Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

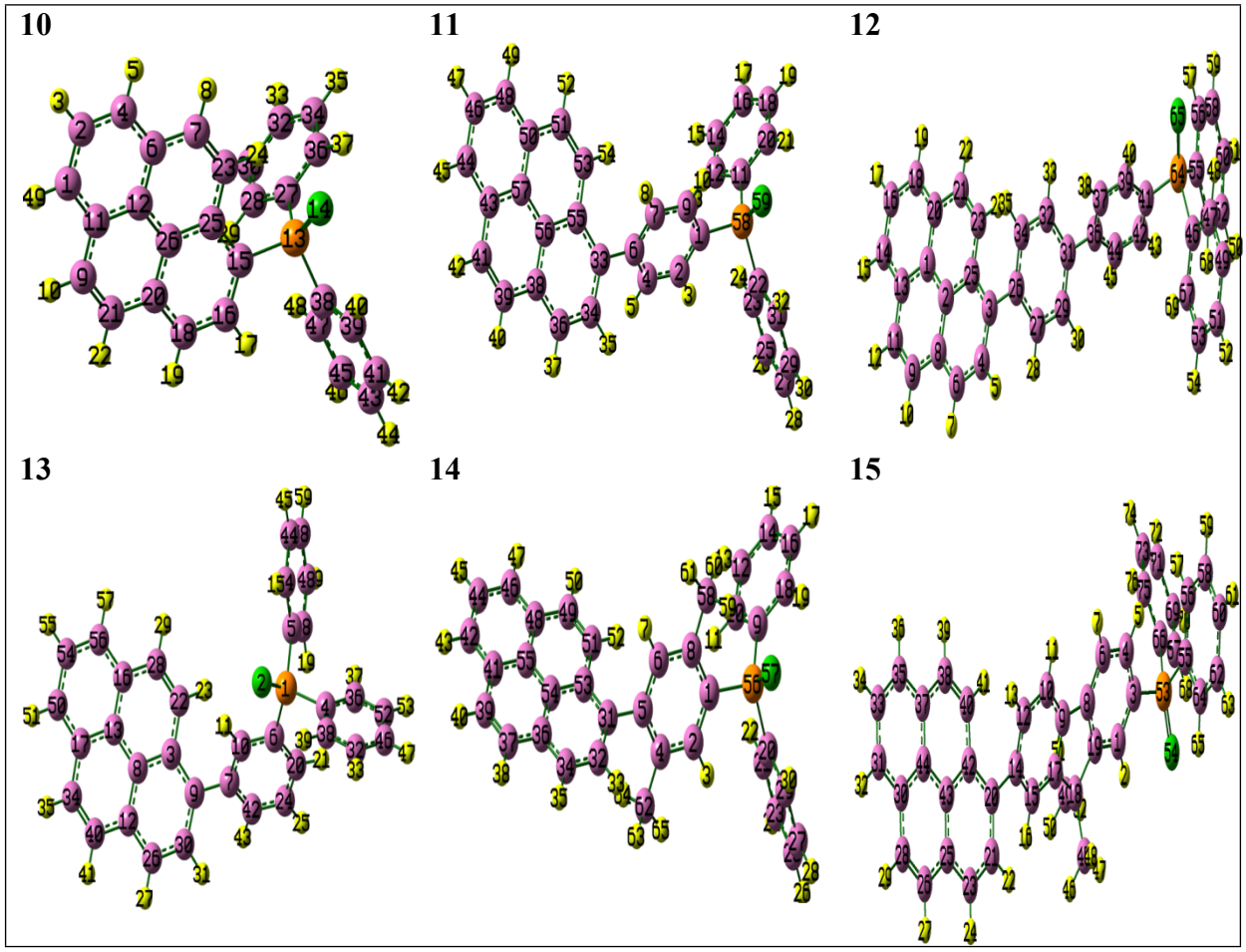
Supporting Information

Phosphine Oxide Functionalized Pyrenes as Efficient Blue Light Emitting Multifunctional Materials for Organic Light Emitting Diodes

Godumala Mallesham,[1,2] Chidirala Swetha,[1,2] Surukonti Niveditha,[2] Maneesha Esther Mohanty,[1] Nanubolu Jagadeesh Babu,[3,*] Arunandan Kumar,[4,*] Kotamarthi Bhanuprakash [2,5,*] and Vaidya Jayathirtha Rao ,[1,5,*]

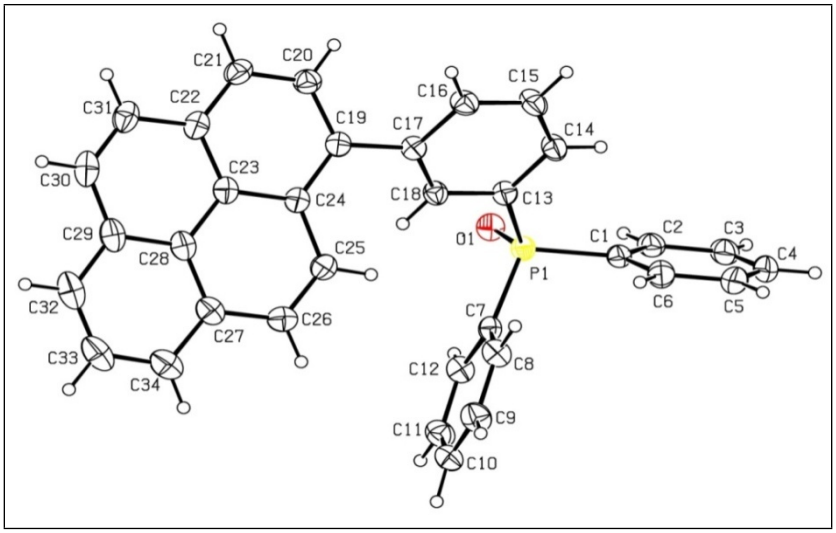
Table S1. Geometrical parameters of **10-15** calculated at B3LYP/6-311G(d,p) level of theory

.



10		11		12		13		14		15	
Torsion angles(^{0})											
C25C15P13O14	47	C9C1P58O59	24	C39C41P64O65	-28	C42C7C9C3	-127 (-136)	C8C1P56O57	51	C4C3P53O54	154
C25C15P13C38	170	C9C1P58C22	148	C39C41P64C46	94	C20C6P1O2	-153(-101)	C8C1P56C20	174	C4C3P53C55	31
C25C15P13C27	-76	C9C1P58C11	-98	C39C41P64C55	-152	C18C5P1O2	-154(-162)	C8C1P56C9	-72	C4C3P53C66	-81
		C55C33C6C4	-128	C25C3C26C27	-128	C36C4P1O2	-155(178)	C53C31C5C4	-105	C42C20C14C15	-127
				C32C31C36C44	-144						
Angles(^{0})											
C15P13O4	114.9	C1P58O51	112.4	C41P64O65	112.5	C6P1C5	106.0(105.7)	C1P56O57	114.3	C3P53O54	112.3
C15P13C38	106.8	C1P58C22	106.3	C41P64C46	106.2	C6P1C4	106.4(106.6)	C1P56C20	107.2	C3P53C55	106.4
C15P13C27	105.2	C1P58OC11	106.4	C41P64C55	106.3	C6P1O2	112.5(113.9)	C1P56C9	105.6	C3P53C56	106.5
Bond lengths(A^0)											
P13O14	1.506	P58O59	1.503	P64O65	1.503	P1O2	1.50(1.48)	P56O57	1.50	P53O54	1.50
P13C15	1.837	P58C1	1.830	P64C41	1.830	P1C6	1.83(1.80)	P56C1	1.835	P53C3	1.829
P13C38	1.833	P58C22	1.831	P64C46	1.831	P1C5	1.83(1.81)	P56C20	1.834	P53C66	1.832
P13C27	1.833	P58C11	1.832	P64C55	1.831	P1C4	1.83(1.80)	P56C9	1.833	P53C55	1.832

Table S2. Prominent intermolecular contacts observed in the crystal structure of **13**.



S.No	D-H…A	D-H /Å	H…A /Å	D…A /Å	∠D-H…A /°
1	C2-H2…O1[i]	0.93	2.66	3.371(2)	133.6
2	C30-H30…O1[ii]	0.93	2.76	3.651(2)	159.7
3	C15-H15…O1[iii]	0.93	2.78	3.472(2)	131.5
4	R1…R4[ii]	-	-	3.825(2)	-
5	R2…R3[ii]	-	-	3.882(2)	-
[i] 1-x, 1-y, -z; [ii] -x, 1-y, 1-z; [iii] -x,1-y,-z; R1 = ring centroid of C19-C20-C21-C22-C23-C24; R2 = ring centroid of C23-C24-C25-C26-C27-C28; R3 = ring centroid of C22-C23-C28-C29-C30-C31; R4 = ring centroid of C27-C28-C29-C32-C33-C34.					

