Electronic Supplementary Information

"Not Quenched" Aggregates of Triphenylene Derivative for the Sensitive Detection of Trinitrotoluene in Aqueous Medium

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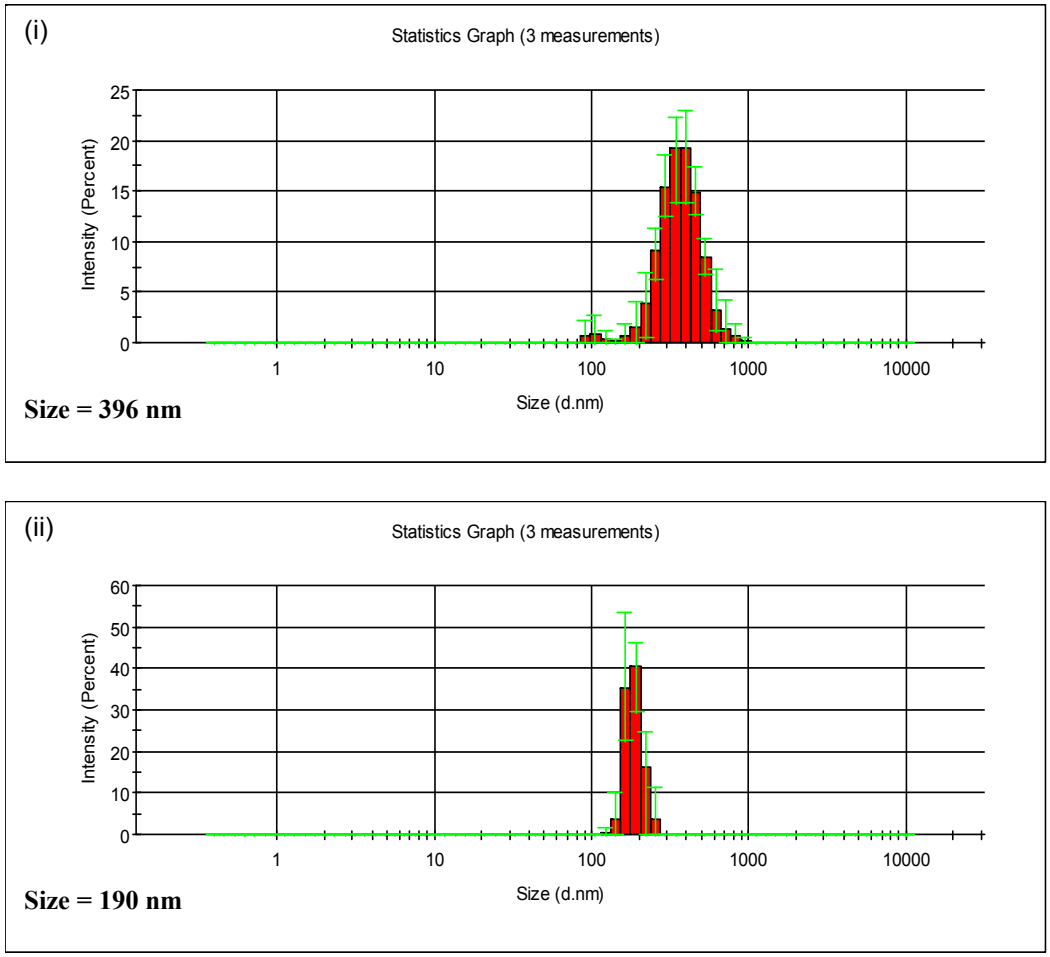

Fig. S1 Dynamic light scattering (DLS) results showing the variation of particle size (diameter) of derivative **4** in (i) H_2O:THF (3:7), (ii) H_2O:THF (1:1) mixture respectively.

