Electronic Supplementary Material (ESI) for Analyst.

An electron-rich small AIEgen as a solid platform for selective and ultrasensitive on-site visual detection of TNT in solid, solution and vapor states

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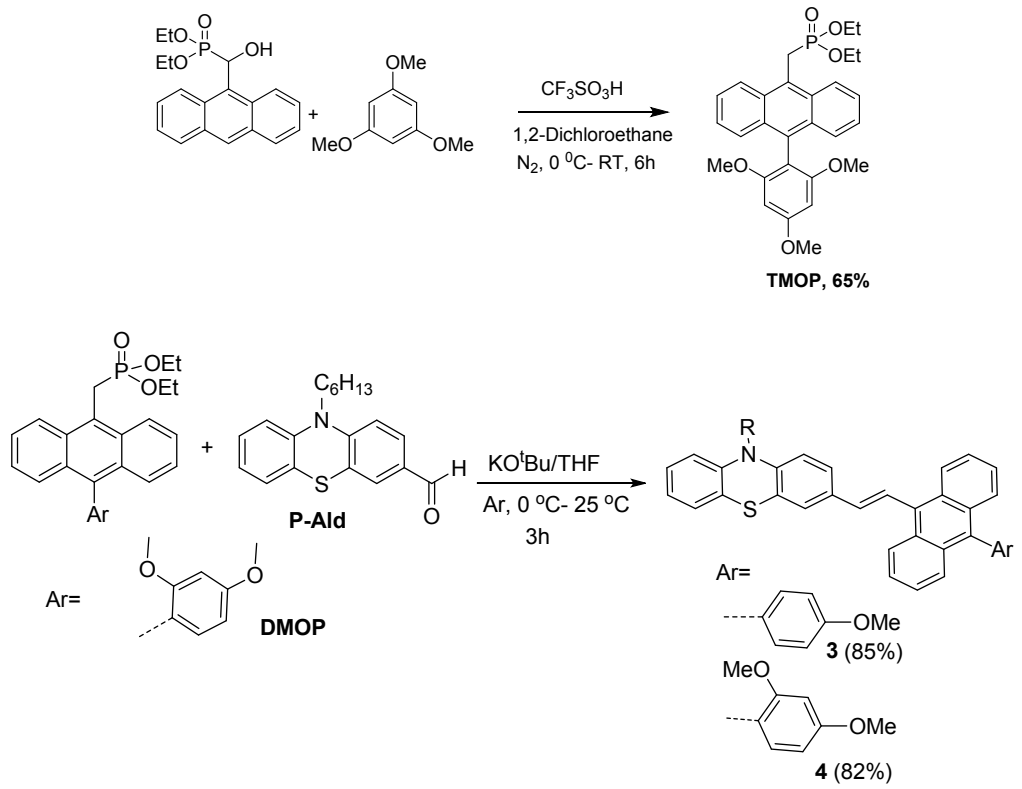
Calculation of optical band gap: The optical bandgap(E_g) of 2 and 3 were estimated from the intercept of the extrapolated linear fit for the plotted experimental data of $(K*E)^{1/2}$ versus incident photon energy (hv) near the absorption edge. Where K = Kubelka Munk constant and E is the energy of electron. Ref: J. Tauc, Amorphous and Liquid Semiconductors, Plenum, New York, 1974.



