), 5.5(s,2H),5.7(s,4H)6.7(t,1H),7.38(t,2H),7.59-7.68(m,7H),7.76-7.84(m,7H),8.02(m,5H),8.29(d,2H). $^{13}\text{CNMR}$ (100MHz, CDCl_3): δ 52.33, 69.90, 73.28, 109.07, 123.84, 124.38, 124.91, 125.37, 125.44, 125.56, 125.62, 125.76, 125.96,126.12,126.59,127.05,127.32,127.9,128.69,128.75,129.17,131.83,132.03,132.86,133.41,133.81,142.59,153.07,166.74.IR(KBr) ν =3131,3042,2969,24821885,1768,1694,1627,1576,1526,1475,1418,1324,and1224 cm^{-1} .ESI-MS : m/z Calcd for $\text{C}_{41}\text{H}_{32}\text{O}_5$: 604.69, found: 627[M+Na] $^+$.

Synthesis of compound C-1

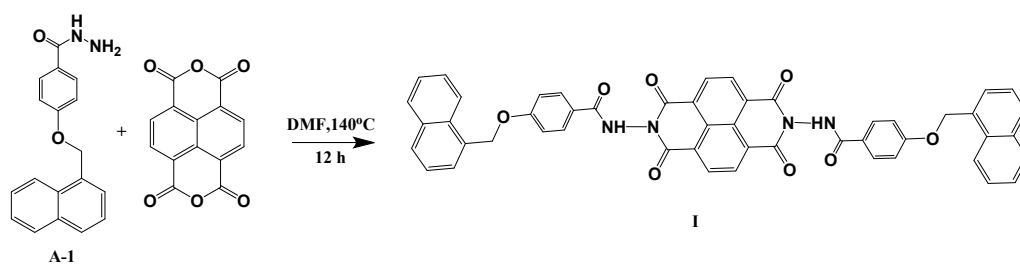


Scheme. S5 Synthetic scheme for compound C-1.

Compound C (2 g, 0.0033 mole) and hydrazine monohydrate (8.0 mL, 0.165 mole) were dissolved in MeOH (30 mL) and THF (15 mL). The reaction mixture was stirred at 60°C for 12 hours. After the reaction mixture was cooled to room

temperature, solvent was evaporated by applying vacuum. The residue was dissolved in DCM and washed many times with water to remove excess of hydrazine mono hydrate. The organic layer was then dried over anhydrous Na_2SO_4 . Crude product was purified by column chromatography 30 % ethyl acetate/Hexane (3:7) mixture as eluent. (1.8g,90%). $^1\text{H NMR}$ (500 MHz, CDCl_3): δ 3.1(s,2H)5.3 (s,2H), 5.52 (s,4H), 7.07(t,2H), 7.2(s,1H), 7.26(s,2H),7.3-7.53 (m,9H),7.65(m,3H)7.8-7.8 (m,5H),8.05(d,2H). $^{13}\text{C NMR}$ (100MHz, CDCl_3): δ 70.03,73.35,106.85,123.7, 124.3, 124.9, 125.35, 125.48, 125.9, 126.62, 126.9, 127.39,127.94,128.71,128.83,129.19,131.55,137.85,131.89,132.79,133.42,133.78,141.71,153.35,. IR(KBr) ν =3323, 3116, 2497, 1812, 1752, 1693, 1621, 1534, 1464 and 1381 cm^{-1} .ESI-MS: m/z Calcd for $\text{C}_{40}\text{H}_{32}\text{N}_2\text{O}_4$: 604.69, found: 627[M+Na] $^+$.

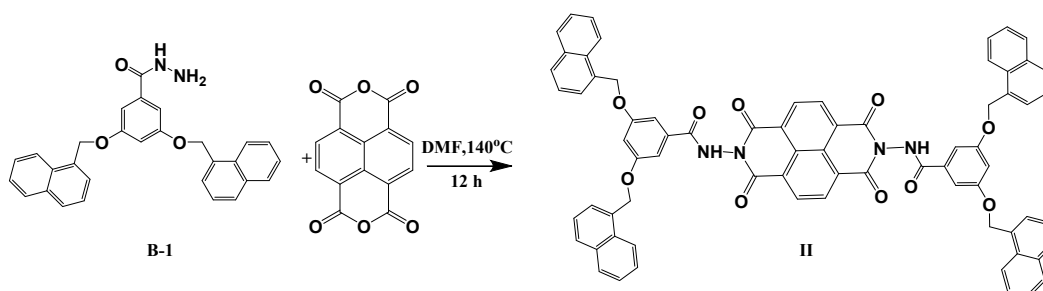
Synthesis of compound I



Scheme .S6 Synthetic scheme for compound I.

Naphthalene dianhydride (1 g, 0.0037 mole) and **A-1**(2.48, 0.0085) were taken in 30 mL of dry DMF and was heated to 140 $^{\circ}\text{C}$ for 12 hours. The reaction mixture was allowed to cool down to room temperature. The reaction mixture was extracted with DCM and washed many times with water. Organic layer was then dried over anhydrous Na_2SO_4 . Solvent The crude product was then purified by column chromatography methanol / CHCl_3 (1:9) mixture as eluent to obtain a brown coloured powder (2.5g, 82% yield). $^1\text{H NMR}$ (500 MHz, DMSO-d_6): δ 5.71(s,4H),7.35(d,4H),7.5-7.65 (m,6H), 7.4(d,2H), 7.9-8.1 (m,14H), 8.8(s,4H), 11.4 (d,2H). $^{13}\text{C NMR}$ (100MHz, DMSO-d_6): δ 68.0, 114.86, 123.81, 123.36, 126.01, 126.5, 126.77,128.49,128.81,129.86,131.05,131.53,131.61,131.97,133.26,160.84,161.83,164.66. IR(KBr) ν =3586, 3277, 3052, 1728, 11690, 1658, 1601, 1508, 1540,1500,1419,1381 and 1355, 1280, 1243, 1202, 1173,1124,1098 cm^{-1} . MS (MALDI-TOF) :m/z Calcd for $\text{C}_{50}\text{H}_{32}\text{N}_4\text{O}_8$: 816.81, found: 839.26[M+Na] $^+$.

Synthesis of compound II

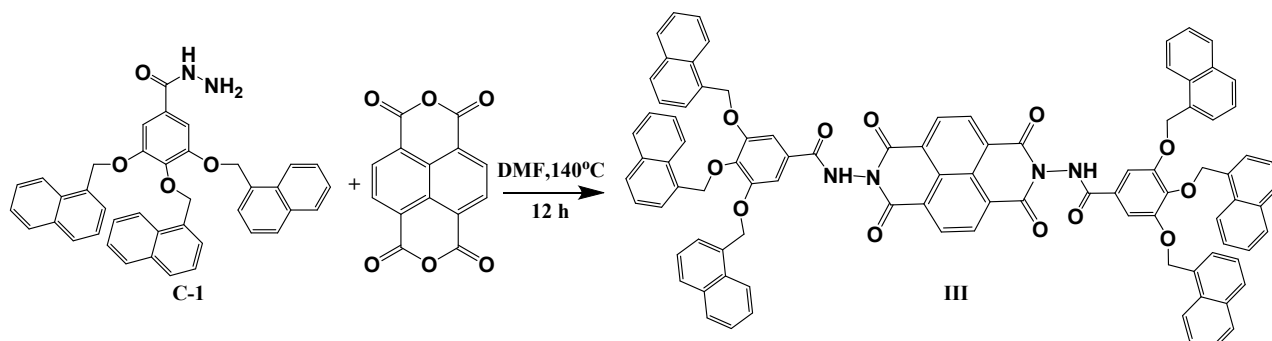


Scheme .S7 Synthetic scheme for compound II.