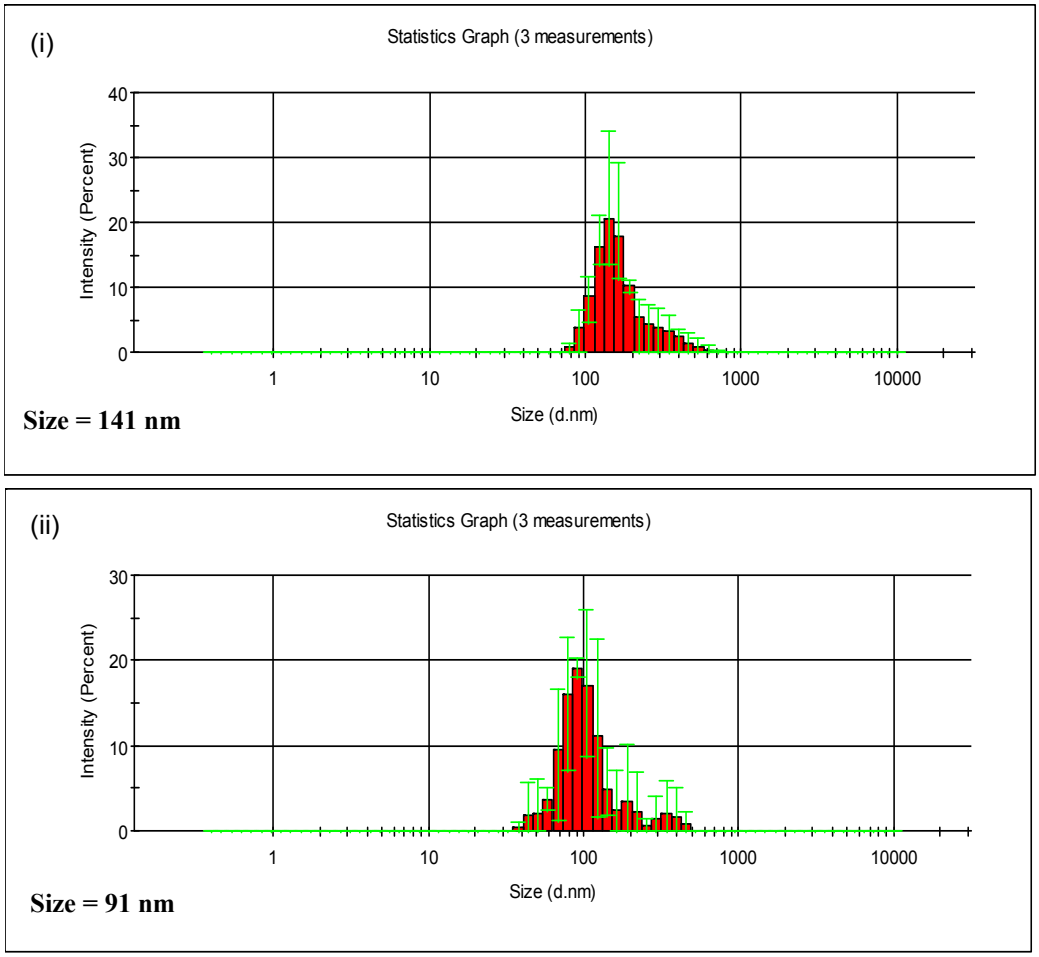

Fig. S2 Dynamic light scattering (DLS) results showing the variation of particle size (diameter) of derivative **4** in (i) H_2O :THF (7:3) and (ii) H_2O :THF (9:1) mixture respectively.

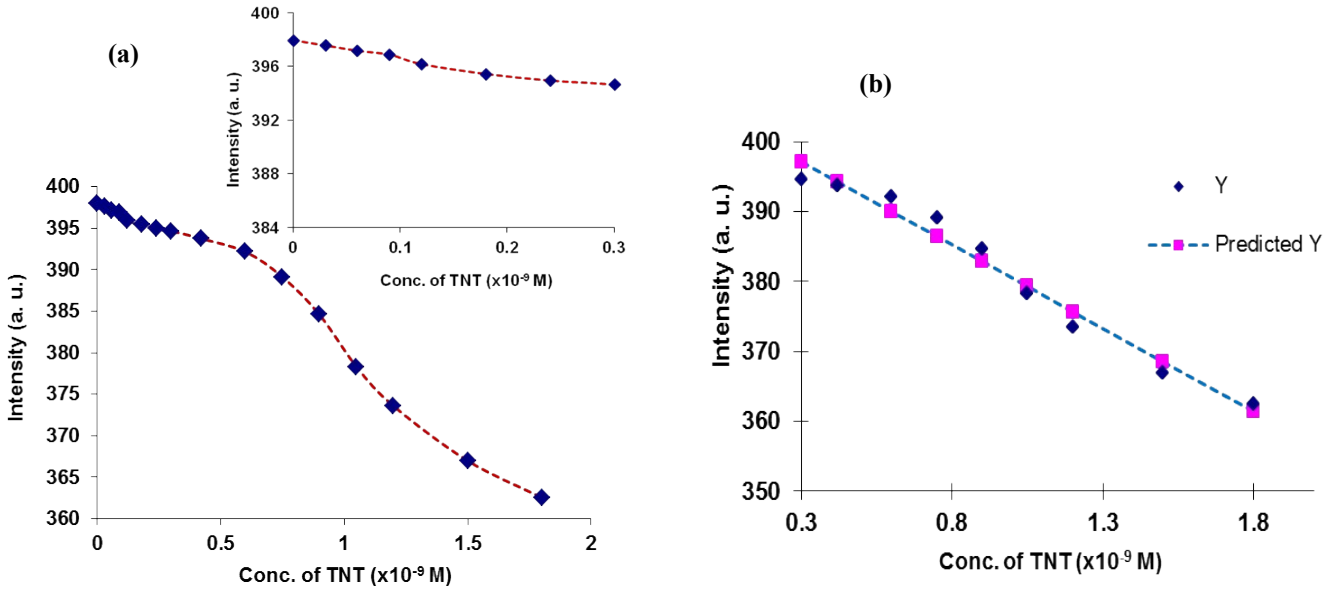

Fig. S3 (a) Showing the fluorescence intensity of compound **4**, inset showing the linear plot at lower concentration 0-0.3×10^{-9} M and (b) Calibrated curve showing the fluorescence intensity of compound **4** at 417 nm as a function of TNT concentration in H_2O/THF (9:1, v/v) buffered with HEPES, pH =7.05, λ_{ex}= 319 nm.