Scheme S1 Synthetic route for **TMOP**, **1**, **2** and **3**

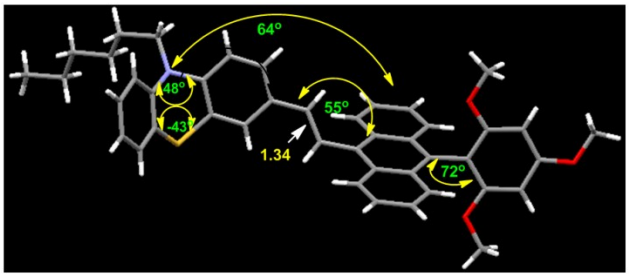


Fig S1 Molecular structure of **1** with some selected bond and torsional angles

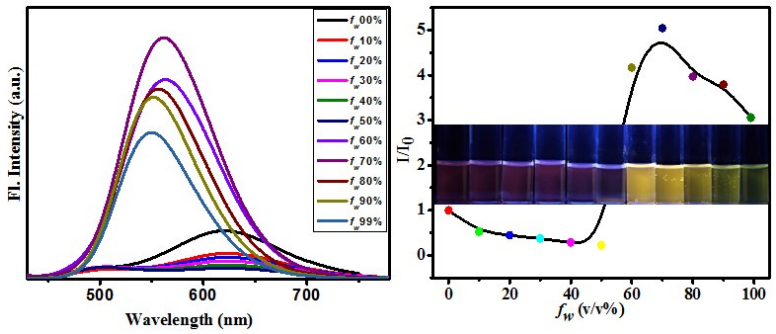


Fig S2 (a) PL spectra of **1** in MeCN (10 µM) by increasing f_w; (b) PL intensity vs f_w (image of gradual change in the intensity and wavelength of **1**). λ_{ex}= 405 nm.

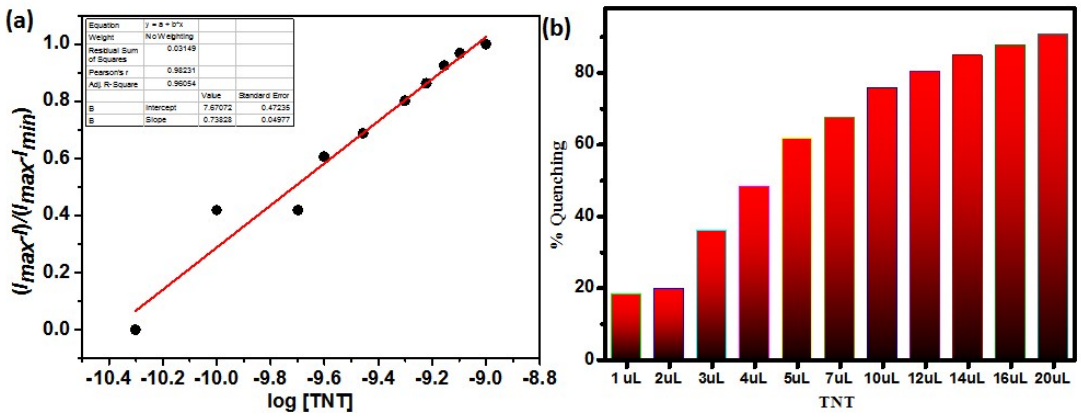


Fig S3 (a) Limit of detection plot, Intercept -10.5; LOD= 31.6 x 10^{-10}= 3.16 x10^{-9} (b) Quenching % of 1 upon incremental addition of TNT (10^{-8}M)

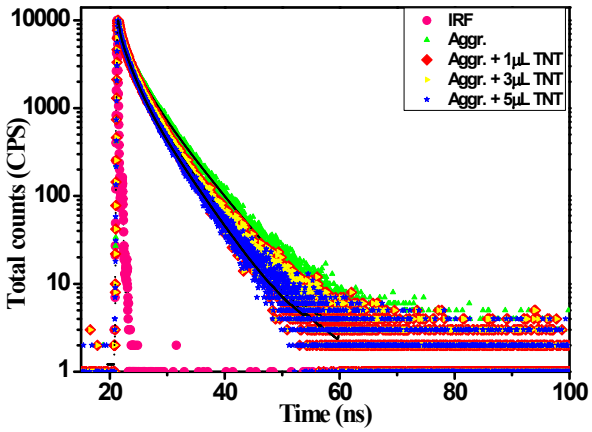


Fig S4 Lifetime decay plots of aggregated compound **1 and** after adding the TNT (10^{-8}M)

Table S1 Lifetime (ns) fluorescence parameters. λ_{ex}= 405 nm

	B_1'	B_2'	B_3'	τ_1	τ_2	τ_3	$<\tau>$	χ^2
Aggregate Of **1**	0.58	0.12	0.30	2.14	0.34	5.19	2.86	1.0
+1 µL TNT	0.56	0.34	0.10	1.98	4.88	0.33	2.80	1.01
+3 µL TNT	0.65	0.24	0.11	2.19	5.33	0.38	2.75	1.11
+5 µL TNT	0.62	0.27	0.11	1.93	4.79	0.34	2.54	1.03