Naphthalene dianhydride (1 g, 0.0037 mole) and **B-1**(3.8g, 0.0085) were taken in 30 mL of dry DMF and was heated to 140 $^{\circ}\text{C}$ for 12 hours. The reaction mixture was allowed to cool down to room temperature. The reaction mixture was extracted with DCM and washed many times with water. Organic layer was then dried over anhydrous Na_2SO_4 . The crude product was then purified by column chromatography methanol/ CHCl_3 (1:9) to obtain a yellowish brown powder (3.4 g, 81% yield). $^1\text{H NMR}$ (500 MHz, DMSO-d_6): δ 5.6(s,8H),7.1(s,1H),7.3(s,4H)8.7(s,4H),7.4-7.56 (m,12H),7.66(m,5H),7.8-7.9(m,10H),8.07(m,5H),8.6(d,4H),11.5(d,2H). $^{13}\text{C NMR}$ (100 MHz, DMSO-d_6): δ 68.77, 70.5, 107.51, 124.2, 125.8, 126.53, 127.0,

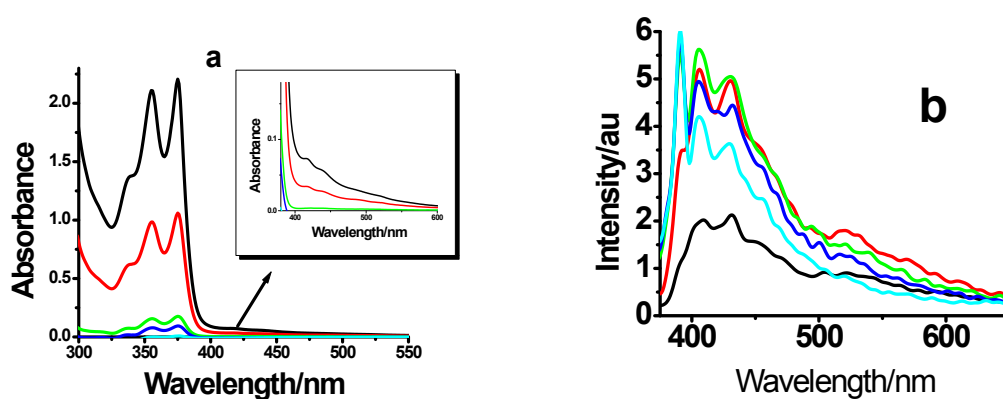
128.79, 129.63, 131.8, 132.47, 133.98, 141.68, 160.2, 161.2. IR(KBr) ν = 3374, 3131, 2999, 1899, 1862, 1767, 1694, 1629, 1548, 1505, 1446, 1369 and 1265 cm^{-1} . MS (MALDI-TOF) : m/z Calcd for $\text{C}_{72}\text{H}_{48}\text{N}_3\text{O}_{11}$: 1129.17, found: 1151.54[M + Na]⁺.

Synthesis of compound III



Scheme. S8 Synthetic scheme for compound III.

Naphthalene dianhydride (1.5 g, 0.0056 mole) and **C-1** (7.77 g, 0.0128 mole) were taken in 30 mL of dry DMF and was heated to 140 °C for 12 hours. The reaction mixture was extracted with DCM and washed many times with water. Organic layer was then dried over anhydrous Na_2SO_4 . The crude product was then purified by column chromatography methanol/ CHCl_3 (1:9) to obtain a dark brown powder (6.5 g, 80 % yield). ¹H NMR (500 MHz, DMSO- d_6) : δ 5.2 (s, 4H), 5.74 (s, 8H), 6.39 (t, 2H), 6.96 (d, 2H), 7.08 (t, 2H), 7.25 (t, 2H), 7.54 (s, 14H), 7.75-7.8 (t, 2H), 8 (s, 9H), 8.23 (s, 5H), 8.84 (s, 4H), 11.63 (d, 2H), (d, 2H). ¹³C NMR (100 MHz, DMSO- d_6) : δ 72.41, 107.01, 124.0, 124.2, 124.7, 125.41, 126.0, 126.56, 127.18, 127.82, 128.48, 128.66, 128.9, 131.2, 131.29, 132.19, 132.5, 132.87, 133.39, 140.38, 152.7, 160.99, 164.58. IR(KBr) ν = 3359, 3142, 2991, 2478, 1908, 1872, 1764, 1684, 1619, 1525, 1446, 1410, and 1316 cm^{-1} . MS (MALDI-TOF) : m/z Calcd for $\text{C}_{94}\text{H}_{64}\text{N}_3\text{O}_{13}$: 1441.53, found: 1464.268[M + Na]⁺.



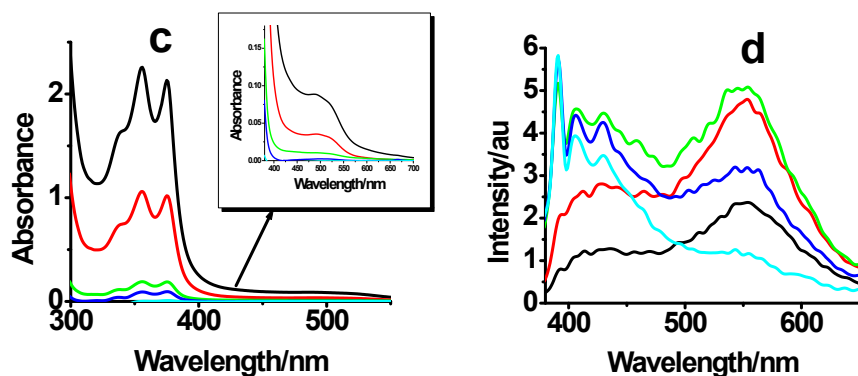


Fig. S1 UV-Vis and emission spectra of compound **II** (a,b) and **III** (c,d) in THF at different concentrations; black- 10^{-4} M, red- 0.5×10^{-4} M, green- 10^{-5} M, sky blue - 0.5×10^{-5} M and navy blue- 10^{-6} M, (Inset of a shows enlarged UV spectra from 400 nm-700 nm).