Multiple R = 0.9864,
R^2 = 0.9731,
Standard deviation = 0.008,
Observation = 10,
Intercept = 404.305,
Slope = 23.83×10^9

Multiple R = 0.9864,
R^2 = 0.9731,
Standard deviation = 0.0084,
Observation = 10,
Intercept = 404.305,
Slope = 23.83×10^9

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, the emission intensity of receptor **4** without TNT was measured by 10 times and the standard deviation of blank measurements was determined. The detection limit is then calculated with the following equation:

DL = 3 × SD/S

Where SD is the standard deviation of the blank solution measured by 10 times; S is the slope of the calibration curve.

From the graph we get slope

S = **23.83×10^9**, and SD value is 0.008

Thus using the formula we get the Detection Limit **(DL) = 3×0.008/23.83×10^9 = 1.007×10^{-12} mol/L = 1.007 pM = 228.59×10^{-12} g/L = 228.59 pg/L = 228.6 ppq**

i.e., probe **4** can detect TNT in this minimum concentration through fluorescence method.

The detection limit was calculated based on the fluorescence titration. To determine the S/N ratio, the emission intensity of 10 separate solution of receptor **4** without TNT was measured by 10 times and the standard deviation of blank measurements was determined to 0.0084. The detection limit is then calculated with the following equation:

DL = 3 × SD/S

Where SD is the standard deviation of 10 separate blank solution measured by 10 times; S is the slope of the calibration curve.

From the graph we get slope

S = **23.83×10^9**, and SD value is 0.0084

Thus using the formula we get the Detection Limit **(DL) = 3×0.0084/23.83×10^9 = 1.057×10^{-12} mol/L = 1.057 pM = 240×10^{-12} g/L = 240 pg/L = 240 ppq**.

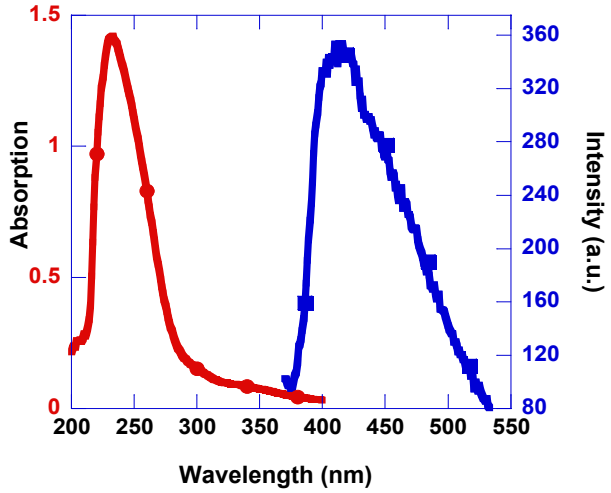

Fig. S4 Spectral overlap of absorption spectrum of 2,4,6-Trinitrotoluene (red line) and emission spectrum (blue line) of derivative **4**

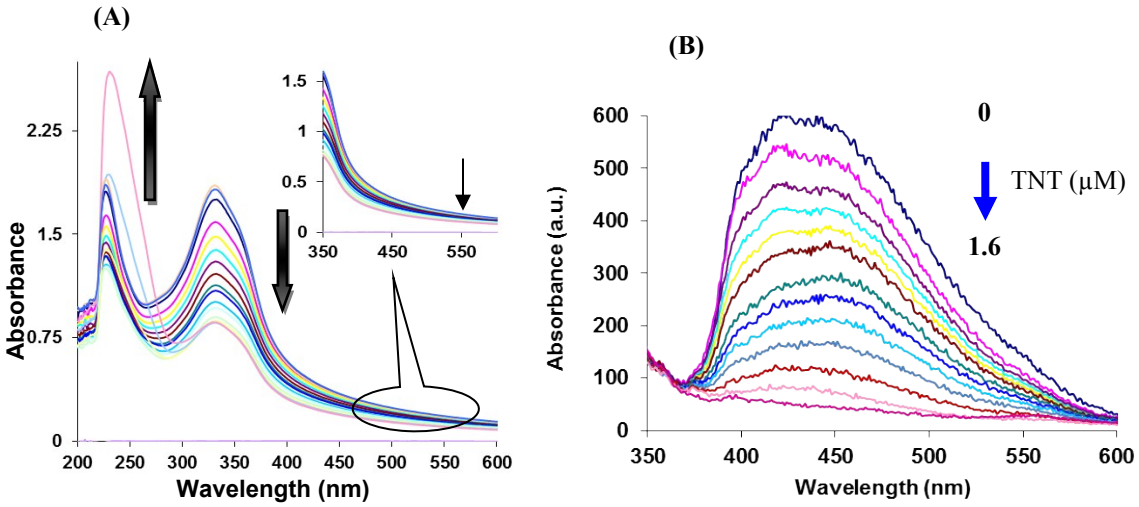

Fig. S5 (A) UV-Vis spectrum of derivative **4** (10 μM) upon the addition of 15 μM of TNT. Inset shows the trail in the absorption spectrum; (B) Fluorescence spectrum of derivative **4** (10 μM) upon the addition of 2,4,6-trinitrotoluene (TNT) from 1 to 1.6 μM in H_2O:DMSO (9:1) mixture.