Table S3. UV-Vis absorption data of compounds **10-15** in different solvents (1 x 10^{-5} M) and in thin film state.

Compound	Hexane (nm)	Toluene (nm)	$CHCl_3$ (nm)	EtOAc (nm)	DMF (nm)	CH_3CN (nm)	CH_3OH (nm)	Film
10	280, 336, 351	282, 339, 353	282, 340, 353	280, 336, 351	281, 337, 352	280, 335, 351	280, 336, 352	292, 347, 350
11	278, 343	283, 348	281, 347	278, 344	281, 347	279, 344	278, 344	292, 354
12	279, 344	284, 350	281, 347	279, 344	280, 347	278, 344	278, 344	296, 358
13	279, 345	282, 348	281, 348	279, 344	281, 347	278, 345	278, 345	291, 354
14	277, 326, 341	282, 330, 345	279, 330, 345	276, 327, 342	278, 329, 344	276, 327, 342	276, 326, 341	334, 350
15	347	350	350	348	350	350	348	360

Table S4: Delayed fluorescence lifetimes of compound 13.

[13]	**Delayed Fluorescence (μs)**	
	τ_1	τ_2
10^{-2} M	9	97
10^{-5}M	7.5	-

Figure S1 . Comparing crystal structure with obtained lowest energy DFT isomers

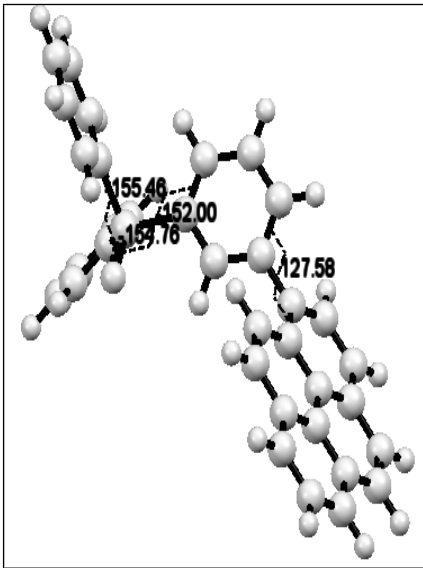
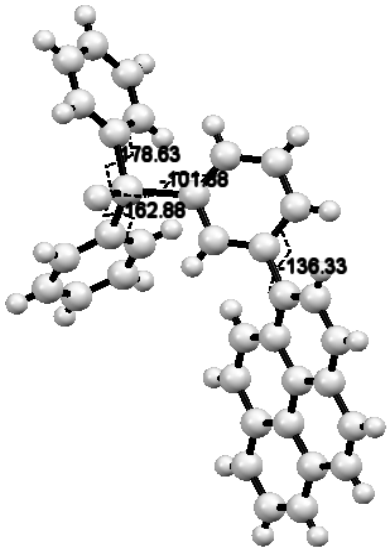
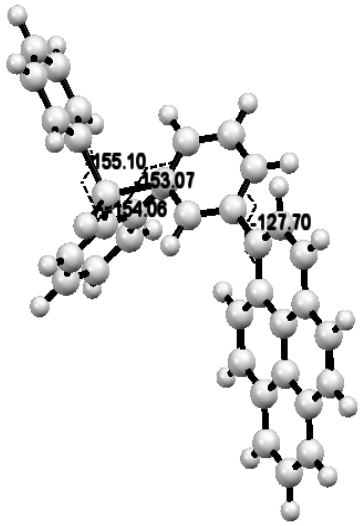
		
DFT-isomer1	X-ray Crystal structure of 13	DFT-isomer2

Figure. S2. Cyclic voltammograms of the compounds **10-15** recorded in dry THF.

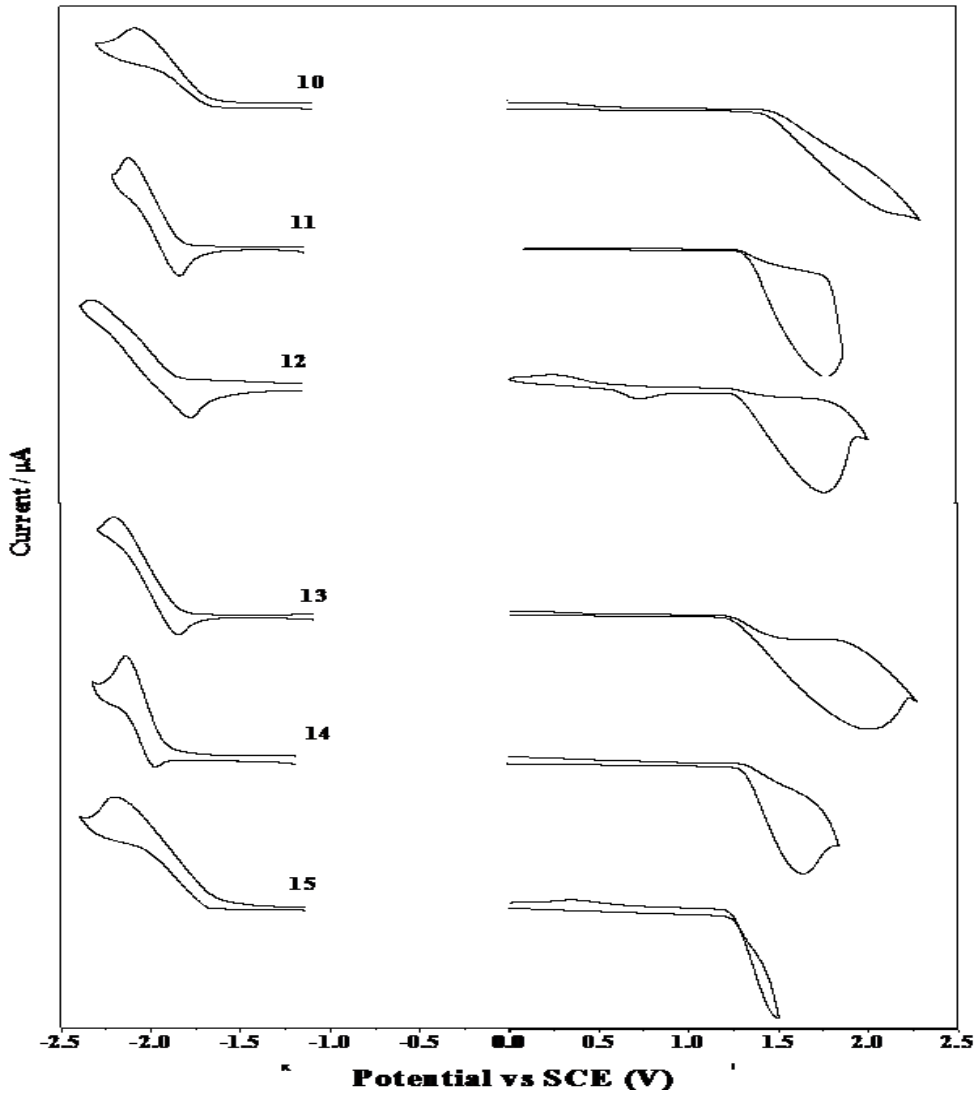


Figure S3. UV-Vis absorption spectra of compounds **10-15** in different polar solvents (1 x 10^{-5} M) and thin film state.

