Electronic Supplementary Material (ESI) for Materials Advances.

Carbazole-Acenaphthene (Donor-Acceptor) based luminophores for picric acid detection: a combined experimental and theoretical study

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NMR data:

8-(4-(9H-carbazol-9-yl)phenyl)-7-phenyl-7H-acenaphtho[1,2-d]imidazole (AC-1): yellow solid (0.75 g, 45%), **^{1}H NMR Data** (400 MHz)**:** 8.15-8.17 (2H, d), 8.01-8.03 (1H, d), 7.76-7.79 (3H, t), 7.60-7.65 (7H, m), 7.53-7.55 (2H, d), 7.40-7.47 (6H, m), 7.30-7.34 (2H, td), 7.27-7.28 (2H, d).**^{13}C NMR Data** (100 MHz): 149.43, 148.03, 140.45, 138.72, 137.82, 137.54, 131.66, 130.38, 129.97, 129.71, 129.44, 129.40, 128.92, 127.81, 127.06, 126.88, 126.76, 126.58, 126.51, 126.08, 125.89, 123.44, 120.74, 120.22, 120.05, 118.79, 109.68. m/z = calcd 509.19, Found: 510.15. Anal. calcd for $C_{37}H_{23}N_3$:C, 87.21; H, 4.55; N, 8.25 Found: C, 87.09; H, 4.37; N, 8.11.

8-(4-(9H-carbazol-9-yl)phenyl)-7-p-tolyl-7H-acenaphtho[1,2-d]imidazole (AC-2): yellow solid (0.80 g, 52%), **^{1}H NMR Data** (400 MHz)**:** 8.14-8.16 (2H, d, J = 8.15), 7.99-8.01 (1H, d, J = 8), 7.78-7.80 (2H, d, J = 7.79), 7.70-7.76 (2H, t, J = 7.74), 7.59-7.62 (1H, d, J = 7.60), 7.50-7.54 (4H, dd, J = 7.52), 7.39-7.54 (8H, m), 7.28-7.33 (2H, m), 7.25-7.27 (1H, d, J = 7.26), 2.53 (3H, s). **^{13}C NMR Data** (100 MHz): 140.51, 139.05, 138.91, 137.48, 135.23, 131.72, 130.61, 129.69, 129.56, 129.47, 127.84, 126.92, 126.87, 126.55, 125.93, 125.85, 123.46, 120.71, 120.26, 118.85, 30.86. m/z = calcd 523.20, Found: 524.20. Anal. calcd for $C_{38}H_{25}N_3$:C, 87.16; H, 4.81; N, 8.02 Found: C, 87.11; H, 4.75; N, 8.13.

8-(4-(9H-carbazol-9-yl)phenyl)-7-(9,9-diethyl-9H-fluoren-2-yl)-7H-acenaphtho[1,2-d]imidazole (AC-3): yellow solid (0.86 g, 59%), **^{1}H NMR Data** (400 MHz)**:** 8.12-8.16 (2H, t, J = 8.14), 7.97-8.05 (2H, dt, J = 8.01), 7.83-7.85 (2H, d, J = 7.84), 7.75-7.77 (3H, d, J = 7.76), 7.62-7.64 (1H, d, J = 7.63), 7.47-7.53 (2H, d, J = 7.63), 7.47-7.53 (2H, dd, J = 7.50), 7.39-7.42 (7H, m), 7.29-7.30 (6H, m), 2.02-2.07 (4H, m), 1.28 (3H, s), 0.87 (3H, s). **^{13}C NMR Data** (100 MHz): 151.94, 149.95, 149.41, 147.89142.32, 140.46, 140.02, 138.83, 137.49, 36.35, 134.13, 131.68, 131.48, 130.35,

129.77, 129.52, 129.46, 128.18, 127.96, 127.87, 127.20, 127.07, 126.92, 126.61, 126.08, 125.86, 124.54, 123.27, 122.98, 121.02, 120.86, 120.23, 120.09, 120.02, 119.92, 118.74, 109.61, 56.50, 32.57, 30.02, 29.61, 8.47. m/z = calcd 653.28, Found: 654.37. Anal. calcd for $C_{45}H_{35}N_3$:C, 88.18; H, 5.40; N, 6.43 Found: C, 88.09; H, 5.28; N, 6.26.

8-(4-(9H-carbazol-9-yl)phenyl)-7-(3-(trifluoromethyl)phenyl)-7H-acenaphtho[1,2-d]imidazole (AC-4): yellow-orange solid (0.45 g, 49%), **^{1}H NMR Data** (400 MHz): 8.67-8.69 (2H, dd, J = 8.68), 8.31-8.33 (2H, dd, J = 8.32), 8.15-8.17 (2H, m), 8.02-8.04 (1H, d, J = 8.03), 7.72-7.81 (7H, m), 7.57 (3H, m), 7.45 (3H, m), 7.30-7.34(2H, m).**^{13}C NMR Data** (100 MHz): 134.48, 132.29, 131.70, 130.65, 129.9, 129.73, 127.90, 127.40, 127.0, 126.78, 125.95, 121.06, 120.23, 120.1, 118.73, 109.76, 109.57. m/z = calcd 577.18, Found:578.35. Anal. calcd for $C_{38}H_{22}F_3N_3$:C, 79.02; H, 3.84; N, 7.27 Found: C, 79.10; H, 3.77; N, 7.16.

8-(4-(9H-carbazol-9-yl)phenyl)-7-(4-(trifluoromethyl)phenyl)-7H-acenaphtho[1,2-d]imidazole (AC-5): yellow solid (0.55 g, 43%), **^{1}H NMR Data** (400 MHz)**:** 8.15-8.17 (1H, d, J = 8.16), 8.0-8.02 (1H, d, J = 8.09), 7.91-7.93 (1H, d, J = 7.92), 7.77-7.81 (3H, dd, J = 7.79), 7.73-7.75 (2H, d, J = 7.74), 7.63-7.67 (4H, t, J = 7.65), 7.57-7.60 (4H, m), 7.43-7.47 (4H, m), 7.28-7.34 (3H, m). **^{13}C NMR Data** (100 MHz): 140.82, 140.31, 138.05, 129.87, 129.51, 128.73, 127.92, 127.48, 127.22, 127.1, 126.95, 126.93, 126.63, 126.40, 126.30, 126.27, 126.1, 125.97, 123.50, 121.07, 120.2, 119.16, 118.91, 109.61. m/z = calcd 577.18, Found: 578.35. Anal. calcd for $C_{38}H_{22}F_3N_3$:C, 79.02; H, 3.84; N, 7.27 Found: C, 79.11; H, 3.86; N, 7.24.

3-(8-(4-(9H-carbazol-9-yl)phenyl)-7H-acenaphtho[1,2-d]imidazol-7-yl)benzonitrile(AC-6): yellow solid (0.72 g, 61%), **^{1}H NMR Data** (400 MHz)**:** 8.15-8.17 (2H, d, J = 8.16), 8.02-8.04 (1H, d, J = 8.03), 7.96 (1H, d, J = 7.96), 7.88-7.91 (2H, m), 7.78-7.82 (3H, m), 7.71-7.74 (2H, d, J = 7.73), 7.62-7.66 (1H, dd, J = 7.64), 7.58-7.60 (2H, d, J = 7.59), 7.44-7.48 (5H, m), 7.30-7.34 (2H,

m), 7.24-7.26 (2H, d, J = 7.25). **^{13}C NMR Data** (100 MHz)**:**140.33, 138.82, 138.20, 134.67, 133.63, 132.66, 132.41, 131.83, 131.07, 130.57, 129.90, 129.83, 129.52, 129.29, 128.93, 128.50, 127.97, 127.55, 127.05, 127.04, 126.93, 126.85, 126.62, 126.12, 126.00, 125.75, 123.51, 121.23, 120.54, 120.40, 120.27, 120.21, 120.13, 119.77, 118.73, 117.18, 114.36, 109.62, 109.57. m/z = calcd 534.17, Found: 535.62. Anal. calcd for $C_{38}H_{22}N_4$:C, 85.37; H, 4.15; N, 10.48 Found: C, 85.28; H, 4.10; N, 10.38.

Single crystal analysis:

Single crystals are grown by slow evaporation method by using dichloromethane solvent. The grown crystals were typically adapting one of only a few possible 3D orientations. When a monochromatic X-ray beam is passed through a single crystal, the radiation interacts with the electrons in the atoms, resulting in scattering of the radiation to produce a unique image pattern. Multiple images are recorded, with an area X-ray detector, as the crystal is rotated in the X-ray beam. Computationally intensive analysis of a set images results in a solution for the 3D structure of the molecule.

Table ST1. Crystal data and structure-refinement parameters of AC-1 and AC-2.

Identification code	**AC-1**	**AC-2**
Empirical formula	$C_{37}H_{23}N_3$	$C_{76}H_{50}N_6$
Formula weight	509.58	1047.22
Temperature/K	293(2)	293(2)
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a/Å	9.2834(3)	10.2146(6)
b/Å	22.7626(5)	11.4653(8)
c/Å	13.0285(3)	11.8920(7)
α/°	90.00	93.271(5)
β/°	106.325(3)	101.152(5)
γ/°	90.00	95.973(6)

Volume/Å^3	2642.13(12)	1354.74(15)
Z	4	1
ρ_{calc}g/cm^3	1.281	1.284
μ/mm^{-1}	0.075	0.075
F(000)	1064.0	548.0
Crystal size/mm^3	0.529 × 0.372 × 0.183	0.413 × 0.246 × 0.198
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.72 to 56.66	3.5 to 56.62
Index ranges	$-12 \le h \le 12$, $-10 \le k \le 28$, $-17 \le l \le 8$	$-13 \le h \le 11$, $-15 \le k \le 15$, $-12 \le l \le 15$
Reflections collected	8939	8282
Independent reflections	5728 [R_{int} = 0.0206, R_{sigma} = 0.0382]	5832 [R_{int} = 0.0156, R_{sigma} = 0.0352]
Data/restraints/parameters	5728/0/361	5832/0/371
Goodness-of-fit on F^2	1.156	1.142
Final R indexes [I>=2σ (I)]	R_1 = 0.0597, wR_2 = 0.1629	R_1 = 0.0556, wR_2 = 0.1333
Final R indexes [all data]	R_1 = 0.0876, wR_2 = 0.1796	R_1 = 0.0794, wR_2 = 0.1472
Largest diff. peak/hole / e Å^{-3}	0.19/-0.26	0.18/-0.19

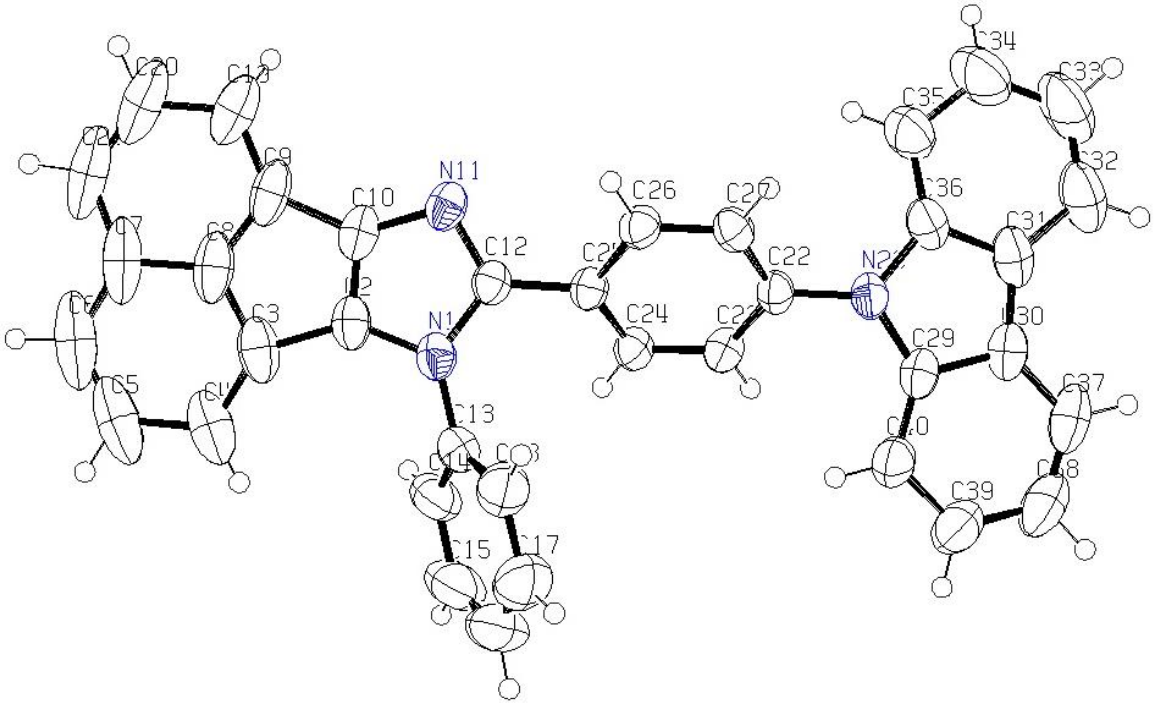


Fig. S1. ORTEP Diagram of AC-1 (eclipsed form 50% probability). N atoms blue, F atoms in green and O atoms in red in color.

Table ST2: Bond Lengths for AC-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N11	C12	1.333(3)	C13	C14	1.380(4)
N11	C10	1.374(3)	C13	C18	1.376(4)
N1	C12	1.384(3)	C9	C8	1.415(4)
N1	C2	1.376(3)	C9	C19	1.364(4)
N1	C13	1.431(3)	C3	C8	1.419(4)
C22	N28	1.420(2)	C3	C4	1.370(4)
C22	C23	1.390(3)	C31	C32	1.402(4)
C22	C27	1.385(3)	C8	C7	1.405(3)
C12	C25	1.467(3)	C40	C39	1.386(4)
N28	C29	1.394(3)	C35	C34	1.387(4)
N28	C36	1.403(3)	C14	C15	1.378(4)
C25	C26	1.397(3)	C7	C21	1.431(6)
C25	C24	1.389(3)	C7	C6	1.395(6)
C26	C27	1.381(3)	C19	C20	1.417(4)
C23	C24	1.380(3)	C39	C38	1.385(4)
C10	C2	1.352(4)	C18	C17	1.388(4)
C10	C9	1.474(3)	C37	C38	1.362(4)
C29	C30	1.402(3)	C21	C20	1.337(6)
C29	C40	1.388(4)	C16	C17	1.366(5)
C2	C3	1.462(3)	C16	C15	1.373(5)
C36	C31	1.404(3)	C4	C5	1.437(5)
C36	C35	1.384(4)	C5	C6	1.371(6)
C30	C31	1.431(4)	C32	C33	1.367(5)
C30	C37	1.398(4)	C34	C33	1.386(5)

Table ST3: Bond Angles for AC-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	N11	C10	103.8(2)	C18	C13	N1	120.3(2)
C12	N1	C13	129.42(18)	C18	C13	C14	121.2(3)
C2	N1	C12	105.41(19)	C8	C9	C10	103.4(2)
C2	N1	C13	125.2(2)	C19	C9	C10	137.9(3)
C23	C22	N28	119.54(19)	C19	C9	C8	118.7(3)
C27	C22	N28	121.26(19)	C8	C3	C2	102.7(2)
C27	C22	C23	119.20(19)	C4	C3	C2	137.9(3)
N11	C12	N1	112.32(18)	C4	C3	C8	119.4(3)
N11	C12	C25	124.1(2)	C36	C31	C30	107.6(2)

N1	C12	C25	123.5(2)	C32	C31	C36	119.3(3)
C29	N28	C22	125.31(19)	C32	C31	C30	133.2(3)
C29	N28	C36	107.91(19)	C9	C8	C3	113.4(2)
C36	N28	C22	126.6(2)	C7	C8	C9	123.5(3)
C26	C25	C12	119.40(19)	C7	C8	C3	123.1(3)
C24	C25	C12	122.36(19)	C39	C40	C29	117.9(3)
C24	C25	C26	118.15(19)	C36	C35	C34	117.3(3)
C27	C26	C25	120.9(2)	C15	C14	C13	119.3(3)
C24	C23	C22	120.3(2)	C8	C7	C21	115.2(4)
C23	C24	C25	121.1(2)	C6	C7	C8	116.7(4)
C26	C27	C22	120.4(2)	C6	C7	C21	128.1(3)
N11	C10	C9	138.8(3)	C9	C19	C20	118.6(4)
C2	C10	N11	111.8(2)	C38	C39	C40	121.2(3)
C2	C10	C9	109.2(2)	C13	C18	C17	118.7(3)
N28	C29	C30	109.3(2)	C38	C37	C30	119.4(3)
C40	C29	N28	129.4(2)	C37	C38	C39	121.0(3)
C40	C29	C30	121.2(2)	C20	C21	C7	121.0(3)
N1	C2	C3	142.0(3)	C17	C16	C15	120.7(3)
C10	C2	N1	106.6(2)	C3	C4	C5	117.5(4)
C10	C2	C3	111.3(2)	C6	C5	C4	122.5(4)
N28	C36	C31	108.4(2)	C21	C20	C19	123.0(4)
C35	C36	N28	129.9(2)	C33	C32	C31	119.0(3)
C35	C36	C31	121.7(2)	C16	C17	C18	120.3(3)
C29	C30	C31	106.8(2)	C33	C34	C35	121.8(4)
C37	C30	C29	119.3(3)	C16	C15	C14	119.8(3)
C37	C30	C31	133.9(3)	C5	C6	C7	120.8(3)
C14	C13	N1	118.5(2)	C32	C33	C34	120.9(3)

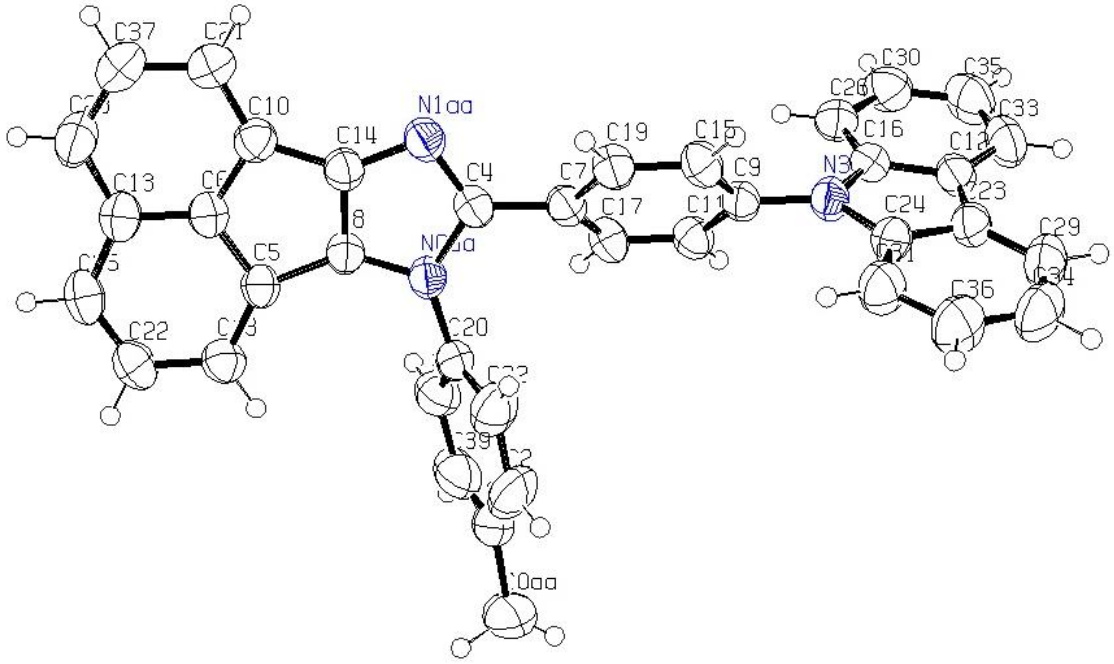


Fig. S2. ORTEP Diagram of AC-2 (eclipsed form 50% probability). N atoms blue in color.

Table ST4: Bond Lengths for AC-2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N0AA	C4	1.388(3)	C13	C25	1.423(3)
N0AA	C8	1.368(3)	C13	C28	1.416(3)
N0AA	C20	1.431(3)	C15	C19	1.382(3)
N1AA	C4	1.330(3)	C16	C26	1.388(3)
N1AA	C14	1.377(3)	C18	C22	1.414(3)
N3	C9	1.424(3)	C20	C27	1.373(3)
N3	C16	1.390(3)	C20	C32	1.369(3)
N3	C24	1.396(3)	C21	C37	1.418(4)
C4	C7	1.473(3)	C22	C25	1.359(3)
C5	C6	1.423(3)	C23	C24	1.401(3)
C5	C8	1.459(3)	C23	C29	1.400(3)
C5	C18	1.367(3)	C24	C31	1.382(3)
C6	C10	1.423(3)	C26	C30	1.379(3)

C6	C13	1.393(3)	C27	C39	1.381(4)
C7	C17	1.391(3)	C28	C37	1.366(4)
C7	C19	1.391(3)	C29	C34	1.365(4)
C8	C14	1.369(3)	C30	C35	1.386(4)
C9	C11	1.382(3)	C31	C36	1.383(3)
C9	C15	1.384(3)	C32	C2	1.386(5)
C10	C14	1.466(3)	C33	C35	1.378(4)
C10	C21	1.367(3)	C34	C36	1.386(4)
C11	C17	1.378(3)	C39	C1	1.361(6)
C12	C16	1.404(3)	C1	C2	1.371(6)
C12	C23	1.440(3)	C1	C0AA	1.523(5)
C12	C33	1.391(3)			

Table ST5: Bond Angles for AC-2.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C4	N0AA	C20	129.74(18)	C8	C14	C10	108.64(19)
C8	N0AA	C4	105.66(17)	C19	C15	C9	119.8(2)
C8	N0AA	C20	124.39(17)	N3	C16	C12	109.16(19)
C4	N1AA	C14	104.36(18)	C26	C16	N3	129.0(2)
C16	N3	C9	125.35(17)	C26	C16	C12	121.9(2)
C16	N3	C24	108.13(18)	C11	C17	C7	120.4(2)
C24	N3	C9	126.41(18)	C5	C18	C22	118.4(2)
N0AA	C4	C7	122.64(19)	C15	C19	C7	120.9(2)
N1AA	C4	N0AA	112.21(19)	C27	C20	N0AA	118.7(2)
N1AA	C4	C7	125.10(19)	C32	C20	N0AA	120.8(2)
C6	C5	C8	102.76(18)	C32	C20	C27	120.3(2)
C18	C5	C6	119.0(2)	C10	C21	C37	118.4(2)
C18	C5	C8	138.1(2)	C25	C22	C18	122.6(2)
C5	C6	C10	113.0(2)	C24	C23	C12	107.10(19)
C13	C6	C5	123.1(2)	C29	C23	C12	134.0(2)
C13	C6	C10	123.8(2)	C29	C23	C24	118.9(2)
C17	C7	C4	120.67(19)	N3	C24	C23	108.9(2)
C17	C7	C19	118.7(2)	C31	C24	N3	129.1(2)
C19	C7	C4	120.63(19)	C31	C24	C23	122.0(2)
N0AA	C8	C5	141.61(19)	C22	C25	C13	120.7(2)
N0AA	C8	C14	106.81(19)	C30	C26	C16	117.7(2)
C14	C8	C5	111.48(19)	C20	C27	C39	118.9(3)
C11	C9	N3	119.4(2)	C37	C28	C13	120.0(2)

C11	C9	C15	119.6(2)	C34	C29	C23	119.2(3)
C15	C9	N3	121.02(19)	C26	C30	C35	121.3(3)
C6	C10	C14	104.08(19)	C24	C31	C36	117.5(3)
C21	C10	C6	118.3(2)	C20	C32	C2	118.9(3)
C21	C10	C14	137.6(2)	C35	C33	C12	119.3(2)
C17	C11	C9	120.6(2)	C29	C34	C36	121.0(3)
C16	C12	C23	106.7(2)	C33	C35	C30	120.9(3)
C33	C12	C16	118.9(2)	C31	C36	C34	121.4(3)
C33	C12	C23	134.4(2)	C28	C37	C21	123.0(2)
C6	C13	C25	116.0(2)	C1	C39	C27	122.4(4)
C6	C13	C28	116.3(2)	C39	C1	C2	117.4(3)
C28	C13	C25	127.6(2)	C39	C1	C0AA	122.8(5)
N1AA	C14	C10	140.4(2)	C2	C1	C0AA	119.8(5)
C8	C14	N1AA	110.95(19)	C1	C2	C32	121.9(3)

NMR Spectroscopy:

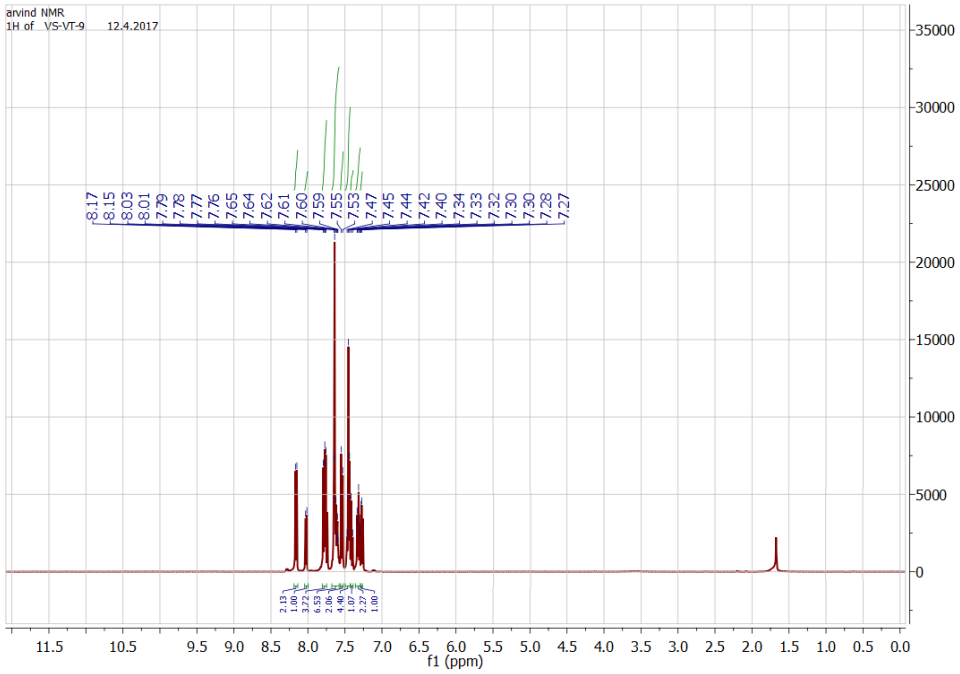


Fig. S3. ^{1}H-NMR spectra of AC-1.