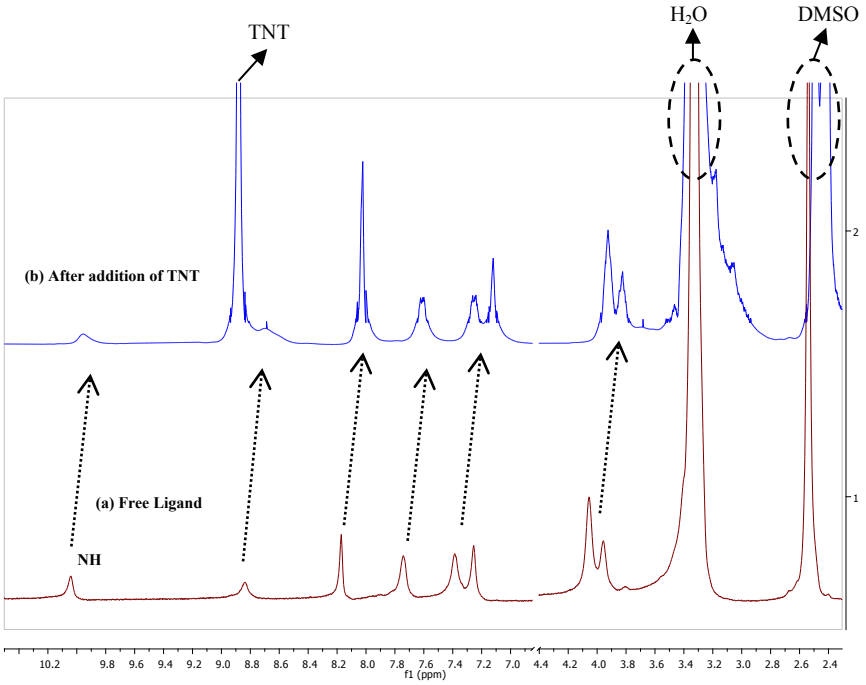

Fig. S6 Partial ^{1}H NMR of derivative **4** (600 µl of 10^{-2} M) (a) before and (b) after the addition of TNT (10 µl of 10^{-2} M) in DMSO-d_6:D_2O (8:2).

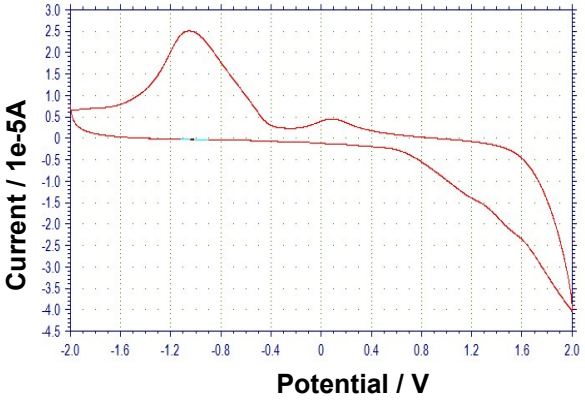

Fig. S7 Cyclic Voltammogram of derivative **4** (1×10^{-3} M) in dichloromethane.

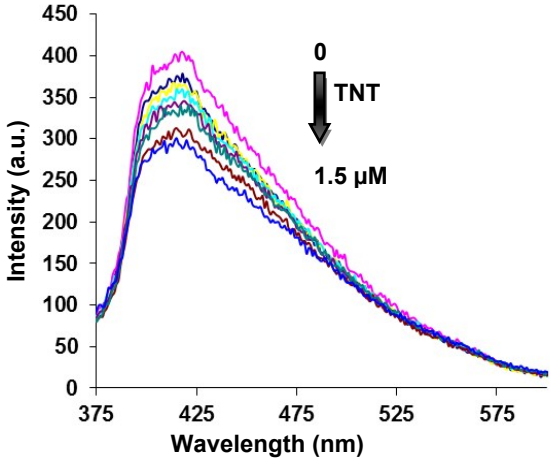

Fig. S8 Fluorescence emission spectrum of derivative **4** (10 µM) upon the addition of 1.5 µM of TNT in pure THF.