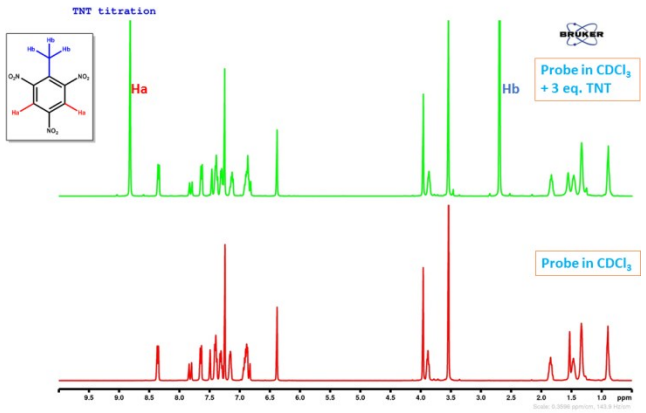


Fig S5a ^{1}H-NMR (400 MHz) spectra of the AIEgen in $CDCl_3$ and after addition of 3eq. TNT solution

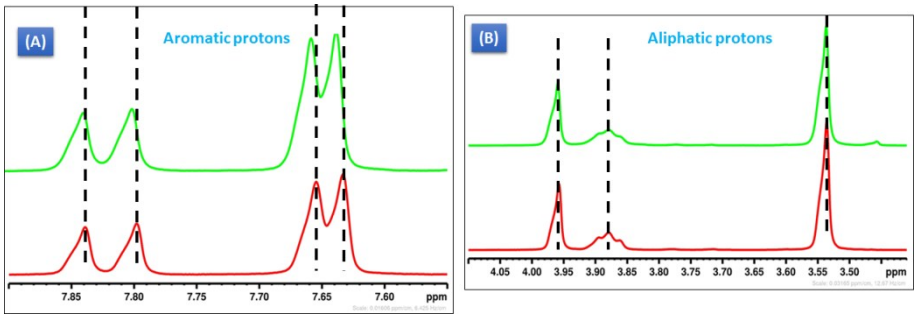


Fig S5b Expanded ^{1}H-NMR (400 MHz) spectra from Fig 4a of the AIEgen in $CDCl_3$ and after addition of 3eq. TNT solution (A) Showing the ^{1}H chemical shift (downfield) after the addition of 3 eq. of TNT; (B) Showing no shift in ^{1}H spectra after the addition of 3 eq. of TNT

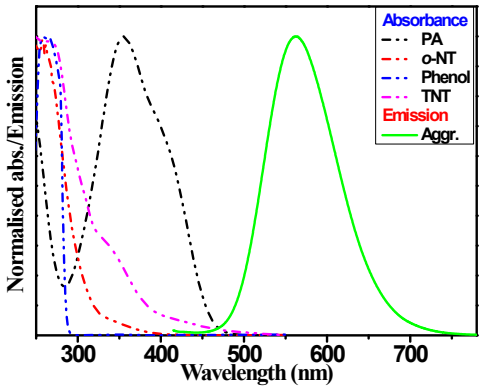


Fig S6 Absorption spectra of few analytes (left) and emission spectrum of AIEgen (green, right)

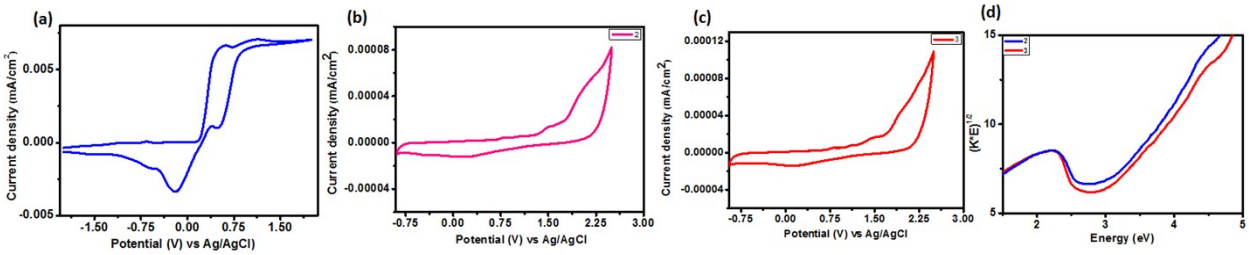


Fig S7 The cyclic voltammograms of compounds (a) **1** (b) **2** (c) **3** in dichloromethane (10^{-5} M) under inert atmosphere N_2 using Ag/AgCl as reference electrode. E_{LUMO} = -(Ered + 4.49), (d) Tauc plot for compounds **2** (blue) and **3** (red).