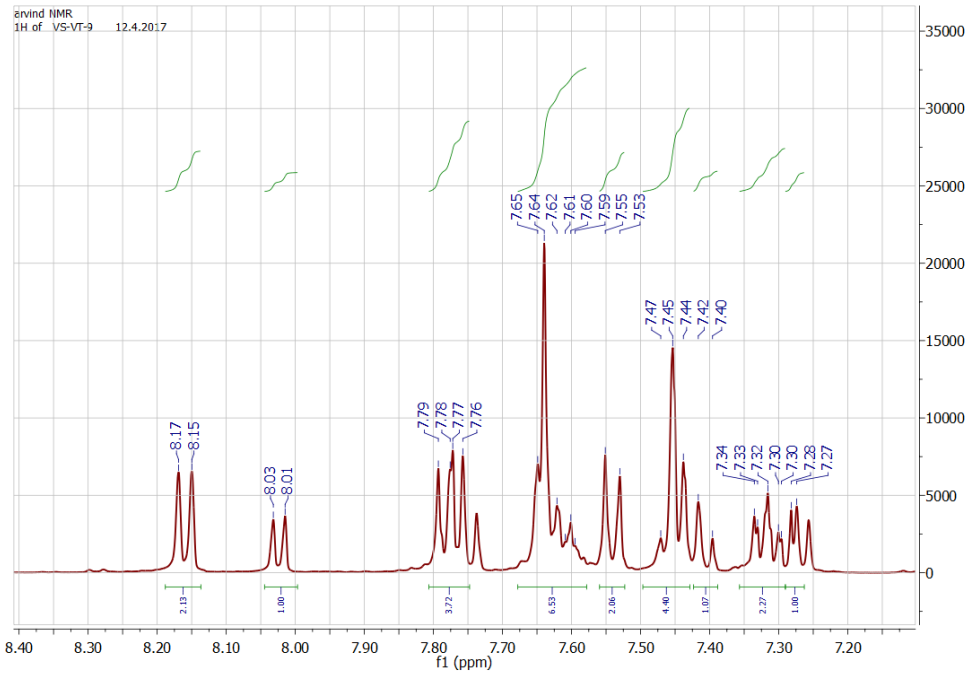


Fig. S4. ^{1}H-NMR spectra of AC-1 (expanded).

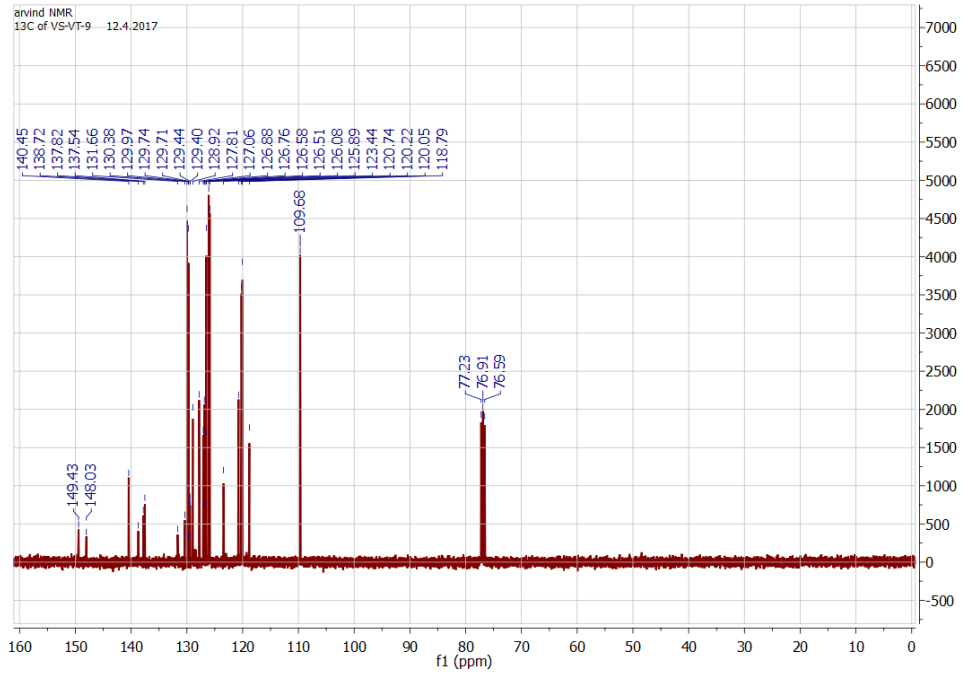


Fig. S5. ^{13}C-NMR spectra of AC-1.

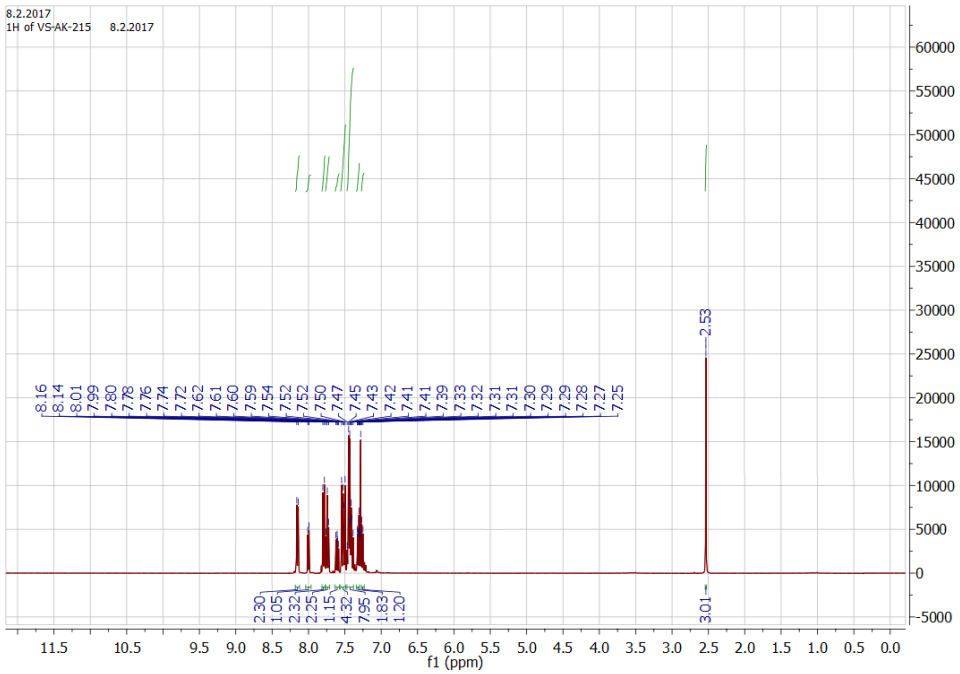


Fig. S6. ^{1}H-NMR spectra of AC-2.

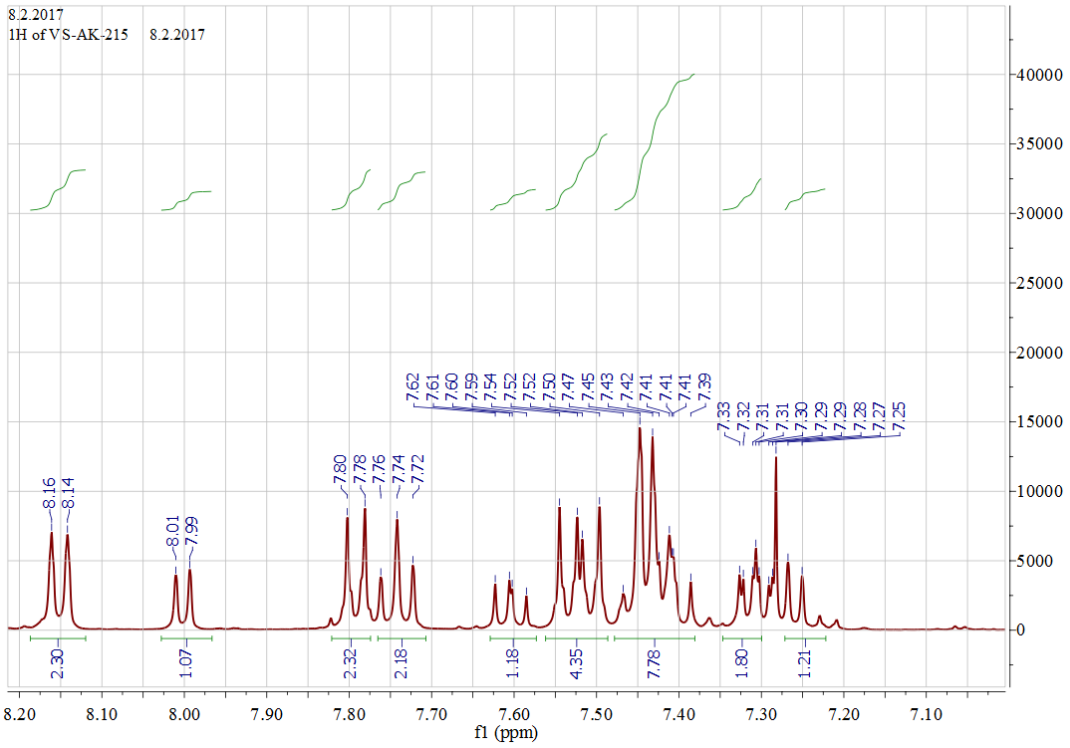


Fig. S7. ^{1}H-NMR spectra of AC-2 (expanded).

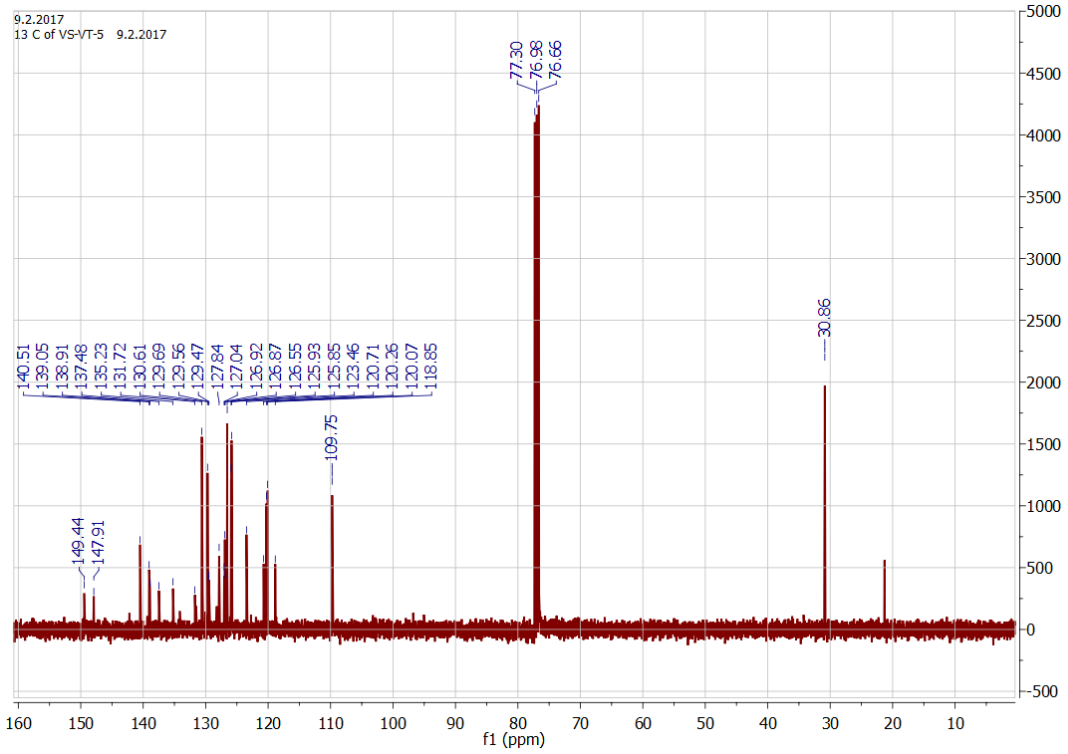


Fig. S8. ^{13}C-NMR spectra of AC-2.

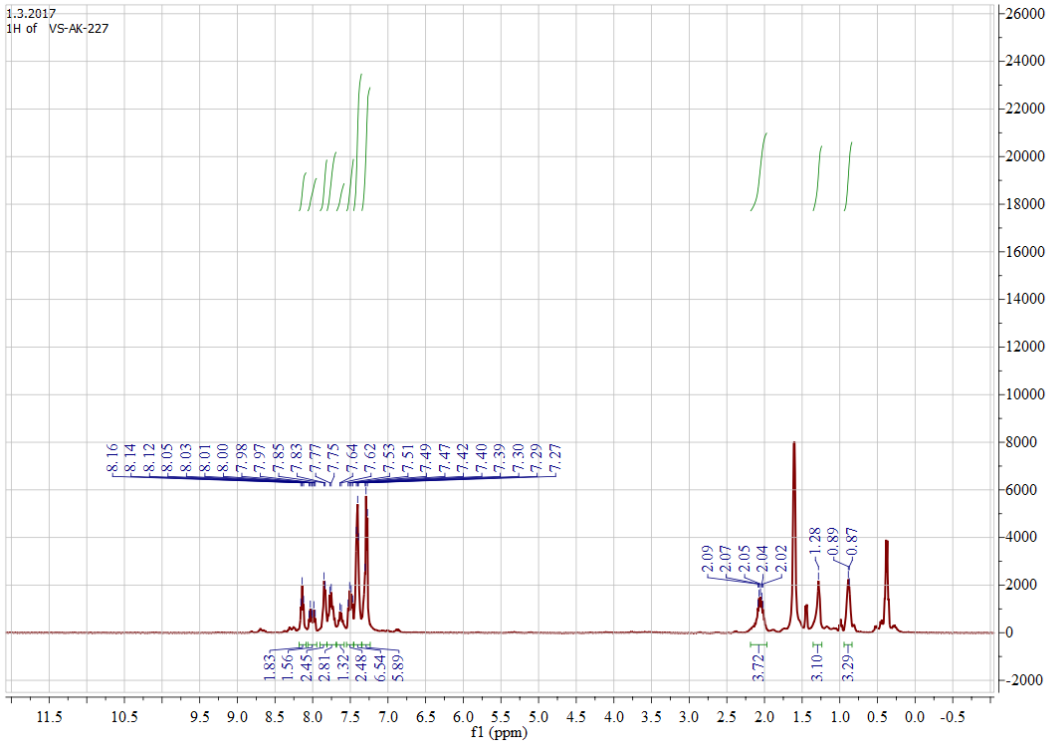


Fig. S9. ^{1}H-NMR spectra of AC-3.

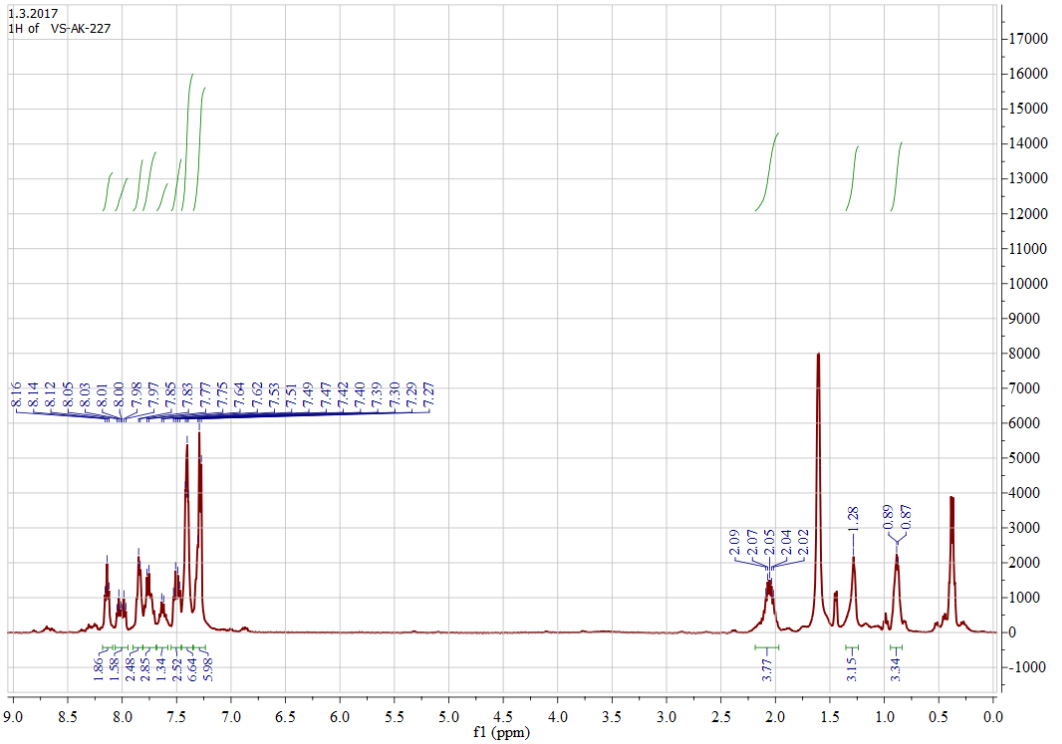


Fig. S10. ^{1}H-NMR spectra of AC-3 (expanded).

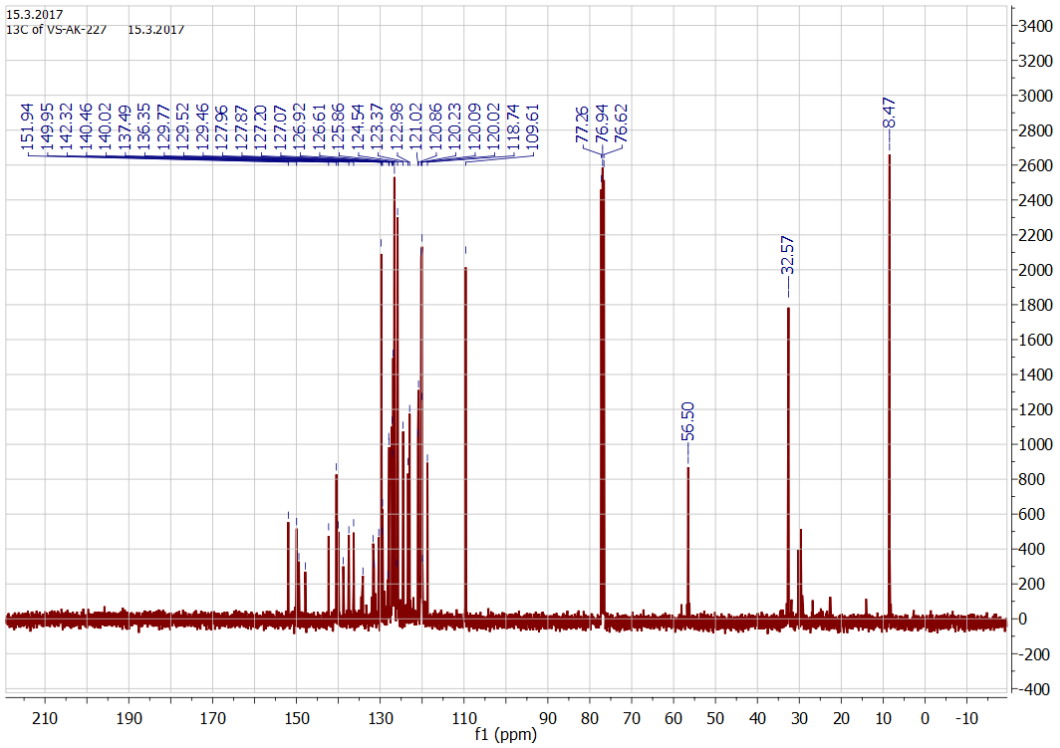


Fig. S11. ^{13}C-NMR spectra of AC-3.

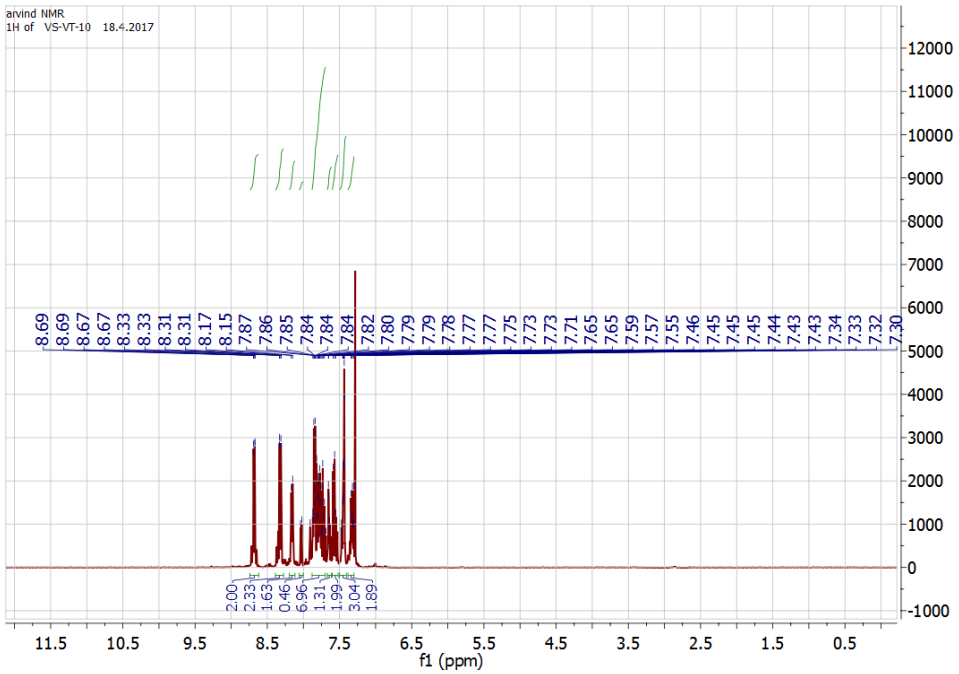


Fig. S12. ^{1}H-NMR spectra of AC-4.