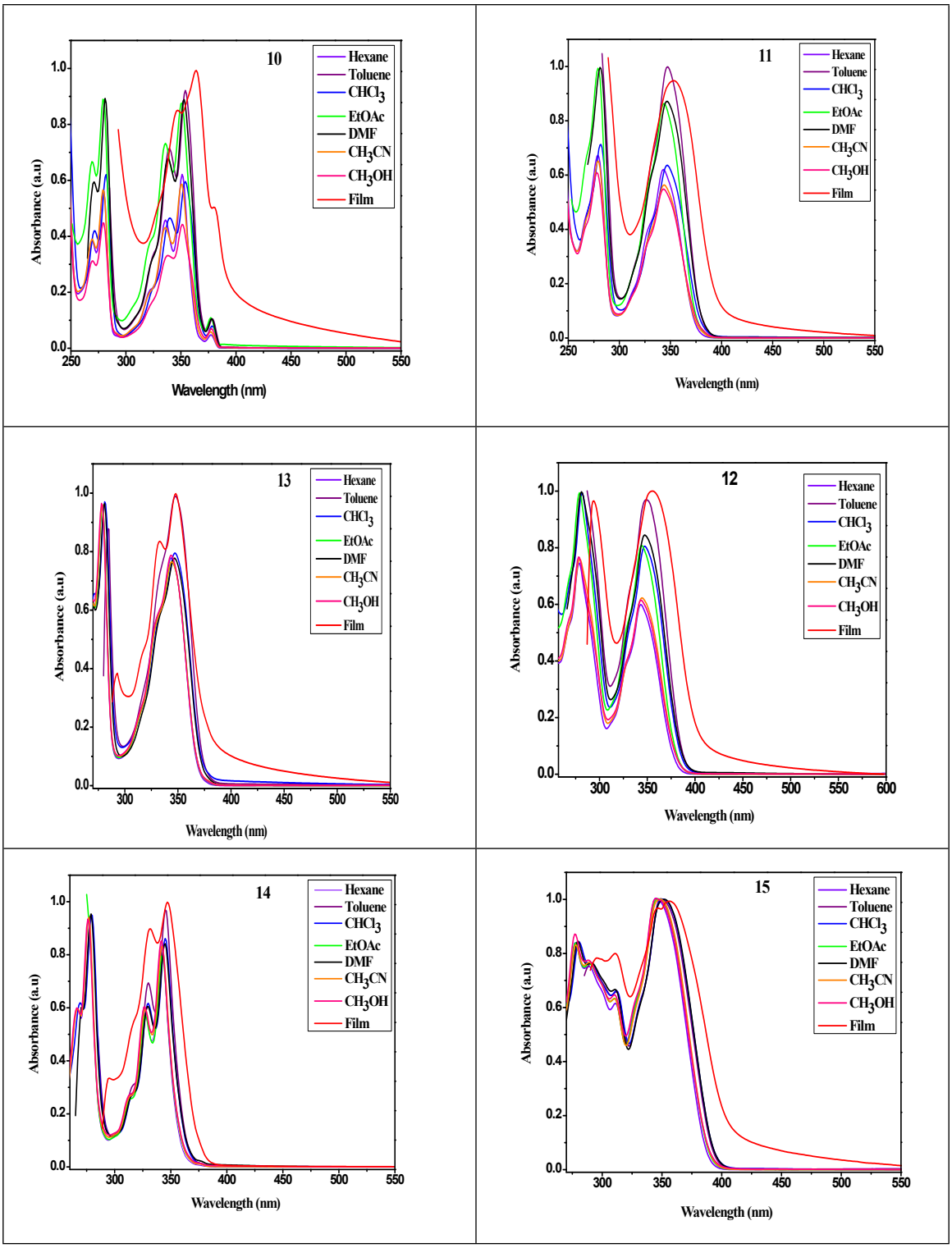

10
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)
11
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)
13
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)
12
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)
14
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)
15
Hexane
Toluene
CHCl3
EtOAc
DMF
CH3CN
CH3OH
Film
Absorbance (a.u)
Wavelength (nm)

Figure S4. Photoluminescence spectra of compounds **10-15** (excited at their maximum absorption wavelengths)in different polar solvents (1 x 10^{-5} M) and thin film state.

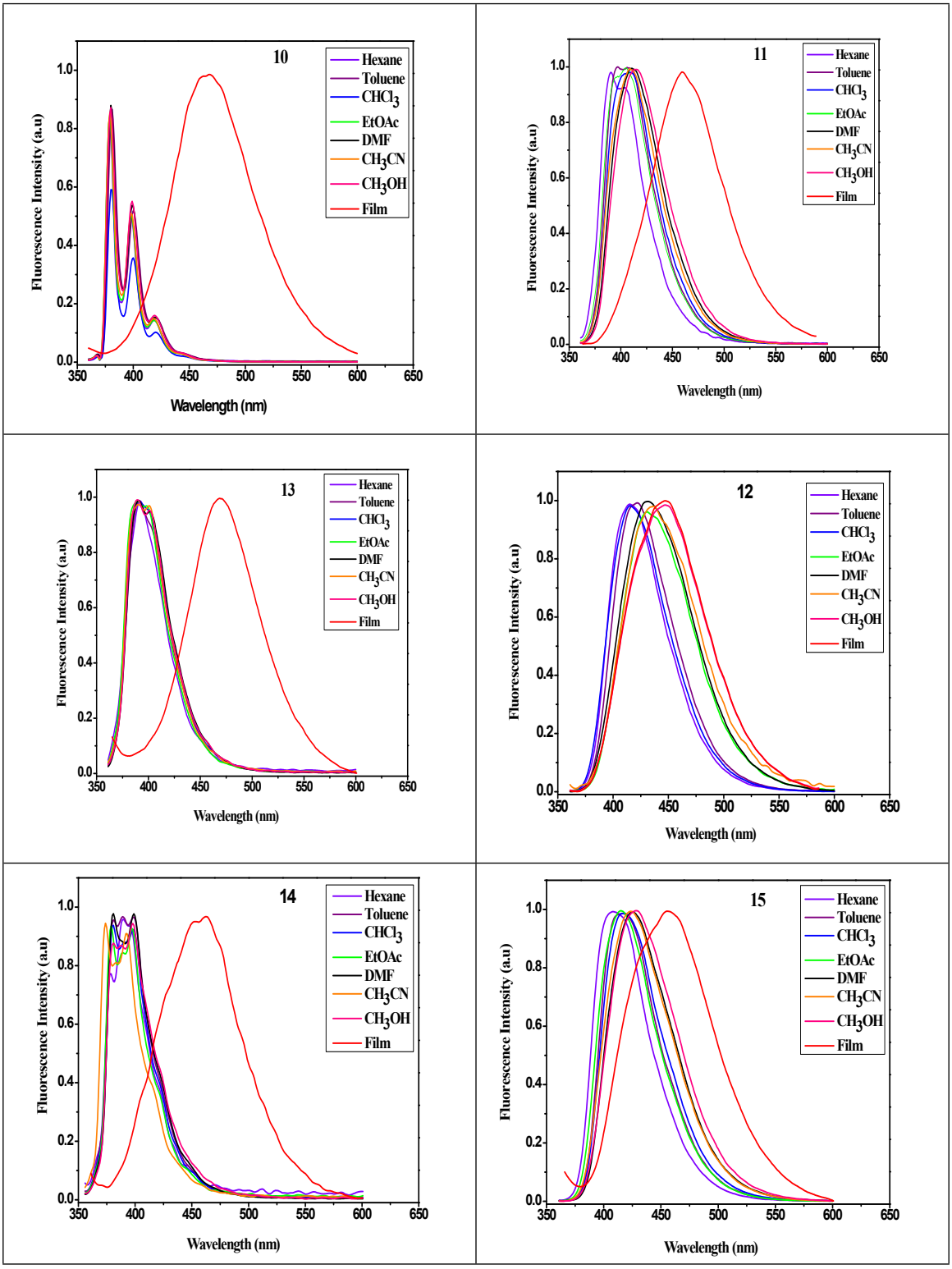


Figure S5. Photoluminescence spectra of compounds **10-15** (excited at their maximum absorption wavelengths) in chloroform at different concentrations.