LUMO calculation for **1**: E^0_{red}= -0.731 vs Ag/AgCl = -1.221 vs Fe/Fe^+; LUMO= -(E^0_{red} + 4.8) =-(-1.221+4.8) = -3.579 eV; LUMO calculation for **2:** E^0_{red}= 0.167 vs Ag/AgCl = -0.323 vs Fe/Fe^+; LUMO= -(E^0_{red} + 4.8) =-(-0.323 +4.8) = -4.477 eV; LUMO calculation for **3:** E^0_{red}= 0.105 vs Ag/AgCl = -0.385 vs Fe/Fe^+ LUMO= -(E^0_{red} + 4.8) =-(-0.385 +4.8) = -4.415 eV. The LUMOs for **2** and **3** look be very low and therefore we have calculated the HOMO from CV and optical band gap from Tauc plot (suggested by one of the reviewers). The calculations are as follows:

HOMO Calculation for **2**: E^0_{oxd}= 2.19 vs Ag/AgCl = 1.7 vs Fe/Fe^+ HOMO= -(E^0_{oxd} + 4.8) =-(1.70 +4.8) = -6.50 eV
HOMO Calculation for **3**: E^0_{oxd}= 2.15 vs Ag/AgCl = 1.66 vs Fe/Fe^+ HOMO= -(E^0_{oxd} + 4.8) =-(1.66 +4.8) = -6.46 eV
From Tauc plot the the optical bandgap (E_g) for **2** was found to be 2.7 and for **3** it was 2.68. Therefore, the calculated LUMOs are: For **2**: E_g = LUMO – HOMO; 2.70 = LUMO – (-6.5), Thus LUMO = -3.80 eV; For **3**: E_g = LUMO – HOMO; 2.68 = LUMO – (-6.46); Thus LUMO = -3.78 eV.

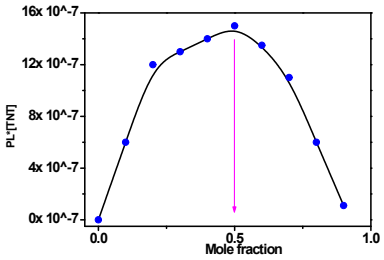


Fig S8 Job's plot confirming the binding of compound 1: TNT is 1:1

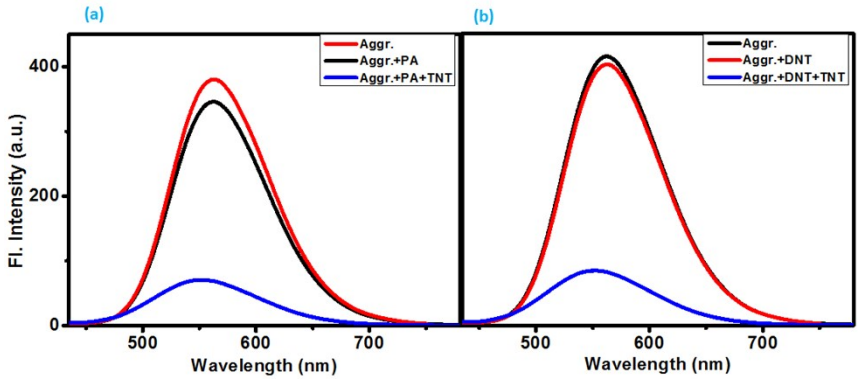


Fig S9 (a) Fl. spectra of aggregate **1** (10^{-5}M) , aggr.+ PA (10 µL, 10^{-3}M) and aggregate **1** +PA (10 µL, 10^{-3}M) + TNT (10 µL, 10^{-3}M); (b) Fl. spectra of aggregate **1** (10^{-5}M) , aggregate **1 +** DNT(10 µL, 10^{-3}M) and aggregate **1+** DNT (10 µL, 10^{-3}M) + TNT (10 µL, 10^{-3}M).