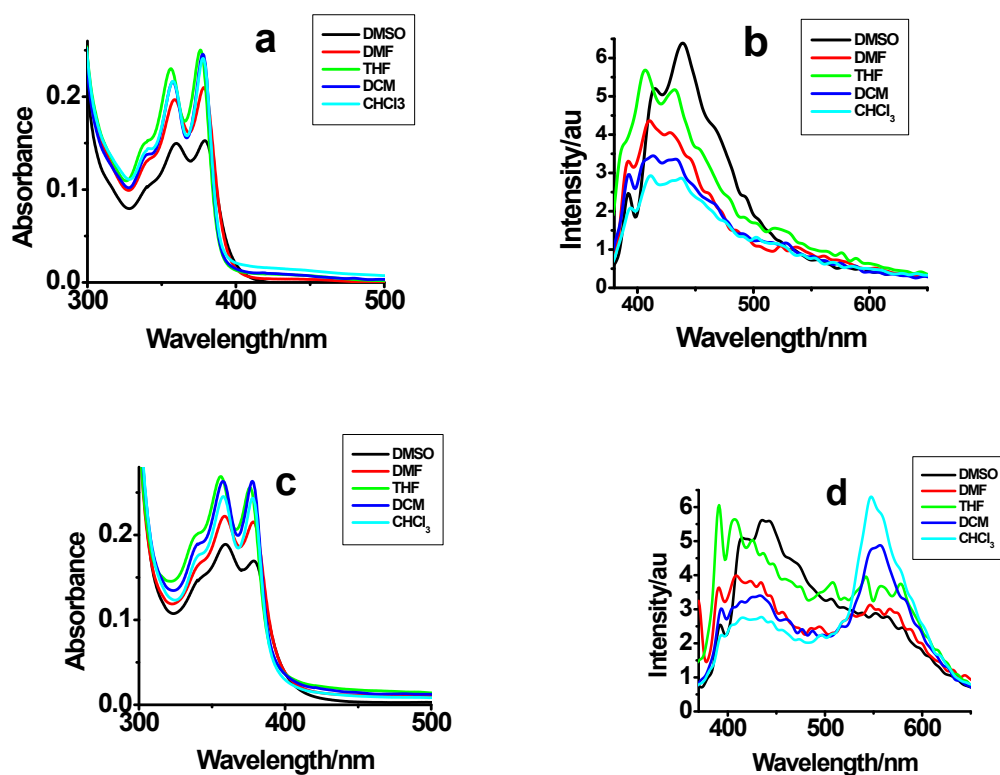
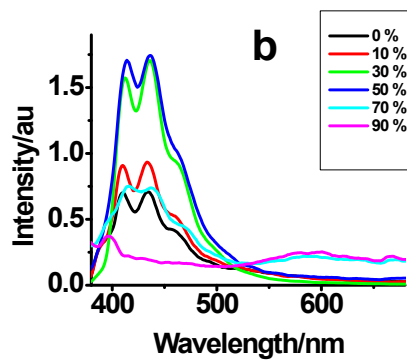
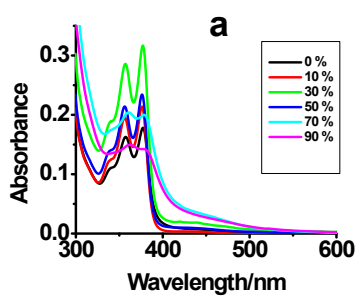


Fig. S2 UV-Vis and emission spectra of compound **II** (a, b) and compound **III** (c, d) [2×10^{-5} M] in different solvents; $\lambda_{\text{ex}} = 350$ nm.

Table S1: Quantum yield measurement of compound **I-III** in different solvents with quinine sulphate 10^{-5} M in 0.05 N

H_2SO_4 as standard ($\phi_R = 0.6 \pm 2$) (Error % ; ± 5)

Solvent	λ_{max} (nm)	λ_{max} (nm)	ϕ_f ($\times 10^{-3}$)
Compound I			
DMSO	378	391	6.78
DMF	379	438	3.42
THF	376	405	3.0
DCM	378	392	2.27
CHCl ₃	378	427	2.09
Compound II			
DMSO	375	442	6.3
DMF	375	410	5.03
THF	372	409	5.78
DCM	374	426	2.28
Chloroform	374	422	1.28
Compound III			
DMSO	378	437	8.99
DMF	378	409	7.5
THF	375	407	7.8
DCM	377	555	2.61
Chloroform	377	547	2.77



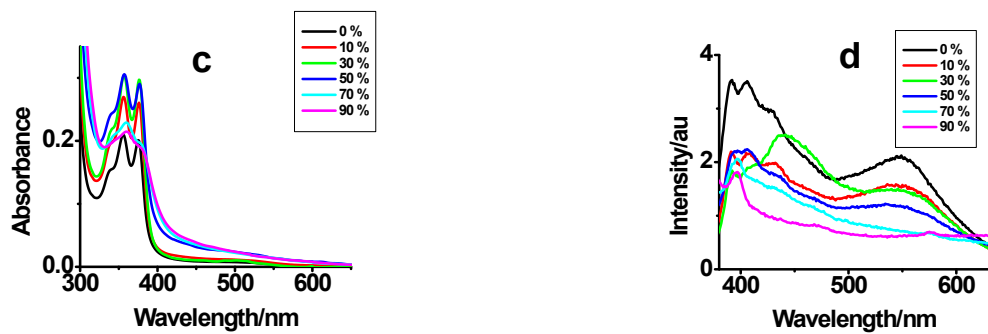


Fig.S3 UV-Vis and emission spectra of compound I (a, b) and compound III (c, d) in THF(10^{-5} M) with different water fraction, λ_{ex} ; 350 nm.

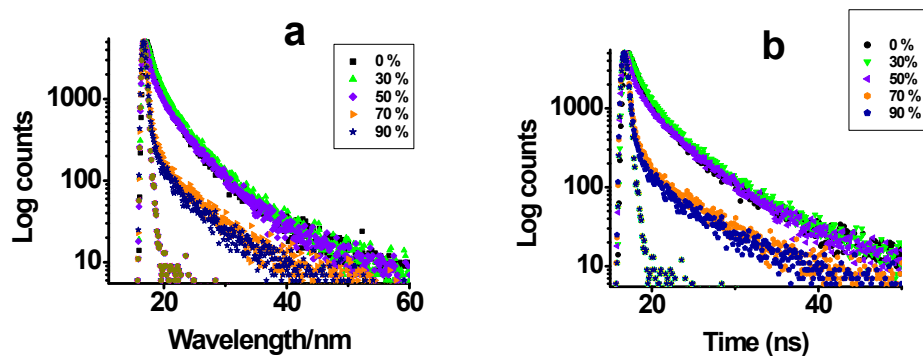


Fig. S4 Lifetime plot for compound I (a), compound II (b) and compound III (c) in THF(10^{-5} M) with different water fraction, λ_{ex} ; 340 nm.

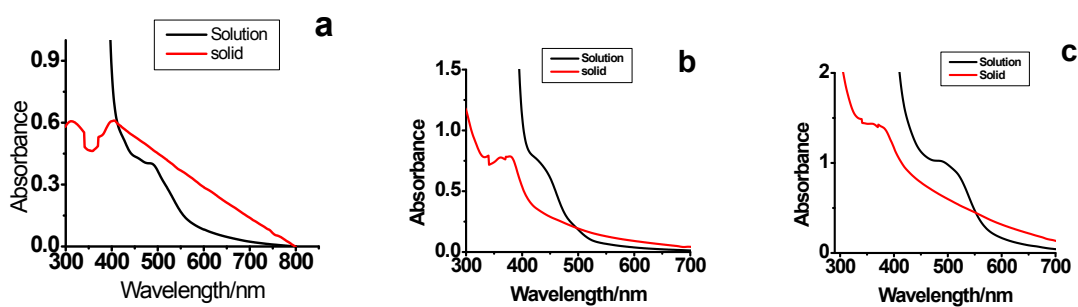


Fig. S5 UV-VIS spectra of compound I (a) II (b) and III (c) [10^{-3} M] in solution and film state.

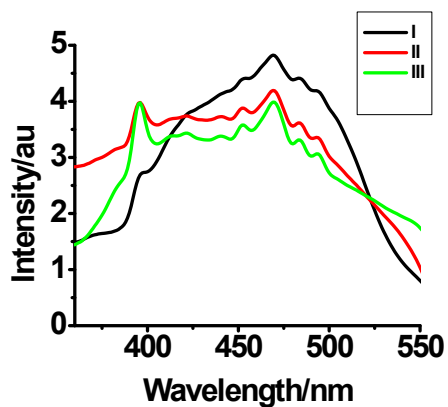


Fig.S6 Excitation spectra of compounds **I-III** in the film state emission collected at 590 nm .