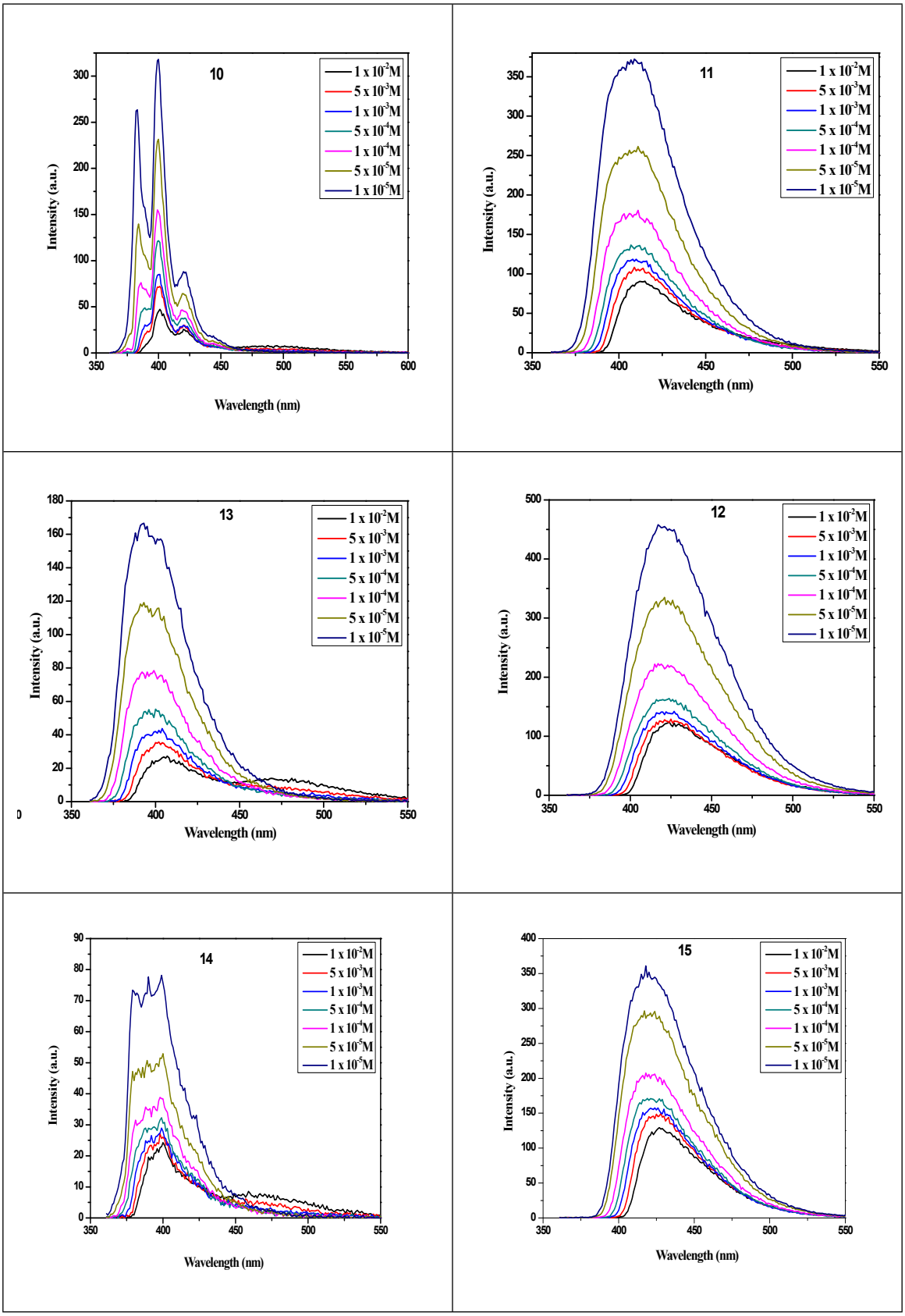


Figure S6: Lifetime decays of **13** at 10^{-5}M concentration

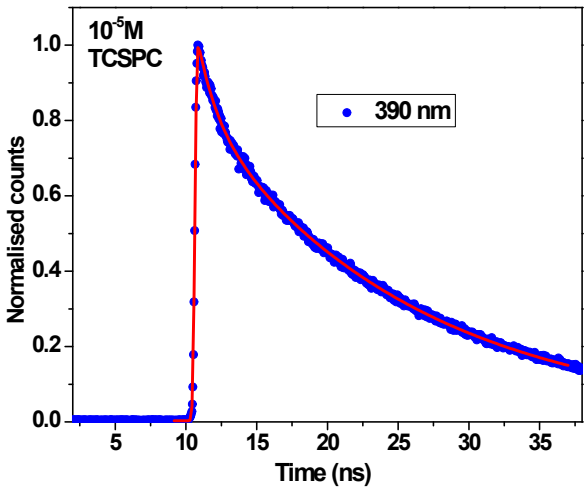


Figure S7 a). TGA plots of compounds **10-15** at a heating rate of 10 ^{o}C min^{-1}.

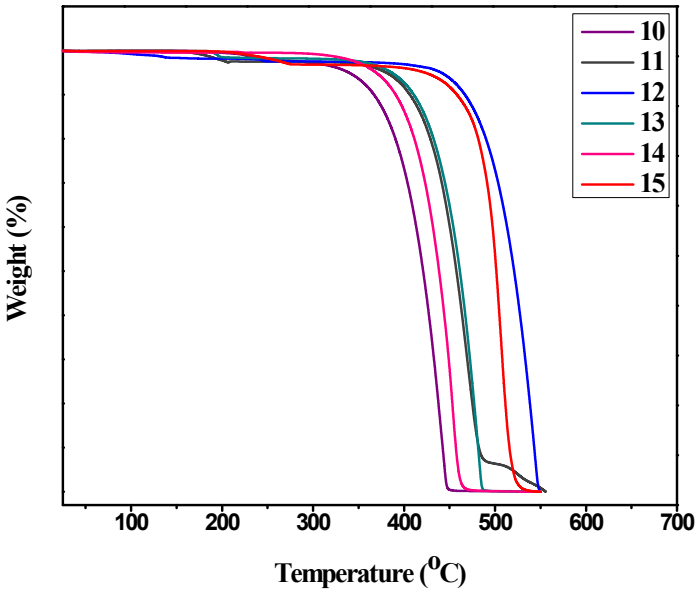


Figure S7 b). DSC traces of derivatives **10-15** at a heating rate of 10 ^{o}C min^{-1}.