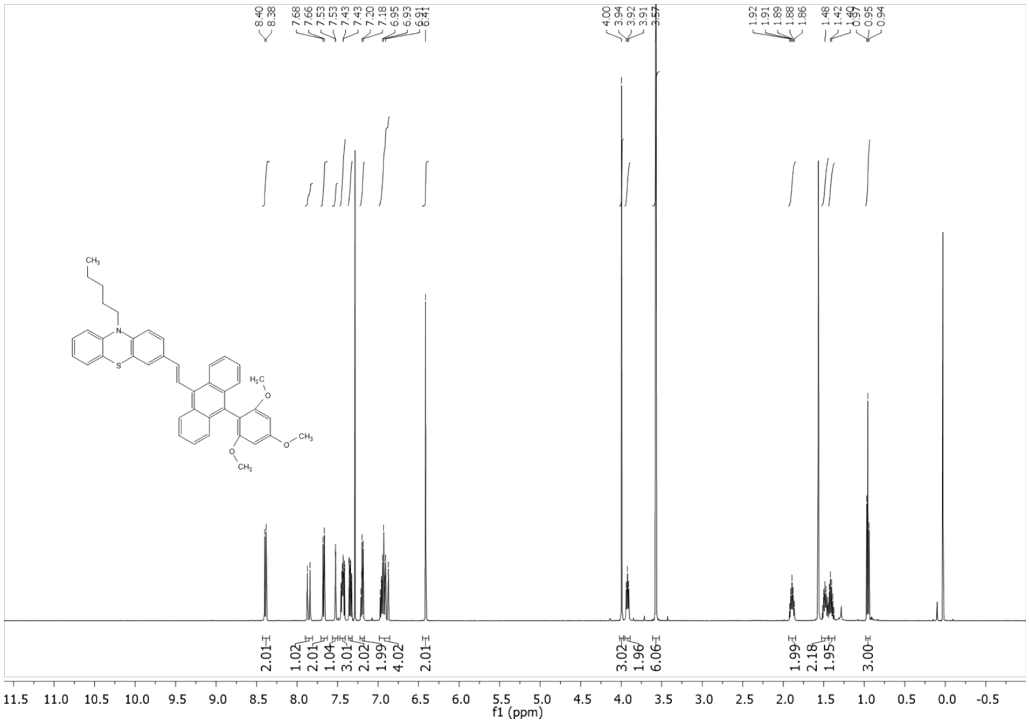


Fig S10 ^{1}H NMR spectrum of **1**

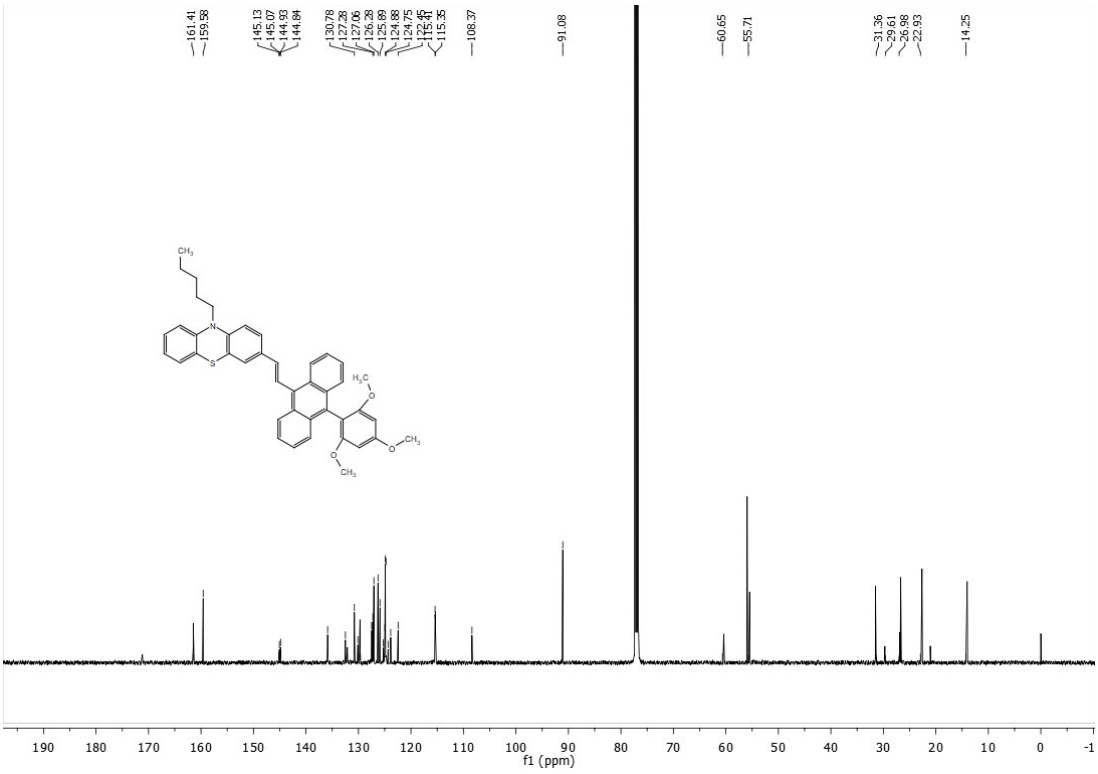