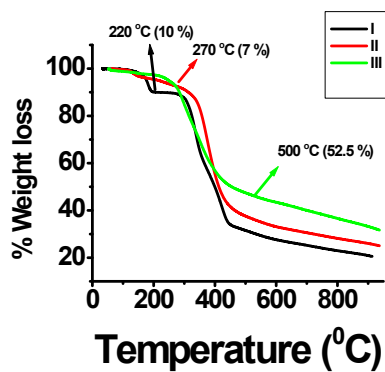
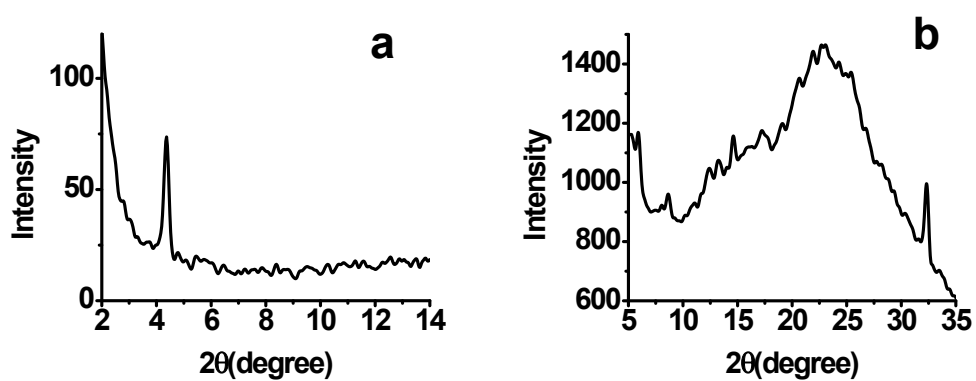


Fig. S7 TGA thermogram of compound **I-III**.



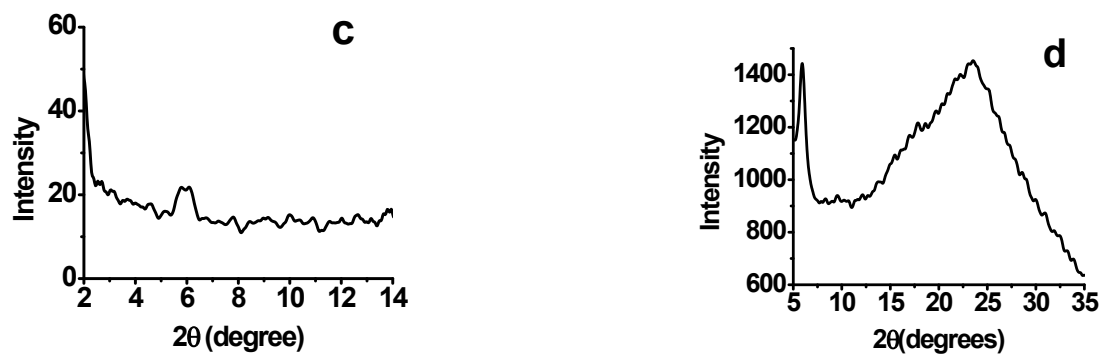


Fig. S8 SXRd ,WXRd pattern of compound **II**(a,b) and compound **III** (c,d).

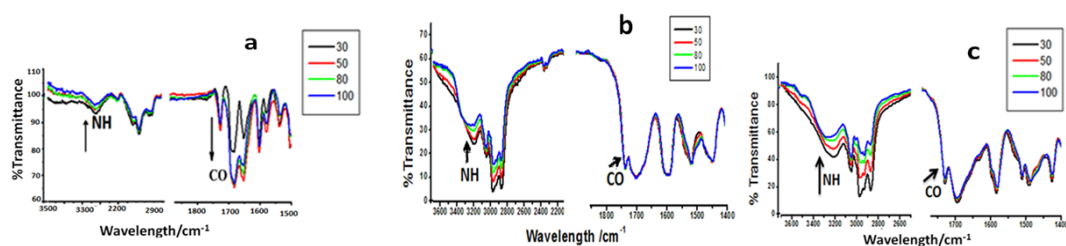


Fig S9 VT-FTIR spectra of compound **I** (a) and compound **III** (b).

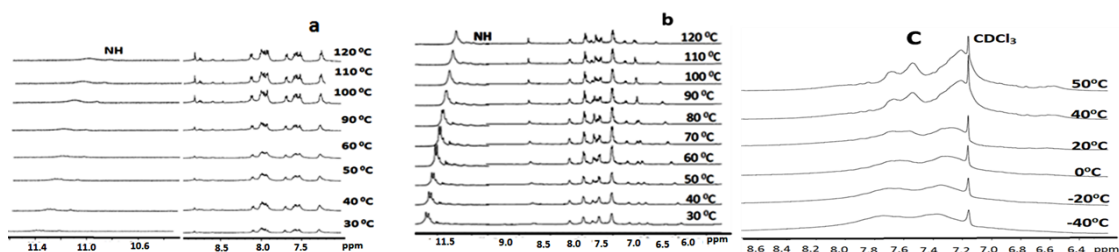


Fig. S10 variable temperature NMR spectra of compound **I** [1.7×10^{-2} M] (a) and compound **II** [3.5×10^{-2} M] (b) in DMSO- d_6 from 30°C to 120°C. variable temperature NMR spectra of compound **II** [5.3×10^{-3} M] in $CDCl_3$ from -40°C to 50°C .

Table .S2 :Lifetime values for compounds **I-II** for the addition of different fraction of water.

Comp.	% water	Lifetime (τ)(ns)	R.A(%)	CIHQ
I	0	2.50, 9.22	46.4, 20.14	1.31
	30	1.9, 9.06	43.63, 34.60	1.31
	50	2.1, 10.03	43.47, 34.19	1.4
	70	1.4, 8.97	37.13, 30	1.4
	90	1.6, 8.8	19.80, 21.06	1.3
II	0	2.38, 7.78	44.34, 25.67	1.04
	30	3.11, 10.09	54.59, 18.27	1.13
	50	1.40, 5.34	17.69, 31.89	1.20
	70	5.33	17.50	1.67
	90	5.67	12.45	1.42