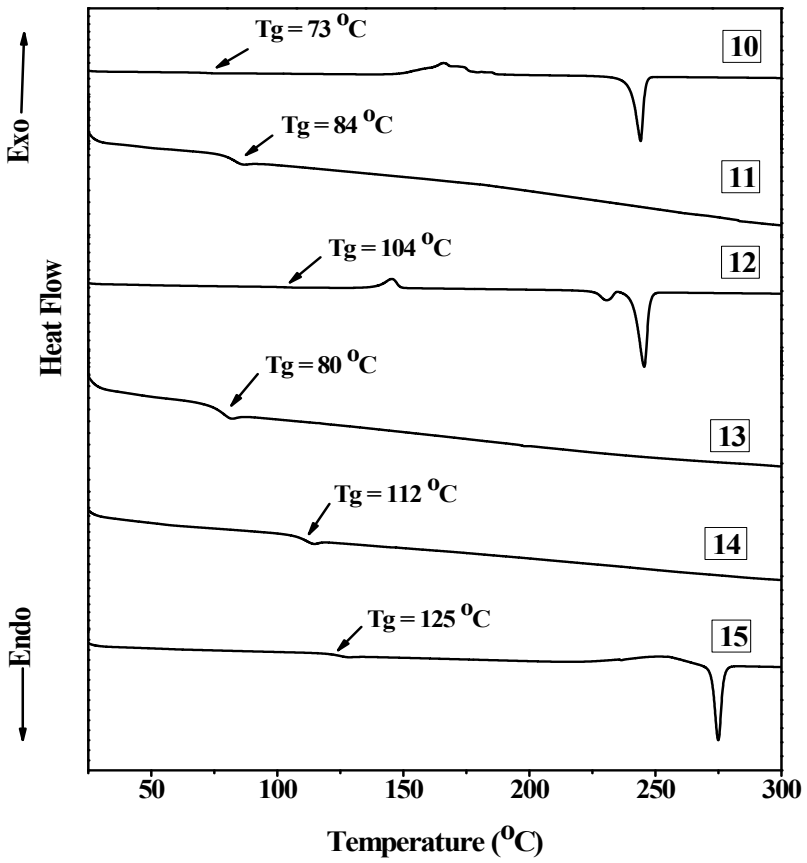


Figure S8. CIE diagram of compounds **10-15**

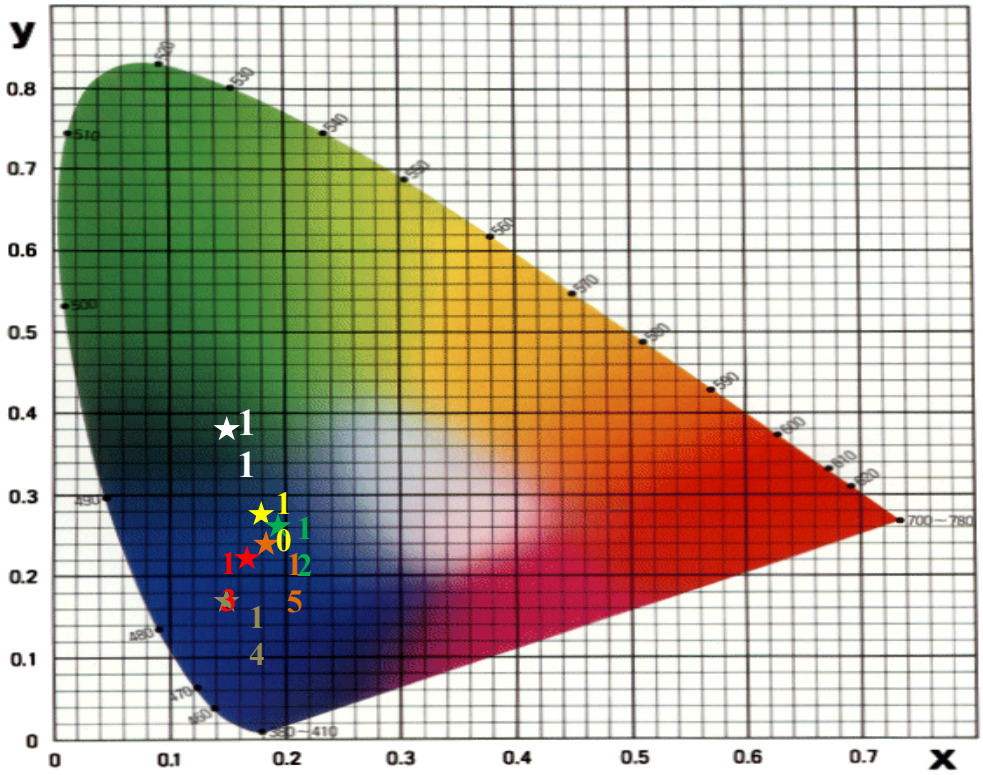


Figure S9a. ^{1}H NMR spectrum of compound **10**.

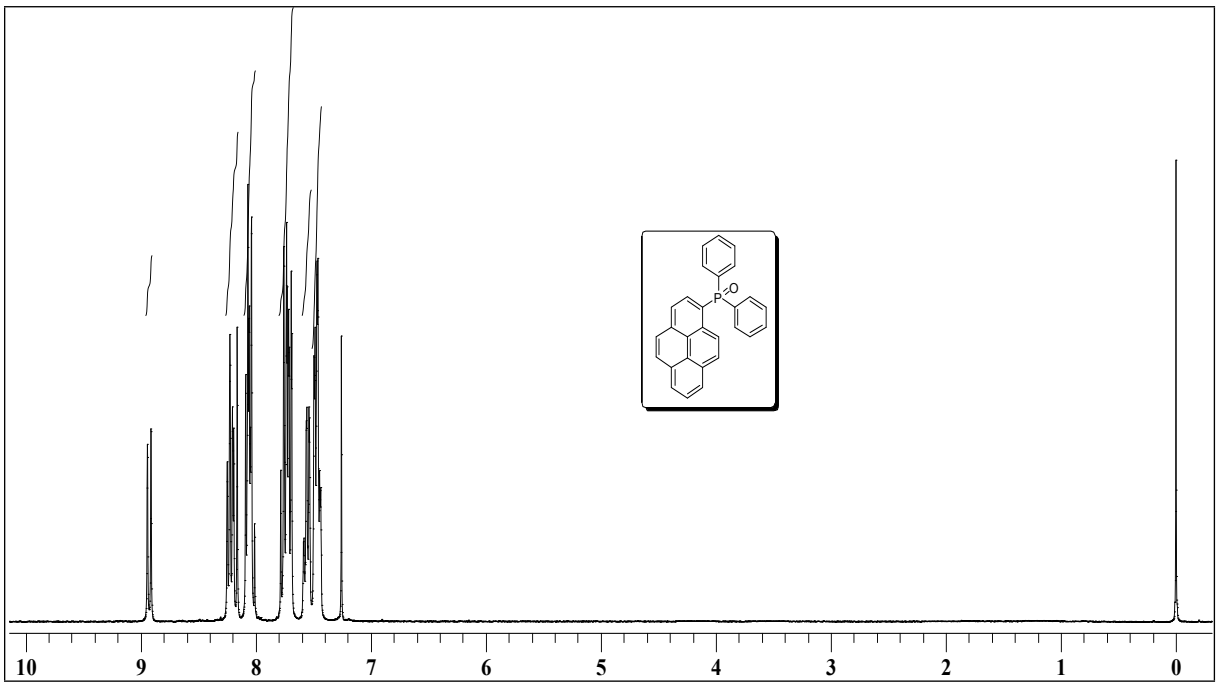


Figure S9b. ^{13}C NMR spectrum of compound **10**.

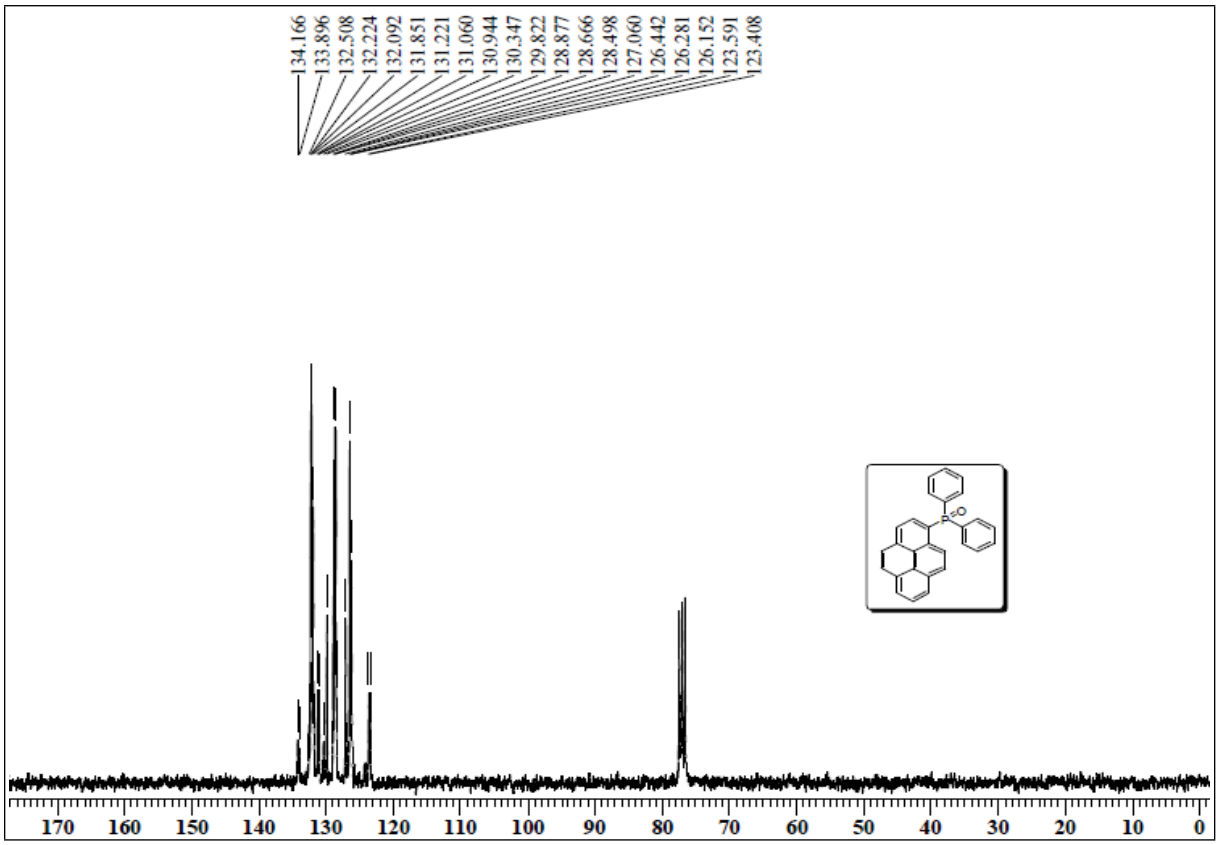


Figure S10a. ^{1}H NMR spectrum of compound **11**.