Fig S11 ^{13}C NMR spectrum of **1**

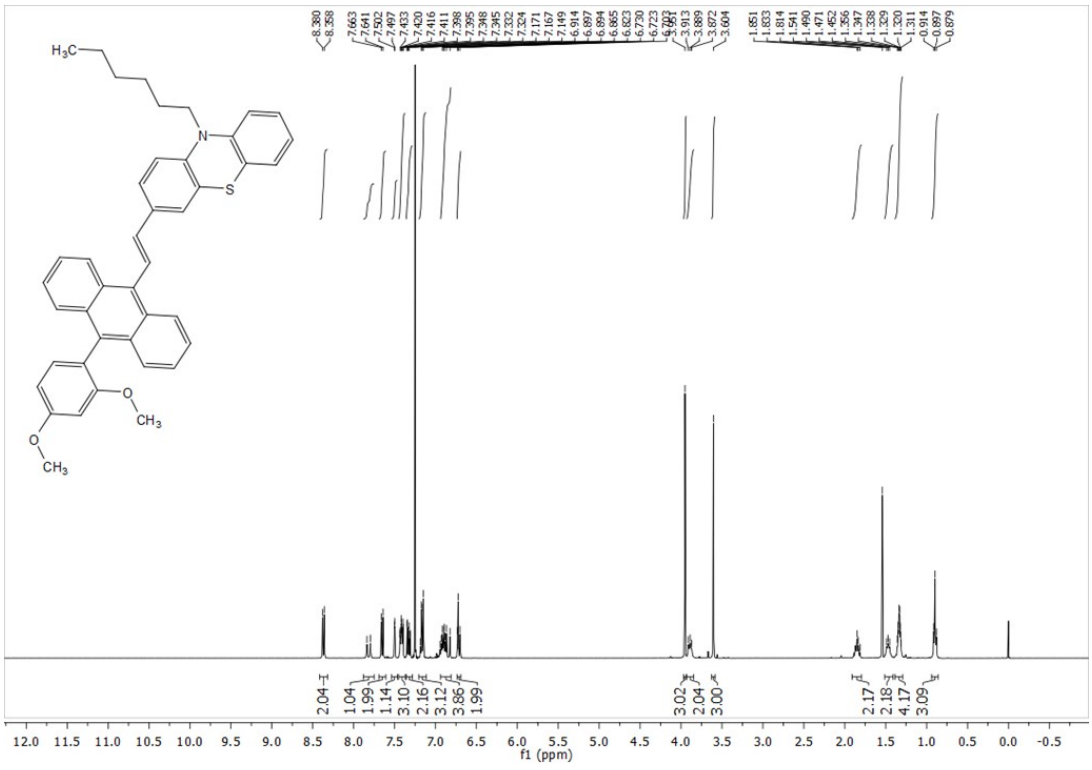


Fig S12 ^{1}H- NMR spectrum of **2.**

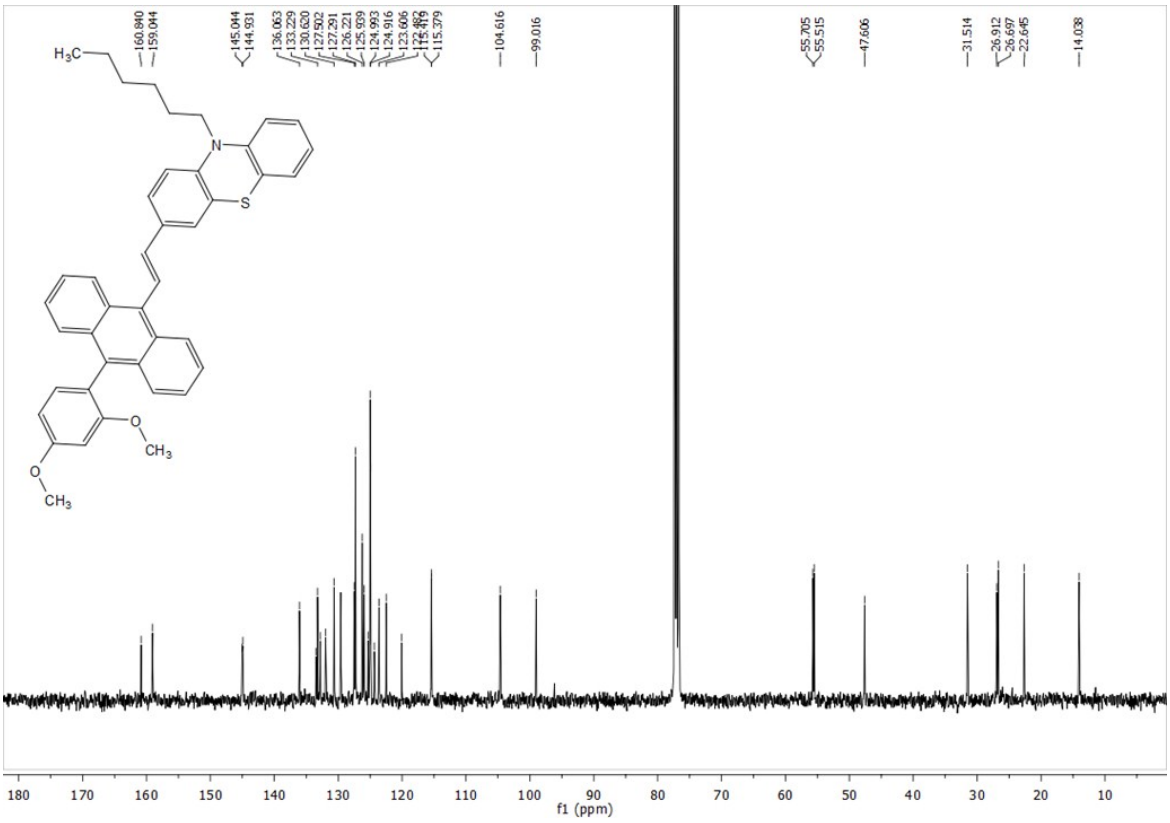