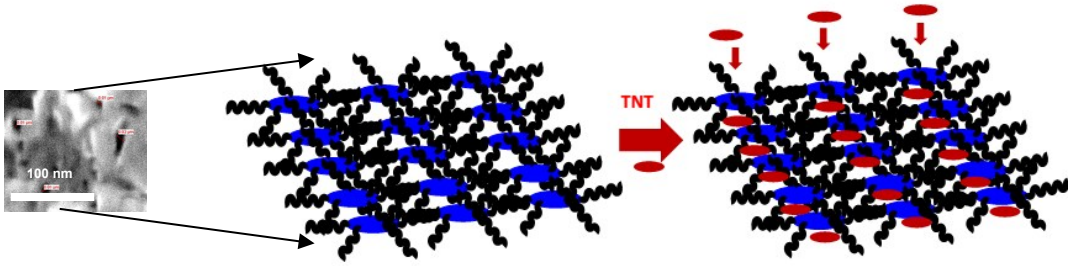

Fig. S9 Schematic representation of sensing of TNT by aggregates of derivative **4**

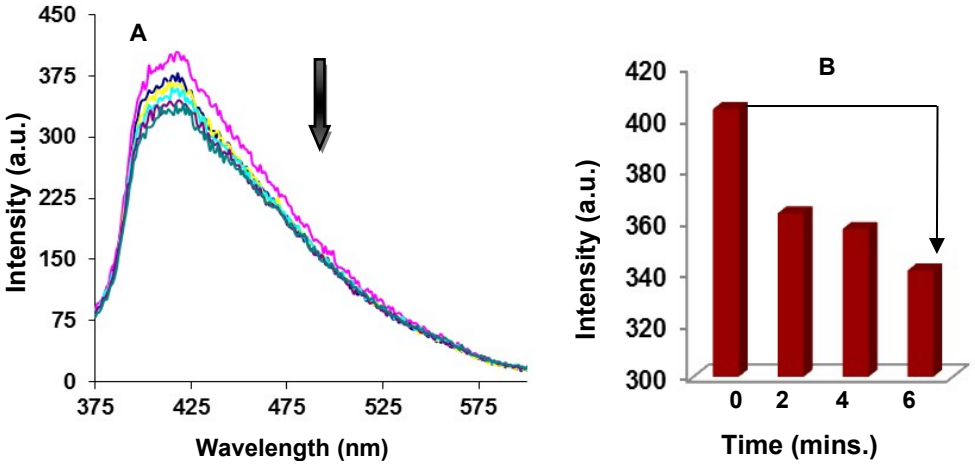

Fig. S10 (A) Fluorescence emission spectrum of derivative **4** (10 μM) in H_2O:THF (9:1) upon exposing it to vapors of 2,4,6-trinitrotoluene (B) Bar diagram showing the change in emission intensity of derivative **7** with time upon exposure to the vapours of TNT.