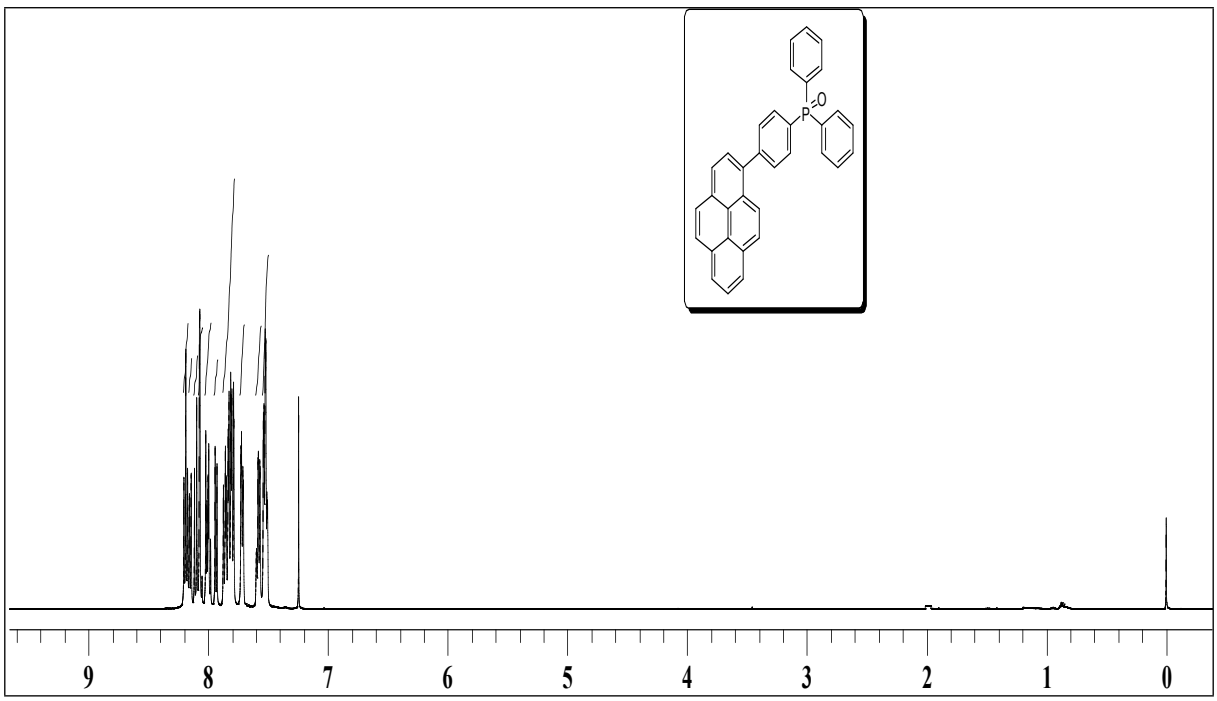


Figure S10b. ^{13}C NMR spectrum of compound **11**.

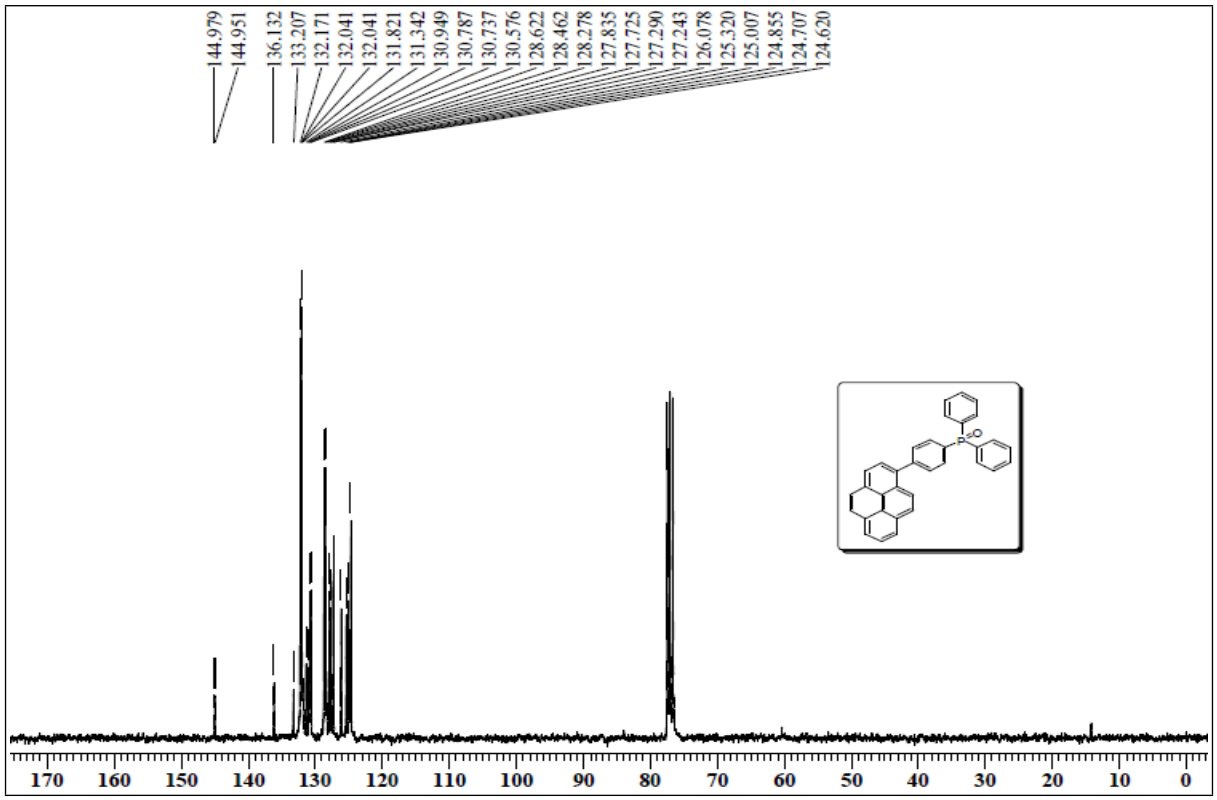


Figure S11a. ^{1}H NMR spectrum of compound **12**.

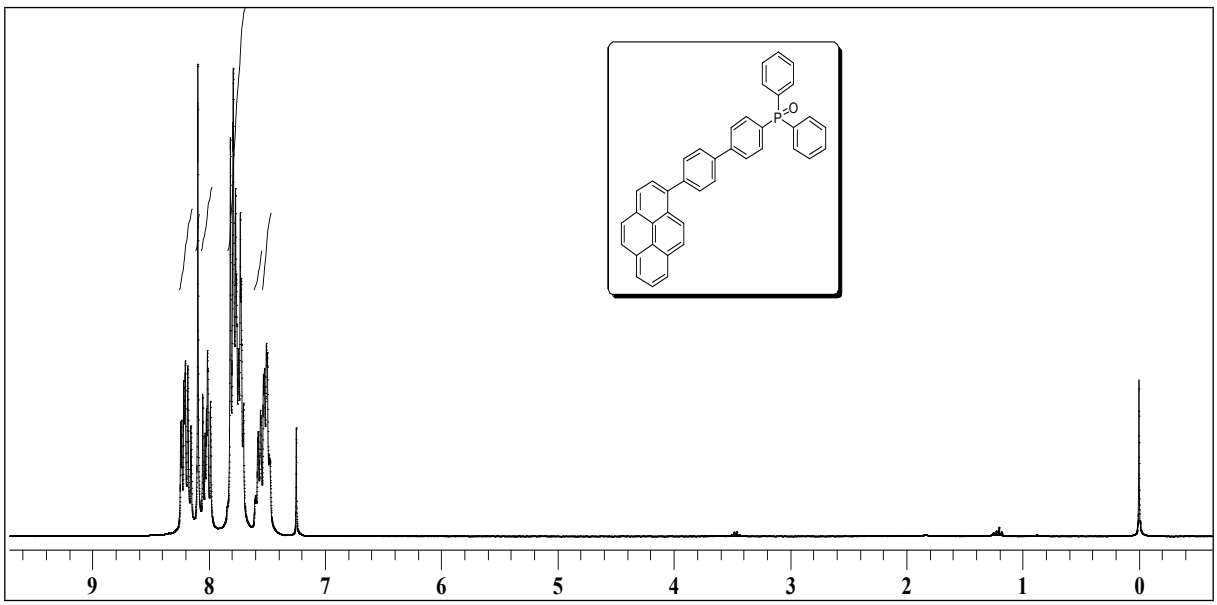


Figure S11b. ^{13}C NMR spectrum of compound **12**.