Fig S13 ^{13}C- NMR spectrum of **2.**

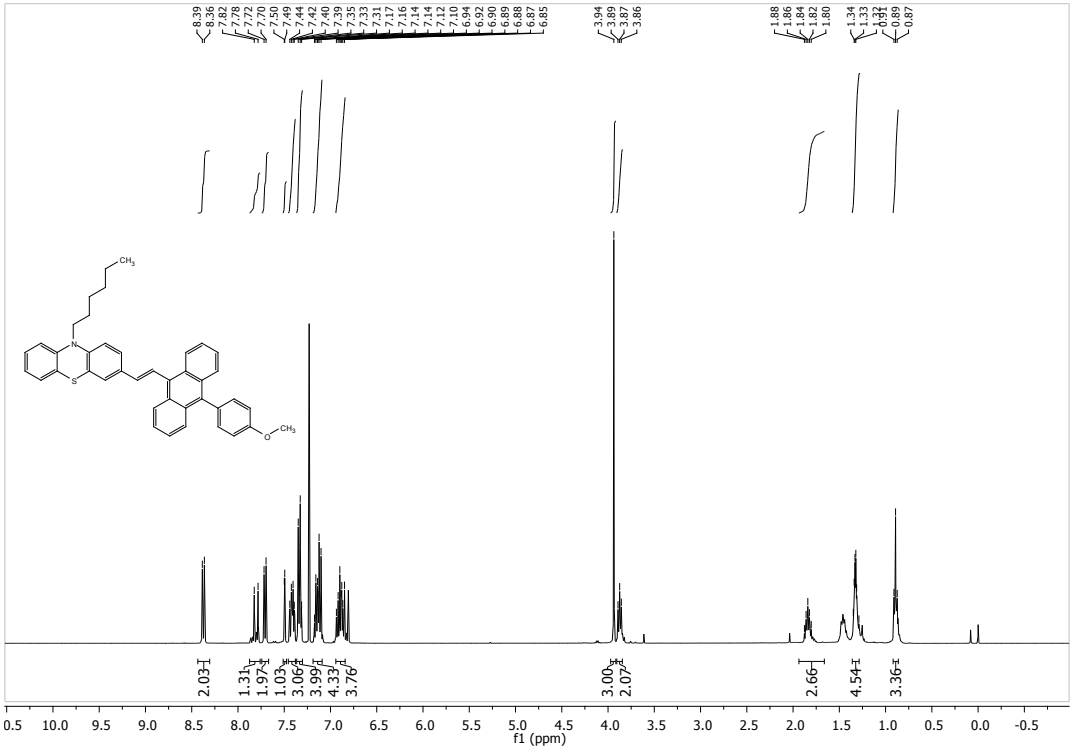


Fig S14 ^{1}H NMR spectrum of **3**