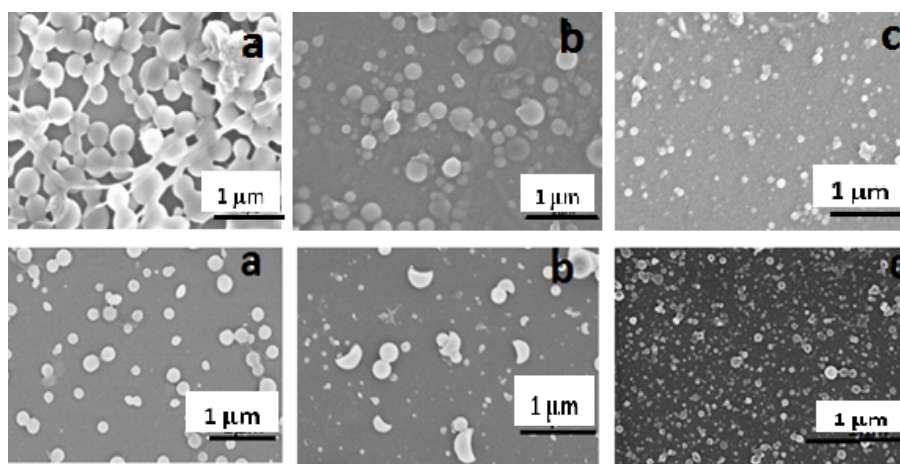
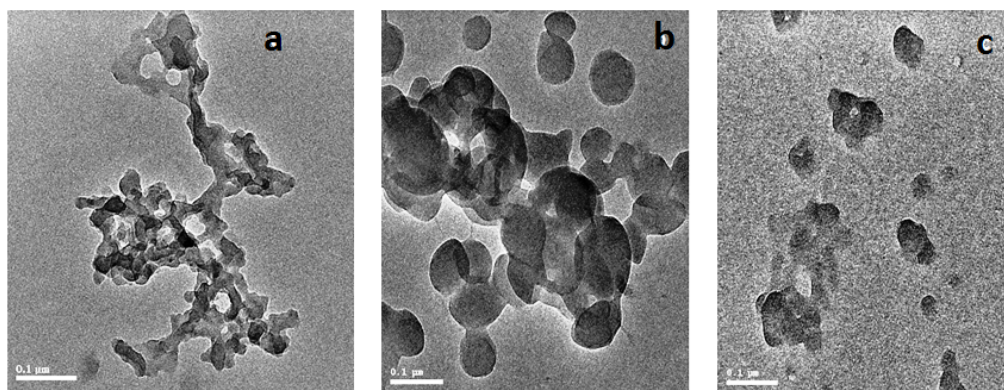


Fig .S11 SEM images of compound **I** (above) and compound **III** (below) with different fraction of water a) 30% water, b) 50% , and c)90% water.



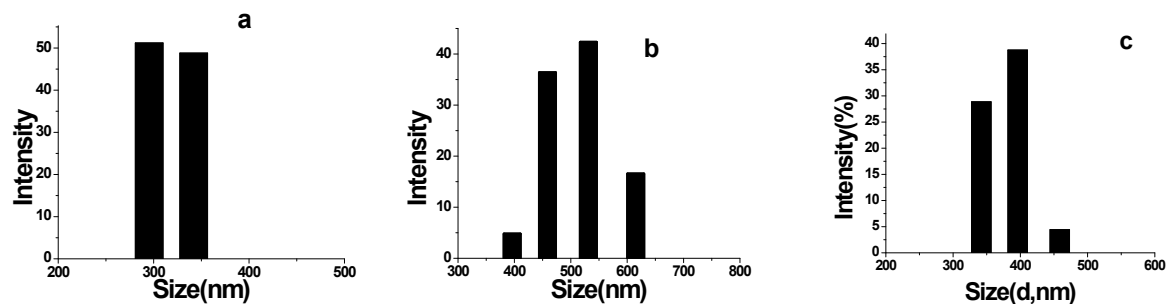


Fig. S12 (Above)TEM images of compound **I** (a), compound **II** (b), and compound **III** (c) with 90% water fraction (scale 0.1 μ m). (Below) DLS spectra of compound a) **I** b) **II** and c) **III** with 90% water fraction (10^{-5} M).

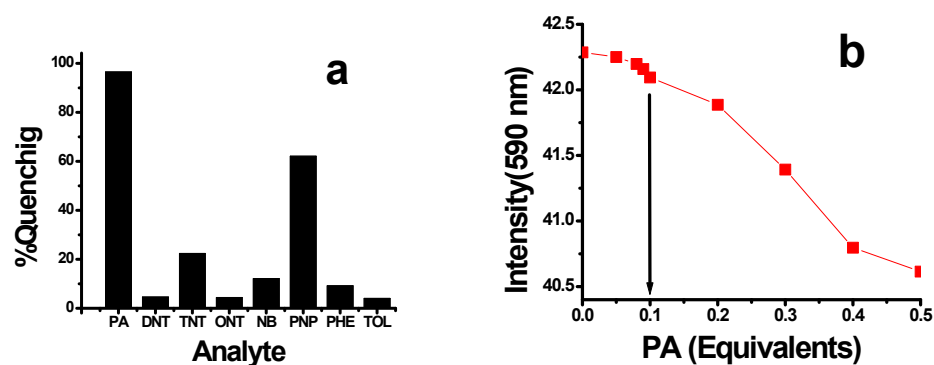


Fig. S13 Quenching percentage and selectivity for different analytes (a). Fluorescence intensity at 590 nm for the addition of different equivalent of PA (b).

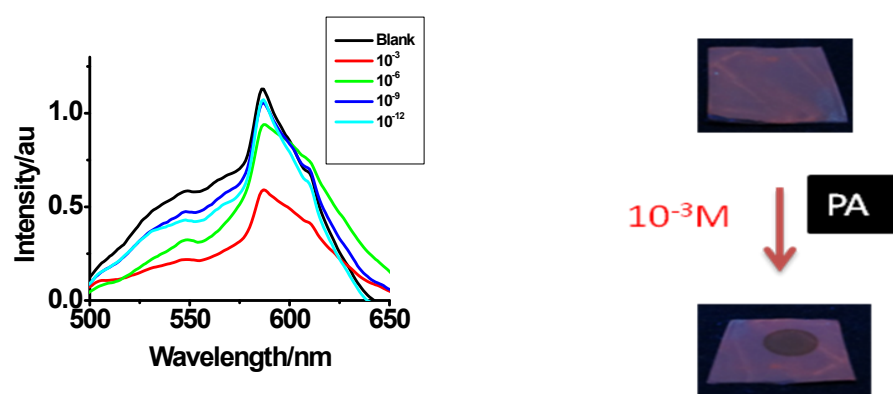


Fig. S14 (Left) Detection of PA in film for compound **II**. (Right) photographs showing quenching in luminescence by the addition of 10^{-3} M PA on TLC stripes under UV illumination.

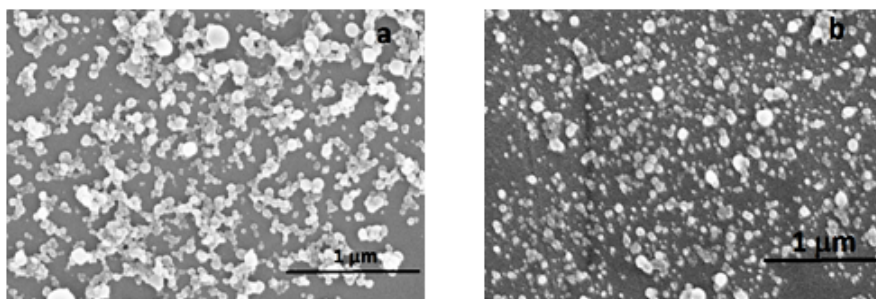
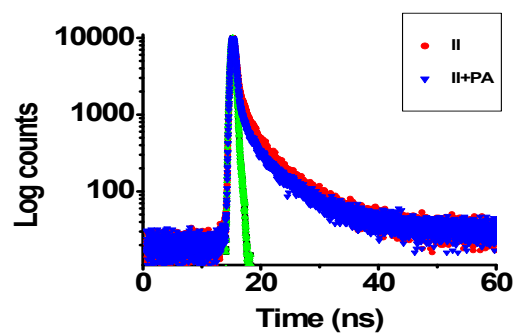


Fig. S15(Above) Lifetime plot for compound II before and after addition of PA. (Below)SEM images of compound II THF /Water(1:9) (a), after the addition of PA (b).