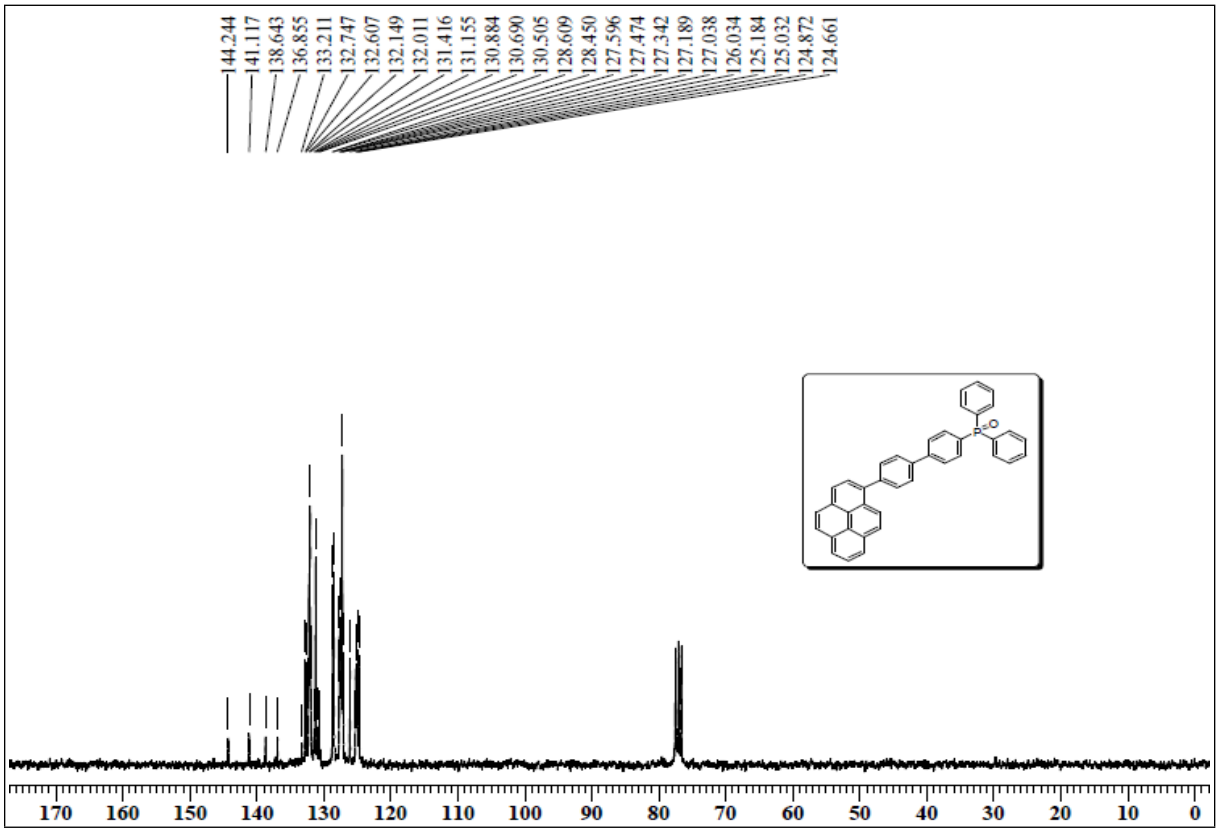


Figure S12a. ^{1}H NMR spectrum of compound **13**.

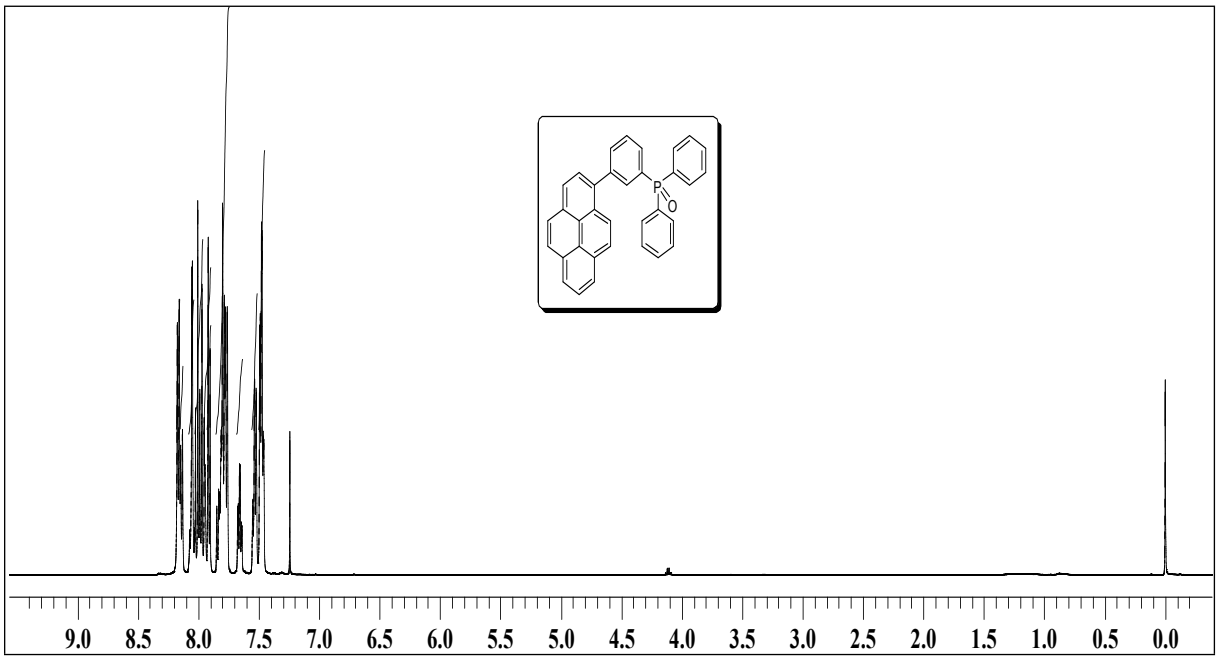


Figure S12b. ^{13}C NMR spectrum of compound **13**.

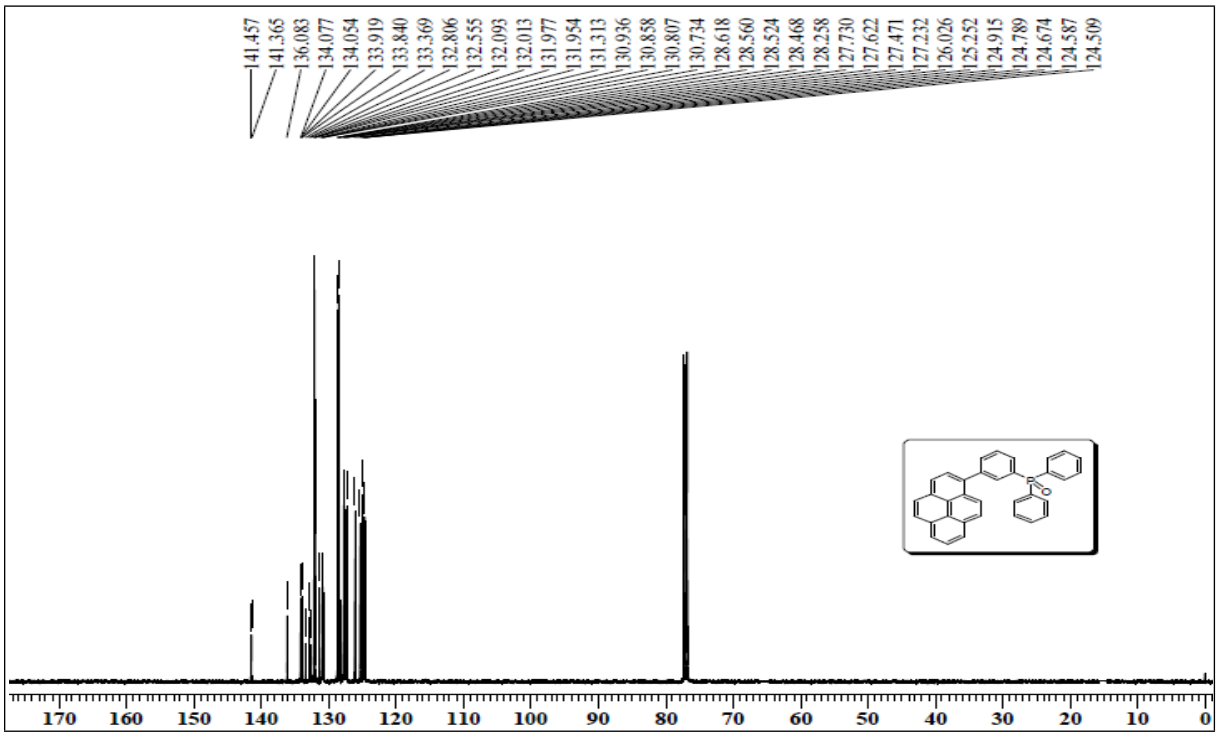


Figure S13a. ^{1}H NMR spectrum of compound **14**.