Fig. S11 ^{1}H NMR of derivative **4** in $CDCl_3$

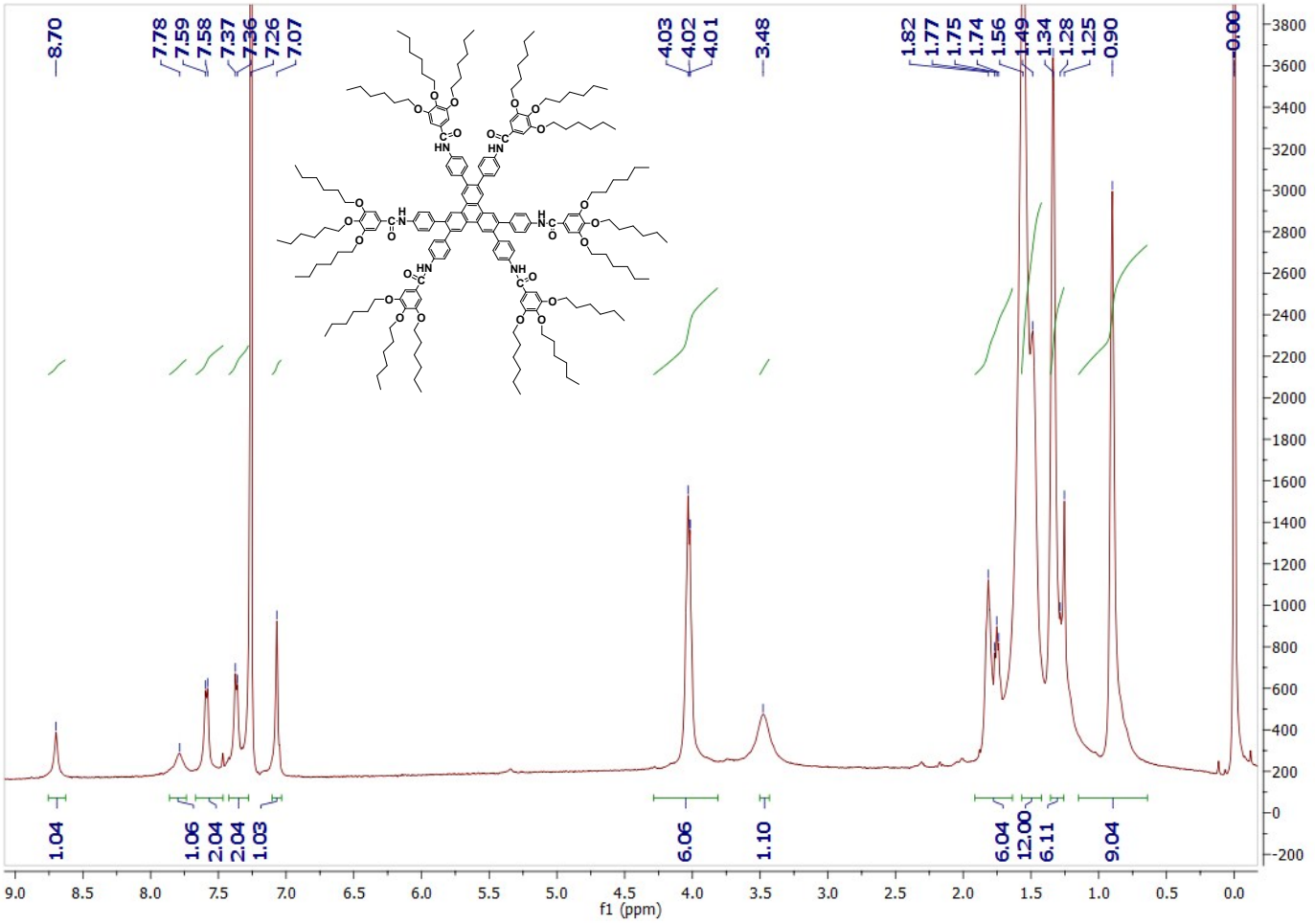

Fig. S12 ^{13}C NMR of derivative **4**

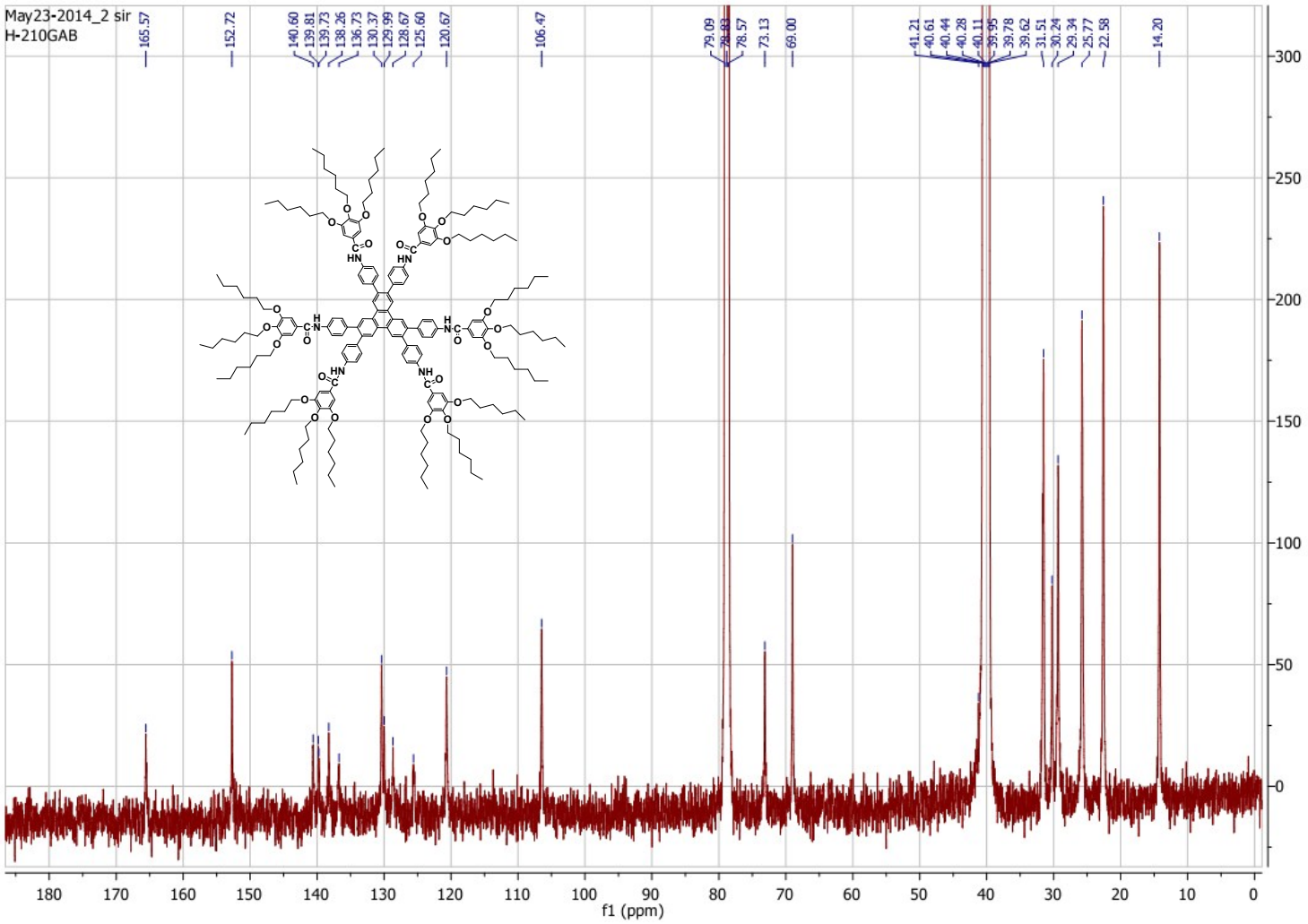

Fig. S13 MALDI-TOF mass spectrum of derivative **4**

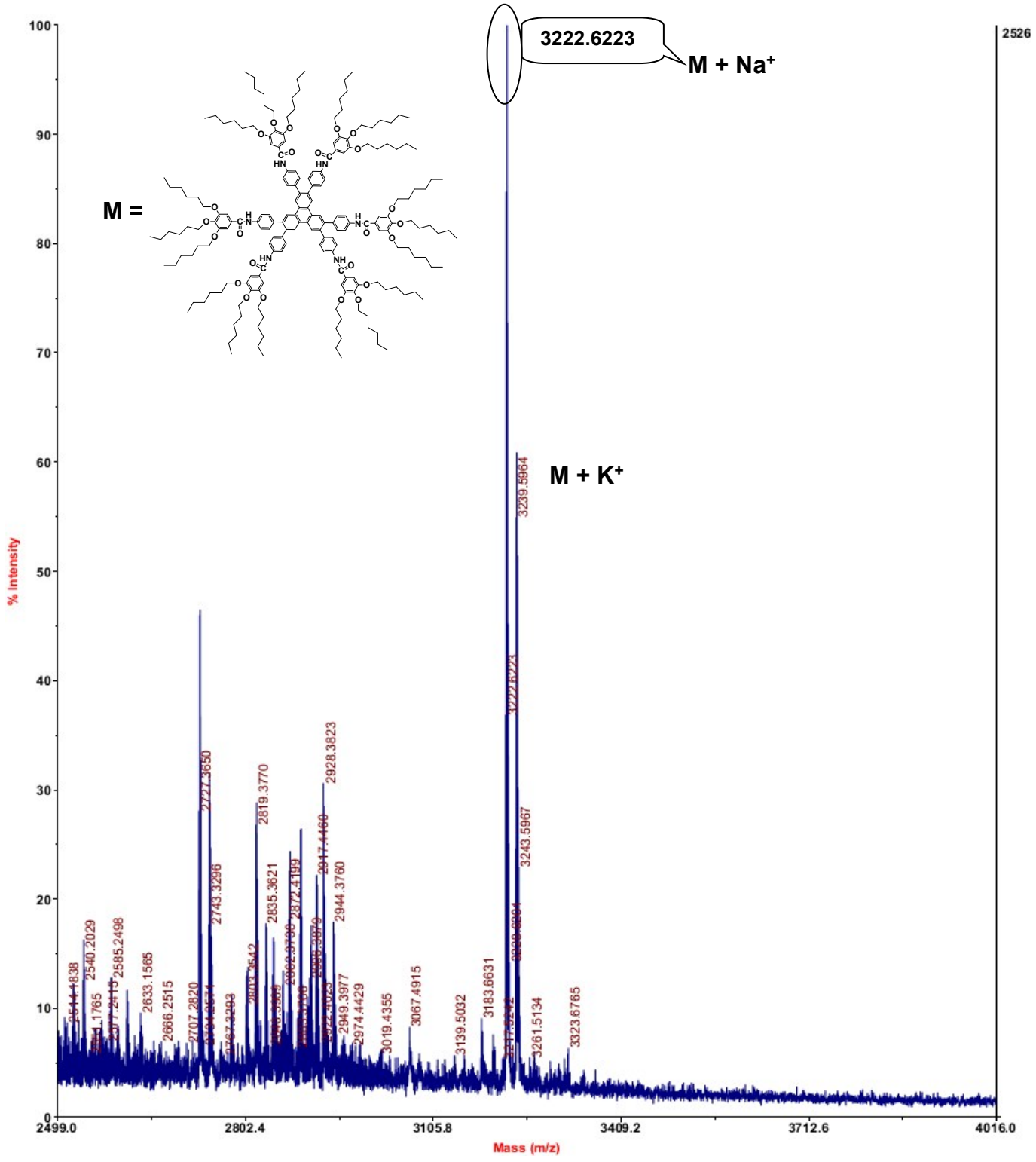

Fig. S14 FT-IR spectrum of derivative **4**

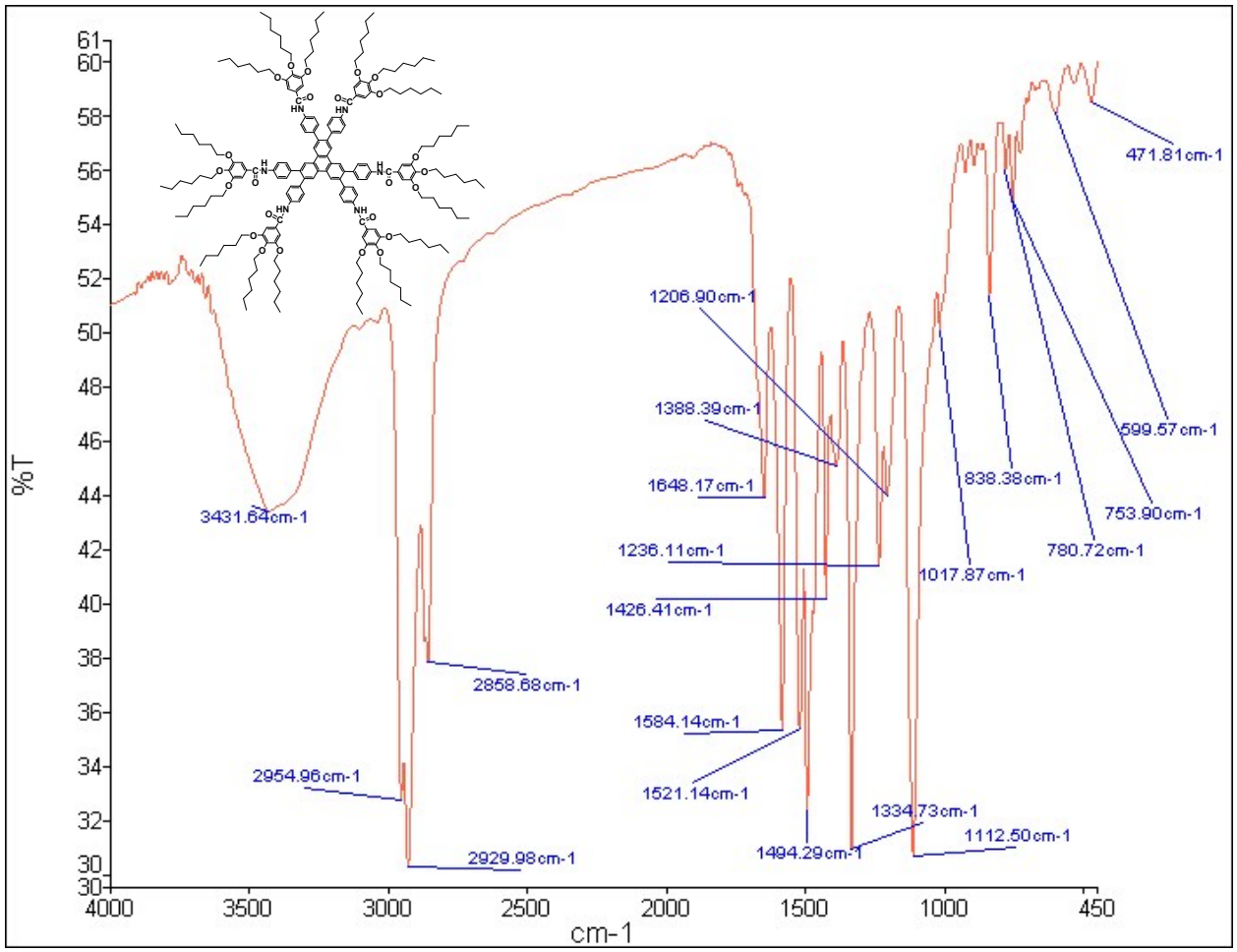

Table S1 Comparison of present manuscript with other literature reports