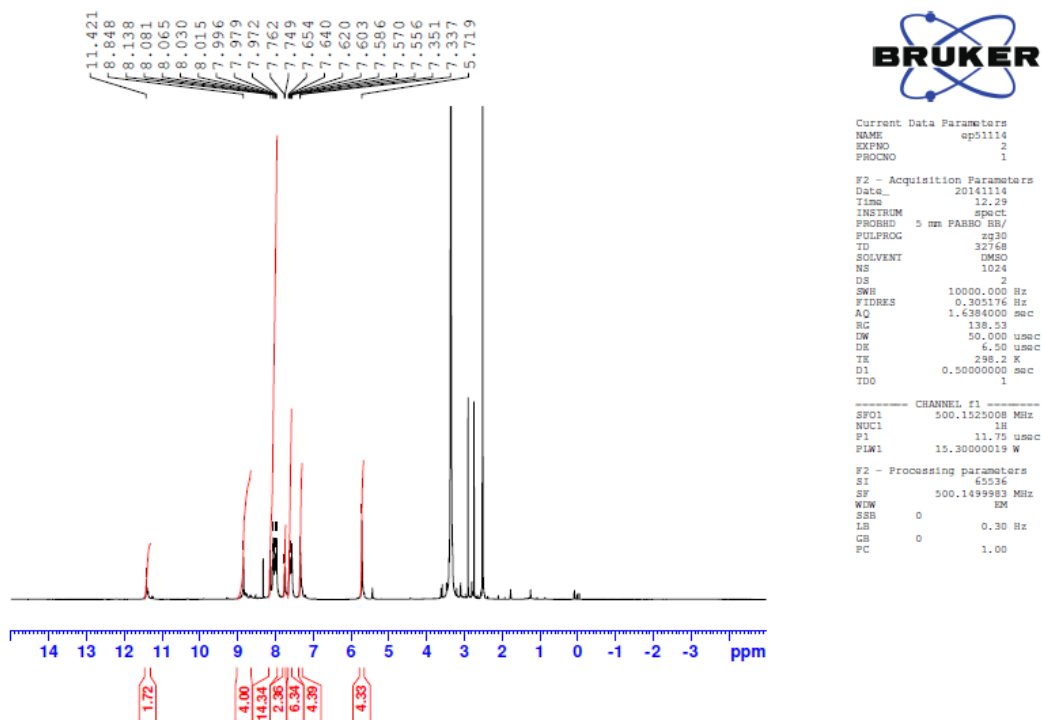


Fig. S 16 ¹H- NMR spectra of **I** DMSO-d₆.

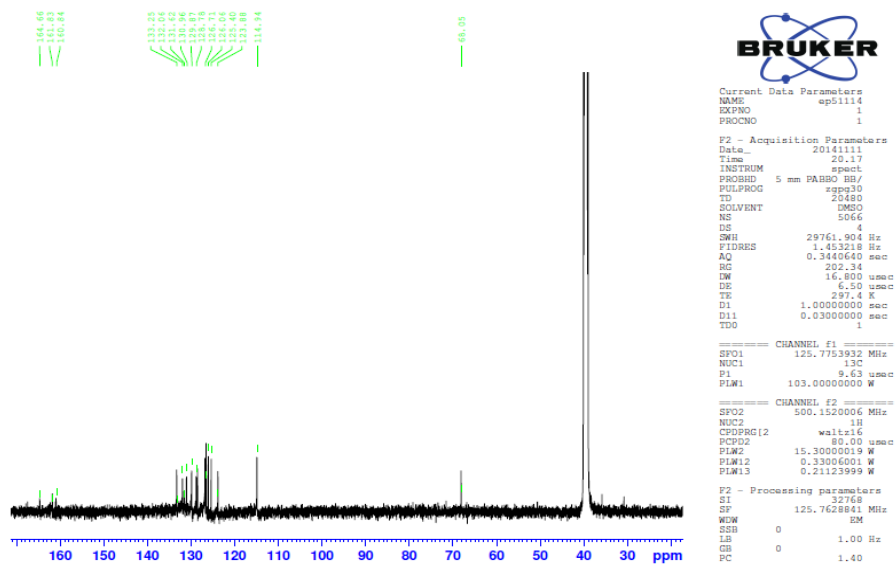
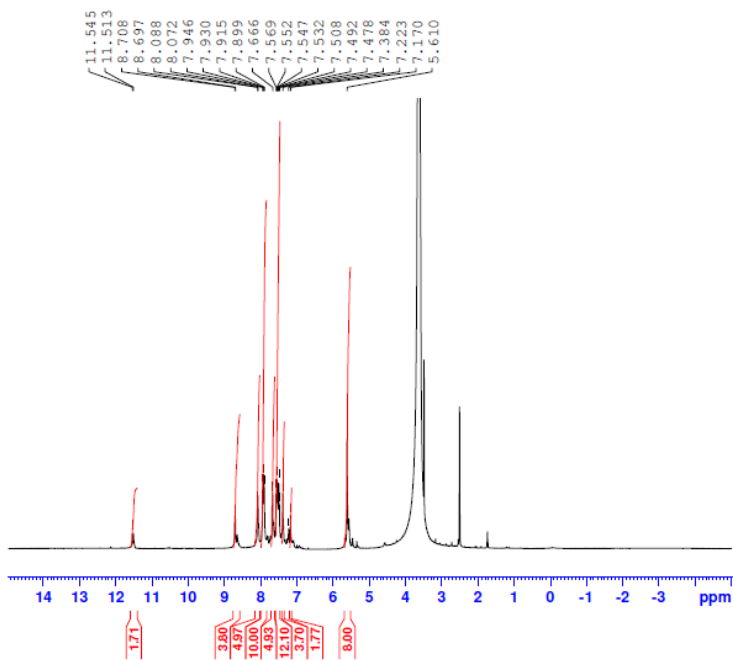


Fig. S 17 ¹³CNMR spectra of **I** DMSO-d₆.



```

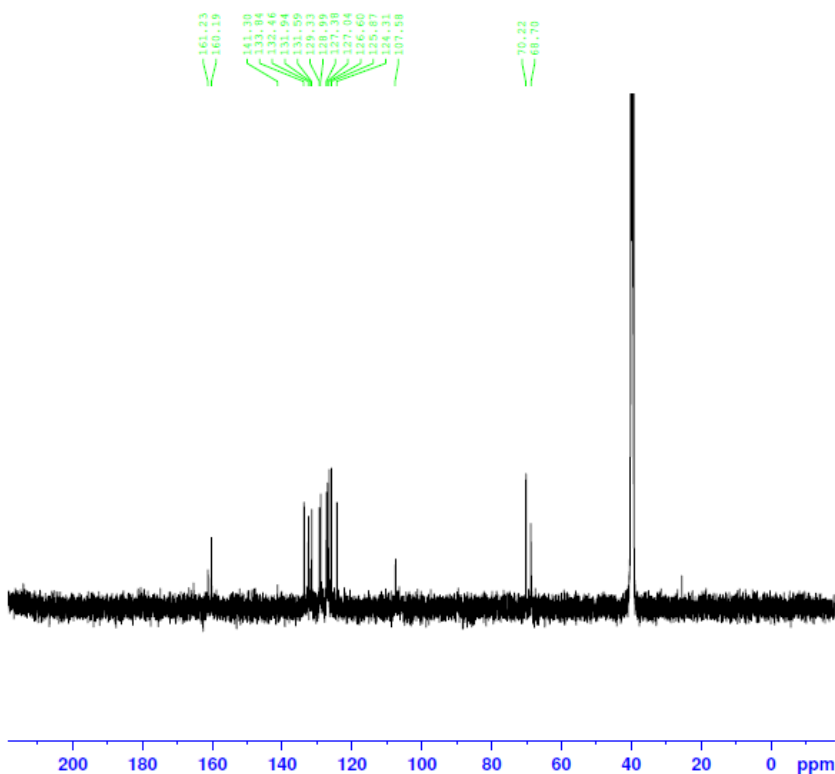
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NAME      ep50814
EXPNO    9
PROCNO   1

F2 - Acquisition Parameters
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INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  DMSO
NS       32
DS       2
SWH      10000.000 Hz
FIDRES   0.305176 Hz
AQ       1.6384000 sec
RG       31.24
DW       50.000 usec
DE       6.50 usec
TE       299.2 K
D1       0.50000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     500.1525008 MHz
NUC1     1H
P1       11.75 usec
PLW1     15.30000019 W

F2 - Processing parameters
SI       65536
SF       500.1500106 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00
  