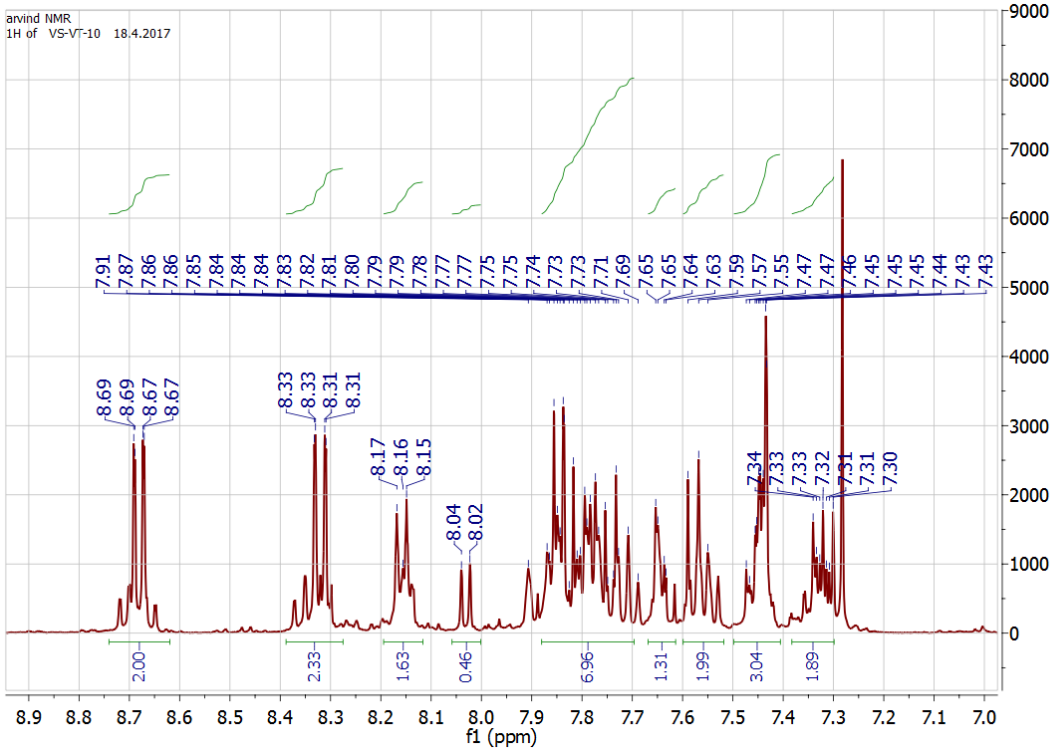


Fig. S13. ^{1}H-NMR spectra of AC-4 (expanded).

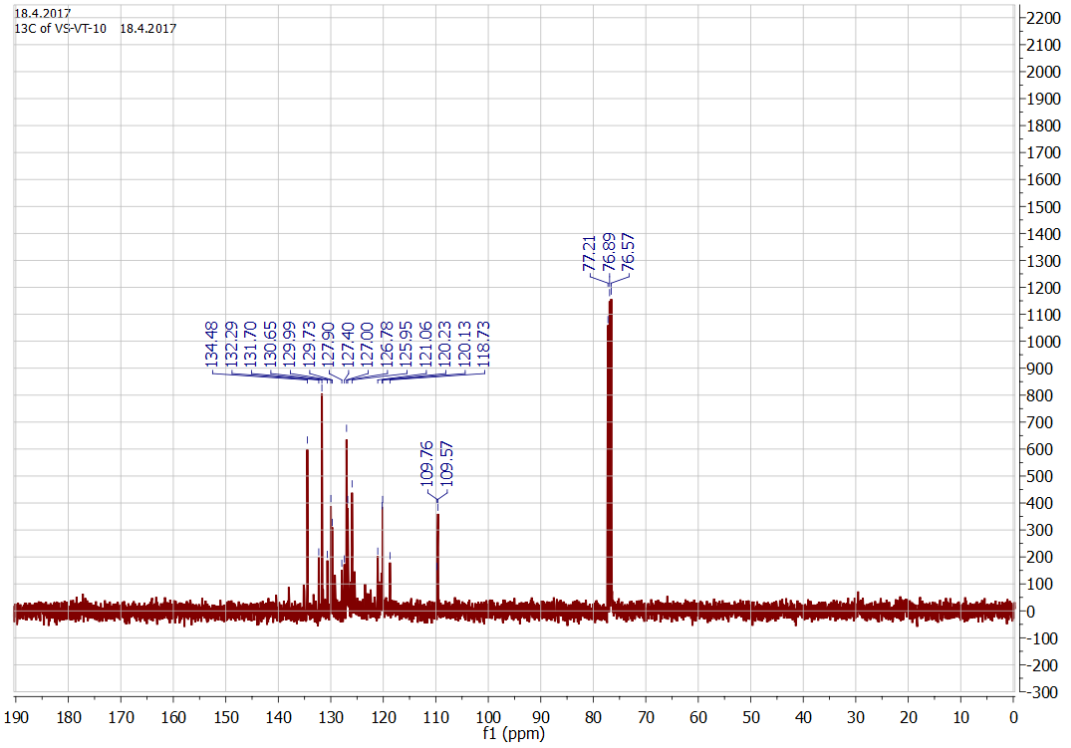


Fig. S14. ^{13}C-NMR spectra of AC-4.

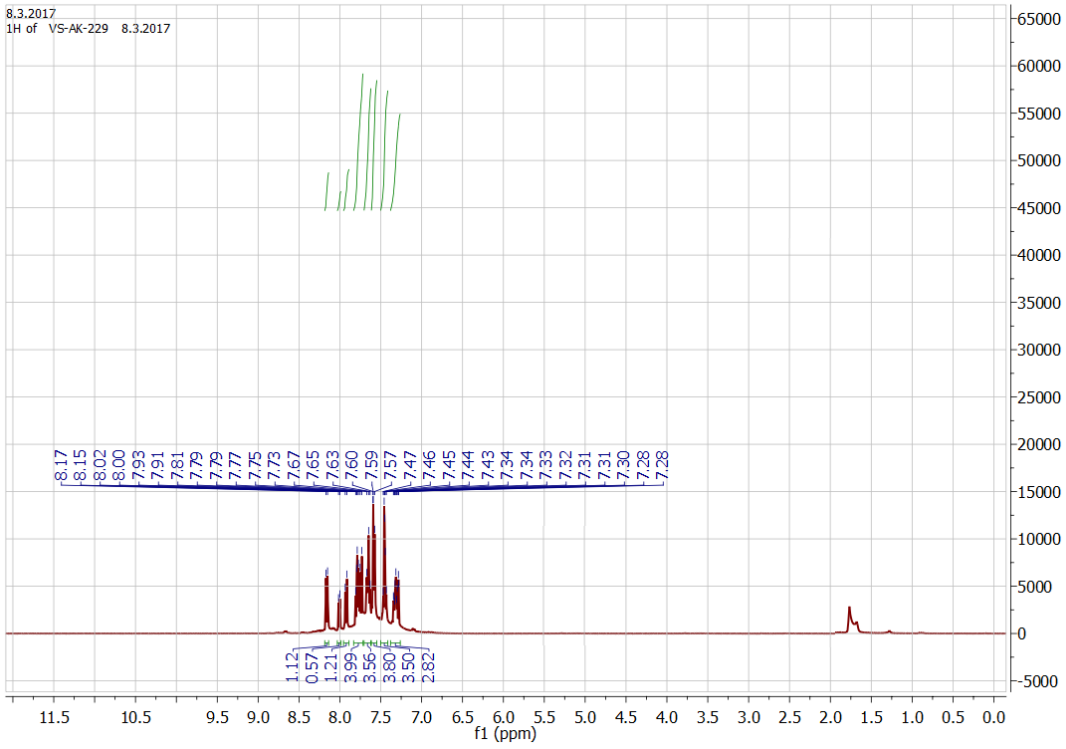


Fig. S15. ^{1}H-NMR spectra of AC-5.

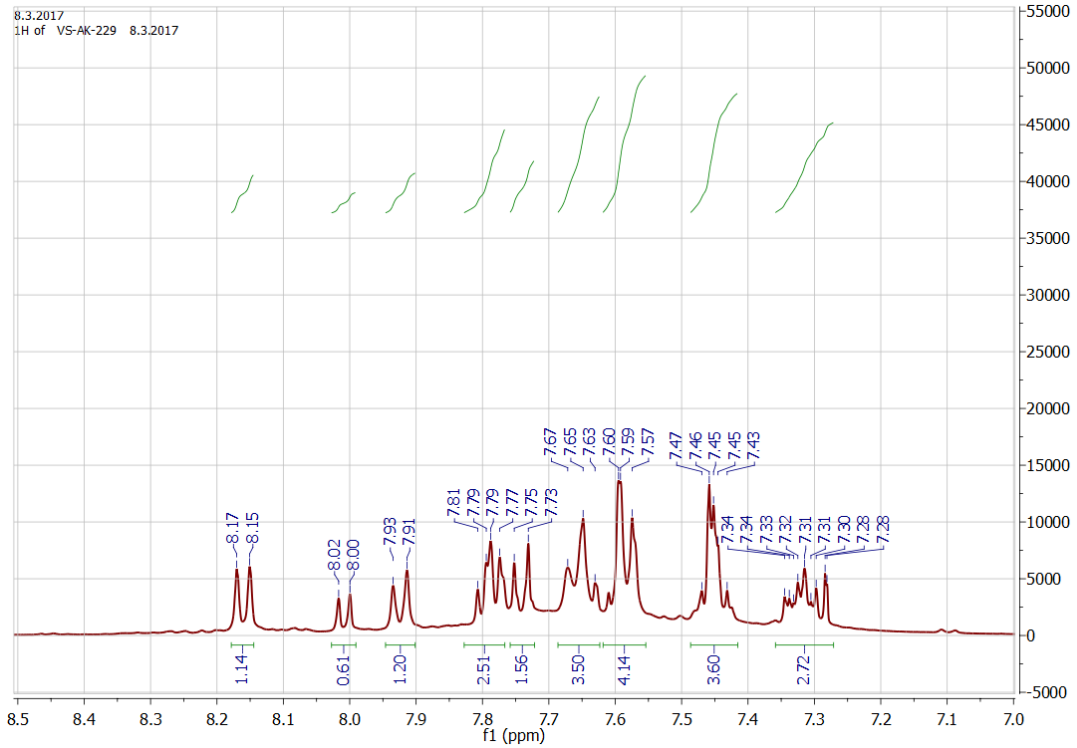


Fig. S16. ^{1}H-NMR spectra of AC-5 (expanded).

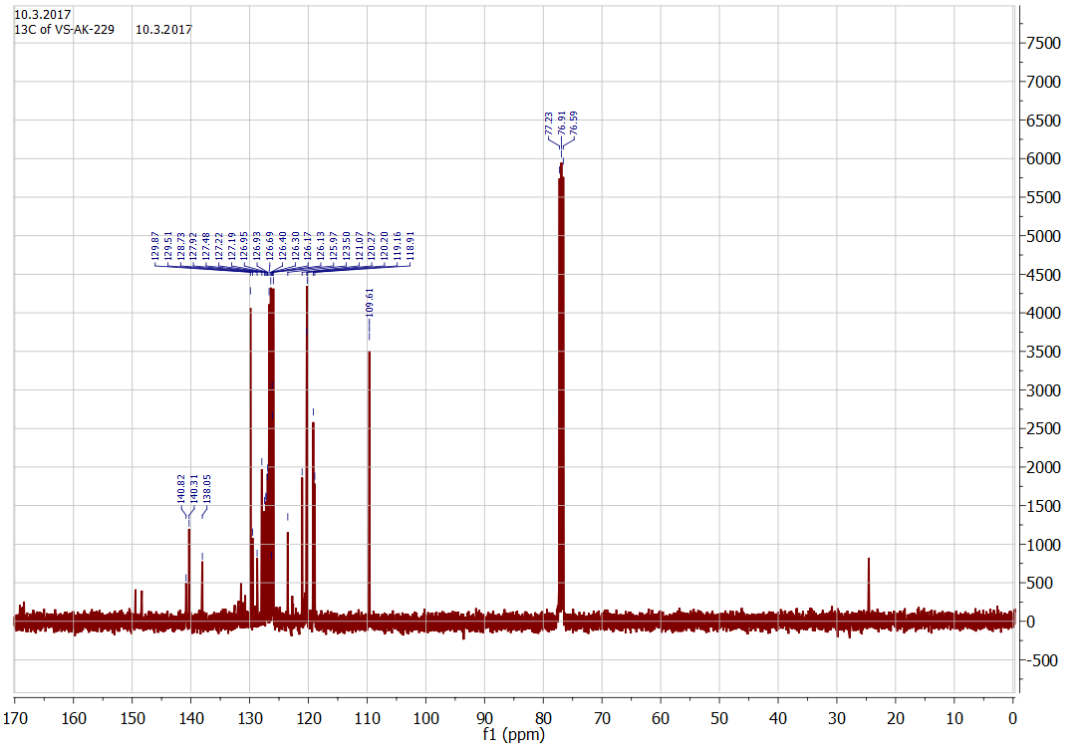


Fig. S17. ^{13}C-NMR spectra of AC-5.

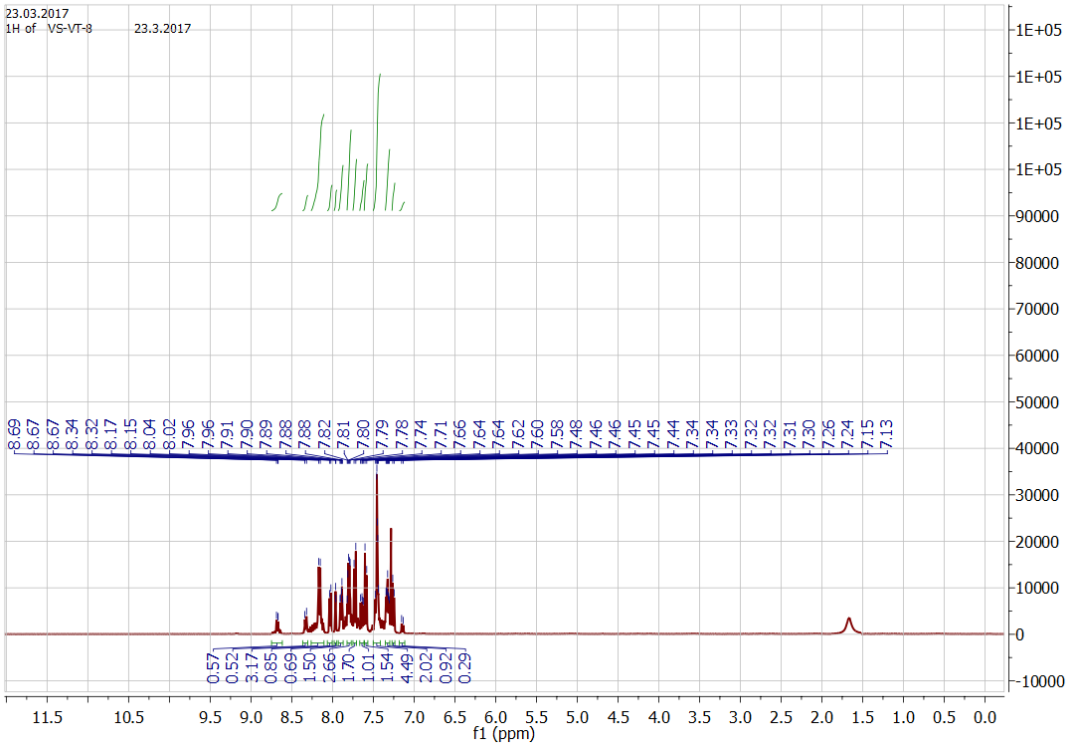


Fig. S18. [1]H-NMR spectra of AC-6.

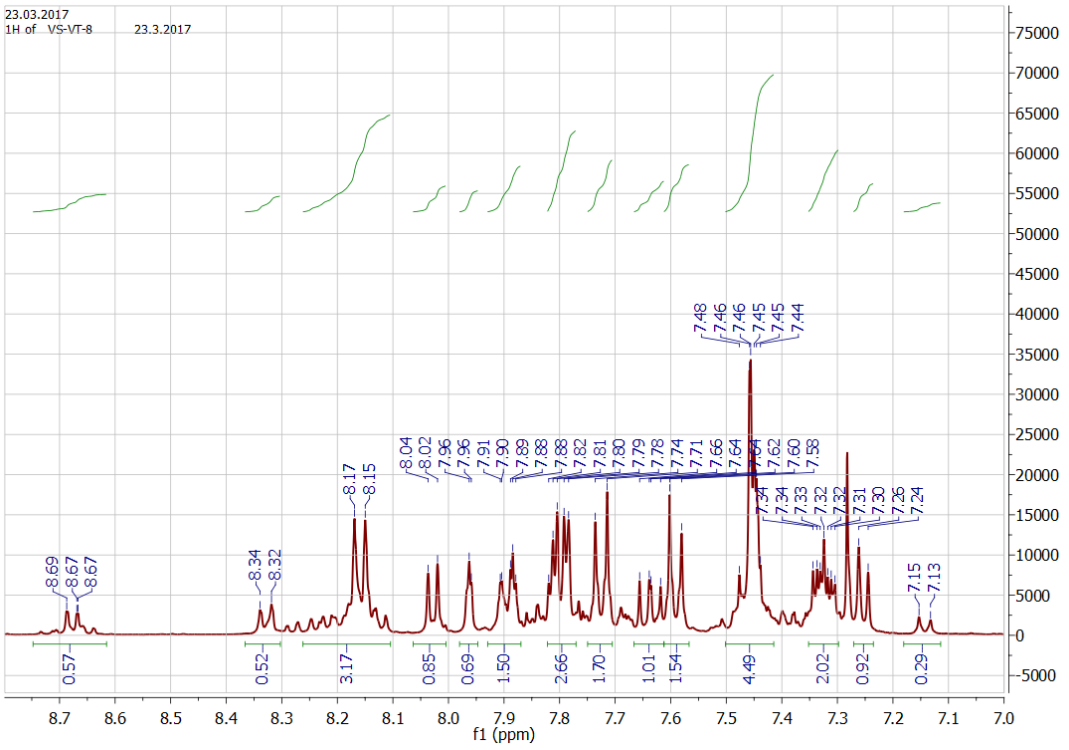


Fig. S19. [1]H-NMR spectra of AC-6 (expanded).

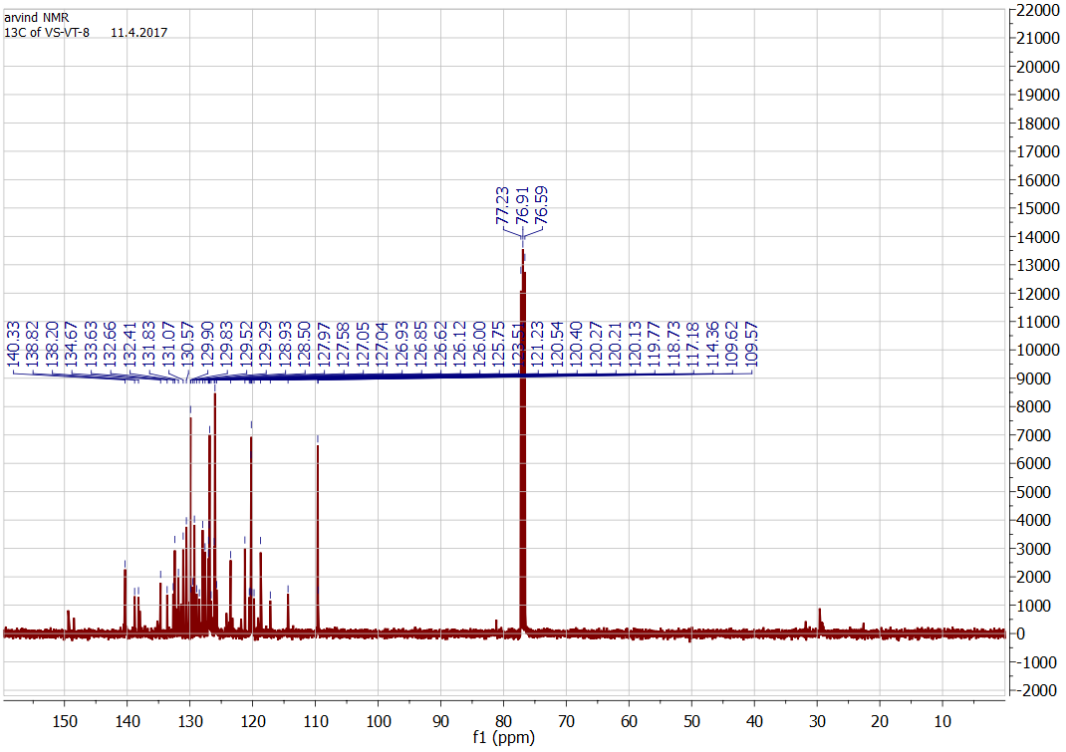


Fig. S20. ^{13}C-NMR spectra of AC-6.

Mass spectral analysis:

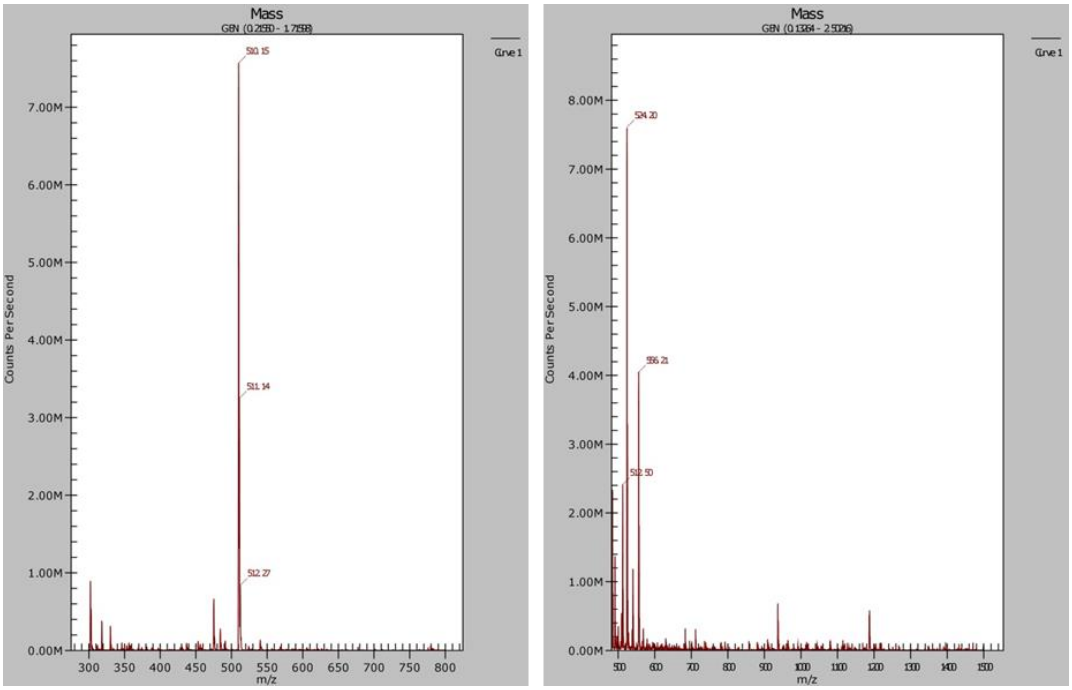


Fig. S21. Mass spectra of AC-1 and AC-2.

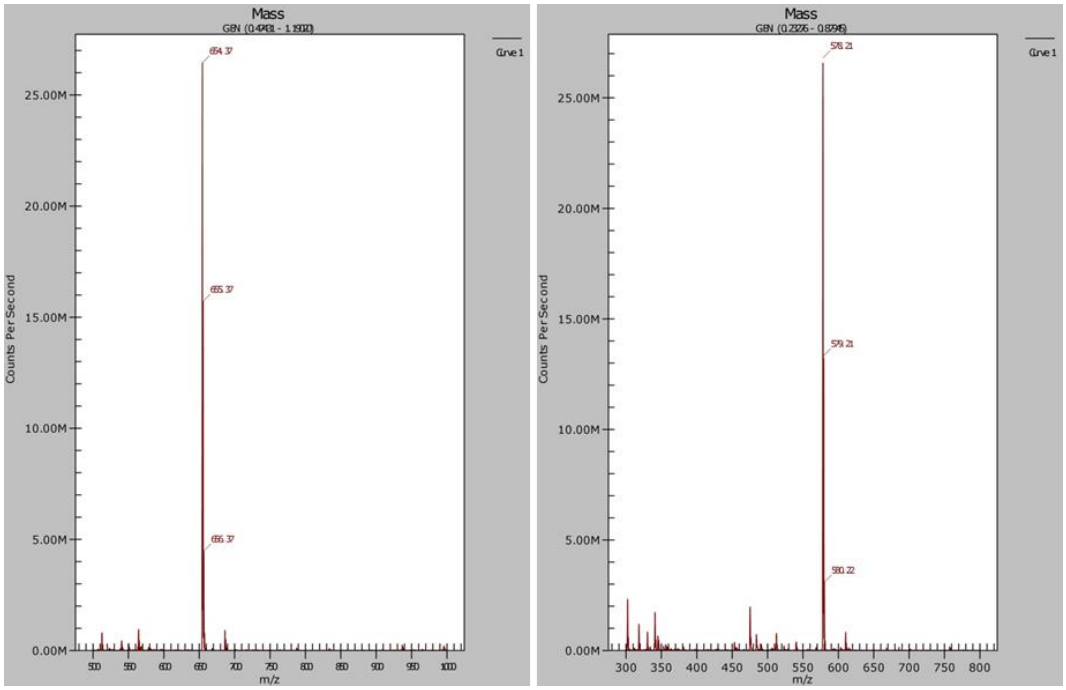


Fig. S22. Mass spectra of AC-3 and AC-4.