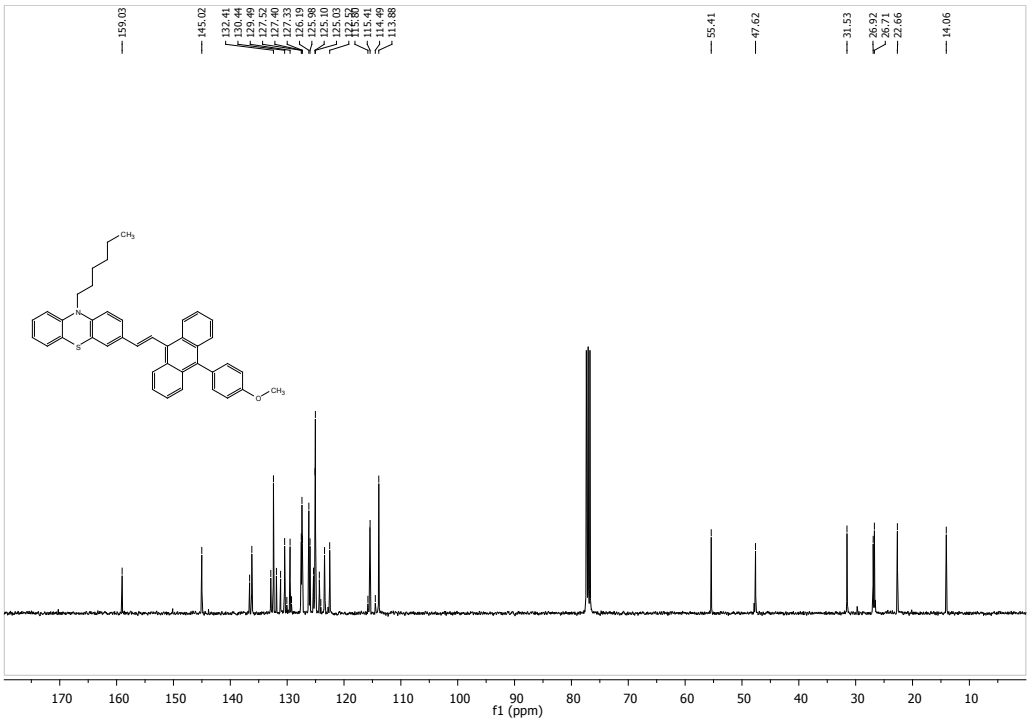


Fig S15 ^{13}C NMR spectrum of **3**

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