```

Fig. S 18 ¹H-NMR spectra of **II** DMSO-d₆.



```

Current Data Parameters
NAME      ep50814
EXPNO    10
PROCNO   1

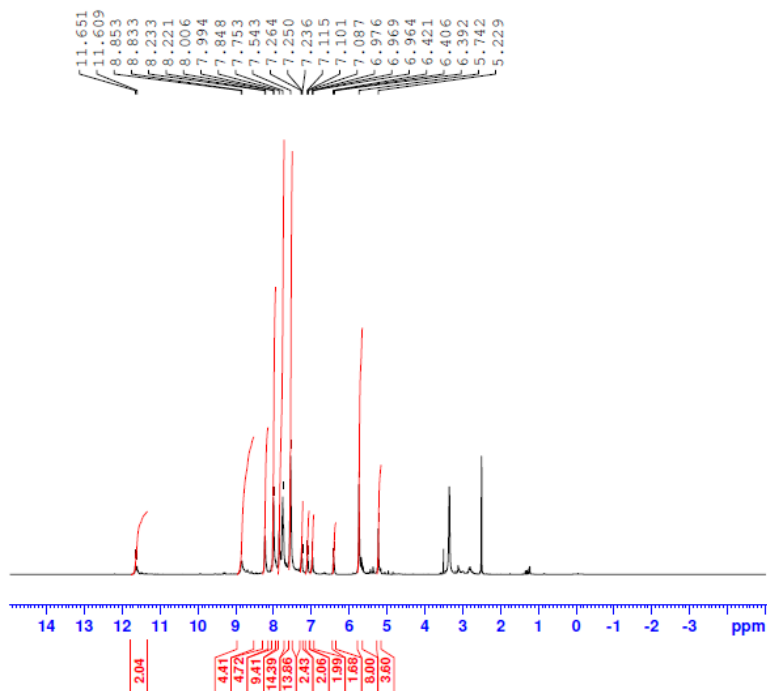
F2 - Acquisition Parameters
Date_    20140819
Time     18.47
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zgpg30
TD       20480
SOLVENT  DMSO
NS       512
DS       4
SWH      29761.904 Hz
FIDRES   1.453218 Hz
AQ       0.3440640 sec
RG       202.34
DW       16.800 usec
DE       6.50 usec
TE       300.0 K
D1       1.00000000 sec
D11      0.03000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     125.7753932 MHz
NUC1     13C
P1       9.63 usec
PLW1     103.00000000 W

===== CHANNEL f2 =====
SFO2     500.1520006 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2     15.30000019 W
PLW12    0.33006001 W
PLW13    0.21123999 W

F2 - Processing parameters
SI       32768
SF       125.7628180 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Fig. S19 ¹³C-NMR spectra of **II** DMSO-d₆.



```

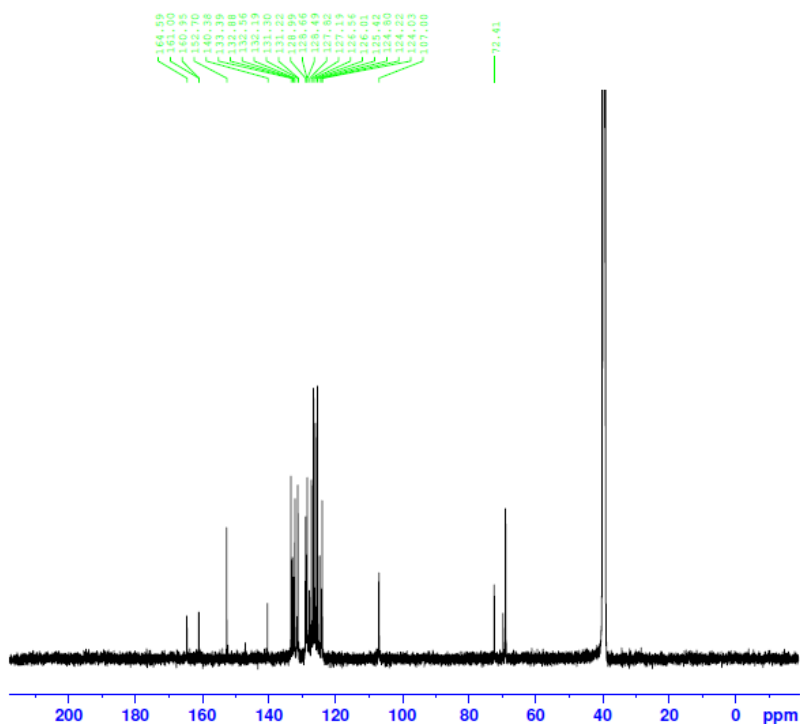
Current Data Parameters
NAME          ep51014
EXPNO        16
PROCNO       1

F2 - Acquisition Parameters
Date_        20141031
Time         20.12
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zg30
TD           32768
SOLVENT      DMSO
NS           204
DS           2
SWH          10000.000 Hz
FIDRES       0.305176 Hz
AQ           1.6384000 sec
RG           101.5
LW           50.000 usec
DE           6.50 usec
TE           298.1 K
D1           0.50000000 sec
TDO          1

==== CHANNEL f1 =====
SFO1         500.1525008 MHz
NUC1         1H
P1           11.75 usec
PLW1         15.30000019 W

F2 - Processing parameters
SI           65536
SF           500.1500120 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