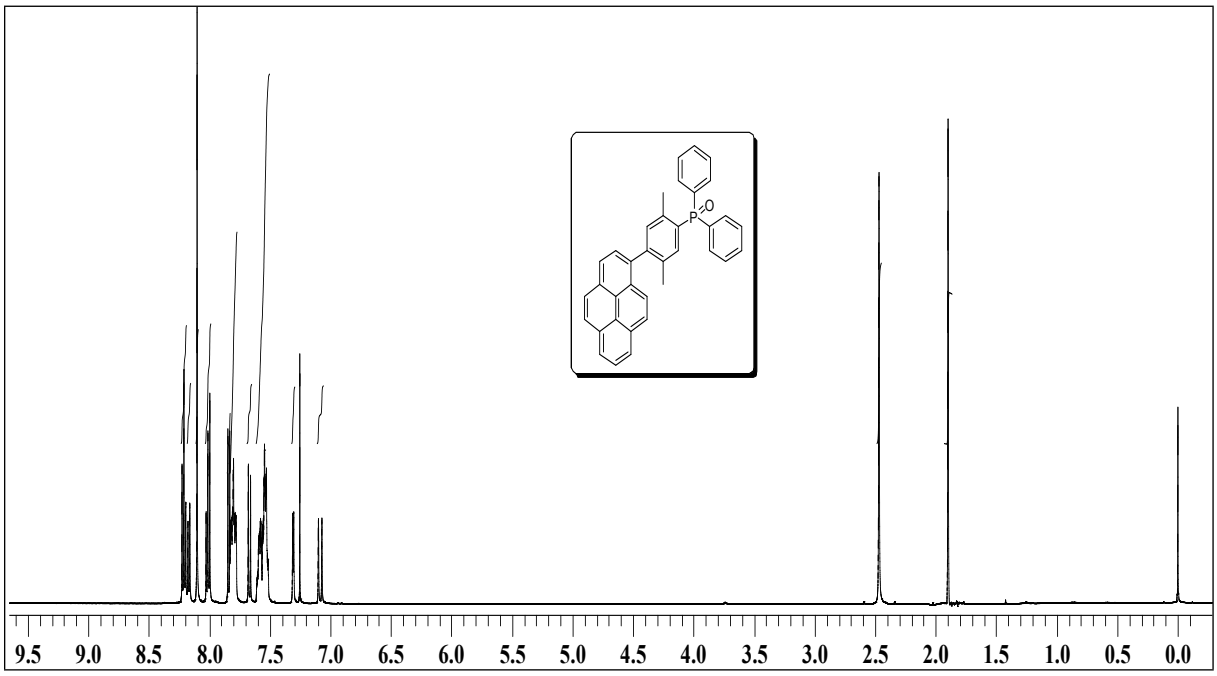


Figure S13b. ^{13}C NMR spectrum of compound **14**.

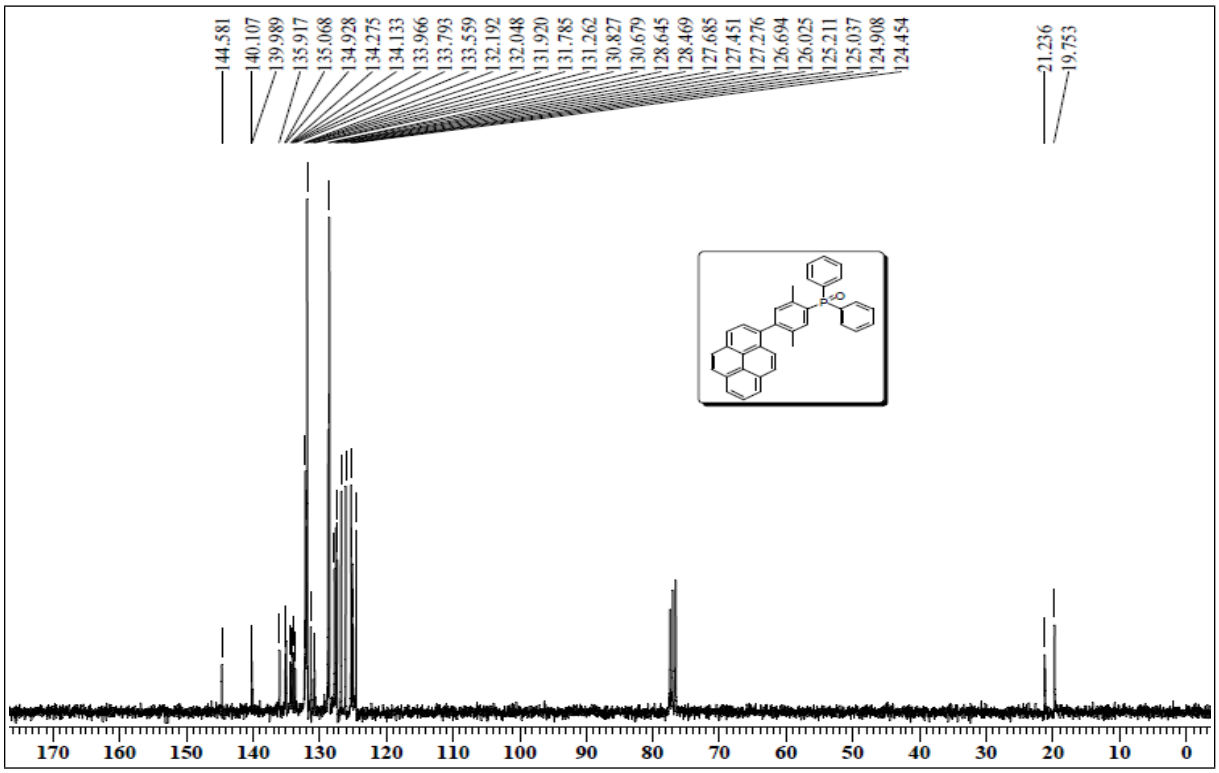


Figure S14a. ^{1}H NMR spectrum of compound **15**.

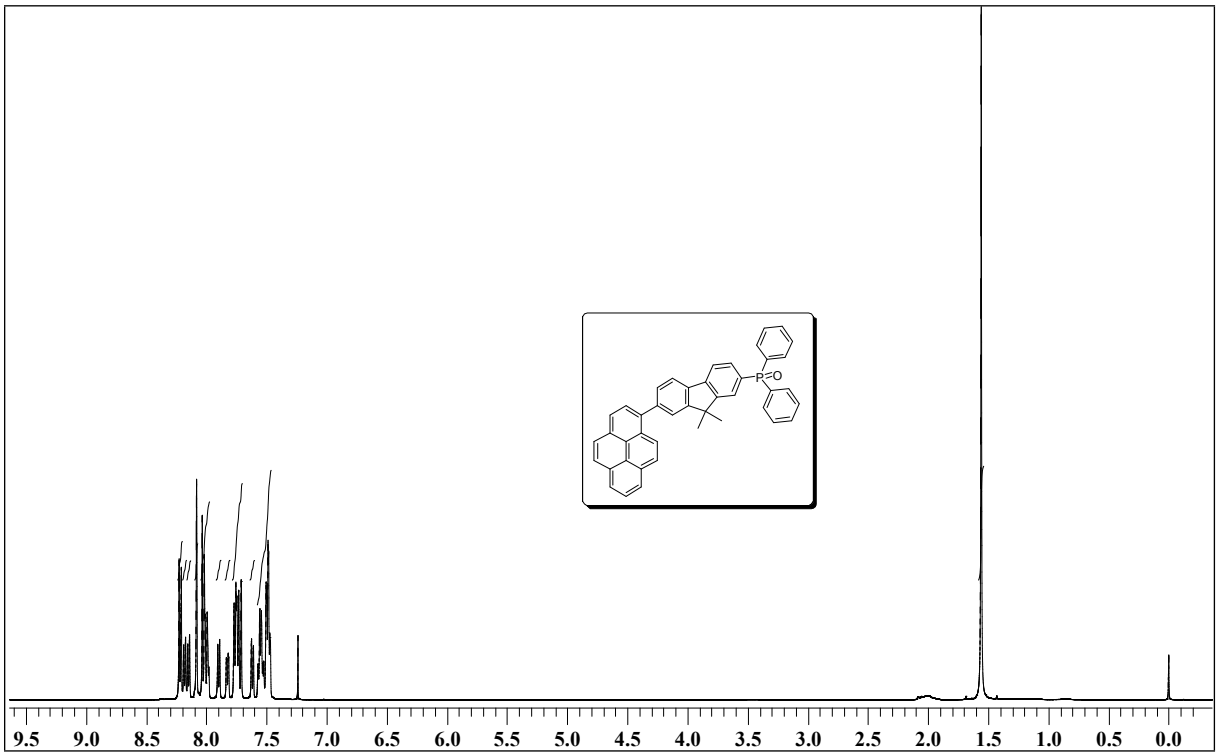


Figure S14b. ^{13}C NMR spectrum of compound **15**.