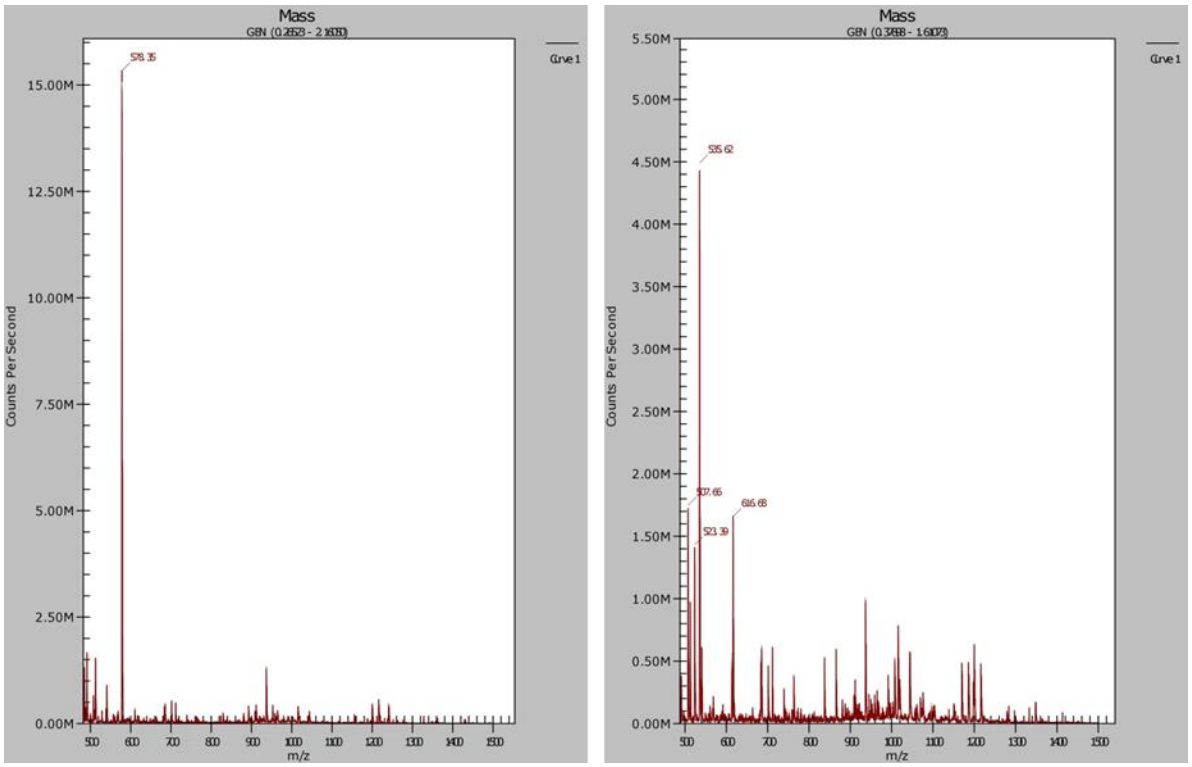


Fig. S23. Mass spectra of AC-5 and AC-6.

Chemosensors:

UV-Vis titrations:

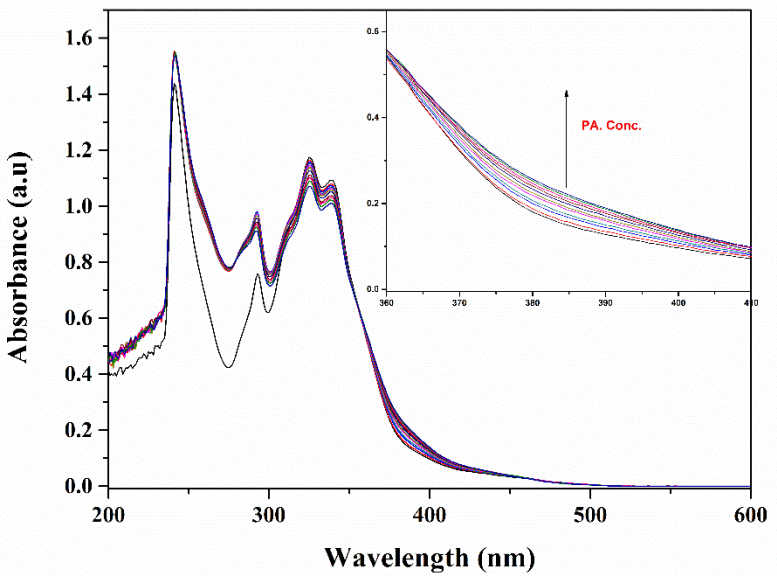


Fig. S24. UV-visible absorption responses of AC-1(5 mM) toward different concentrations of PA in THF (0–15 equivalents).

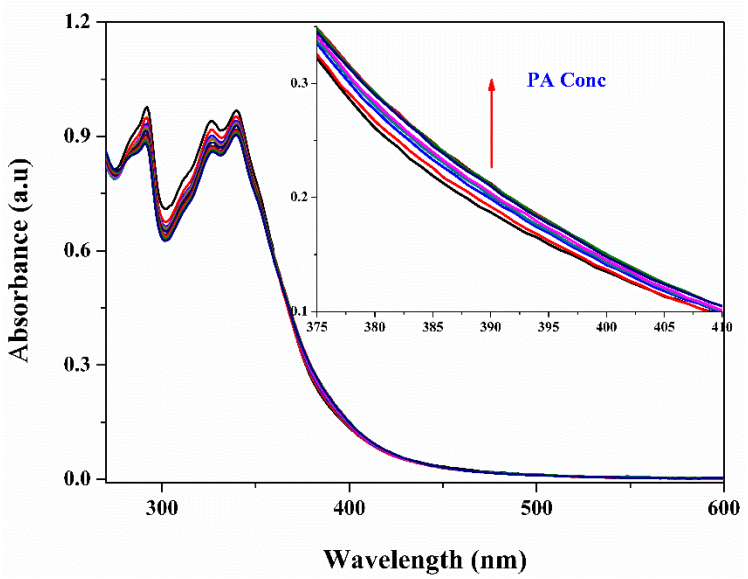


Fig. S25. UV-visible absorption responses of AC-2 (5 mM) toward different concentrations of PA in THF (0–15 equivalents).

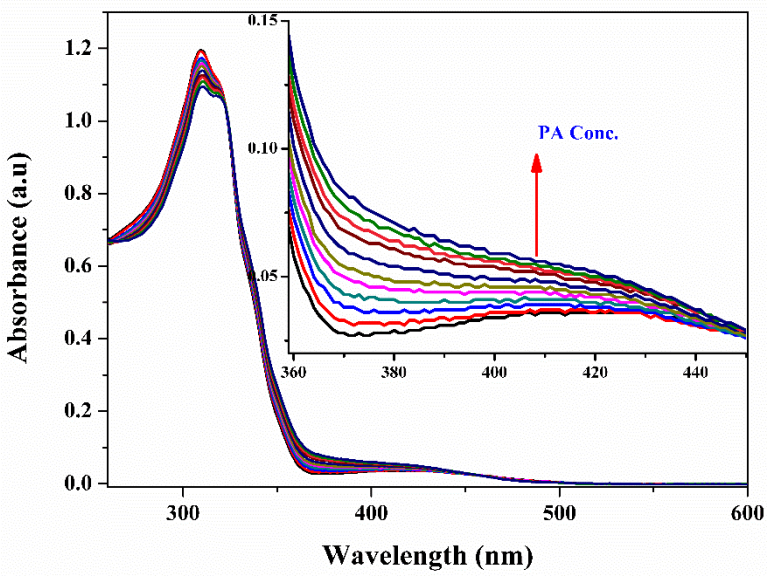


Fig. S26. UV-visible absorption responses of AC-3 (5 mM) toward different concentrations of PA in THF (0–15 equivalents).

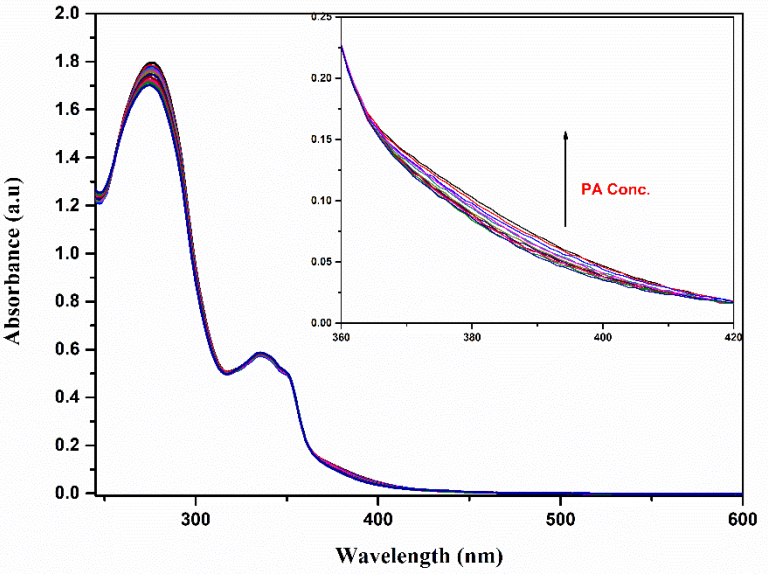


Fig. S27. UV-visible absorption responses of AC-4 (5 mM) toward different concentrations of PA in THF (0–15 equivalents).

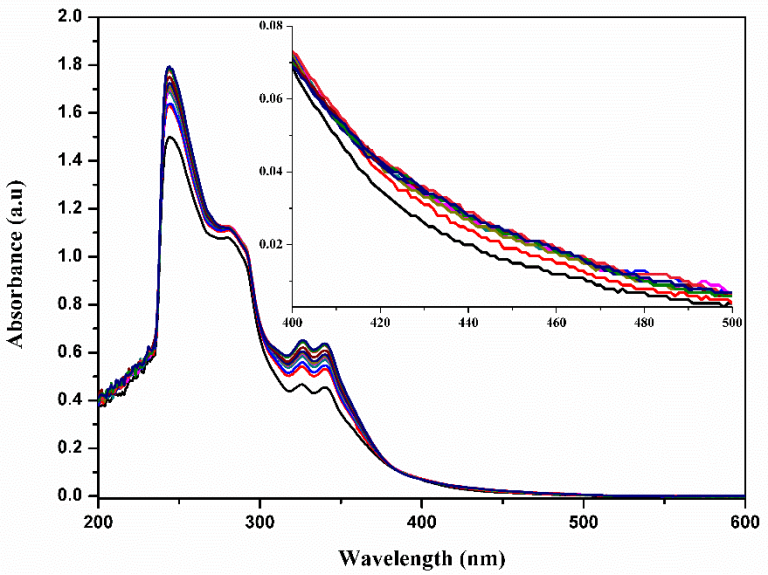


Fig. S28. UV-visible absorption responses of AC-5 (5 mM) toward different concentrations of PA in THF (0–15 equivalents).

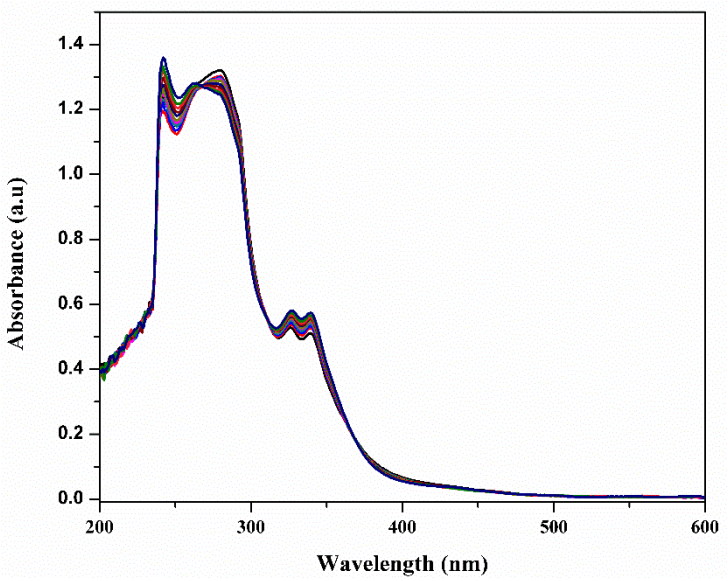


Fig. S29. UV-visible absorption responses of AC-6 (5 mM) toward different concentrations of PA in THF (0–15 equivalents).

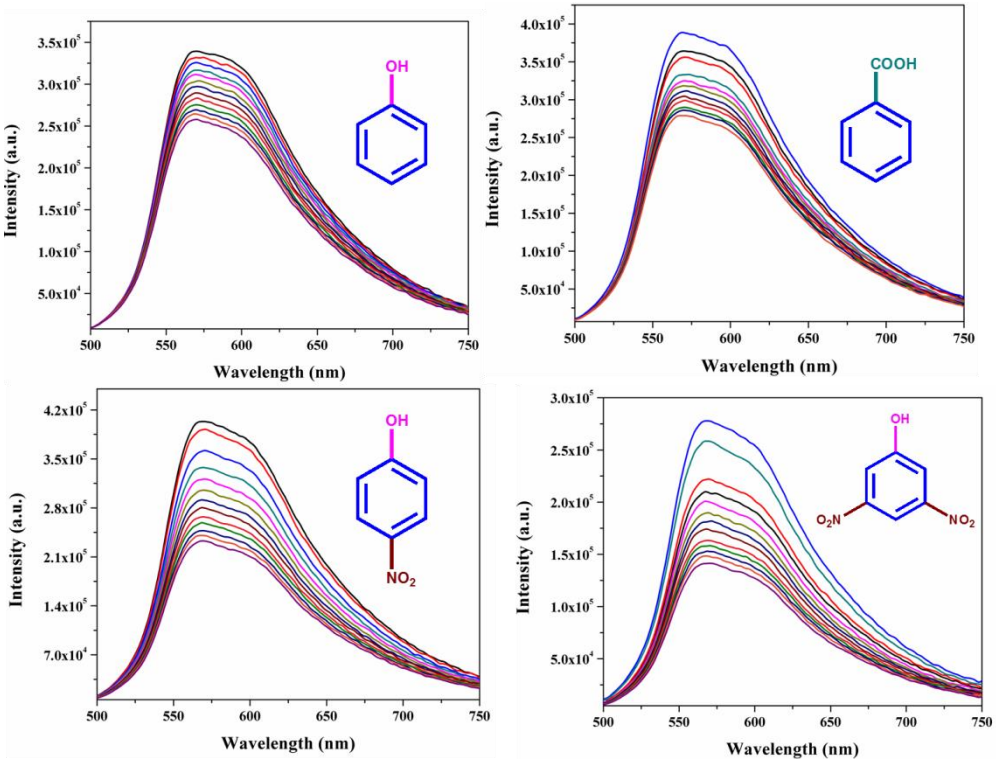


Fig. S30. The fluorescence spectra of different nitroaromatics to AC-1 in THF. Upon addition of (a) 2,4-Dinitrophenol (2,4-DNP), (b) 4-nitro phenol(NP), (c) benzoic acid (BA), (d) phenol (PH).

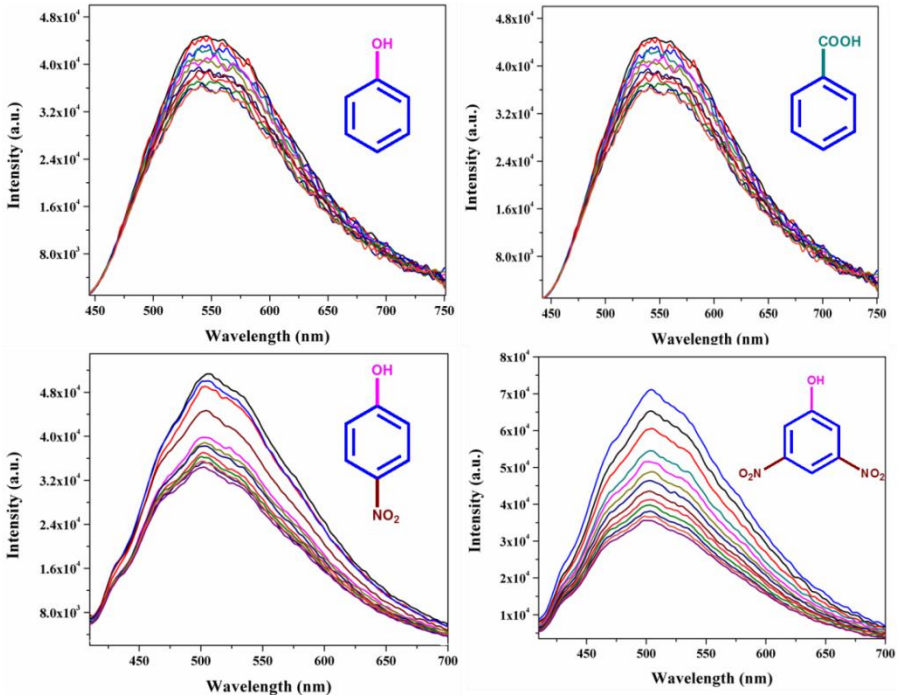


Fig. S31. The fluorescence spectra of different nitroaromatics to AC-2 in THF. Upon addition of (a) 2,4-Dinitrophenol (2,4-DNP), (b) 4-nitro phenol(NP), (c) benzoic acid (BA), (d) phenol (PH).

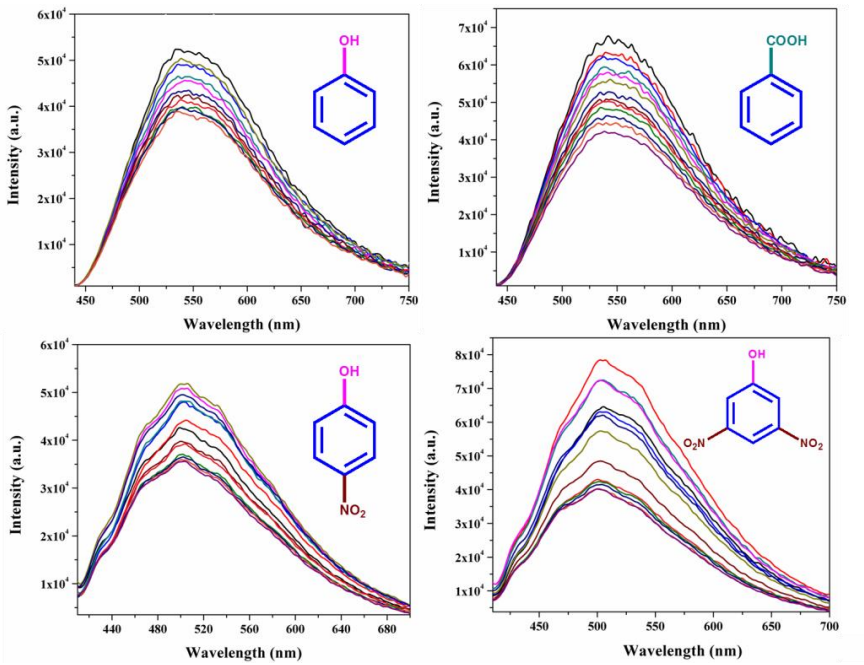


Fig. S32. The fluorescence spectra of different nitroaromatics to AC-3 in THF. Upon addition of (a) 2,4-Dinitrophenol (2,4-DNP), (b) 4-nitro phenol(NP), (c) benzoic acid (BA), (d) phenol (PH).

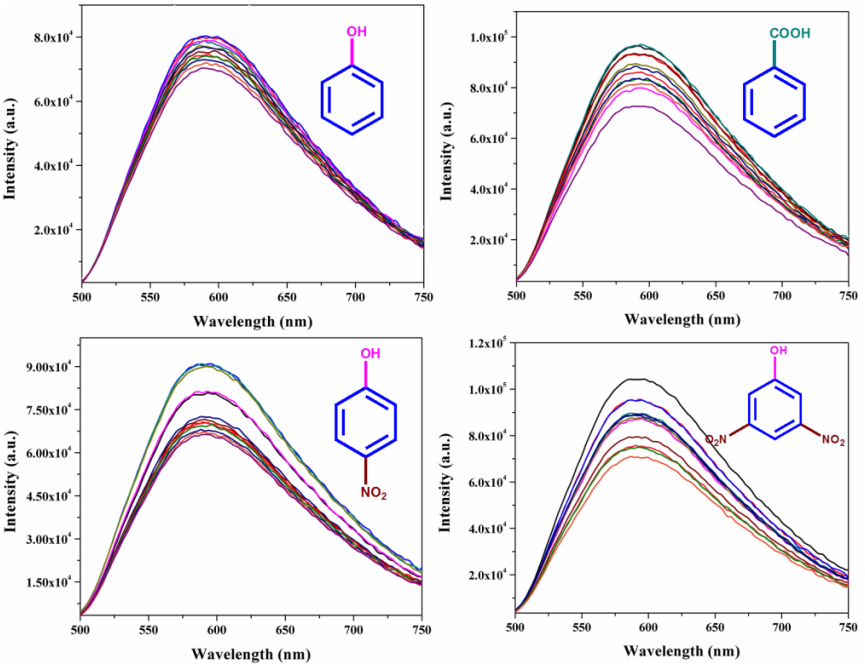


Fig. S33. The fluorescence spectra of different nitroaromatics to AC-5 in THF. Upon addition of (a) 2,4-Dinitrophenol (2,4-DNP), (b) 4-nitro phenol(NP), (c) benzoic acid (BA), (d) phenol (PH).

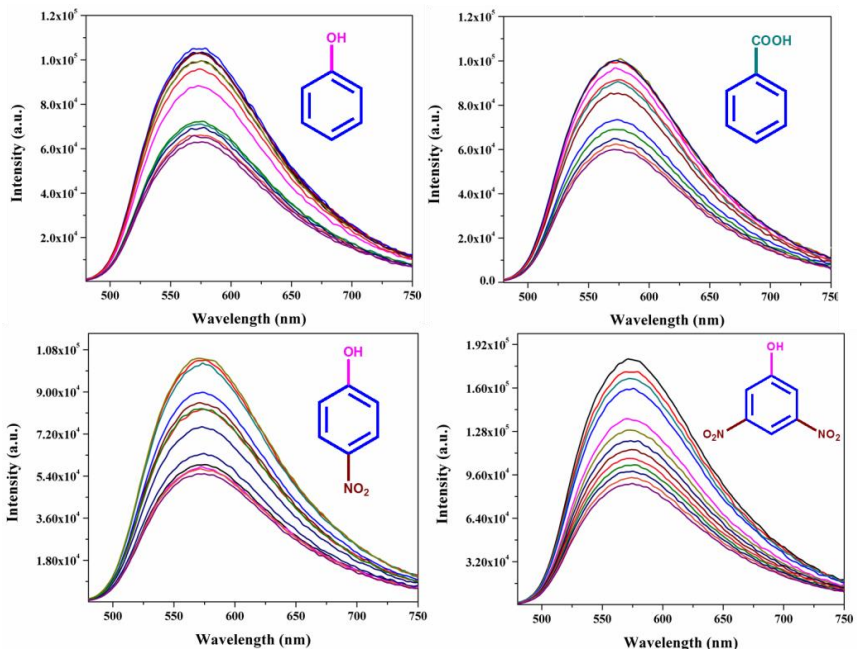


Fig. S34. The fluorescence spectra of different nitroaromatics to AC-6 in THF. Upon addition of (a) 2,4-Dinitrophenol (2,4-DNP), (b) 4-nitro phenol(NP), (c) benzoic acid (BA), (d) phenol (PH).1

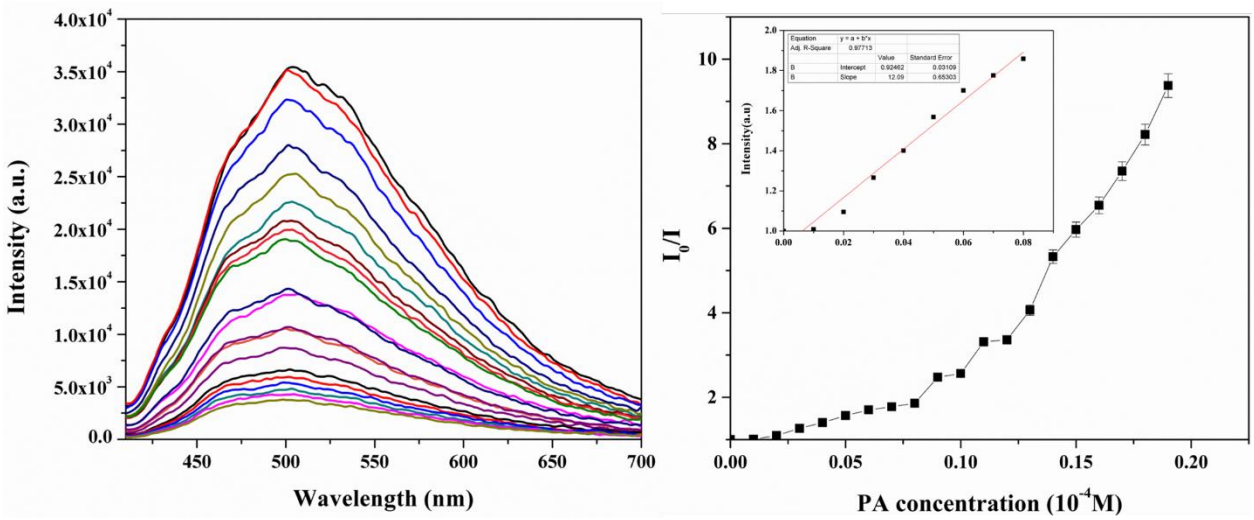


Fig. S35. Change in the fluorescence of AC-2 upon the addition of PA. b) Stern–Volmer plots of AC-1 using PA as a quencher. Inset:Stern–Volmer plots at lower concentration region of PA.