S.No.	Publication	K_{SV} (M^{-1})	Phase	Detection limit in solution phase	Solid state Detection limit
1	**Present Manuscript**	**13.33×10^5**	**Solution, solid and vapor**	**228.6 ppq**	**22.7 ag.cm^{-2}**
2	*ACS Appl. Mater. Interfaces*, 2014, **6**, 20067	1.37×10^5	Solution and solid	0.22 ppb	0.45 pg cm^{-2}
3	*Chem. Commun.,* 2014, **50**, 9683	8.4×10^4	Solution and vapor	2-14 ppb	-
4	*Chem. Eur. J.,* 2014, **20**, 2276	2.8×10^3 1.55×10^3 1.62×10^3	Only solution	0.9 ppb, 3.63 ppb, 2.27 ppb	-
5	*Polym. Chem.,* 2014, **5**, 4521	1.38×10^3	Solution and solid	10 μM	0.5 ng mm^{-2}
6	*J. Mater. Chem. C,* 2014, **2**, 515	7.4×10^4	Solution and solid	-	22.7 ng ml^{-1}
7	*Analyst,* 2014, **139,** 2379	-	Solution and solid	-	5.68 ng mm^{-2}
8	*Sensors and Actuators B,* 2014, **199**, 148	1.04	Only solution	423 ppb	-
9	*Dyes and Pigments,* 2014, **101**, 122	2.37×10^5	Only solution	1.3×10^{-7} M	-
10	*Chem. Commun.,*2013, **49**, 780	1.7×10^4	Solution and solid	-	0.58 ng mm^{-2}