Fig. S20 ¹H-NMR spectra of **III** DMSO-d₆.



```

Current Data Parameters
NAME          ep51014
EXPNO        17
PROCNO       1

F2 - Acquisition Parameters
Date_        20141031
Time         22.13
INSTRUM      spect
PROBHD       5 mm PABBO BB/
PULPROG      zgpg30
TD           20480
SOLVENT      DMSO
NS           5120
DS           4
SWH          29761.904 Hz
FIDRES       1.453218 Hz
AQ           0.3440640 sec
RG           202.34
LW           16.800 usec
DE           6.50 usec
TE           298.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TDO          1

==== CHANNEL f1 =====
SFO1         125.7753932 MHz
NUC1         13C
P1           9.63 usec
PLW1         103.00000000 W

==== CHANNEL f2 =====
SFO2         500.1520006 MHz
NUC2         1H
CPDPRG2      waltz16
PCPD2        80.00 usec
PLW2         15.30000019 W
PLW12        0.33006001 W
PLW13        0.21123999 W

F2 - Processing parameters
SI           32768
SF           125.7628831 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

Fig. S21 ¹³C-NMR spectra of **III** DMSO-d₆.

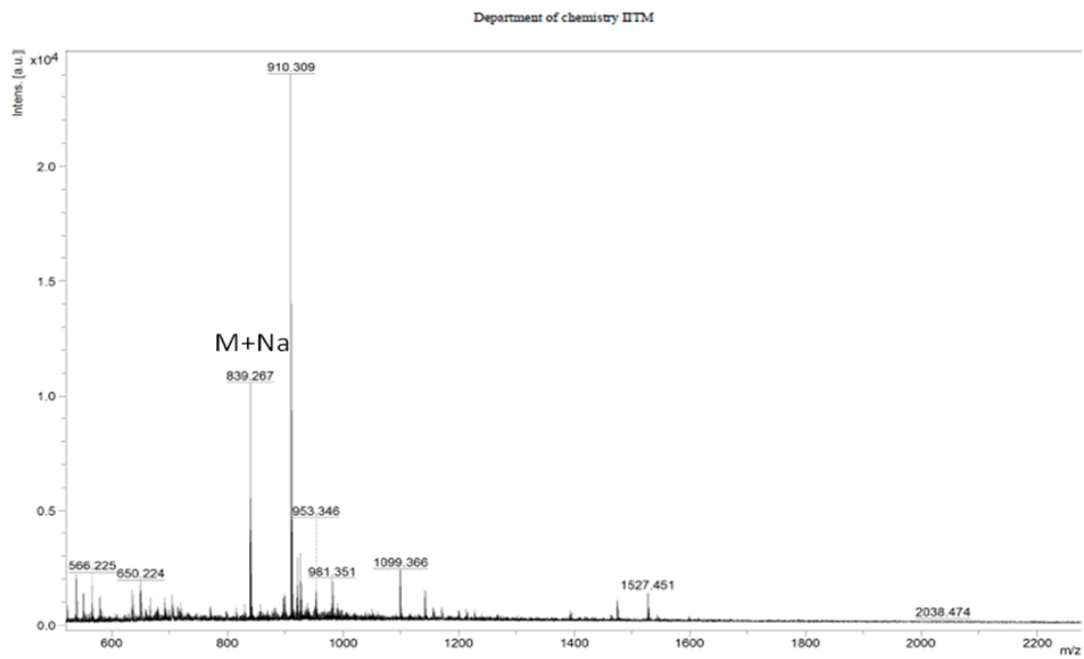


Fig. S22 MALDI-TOF of compound I.

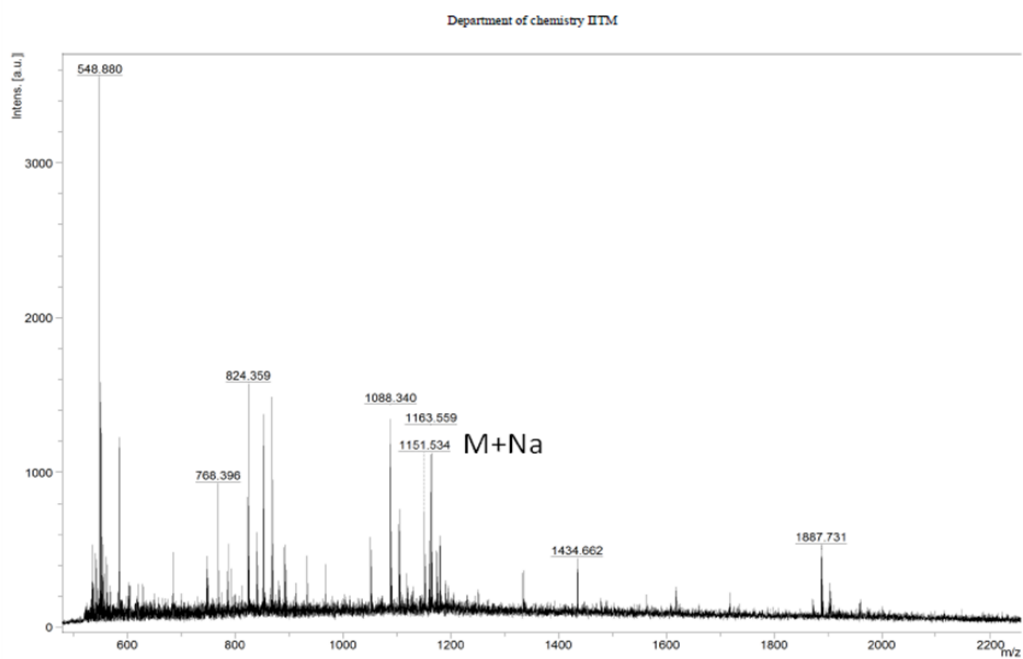


Fig. S23 MALDI-TOF of compound II.

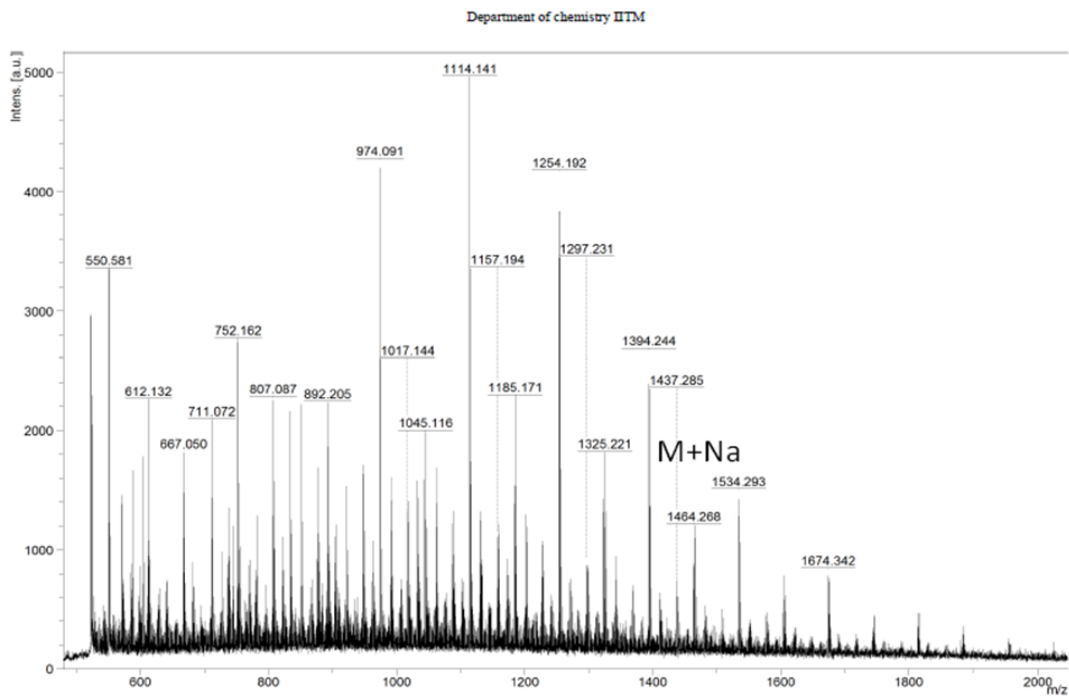


Fig. S24 MALDI-TOF of compound **III**.