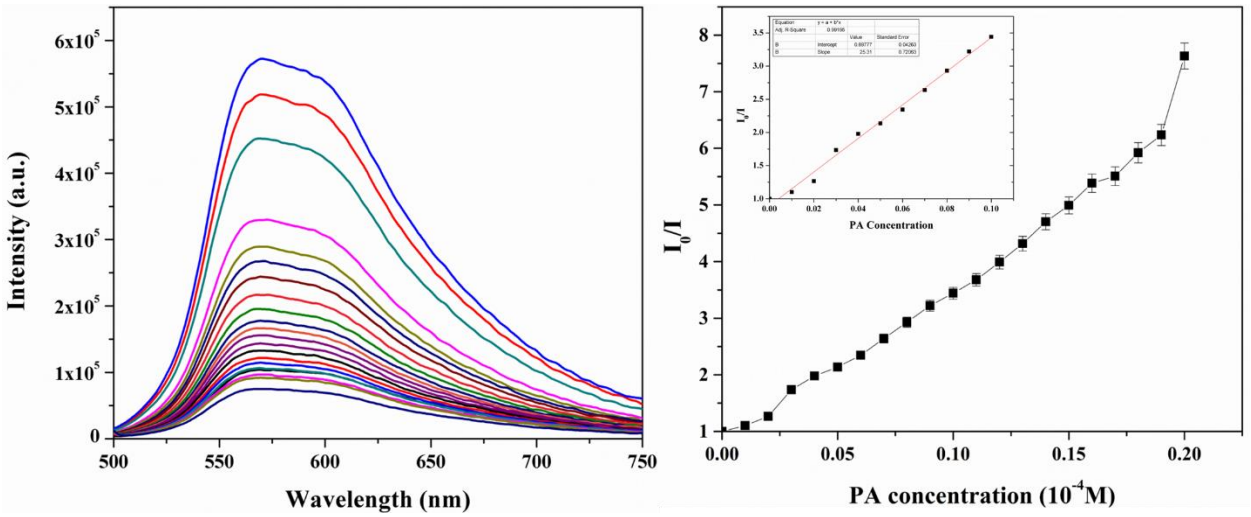


Fig. S36. Change in the fluorescence of AC-3 upon the addition of PA. b) Stern–Volmer plots of AC-3 using PA as a quencher. Inset:Stern–Volmer plots at lower concentration region of PA.

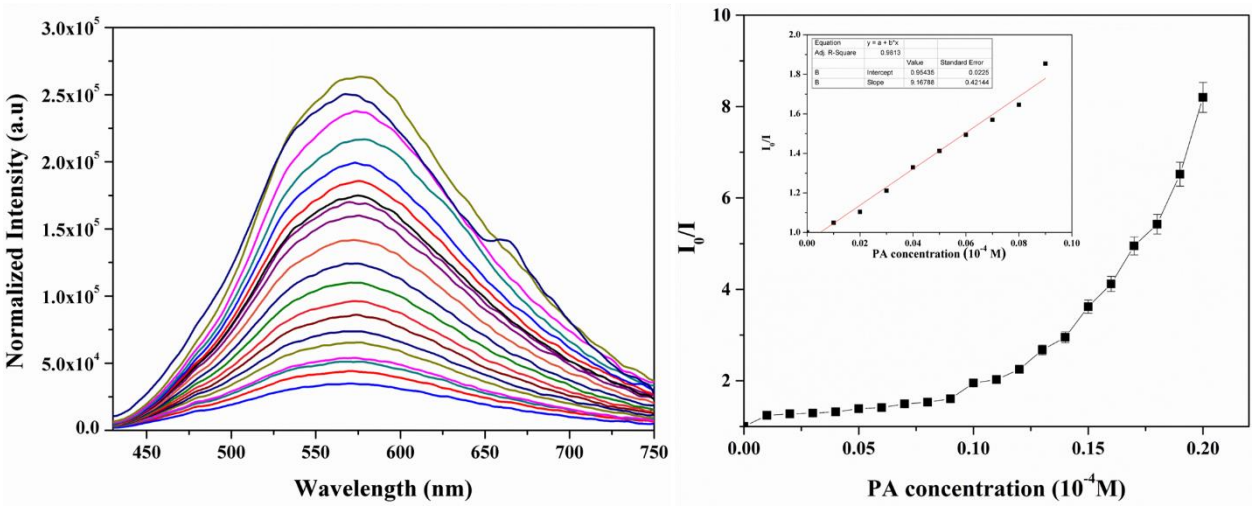


Fig. S37. Change in the fluorescence of AC-4 upon the addition of PA. b) Stern–Volmer plots of AC-3 using PA as a quencher. Inset:Stern–Volmer plots at lower concentration region of PA.

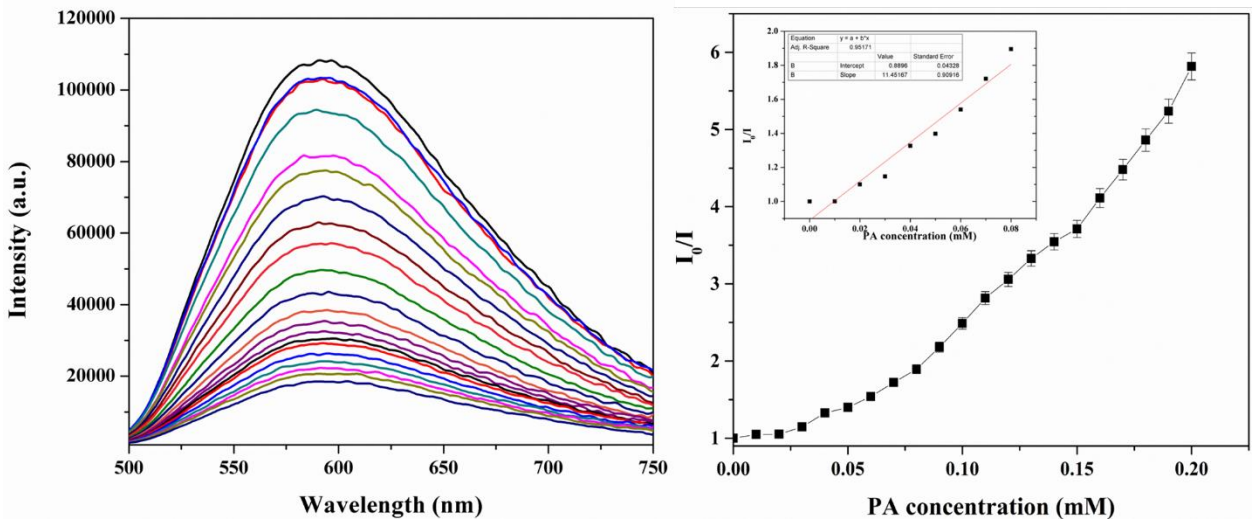


Fig. S38. Change in the fluorescence of AC-5 upon the addition of PA. b) Stern–Volmer plots of AC-6 using PA as a quencher. Inset:Stern–Volmer plots at lower concentration region of PA.

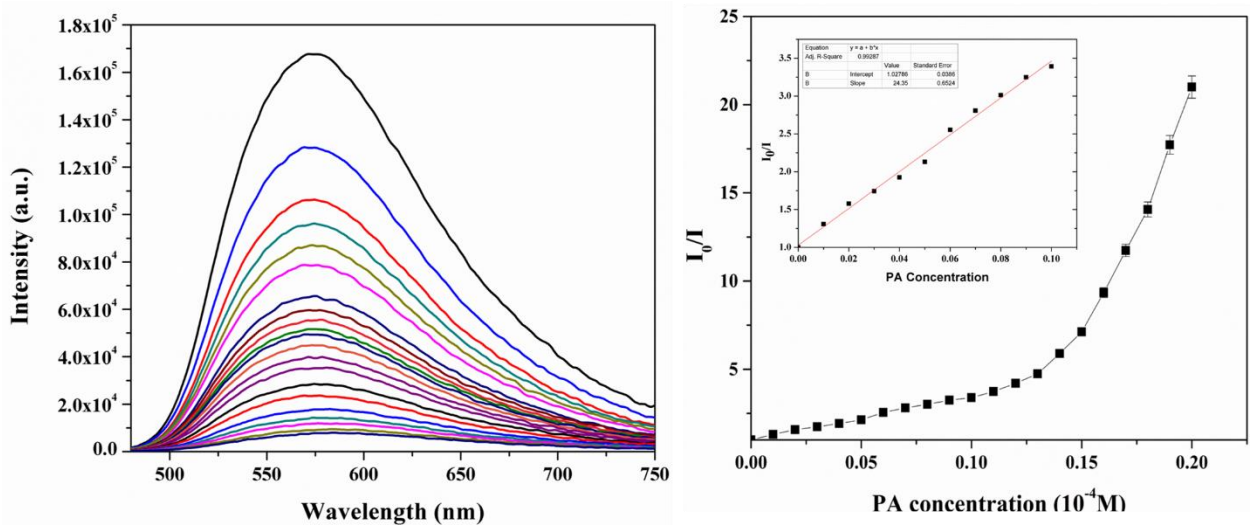


Fig. S39. Change in the fluorescence of AC-6 upon the addition of PA. b) Stern–Volmer plots of AC-6 using PA as a quencher. Inset:Stern–Volmer plots at lower concentration region of PA.

Table ST6 The Stern – Volmer quenching constants and detection limits data of luminophores in THF at 298 K.

Luminophore	Stern – Volmer constant (k_{SV}) ($10^4 x M^{-1}$)	Detection limit (ppb)
AC-1	12.66	100
AC-2	25.31	450
AC-3	12.09	150
AC-4	9.16	200
AC-5	11.45	200
AC-6	24.35	50

Lifetime measurements:

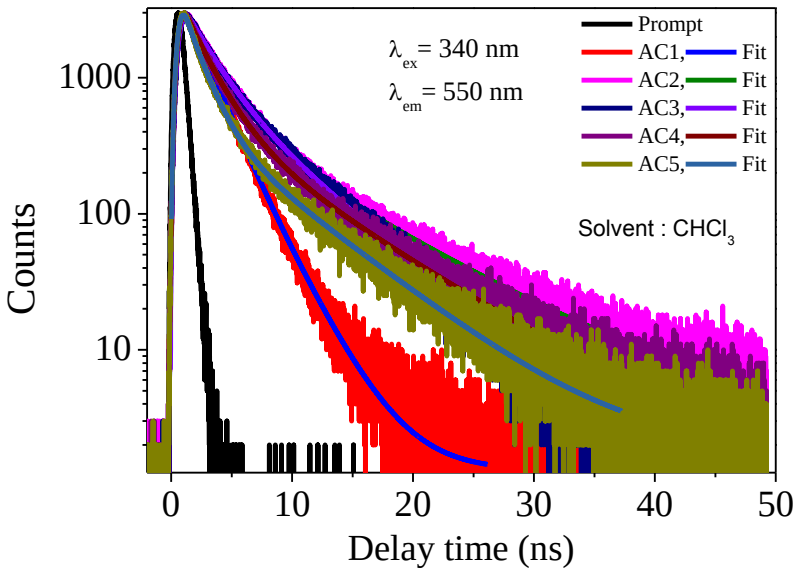


Fig. S40. Lifetime spectra of the AC compounds.

Lifetime measurements of luminophores with PA:

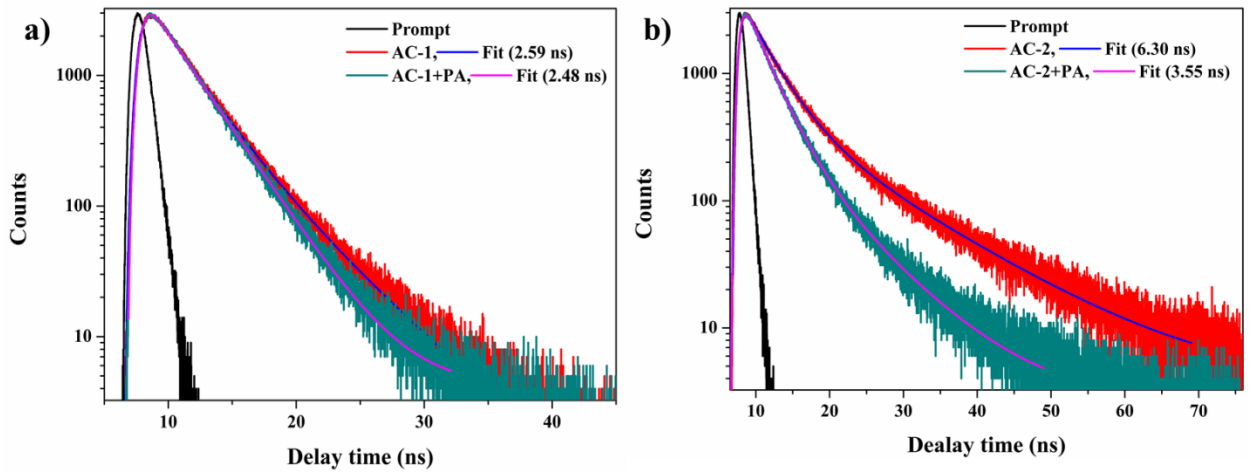


Fig. S41. Lifetime spectra of AC-1 (a) and AC-2 (b) luminophores with and without PA.

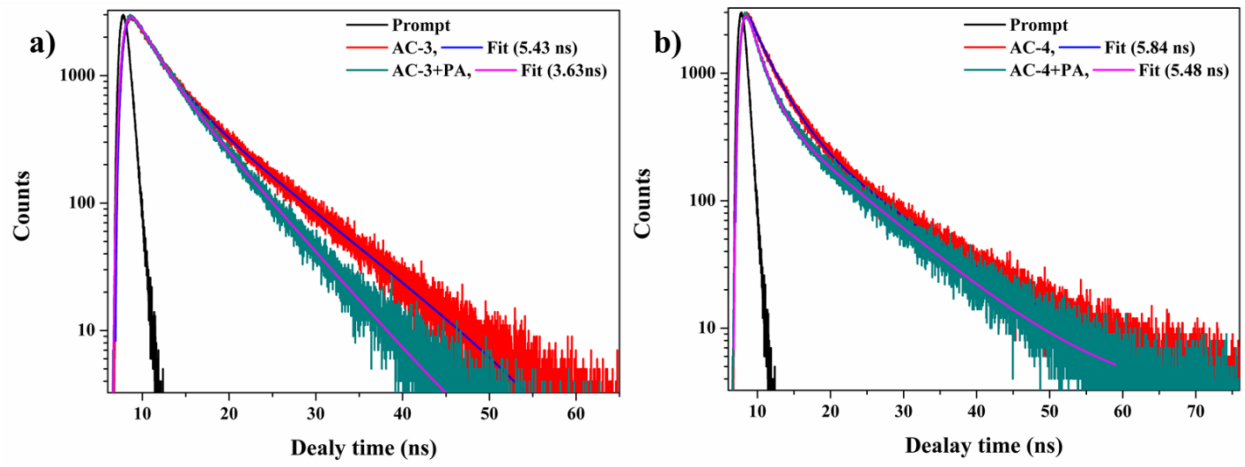


Fig. S42. Lifetime spectra of AC-3 (a) and AC-4 (b) luminophores with and without PA.

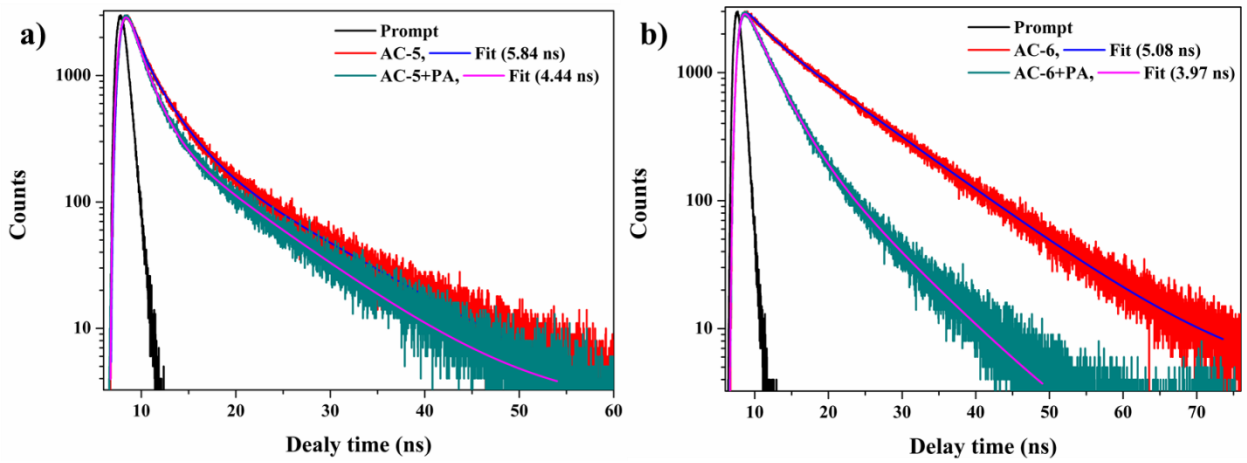


Fig. S43. Lifetime spectra of AC-5 (a) and AC-6 (b) luminophores with and without PA.

Table ST7: Excited state time constants of AC compounds

Compounds	λ_{ex}(nm)	λ_{em}(nm)	τ_1 (ns)	B_1	τ_2 (ns)	B_2	<τ>(ns)	χ^2
AC-1	340	550	1.79	68.52	3.48	31.48	2.59	1.09
AC-1+PA			1.72	62.92	3.18	37.08	2.48	1.05
AC-2			2.45	61.67	8.56	38.33	6.30	1.07
AC-2+PA			1.93	75.98	5.39	24.02	3.55	1.04
AC-3			2.32	52.63	6.64	47.37	5.43	1.18
AC-3+PA			1.71	32.61	4.02	67.39	3.63	1.08
AC-4			2.04	60.65	7.44	39.35	5.84	1.11
AC-4+PA			1.30	52.87	6.43	47.13	5.48	1.15
AC-5			2.04	60.65	7.44	39.35	5.84	1.11
AC-5+PA			1.14	63.92	5.62	36.08	4.44	1.16
AC-6			1.49	61.03	6.39	38.97	5.08	1.18
AC-6+PA			2.05	68.13	5.50	31.87	3.97	1.08

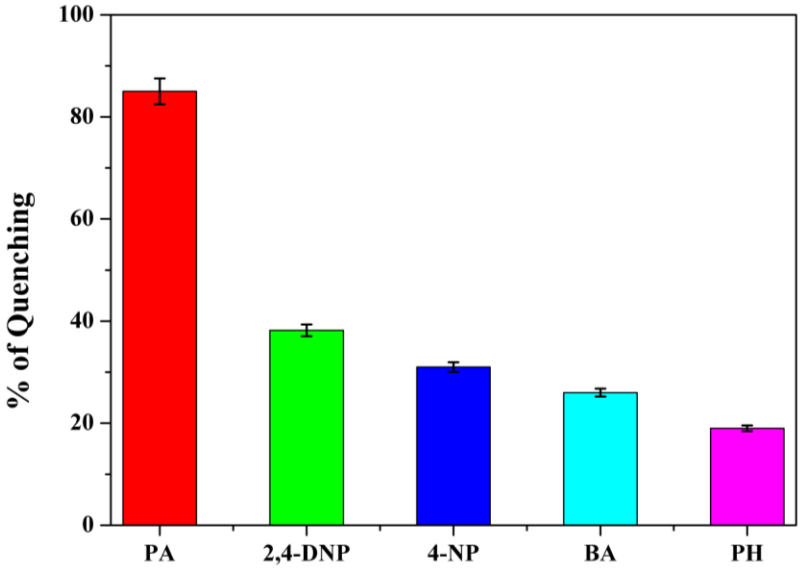


Fig. S44. Fluorescence quenching efficiencies of AC-1 towards different analytes.

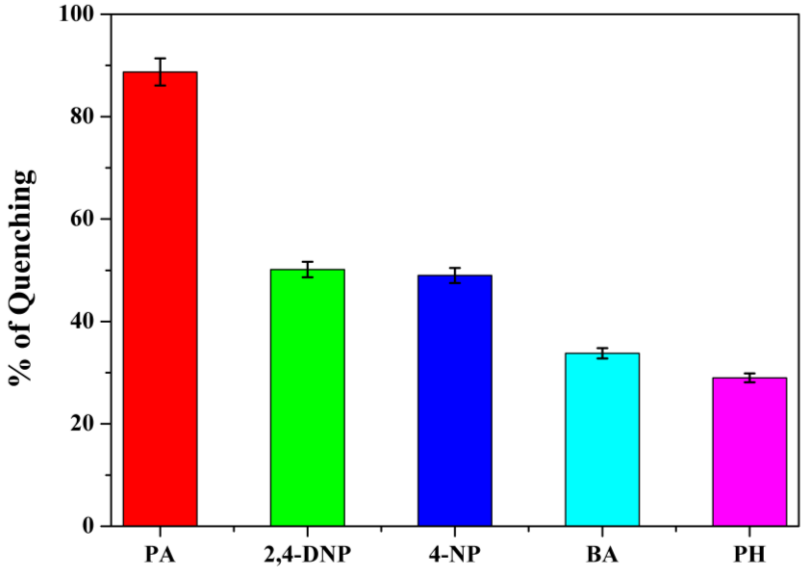


Fig. S45. Fluorescence quenching efficiencies of AC-2 towards different analytes.

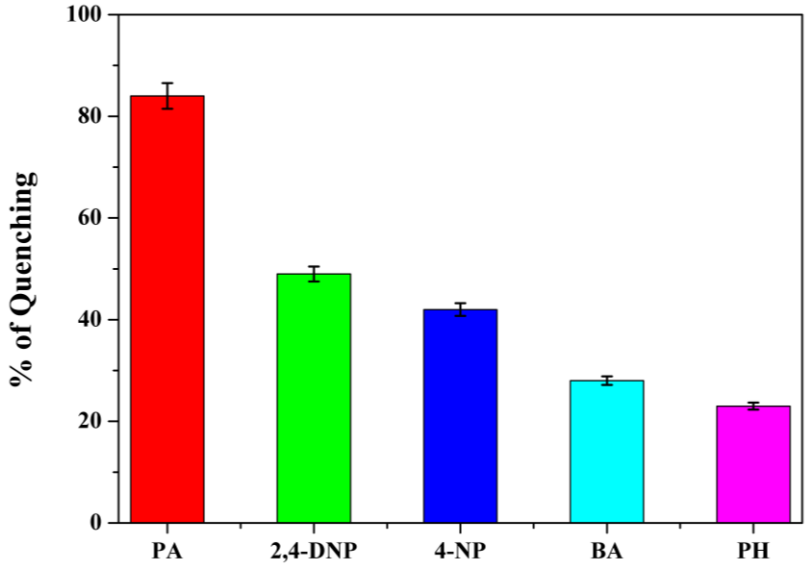


Fig. S46. Fluorescence quenching efficiencies of AC-3 towards different analytes.

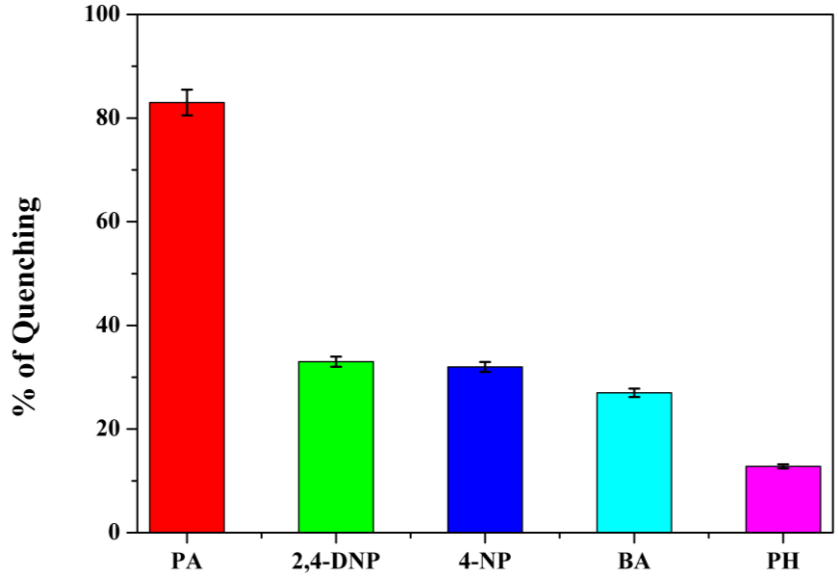


Fig. S47. Fluorescence quenching efficiencies of AC-5 towards different analytes.

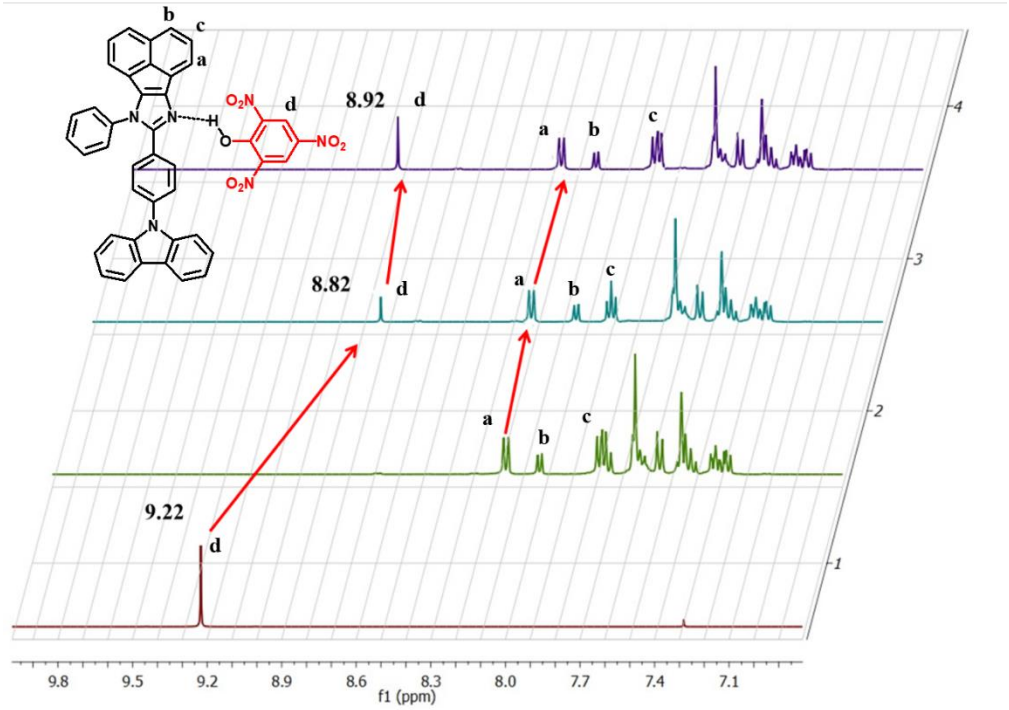


Fig. S48. ^{1}H-NMR spectra of AC-1, with PA (0, 0.5, 1.0 equiv) in $CDCI_3$.

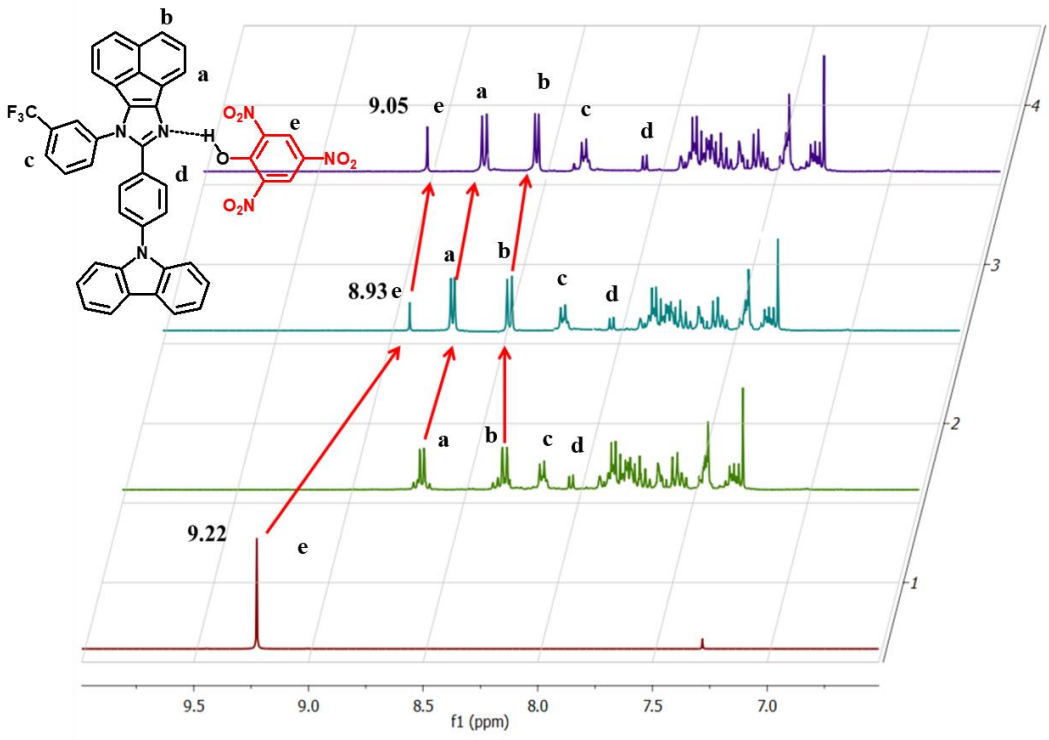


Fig. S49. ^{1}H-NMR spectra of AC-4, with PA (0, 0.5, 1.0 equiv) in $CDCI_3$.

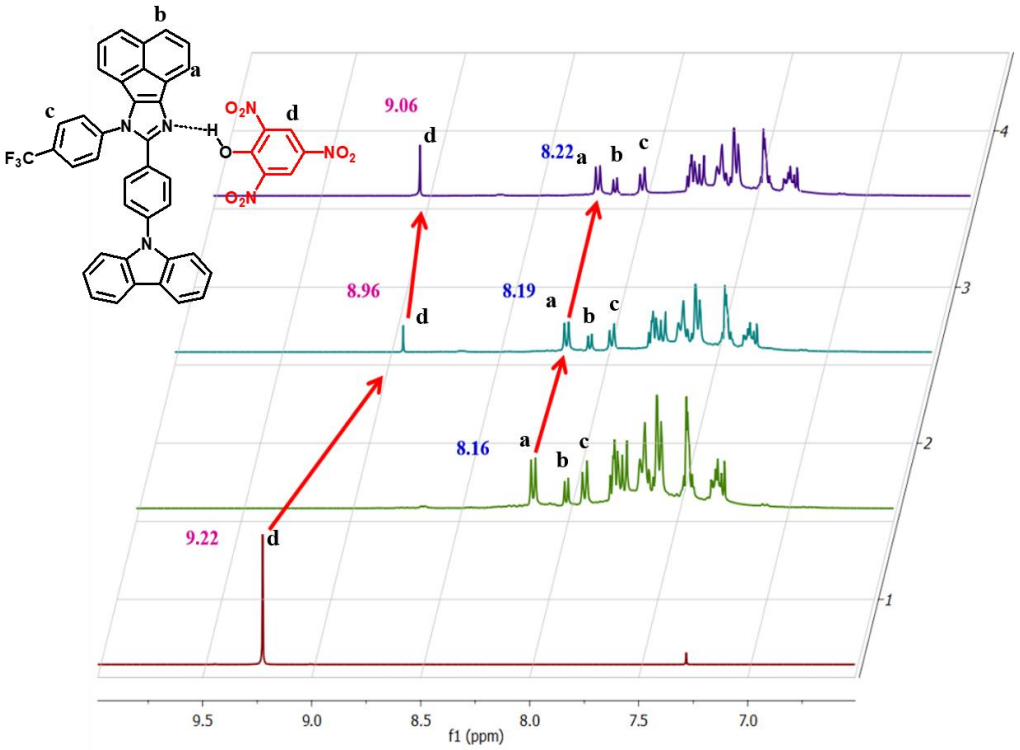


Fig. S50. ^{1}H-NMR spectra of AC-5, with PA (0, 0.5, 1.0 equiv) in $CDCI_3$.

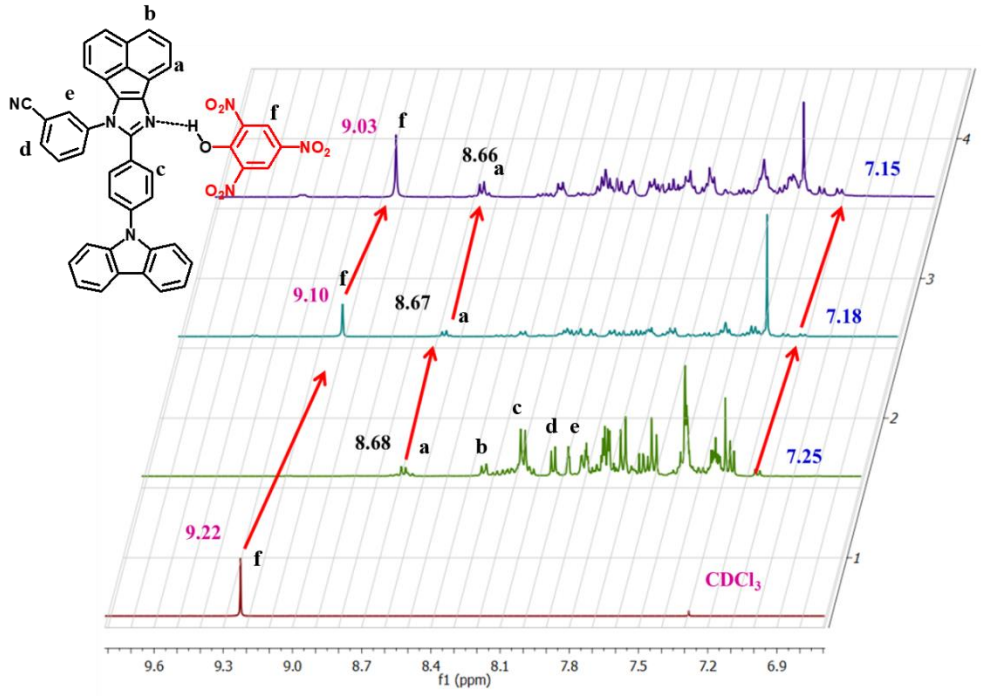


Fig. S51. ^{1}H-NMR spectra of AC-6, with PA (0, 0.5, 1.0 equiv) in $CDCI_3$.

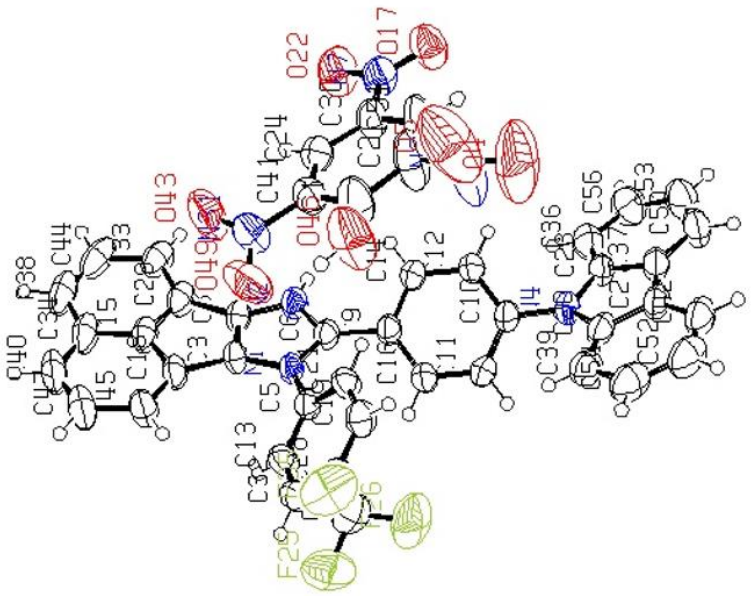


Fig. S52. ORTEP Diagram of AC-5 with Picric acid (eclipsed form 50% f probability). N atoms blue, F atoms in green and O atoms in red in color.

Table ST8: Crystal data and structure refinement for AC-5 with PA.

Identification code	AC-5 with PA	AC-6 with PA
Empirical formula	$C_{3.38}H_2F_{0.23}N_{0.46}O_{0.54}$	$C_{54}H_{45}N_{12}O_{16}$
Formula weight	62.13	1118.02
Temperature/K	293(2)	293(2)
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a/Å	11.4803(6)	10.8260(6)
b/Å	13.3395(9)	15.7882(8)
c/Å	14.9477(8)	17.3646(9)
α/°	96.499(5)	65.809(5)
β/°	111.425(5)	79.459(4)
γ/°	114.287(6)	80.439(4)
Volume/$Å^3$	1846.35(19)	2647.9(2)
Z	26	2
$\rho_{calc}g/cm^3$	1.453	1.402
μ/mm^{-1}	0.935	0.893
F(000)	830.0	1162.0

Crystal size/mm^3	0.217 × 0.103 × 0.074	0.149 × 0.085 × 0.064
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.64 to 133.84	6.52 to 137.16
Index ranges	-13 ≤ h ≤ 13, -12 ≤ k ≤ 15, -17 ≤ l ≤ 17	-9 ≤ h ≤ 12, -18 ≤ k ≤ 18, -19 ≤ l ≤ 20
Reflections collected	11187	15913
Independent reflections	6475 [R_{int} = 0.0218, R_{sigma} = 0.0302]	9192 [R_{int} = 0.0784, R_{sigma} = 0.0993]
Data/restraints/parameters	6475/0/542	9192/0/746
Goodness-of-fit on F^2	1.037	1.752
Final R indexes [I>=2σ (I)]	R_1 = 0.0710, wR_2 = 0.2075	R_1 = 0.1765, wR_2 = 0.4621
Final R indexes [all data]	R_1 = 0.0844, wR_2 = 0.2268	R_1 = 0.2214, wR_2 = 0.5056
Largest diff. peak/hole / e Å^{-3}	1.00/-0.59	2.43/-0.51

Table ST9: Bond Lengths for AC-5 with PA.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C3	1.383(3)	C27	C42	1.396(5)
N1	C5	1.439(3)	C28	C32	1.385(4)
N1	C6	1.366(3)	C28	C48	1.488(4)
N2	C6	1.334(3)	C29	C33	1.369(4)
N2	C8	1.369(3)	C33	C44	1.432(5)
C3	C8	1.361(4)	C34	C38	1.404(6)
C3	C18	1.468(3)	C34	C40	1.410(6)
N4	C10	1.421(3)	F35	C48	1.320(4)
N4	C20	1.401(4)	C36	C56	1.381(5)
N4	C23	1.404(4)	C37	C50	1.394(5)
C5	C13	1.374(4)	C38	C44	1.355(6)
C5	C21	1.386(4)	C39	C54	1.381(5)
C6	C9	1.465(3)	C40	C47	1.351(6)
C8	C29	1.466(4)	C42	C52	1.364(6)
C9	C14	1.389(4)	C45	C47	1.417(5)
C9	C16	1.392(4)	C50	C53	1.360(6)
C10	C11	1.393(4)	C52	C54	1.390(6)
C10	C12	1.383(4)	C53	C56	1.398(6)
C11	C16	1.381(4)	N7	O17	1.223(3)
C12	C14	1.380(4)	N7	O22	1.222(3)
C13	C32	1.378(4)	N7	C30	1.435(4)
C15	C18	1.421(4)	C24	C30	1.375(4)

C15	C29	1.412(5)	C24	C41	1.378(4)
C15	C34	1.398(4)	C30	C51	1.380(4)
C18	C45	1.359(5)	N31	C41	1.432(4)
C19	C21	1.379(4)	N31	O43	1.213(4)
C19	C28	1.383(4)	N31	O49	1.216(4)
C20	C27	1.413(4)	C41	C1	1.440(5)
C20	C39	1.379(5)	O46	C1	1.241(4)
C23	C36	1.381(5)	C51	C2	1.340(5)
C23	C37	1.406(4)	C1	C2	1.453(5)
F25	C48	1.332(5)	C2	N3	1.457(6)
F26	C48	1.321(4)	N3	O4	1.104(7)
C27	C37	1.432(5)	N3	O5	1.279(10)

Table ST10: Bond Angles for AC-5 with PA.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C3	N1	C5	125.0(2)	C33	C29	C15	119.3(3)
C6	N1	C3	107.3(2)	C13	C32	C28	119.7(3)
C6	N1	C5	127.2(2)	C29	C33	C44	117.1(4)
C6	N2	C8	108.7(2)	C15	C34	C38	116.4(4)
N1	C3	C18	141.9(3)	C15	C34	C40	116.2(3)
C8	C3	N1	107.4(2)	C38	C34	C40	127.3(3)
C8	C3	C18	110.4(2)	C56	C36	C23	117.3(3)
C20	N4	C10	125.4(2)	C23	C37	C27	107.1(3)
C20	N4	C23	108.3(2)	C50	C37	C23	119.3(3)
C23	N4	C10	125.0(2)	C50	C37	C27	133.6(3)
C13	C5	N1	119.4(2)	C44	C38	C34	120.5(3)
C13	C5	C21	121.1(2)	C20	C39	C54	117.1(3)
C21	C5	N1	119.4(2)	C47	C40	C34	120.9(3)
N1	C6	C9	126.6(2)	C52	C42	C27	119.2(3)
N2	C6	N1	108.7(2)	C38	C44	C33	123.2(3)
N2	C6	C9	124.6(2)	C18	C45	C47	118.3(4)
N2	C8	C29	142.0(3)	C40	C47	C45	122.6(4)
C3	C8	N2	107.8(2)	F25	C48	C28	113.6(3)
C3	C8	C29	110.0(3)	F26	C48	F25	105.2(3)
C14	C9	C6	118.1(2)	F26	C48	C28	112.7(3)
C14	C9	C16	119.6(2)	F35	C48	F25	104.7(3)
C16	C9	C6	122.3(2)	F35	C48	F26	107.5(3)
C11	C10	N4	120.4(2)	F35	C48	C28	112.4(3)

C12	C10	N4	119.8(2)	C53	C50	C37	119.1(3)
C12	C10	C11	119.8(2)	C42	C52	C54	120.8(3)
C16	C11	C10	119.7(2)	C50	C53	C56	121.0(4)
C14	C12	C10	120.6(2)	C39	C54	C52	121.9(4)
C5	C13	C32	119.8(3)	C36	C56	C53	121.4(4)
C12	C14	C9	119.9(2)	O17	N7	O22	122.4(3)
C29	C15	C18	113.9(2)	O17	N7	C30	119.1(2)
C34	C15	C18	122.8(3)	O22	N7	C30	118.5(3)
C34	C15	C29	123.3(3)	C30	C24	C41	119.2(3)
C11	C16	C9	120.4(2)	C24	C30	N7	120.2(3)
C15	C18	C3	102.5(2)	C24	C30	C51	121.4(3)
C45	C18	C3	138.3(3)	C51	C30	N7	118.4(3)
C45	C18	C15	119.1(3)	O43	N31	C41	118.1(3)
C21	C19	C28	120.0(3)	O43	N31	O49	122.6(3)
N4	C20	C27	108.2(3)	O49	N31	C41	119.3(3)
C39	C20	N4	129.8(3)	C24	C41	N31	117.1(3)
C39	C20	C27	122.0(3)	C24	C41	C1	123.5(3)
C19	C21	C5	119.2(3)	N31	C41	C1	119.4(3)
N4	C23	C37	108.8(3)	C2	C51	C30	119.1(3)
C36	C23	N4	129.3(3)	C41	C1	C2	111.8(3)
C36	C23	C37	121.9(3)	O46	C1	C41	127.7(4)
C20	C27	C37	107.7(3)	O46	C1	C2	120.5(4)
C42	C27	C20	118.9(3)	C51	C2	C1	124.9(4)
C42	C27	C37	133.4(3)	C51	C2	N3	117.0(4)
C19	C28	C32	120.4(3)	C1	C2	N3	118.0(3)
C19	C28	C48	118.5(3)	O4	N3	C2	124.1(7)
C32	C28	C48	121.1(3)	O4	N3	O5	116.6(6)
C15	C29	C8	103.1(2)	O5	N3	C2	117.7(6)
C33	C29	C8	137.4(3)				

Table ST11: Hydrogen Bonds for AC-5 with PA.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2	O46[1]	0.86	1.81	2.657(3)	167.2

[1]+X,-1+Y,+Z

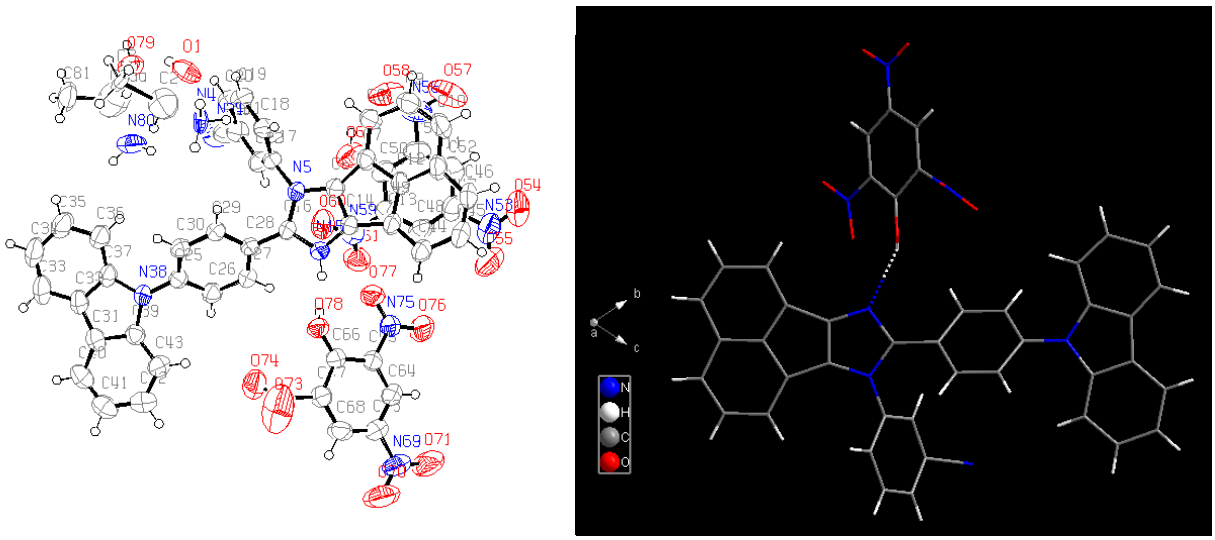


Fig. S53. (left) ORTEP Diagram of AC-6 with Picric acid. (Right) wire and stick structures of AC-6 with Picric acid by using Diamond software (solvent molecules is vomited). N atoms blue, F atoms in green and O atoms in red in color.

Table ST12: Crystal data and structure refinement for AC-6 with PA.

Table 1 Crystal data and structure refinement for AC_6_PA_RT_CU.	
Identification code	AC_6_PA_RT_CU
Empirical formula	$C_{54}H_{45}N_{12}O_{16}$
Formula weight	1118.02
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.8260(6)
b/Å	15.7882(8)
c/Å	17.3646(9)
α/°	65.809(5)
β/°	79.459(4)
γ/°	80.439(4)
Volume/Å^3	2647.9(2)
Z	2
ρ_{calc}g/cm^3	1.402

μ/mm^{-1}	0.893
F(000)	1162.0
Crystal size/mm^3	0.149 × 0.085 × 0.064
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.52 to 137.16
Index ranges	$-9 \leq h \leq 12$, $-18 \leq k \leq 18$, $-19 \leq l \leq 20$
Reflections collected	15913
Independent reflections	9192 [R_{int} = 0.0784, R_{sigma} = 0.0993]
Data/restraints/parameters	9192/0/746
Goodness-of-fit on F^2	1.752
Final R indexes [I>=2σ (I)]	R_1 = 0.1765, wR_2 = 0.4621
Final R indexes [all data]	R_1 = 0.2214, wR_2 = 0.5056
Largest diff. peak/hole / e $Å^{-3}$	2.43/-0.51

Table ST13: Bond Lengths for AC-6 with PA

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N4	C2	1.776(15)	N59	O60	1.221(10)
C3	C2	1.718(14)	C49	C50	1.401(12)
N15	C16	1.351(8)	C49	C48	1.382(12)
N15	C14	1.365(9)	C50	O62	1.343(11)
O1	C2	1.714(15)	C50	C51	1.393(14)
N38	C39	1.406(9)	C20	C19	1.366(13)
N38	C37	1.409(8)	C32	C33	1.395(11)
N38	C25	1.416(9)	C36	C35	1.403(12)
N5	C6	1.376(8)	C46	C45	1.325(13)
N5	C16	1.360(8)	C40	C41	1.336(15)
N5	C17	1.440(8)	C51	N56	1.454(13)
C6	C14	1.360(9)	C51	C52	1.409(14)
C6	C7	1.451(9)	C8	C9	1.416(12)
C39	C31	1.418(10)	C42	C41	1.393(14)
C39	C43	1.389(11)	C10	C9	1.349(13)
C16	C28	1.455(9)	C47	C48	1.371(14)
C37	C32	1.396(11)	C47	N53	1.475(12)
C37	C36	1.379(11)	C47	C52	1.351(14)
C13	C12	1.407(10)	C33	C34	1.357(15)
C13	C14	1.467(9)	N53	O55	1.180(14)
C13	C44	1.382(9)	N53	O54	1.224(14)
C30	C25	1.394(10)	C23	N24	1.130(15)
C30	C29	1.377(10)	O58	N56	1.202(15)

C25	C26	1.379(10)	N56	O57	1.264(16)
C26	C27	1.378(10)	C35	C34	1.389(16)
C12	C11	1.400(10)	O78	C66	1.255(8)
C12	C7	1.430(9)	O77	N75	1.223(9)
C28	C29	1.385(10)	C66	C67	1.439(10)
C28	C27	1.378(10)	C66	C65	1.441(10)
C17	C18	1.377(10)	N75	C65	1.452(9)
C17	C22	1.379(11)	N75	O76	1.199(10)
C31	C32	1.442(12)	C67	N72	1.442(10)
C31	C40	1.391(12)	C67	C68	1.355(11)
O61	N59	1.215(10)	C65	C64	1.366(10)
C43	C42	1.380(12)	O74	N72	1.229(11)
C18	C19	1.380(10)	N72	O73	1.224(13)
C21	C22	1.391(10)	C68	C63	1.388(13)
C21	C20	1.382(12)	C63	C64	1.385(13)
C21	C23	1.458(14)	C63	N69	1.421(11)
C11	C46	1.435(11)	O71	N69	1.230(14)
C11	C10	1.412(12)	O70	N69	1.235(14)
C7	C8	1.370(10)	O79	C0AA	1.73(2)
C44	C45	1.426(12)	N80	C0AA	1.77(2)
N59	C49	1.461(12)	C81	C0AA	1.65(2)

Table ST14: Bond Angles for AC-6 with PA.

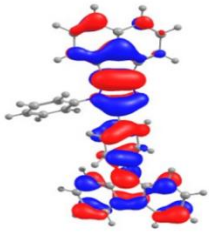
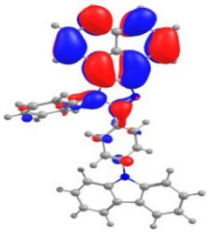
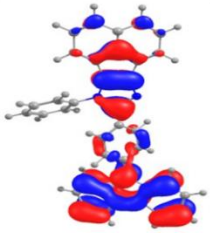
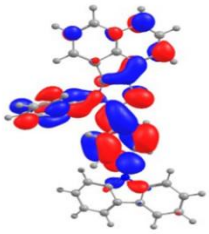
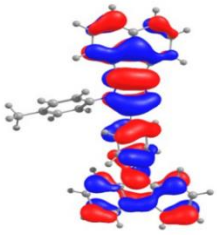
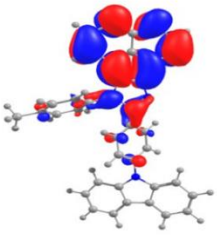
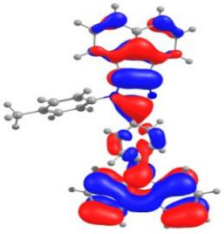
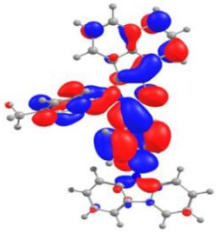
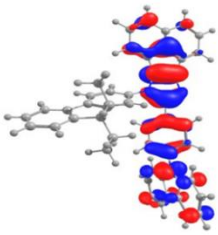
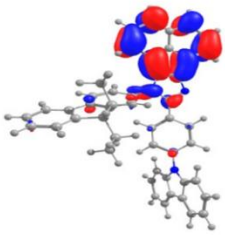
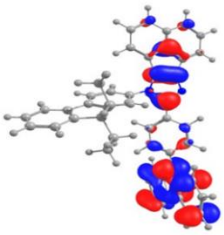
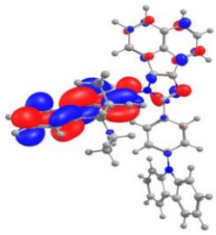
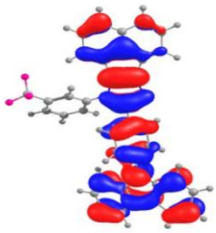
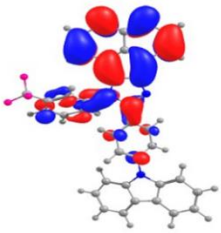
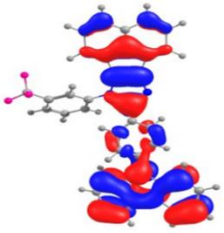
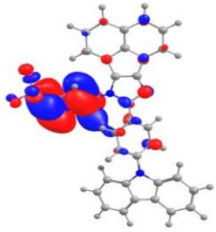
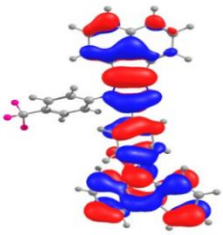
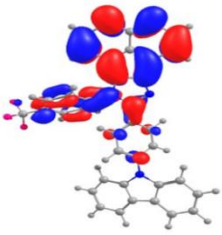
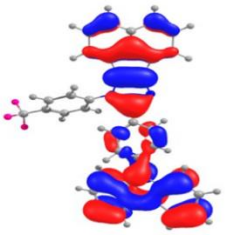
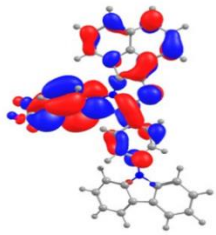
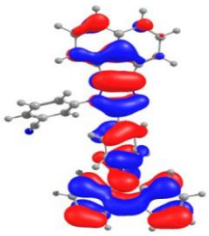
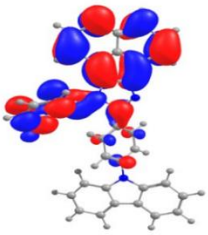
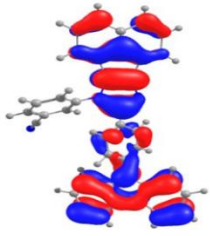
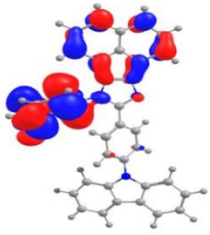
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C16	N15	C14	108.1(5)	O62	C50	C51	123.6(8)
C39	N38	C37	108.0(6)	C51	C50	C49	117.3(8)
C39	N38	C25	125.4(5)	C19	C20	C21	119.6(7)
C37	N38	C25	126.4(6)	C20	C19	C18	120.0(7)
C6	N5	C17	125.6(5)	C37	C32	C31	107.9(6)
C16	N5	C6	108.2(5)	C37	C32	C33	120.8(8)
C16	N5	C17	125.4(5)	C33	C32	C31	131.3(8)
N5	C6	C7	142.4(6)	C37	C36	C35	117.4(8)
C14	C6	N5	107.0(6)	C45	C46	C11	121.5(7)
C14	C6	C7	110.4(6)	C41	C40	C31	121.0(9)
N38	C39	C31	108.6(6)	C50	C51	N56	119.0(9)
C43	C39	N38	130.5(7)	C50	C51	C52	121.3(8)
C43	C39	C31	120.9(7)	C52	C51	N56	119.7(10)
N15	C16	N5	108.2(5)	C7	C8	C9	118.6(7)
N15	C16	C28	124.9(5)	C43	C42	C41	122.2(8)
N5	C16	C28	126.9(5)	C9	C10	C11	120.7(7)

C32	C37	N38	108.8(6)	C48	C47	N53	117.7(9)
C36	C37	N38	130.1(7)	C52	C47	C48	124.1(8)
C36	C37	C32	121.0(7)	C52	C47	N53	118.1(9)
C12	C13	C14	103.1(5)	C47	C48	C49	117.4(8)
C44	C13	C12	119.6(6)	C34	C33	C32	118.2(9)
C44	C13	C14	137.3(7)	C46	C45	C44	124.1(7)
C29	C30	C25	119.6(6)	C10	C9	C8	122.9(8)
C30	C25	N38	120.2(6)	O55	N53	C47	118.9(10)
C26	C25	N38	120.5(6)	O55	N53	O54	124.4(11)
C26	C25	C30	119.3(6)	O54	N53	C47	116.7(11)
C27	C26	C25	120.6(7)	N24	C23	C21	176.7(14)
C13	C12	C7	113.3(6)	O58	N56	C51	120.8(11)
C11	C12	C13	124.0(6)	O58	N56	O57	123.3(11)
C11	C12	C7	122.6(7)	O57	N56	C51	115.9(12)
C29	C28	C16	119.6(6)	C40	C41	C42	120.0(8)
C27	C28	C16	121.2(6)	C34	C35	C36	120.9(9)
C27	C28	C29	119.1(6)	C33	C34	C35	121.6(8)
C18	C17	N5	120.1(7)	C3	C2	N4	109.6(8)
C22	C17	N5	119.0(6)	O1	C2	N4	109.2(8)
C22	C17	C18	120.8(6)	O1	C2	C3	114.5(8)
C39	C31	C32	106.7(6)	O78	C66	C67	120.7(6)
C40	C31	C39	118.6(8)	O78	C66	C65	127.4(6)
C40	C31	C32	134.7(8)	C65	C66	C67	111.9(6)
N15	C14	C6	108.5(6)	O77	N75	C65	120.1(6)
N15	C14	C13	141.4(6)	O76	N75	O77	121.7(7)
C6	C14	C13	110.1(6)	O76	N75	C65	118.2(7)
C42	C43	C39	117.3(8)	C66	C67	N72	115.4(6)
C19	C18	C17	120.2(7)	C68	C67	C66	125.3(7)
C22	C21	C23	118.4(7)	C68	C67	N72	119.3(7)
C20	C21	C22	121.2(7)	C66	C65	N75	120.2(6)
C20	C21	C23	120.3(7)	C64	C65	C66	123.4(7)
C30	C29	C28	120.9(7)	C64	C65	N75	116.4(7)
C12	C11	C46	114.5(7)	O74	N72	C67	119.7(9)
C12	C11	C10	116.7(7)	O73	N72	C67	118.9(9)
C10	C11	C46	128.8(7)	O73	N72	O74	121.2(10)
C12	C7	C6	103.0(6)	C67	C68	C63	118.9(7)
C8	C7	C6	138.4(6)	C68	C63	C64	120.1(7)
C8	C7	C12	118.5(6)	C68	C63	N69	119.9(9)
C13	C44	C45	116.4(7)	C64	C63	N69	120.0(9)
C26	C27	C28	120.4(6)	C65	C64	C63	120.3(8)
O61	N59	C49	117.6(7)	C47	C52	C51	117.7(9)
O61	N59	O60	123.9(8)	O71	N69	C63	119.1(10)

O60	N59	C49	118.4(8)	O71	N69	O70	123.1(9)
C17	C22	C21	118.1(7)	O70	N69	C63	117.8(10)
C50	C49	N59	119.9(7)	O79	C0AA	N80	107.6(13)
C48	C49	N59	117.8(8)	C81	C0AA	O79	116.1(12)
C48	C49	C50	122.2(8)	C81	C0AA	N80	116.4(15)
O62	C50	C49	119.1(8)				

DFT Analysis:

Table ST15. FMO orbitals of the luminophores (AC-1 –AC-6).

Compound	HOMO	LUMO	HOMO-1	LUMO+1
AC-1				
AC-2				
AC-3				
AC-4				
AC-5				
AC-6				

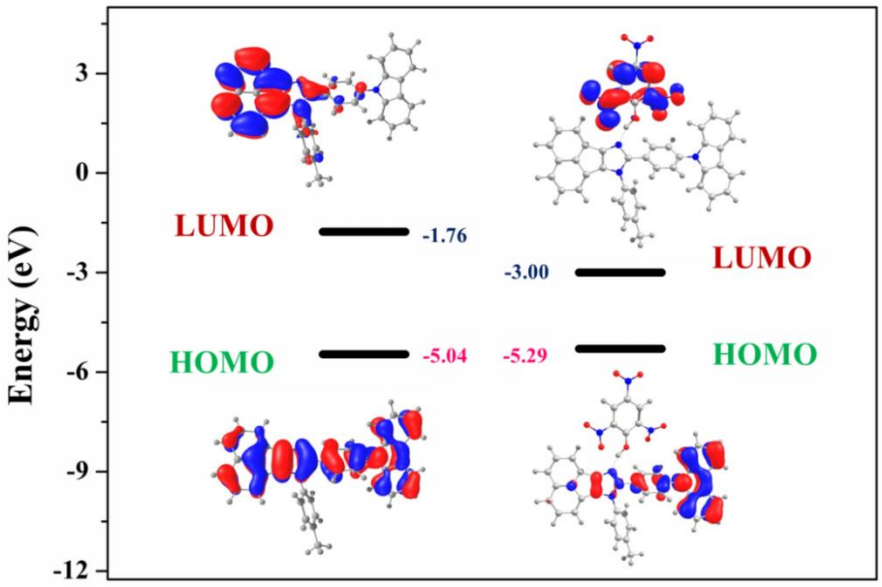


Fig. S54. Frontier molecular orbitals of AC-2 and AC-2 + PA obtained from the DFT calculations using Gaussian 09 program.

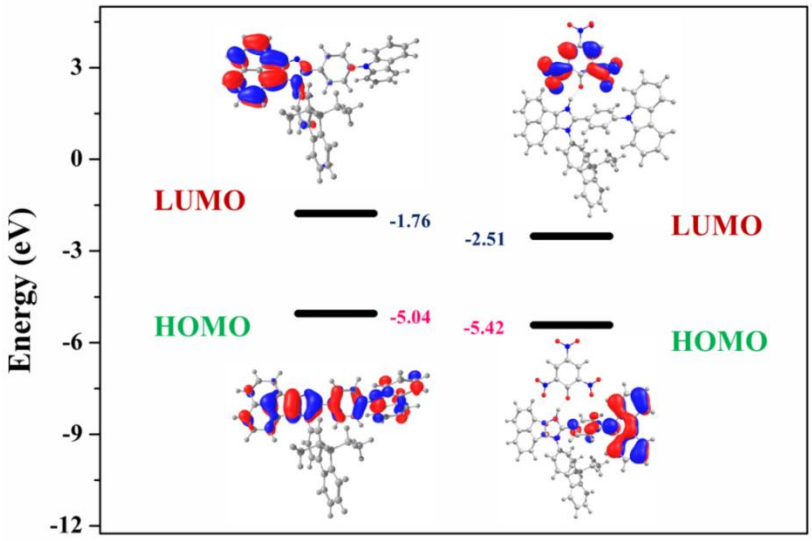


Fig. S55. Frontier molecular orbitals of AC-3 and AC-3 + PA obtained from the DFT calculations using Gaussian 09 program.

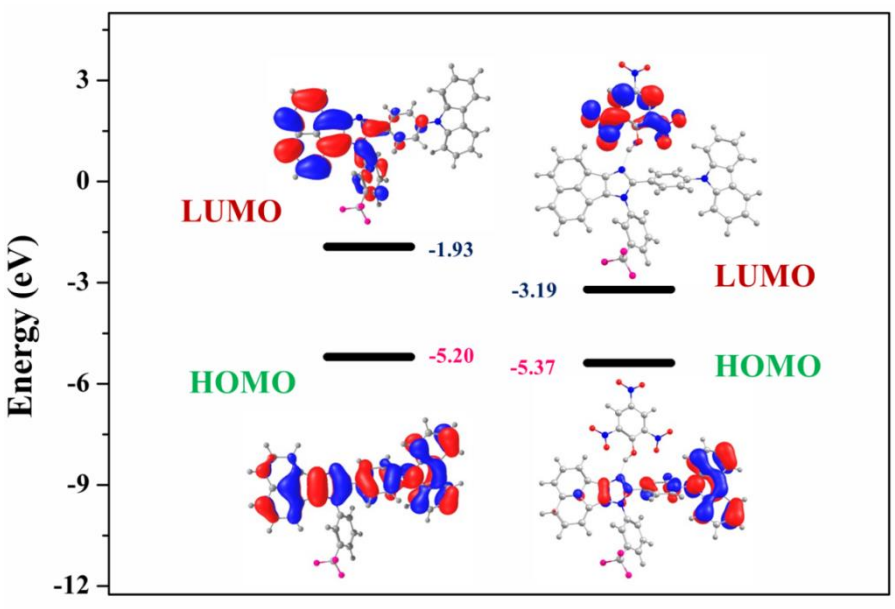


Fig. S56. Frontier molecular orbitals of AC-4 and AC-4 + PA obtained from the DFT calculations using Gaussian 09 program.

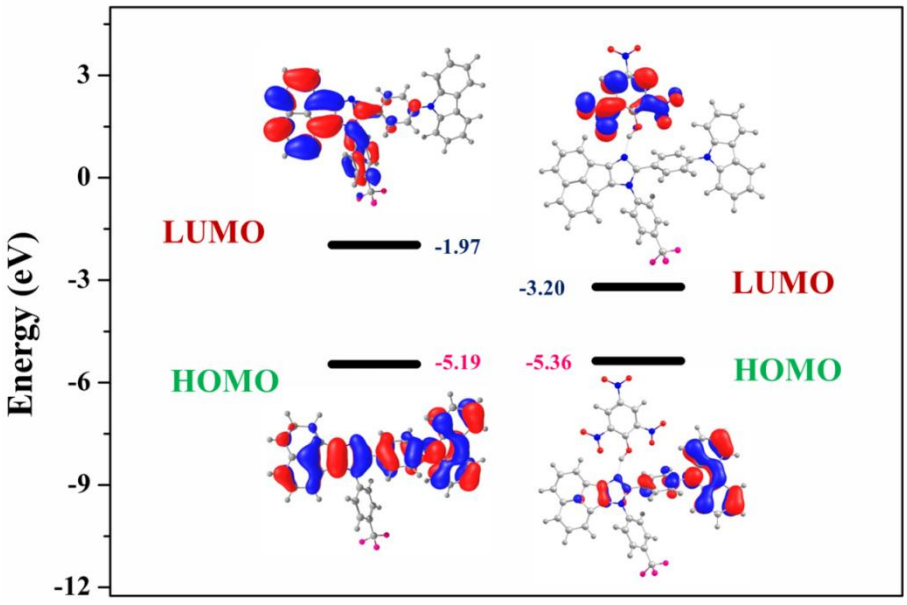


Fig. S57. Frontier molecular orbitals of AC-5 and AC-5 + PA obtained from the DFT calculations using Gaussian 09 program.

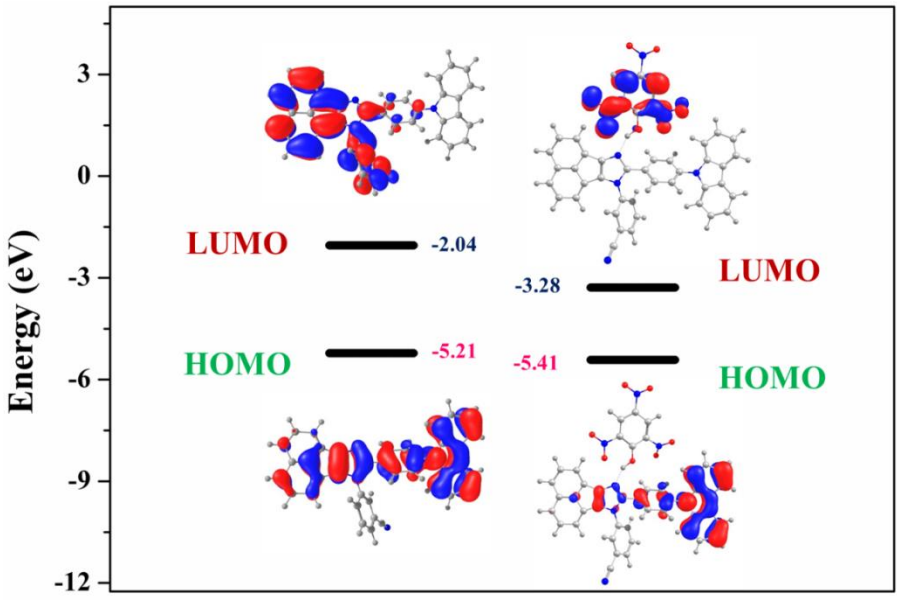


Fig. S58. Frontier molecular orbitals of AC-6 and AC-6 + PA obtained from the DFT calculations using Gaussian 09 program.

Absorption and emission spectra:

By using the optimized geometry of ground-state, the absorption spectra of the studied luminophores were calculated with the help of TDDFT/B3LYP method. The related absorption wavelength (nm), oscillator strength, major configuration, and their assignment are collected in Table ST17. Orbital composition of each excited state has also been calculated. These results give complete information about the absorption spectra. Simulated absorption spectra of these materials based on these calculated results are shown in Fig. S55. Table ST16 shows the calculated results of all materials are in good agreement with the experimental values. For example, the calculated absorption spectra at 320 nm and 425 nm are consistent with the experimental values of 327 nm and 420 nm, respectively. In addition, as reported by experimental data, the absorption spectra of all materials exhibit strong absorption bands in the 300-350 nm region and less intense absorption bands in the region of 400–450 nm. By using TD-DFT calculations we calculated singlet energy

levels of the synthesized luminophores. The detailed information of the corresponding transition and their oscillator strength were tabulated in Table ST16.

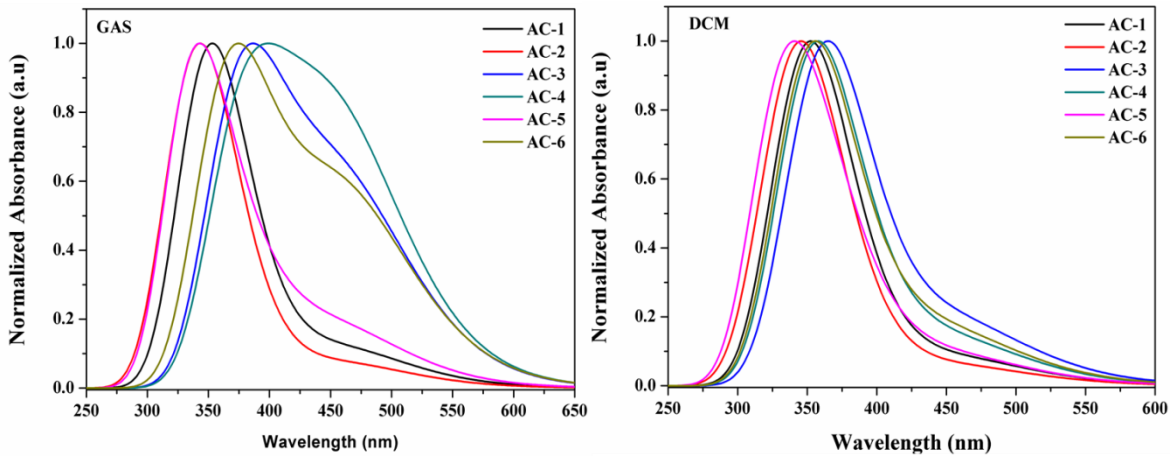


Fig. S59.UV-Visible spectra of luminophores (AC-1-AC-6) in gas and DCM phase.

Table ST16: Singlet Energy Levels of the Compounds in Various Solvents:

Luminophore	State	λ_{max} nm	*f*	Configuration
AC-1	Gas	464.59	0.0589	HOMO → LUMO (24.32%)
		371.21	0.1	HOMO-1 → LUMO (64.05%)
				HOMO → LUMO (24.32%)
		350.83	0.5179	HOMO-1 → LUMO (15.92%)
				HOMO → LUMO+1 (67.17%)
	DCM	460.52	0.0679	HOMO → LUMO (66.47%)
		369.14	0.1525	HOMO-1 → LUMO (63.12%)
				HOMO → LUMO (22.14%)
		349.75	0.8006	HOMO-1 → LUMO (21.42%)
				HOMO → LUMO+1 (66.53%)
AC-2	DCM	461.01	0.0656	HOMO → LUMO (66.61%)
		369.76	0.2083	HOMO -1→ LUMO (57.48%)
				HOMO → LUMO (21.08%)
		358.58	0.1873	HOMO -3→ LUMO (12.51%)
				HOMO-1 → LUMO (33.57%)
				HOMO → LUMO+1 (59.64%)
	Gas	464.91	0.0557	HOMO → LUMO (66.06%)

		381.61	0.0855	HOMO → LUMO+1 (60.17%) HOMO-1 → LUMO (58.82%) HOMO → LUMO (15.64%) HOMO → LUMO+1 (33.54%)
		371.49		
AC-3	DCM	458.69	0.0813	HOMO → LUMO (65.61%)
		375.48	0.1426	HOMO-1 → LUMO (61.85%) HOMO → LUMO (24.42%)
		354.14	0.5625	HOMO-1 → LUMO (22.66%) HOMO → LUMO+1 (65.79%)
	Gas	461.22	0.0725	HOMO → LUMO (64.74%)
		383.79	0.0838	HOMO-1 → LUMO (60.97%) HOMO → LUMO (26.46%)
		369.32		HOMO-1 → LUMO (13.52%) HOMO → LUMO+1 (67.08%)
AC-4	DCM	458.92	0.0840	HOMO → LUMO (65.04%)
		409.79		HOMO-1 → LUMO (62.82%) HOMO → LUMO (24.51%)
		377.49		HOMO-1 → LUMO (62.82%) HOMO → LUMO (24.51%)
	Gas	467.30	0.0801	HOMO-1 → LUMO (27.51%) HOMO → LUMO (62.52%) HOMO → LUMO (11%)
		441.23		HOMO-1 → LUMO+1 (19.02%) HOMO → LUMO+1 (66.06%)
		397.78		HOMO-1 → LUMO (62.57%) HOMO → LUMO+2 (12.88%)
AC-5	DCM	459.98	0.0821	HOMO → LUMO (65.76%)
		376.38	0.1706	HOMO-1 → LUMO (59.09%) HOMO → LUMO (23.74%)
		360.31	0.3006	HOMO-1 → LUMO (29.20%) HOMO → LUMO+1 (62.56%)
	Gas	460.18	0.0820	HOMO → LUMO (65.72%)
		376.84	0.1669	HOMO-1 → LUMO (59.02%) HOMO → LUMO (23.84%) HOMO → LUMO+1 (29.25%)
		360.81	0.2839	HOMO → LUMO+1 (62.46%)

AC-6	DCM	461.17	0.0656	HOMO → LUMO (66.67%)
		367.94	0.1579	HOMO-1 → LUMO (63.22%) HOMO → LUMO (21.55%) HOMO → LUMO+1 (21.15%)
		349.36	0.8075	HOMO → LUMO+1 (66.35%)
	Gas	465.17	0.0566	HOMO → LUMO (66%)
		375.07		HOM0-1 → LUMO (64.47%) HOMO → LUMO (23.36%)
		349.26	0.5583	HOMO-1 → LUMO (15.56%) HOMO → LUMO+1 (67.24%)
		349.31	0.8013	HOMO → LUMO+1 (66.42%)

Optimized Cartesian coordinates and energies of luminophores:

AC-1

Total Energy (a.u.): -1588.1204

Table ST17: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.820606	1.411979	0.317374
2	6	0	5.024699	0.302325	0.118091
3	6	0	5.661340	-0.962633	-0.106966
4	6	0	7.048928	-1.137058	-0.133290
5	6	0	7.842569	0.029528	0.077740
6	6	0	7.235696	1.252884	0.292636
7	1	0	5.395354	2.395729	0.489311
8	6	0	4.723504	-2.021066	-0.307389
9	6	0	7.517699	-2.463446	-0.374114
10	1	0	8.926494	-0.046274	0.067254
11	1	0	7.855049	2.131261	0.449349
12	6	0	6.616593	-3.493217	-0.568099
13	6	0	5.206127	-3.290092	-0.538989
14	1	0	8.585949	-2.659890	-0.405558
15	1	0	6.990511	-4.496552	-0.750573

16	1	0	4.536198	-4.129516	-0.697942
17	6	0	3.604061	-0.021770	0.057688
18	6	0	3.411558	-1.371668	-0.200636
19	6	0	1.450400	-0.525150	-0.096832
20	7	0	2.345979	0.535803	0.121385
21	7	0	2.090241	-1.676840	-0.295897
22	6	0	-0.013275	-0.427268	-0.068165
23	6	0	-0.719233	0.526154	0.686145
24	6	0	-0.751963	-1.380949	-0.793587
25	6	0	-2.110927	0.532748	0.704891
26	1	0	-0.185669	1.248589	1.291881
27	6	0	-2.140729	-1.367695	-0.787269
28	1	0	-0.212551	-2.126542	-1.366521
29	6	0	-2.834841	-0.407623	-0.037511
30	1	0	-2.643141	1.254313	1.315600
31	1	0	-2.696691	-2.090702	-1.374747
32	6	0	-5.082596	-1.474496	0.297384
33	6	0	-5.064468	0.705578	-0.336820
34	6	0	-4.737664	-2.765542	0.707012
35	6	0	-6.436478	-1.065494	0.192533
36	6	0	-4.699493	1.990151	-0.749430
37	6	0	-6.425119	0.324055	-0.214384
38	6	0	-5.773062	-3.652597	0.992505
39	1	0	-3.700843	-3.066866	0.805760
40	6	0	-7.457266	-1.977545	0.484842
41	6	0	-5.720243	2.898378	-1.021197
42	1	0	-3.657859	2.270349	-0.859634
43	6	0	-7.430741	1.256878	-0.492838
44	6	0	-7.120221	-3.268430	0.880037
45	1	0	-5.530205	-4.661903	1.311557
46	1	0	-8.498807	-1.678480	0.408588
47	6	0	-7.073182	2.541235	-0.891794
48	1	0	-5.461554	3.903163	-1.342391
49	1	0	-8.477014	0.978807	-0.403148
50	1	0	-7.902818	-3.985368	1.108392
51	1	0	-7.844237	3.273798	-1.109629
52	7	0	-4.253838	-0.392593	-0.025471
53	6	0	2.082134	1.937292	0.232088
54	6	0	1.442223	2.616147	-0.809015
55	6	0	2.503448	2.626009	1.373577
56	6	0	1.212325	3.986638	-0.696554
57	1	0	1.132711	2.069342	-1.693049
58	6	0	2.280012	3.999927	1.471432
59	1	0	2.994575	2.081644	2.173699
60	6	0	1.631393	4.681366	0.440086
61	1	0	0.713520	4.513476	-1.504203

62	1	0	2.606874	4.534412	2.358125
63	1	0	1.454631	5.749434	0.520685

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Total Energy (a.u.): – 1627.4413

Table ST18: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.797195	1.145511	-0.277592
2	6	0	-4.985557	0.044538	-0.094577
3	6	0	-5.603864	-1.232887	0.110289
4	6	0	-6.988775	-1.427802	0.132931
5	6	0	-7.799099	-0.269578	-0.060329
6	6	0	-7.209868	0.965566	-0.256143
7	1	0	-5.385721	2.137549	-0.435021
8	6	0	-4.650554	-2.280754	0.293519
9	6	0	-7.438353	-2.764612	0.351888
10	1	0	-8.881833	-0.361181	-0.051777
11	1	0	-7.841925	1.837104	-0.399988
12	6	0	-6.522365	-3.784183	0.529266
13	6	0	-5.114928	-3.560215	0.503954
14	1	0	-8.503652	-2.977042	0.379673
15	1	0	-6.881683	-4.795728	0.695084
16	1	0	-4.433024	-4.392479	0.649106
17	6	0	-3.560528	-0.259578	-0.038611
18	6	0	-3.348097	-1.610701	0.197133
19	6	0	-1.400222	-0.733013	0.103724
20	7	0	-2.311539	0.317542	-0.095656
21	7	0	-2.022445	-1.897705	0.285531
22	6	0	0.061858	-0.613455	0.076163
23	6	0	0.753844	0.368984	-0.653583
24	6	0	0.814780	-1.574989	0.776351
25	6	0	2.145351	0.395008	-0.673441
26	1	0	0.209541	1.099984	-1.238975
27	6	0	2.203174	-1.542403	0.769290
28	1	0	0.286279	-2.342419	1.330272
29	6	0	2.883112	-0.554065	0.043652
30	1	0	2.666733	1.139417	-1.265840
31	1	0	2.769627	-2.272542	1.337636
32	6	0	5.144642	-1.581197	-0.322055
33	6	0	5.098275	0.580711	0.369410
34	6	0	4.816336	-2.865721	-0.764525
35	6	0	6.493136	-1.156991	-0.208442

36	6	0	4.716774	1.848972	0.816189
37	6	0	6.463792	0.221129	0.234831
38	6	0	5.862973	-3.731222	-1.074104
39	1	0	3.783472	-3.178119	-0.869788
40	6	0	7.525521	-2.047471	-0.525581
41	6	0	5.725668	2.763520	1.110118
42	1	0	3.671631	2.111867	0.935354
43	6	0	7.457227	1.159913	0.536048
44	6	0	7.205096	-3.332147	-0.953486
45	1	0	5.633004	-4.735142	-1.418686
46	1	0	8.563118	-1.736627	-0.442831
47	6	0	7.083089	2.428410	0.969146
48	1	0	5.454020	3.755893	1.458140
49	1	0	8.506984	0.898501	0.437349
50	1	0	7.996833	-4.032466	-1.201110
51	1	0	7.844578	3.165442	1.204860
52	7	0	4.301976	-0.519544	0.030300
53	6	0	-2.069497	1.724690	-0.186182
54	6	0	-1.451037	2.404960	0.866321
55	6	0	-2.485414	2.425723	-1.320391
56	6	0	-1.240707	3.778075	0.770289
57	1	0	-1.137063	1.856350	1.747860
58	6	0	-2.279225	3.803050	-1.396609
59	1	0	-2.957467	1.889299	-2.137341
60	6	0	-1.653596	4.502908	-0.357005
61	1	0	-0.753713	4.297849	1.591095
62	1	0	-2.602660	4.339630	-2.284455
63	6	0	-1.451554	5.997319	-0.433474
64	1	0	-2.250228	6.531182	0.096092
65	1	0	-0.504050	6.296577	0.024583
66	1	0	-1.454025	6.349044	-1.468812

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Total Energy (a.u.): -2014.5655

Table ST19: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.645636	-0.472425	-0.640166
2	6	0	4.777281	-1.498375	-0.328056
3	6	0	5.326134	-2.777745	0.015133
4	6	0	6.698289	-3.046757	0.050046
5	6	0	7.568749	-1.965110	-0.278411

6	6	0	7.046343	-0.728346	-0.608384
7	1	0	5.287022	0.516993	-0.906190
8	6	0	4.318360	-3.742195	0.323345
9	6	0	7.075901	-4.373514	0.416552
10	1	0	8.644760	-2.116238	-0.266893
11	1	0	7.723763	0.084329	-0.854148
12	6	0	6.107095	-5.312737	0.715570
13	6	0	4.713975	-5.013769	0.674923
14	1	0	8.128022	-4.641556	0.460823
15	1	0	6.411812	-6.317691	0.993191
16	1	0	3.989152	-5.784383	0.918921
17	6	0	3.338700	-1.712211	-0.226777
18	6	0	3.053979	-3.013916	0.162082
19	6	0	1.158537	-2.039961	-0.010210
20	7	0	2.124069	-1.073374	-0.336461
21	7	0	1.715614	-3.211307	0.296269
22	6	0	-0.294069	-1.834641	-0.038809
23	6	0	-0.935504	-0.916112	-0.888164
24	6	0	-1.093305	-2.645291	0.788879
25	6	0	-2.321889	-0.788930	-0.884528
26	1	0	-0.355239	-0.298948	-1.563494
27	6	0	-2.478100	-2.534878	0.778684
28	1	0	-0.605607	-3.376813	1.423120
29	6	0	-3.105766	-1.595400	-0.050829
30	1	0	-2.803091	-0.062911	-1.531142
31	1	0	-3.082620	-3.180451	1.407111
32	6	0	1.957689	0.330598	-0.562245
33	6	0	1.430019	1.141134	0.452855
34	6	0	2.361396	0.879145	-1.785518
35	6	0	1.300281	2.503947	0.222159
36	1	0	1.137553	0.690888	1.396290
37	6	0	2.238112	2.250721	-2.012747
38	1	0	2.763195	0.224084	-2.551785
39	6	0	0.767784	3.583545	1.163199
40	6	0	1.703269	3.061079	-1.009477
41	1	0	2.551824	2.671568	-2.963485
42	6	0	0.913553	4.829950	0.291462
43	6	0	1.458920	4.508026	-0.967454
44	6	0	0.588698	6.148176	0.593798
45	6	0	1.680152	5.499500	-1.925416
46	6	0	0.810088	7.142827	-0.365891
47	1	0	0.166992	6.410406	1.560607
48	6	0	1.351281	6.820253	-1.614805
49	1	0	2.099735	5.253109	-2.896840
50	1	0	0.558721	8.174733	-0.139040
51	1	0	1.516315	7.603687	-2.348510

52	6	0	-0.713147	3.326704	1.569271
53	1	0	-0.740772	2.423439	2.192134
54	1	0	-1.026053	4.152468	2.220915
55	6	0	1.617000	3.683560	2.465562
56	1	0	1.476818	2.753118	3.030615
57	1	0	1.184587	4.480037	3.084549
58	6	0	3.113585	3.943576	2.274143
59	1	0	3.293117	4.888010	1.752191
60	1	0	3.615943	3.997312	3.245092
61	1	0	3.589947	3.144779	1.697894
62	6	0	-1.710675	3.179507	0.417551
63	1	0	-2.721396	3.029398	0.809368
64	1	0	-1.726412	4.070393	-0.217216
65	1	0	-1.469866	2.317978	-0.211839
66	6	0	-5.318405	-1.216321	1.071730
67	6	0	-5.350966	-1.543933	-1.174516
68	6	0	-4.943302	-1.026156	2.404660
69	6	0	-6.674288	-1.132969	0.663615
70	6	0	-5.020717	-1.810343	-2.506336
71	6	0	-6.695217	-1.343765	-0.768739
72	6	0	-5.950993	-0.769550	3.331701
73	1	0	-3.903651	-1.072663	2.708945
74	6	0	-7.666794	-0.874106	1.615947
75	6	0	-6.058149	-1.853311	-3.434958
76	1	0	-3.993869	-1.984936	-2.807586
77	6	0	-7.718217	-1.391766	-1.722863
78	6	0	-7.300548	-0.697045	2.946765
79	1	0	-5.684018	-0.620921	4.373934
80	1	0	-8.709299	-0.808585	1.317670
81	6	0	-7.393981	-1.642520	-3.052641
82	1	0	-5.826369	-2.057788	-4.476111
83	1	0	-8.752313	-1.239769	-1.426860
84	1	0	-8.061598	-0.497776	3.694897
85	1	0	-8.178451	-1.681156	-3.802126
86	7	0	-4.519585	-1.465753	-0.050543

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Total Energy (a.u.): -1925.1550

Table ST20: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.508117	0.247989	0.176920

2	6	0	-4.589565	-0.783510	0.170561
3	6	0	-5.079382	-2.131609	0.163033
4	6	0	-6.438771	-2.462193	0.164421
5	6	0	-7.360150	-1.373678	0.175857
6	6	0	-6.895861	-0.071804	0.181401
7	1	0	-5.207275	1.290865	0.170503
8	6	0	-4.029002	-3.098734	0.153149
9	6	0	-6.754393	-3.853857	0.157094
10	1	0	-8.428640	-1.571024	0.178618
11	1	0	-7.610436	0.745915	0.187374
12	6	0	-5.742815	-4.795554	0.148367
13	6	0	-4.364360	-4.434680	0.146040
14	1	0	-7.793951	-4.170082	0.158770
15	1	0	-6.001223	-5.850465	0.142572
16	1	0	-3.603079	-5.208634	0.137612
17	6	0	-3.139786	-0.956563	0.159153
18	6	0	-2.798092	-2.300813	0.157768
19	6	0	-0.938239	-1.246721	0.205003
20	7	0	-1.945372	-0.264141	0.199631
21	7	0	-1.448373	-2.474828	0.185111
22	6	0	0.503867	-0.981224	0.161868
23	6	0	1.065781	0.132323	-0.486051
24	6	0	1.372610	-1.923996	0.741316
25	6	0	2.445605	0.303690	-0.542669
26	1	0	0.427985	0.852090	-0.986266
27	6	0	2.749908	-1.747774	0.699246
28	1	0	0.945288	-2.792573	1.229648
29	6	0	3.300570	-0.629961	0.056237
30	1	0	2.867462	1.149095	-1.075579
31	1	0	3.407177	-2.466868	1.176435
32	6	0	5.635707	-1.389702	-0.464781
33	6	0	5.403564	0.693555	0.410678
34	6	0	5.419516	-2.658902	-1.008603
35	6	0	6.938706	-0.841056	-0.356513
36	6	0	4.917968	1.876484	0.974865
37	6	0	6.791125	0.485991	0.203663
38	6	0	6.533992	-3.384262	-1.423891
39	1	0	4.419920	-3.065621	-1.112519
40	6	0	8.041200	-1.591606	-0.781163
41	6	0	5.843017	2.862200	1.311832
42	1	0	3.857968	2.022687	1.149759
43	6	0	7.698925	1.492846	0.551141
44	6	0	7.833490	-2.862113	-1.309216
45	1	0	6.391067	-4.373525	-1.848514
46	1	0	9.045106	-1.183941	-0.703789
47	6	0	7.219873	2.678428	1.100258

48	1	0	5.489226	3.791014	1.749713
49	1	0	8.764400	1.347522	0.397537
50	1	0	8.680537	-3.454624	-1.640820
51	1	0	7.914158	3.467478	1.372079
52	7	0	4.706400	-0.451303	0.004136
53	6	0	-1.838759	1.141068	0.409158
54	6	0	-1.109369	1.651287	1.490419
55	6	0	-2.526241	2.005209	-0.442156
56	6	0	-1.069695	3.026163	1.706937
57	1	0	-0.588520	0.970394	2.153860
58	6	0	-2.507614	3.379499	-0.192928
59	1	0	-3.078535	1.606189	-1.285714
60	6	0	-1.775698	3.897378	0.875050
61	1	0	-0.501506	3.420375	2.543236
62	1	0	-1.762678	4.965997	1.054030
63	6	0	-3.348192	4.272639	-1.065426
64	9	0	-3.189762	3.983693	-2.375455
65	9	0	-4.666943	4.114251	-0.789543
66	9	0	-3.057849	5.577723	-0.894881

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Total Energy (a.u.): 1925.1546

Table ST21: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.715573	0.360567	-0.227288
2	6	0	-4.850593	-0.705441	-0.083910
3	6	0	-5.406500	-2.017558	0.075357
4	6	0	-6.780471	-2.280198	0.087521
5	6	0	-7.646087	-1.156824	-0.065584
6	6	0	-7.117661	0.111897	-0.214638
7	1	0	-5.355295	1.377625	-0.345286
8	6	0	-4.404746	-3.023652	0.226285
9	6	0	-7.164615	-3.644042	0.258286
10	1	0	-8.723022	-1.301031	-0.062412
11	1	0	-7.790880	0.956676	-0.326913
12	6	0	-6.200657	-4.623806	0.403336
13	6	0	-4.805964	-4.330856	0.391296
14	1	0	-8.218328	-3.908684	0.275416
15	1	0	-6.510739	-5.656606	0.532919
16	1	0	-4.084385	-5.133191	0.510514

17	6	0	-3.412062	-0.943481	-0.037198
18	6	0	-3.136308	-2.289157	0.156966
19	6	0	-1.228841	-1.323372	0.107494
20	7	0	-2.187766	-0.307201	-0.064030
21	7	0	-1.798079	-2.517831	0.245398
22	6	0	0.225711	-1.132742	0.079744
23	6	0	0.865097	-0.135750	-0.677271
24	6	0	1.026490	-2.036707	0.801844
25	6	0	2.253035	-0.038439	-0.701994
26	1	0	0.282527	0.547987	-1.283594
27	6	0	2.411484	-1.932527	0.791007
28	1	0	0.539579	-2.816194	1.376907
29	6	0	3.039579	-0.929750	0.038275
30	1	0	2.734658	0.714163	-1.316961
31	1	0	3.014790	-2.616934	1.377734
32	6	0	5.350105	-1.857760	-0.280377
33	6	0	5.192703	0.333252	0.299909
34	6	0	5.090129	-3.178327	-0.657336
35	6	0	6.674330	-1.358643	-0.192717
36	6	0	4.748416	1.601339	0.684730
37	6	0	6.574266	0.037227	0.178993
38	6	0	6.180896	-4.002659	-0.924633
39	1	0	4.075660	-3.550235	-0.746437
40	6	0	7.752151	-2.208496	-0.466473
41	6	0	5.709968	2.579804	0.927492
42	1	0	3.692039	1.818422	0.796404
43	6	0	7.519386	1.038938	0.427963
44	6	0	7.500046	-3.528551	-0.827132
45	1	0	6.003662	-5.033267	-1.217624
46	1	0	8.771791	-1.839401	-0.402518
47	6	0	7.082190	2.307376	0.797392
48	1	0	5.388454	3.573373	1.225750
49	1	0	8.580784	0.825875	0.338464
50	1	0	8.327540	-4.198103	-1.040378
51	1	0	7.805565	3.093179	0.991705
52	7	0	4.453217	-0.823494	0.020118
53	6	0	-2.005008	1.106501	-0.097073
54	6	0	-1.335129	1.756211	0.944711
55	6	0	-2.528560	1.842025	-1.165659
56	6	0	-1.180288	3.138808	0.909066
57	1	0	-0.940811	1.177491	1.772090
58	6	0	-2.381716	3.226716	-1.190848
59	1	0	-3.036321	1.324745	-1.972733
60	6	0	-1.703887	3.876163	-0.156278
61	1	0	-0.655112	3.646662	1.710175
62	1	0	-2.776865	3.800319	-2.021842

63	6	0	-1.588940	5.377405	-0.161240
64	9	0	-2.646704	5.959530	0.449644
65	9	0	-0.480317	5.797058	0.486081
66	9	0	-1.540886	5.870507	-1.418156

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Total Energy (a.u.): -1680.3586

Table ST22: Optimized Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.823046	1.177556	0.487371
2	6	0	5.028730	0.081386	0.217526
3	6	0	5.668761	-1.162469	-0.097972
4	6	0	7.056851	-1.329409	-0.142907
5	6	0	7.847850	-0.177780	0.144399
6	6	0	7.238297	1.026019	0.445095
7	1	0	5.398180	2.147736	0.725147
8	6	0	4.734663	-2.207185	-0.370196
9	6	0	7.528930	-2.633671	-0.478971
10	1	0	8.931858	-0.248660	0.123067
11	1	0	7.855312	1.894143	0.657476
12	6	0	6.630740	-3.650543	-0.742230
13	6	0	5.219906	-3.454941	-0.693723
14	1	0	8.597636	-2.823283	-0.528806
15	1	0	7.007268	-4.636791	-0.997352
16	1	0	4.551918	-4.282856	-0.910370
17	6	0	3.608881	-0.244333	0.140527
18	6	0	3.421111	-1.572083	-0.213977
19	6	0	1.453183	-0.749107	-0.052545
20	7	0	2.344647	0.300921	0.241653
21	7	0	2.100326	-1.876954	-0.331327
22	6	0	-0.010718	-0.656896	-0.016535
23	6	0	-0.717508	0.203233	0.841616
24	6	0	-0.747855	-1.520983	-0.847438
25	6	0	-2.108956	0.212143	0.855930
26	1	0	-0.185533	0.845307	1.533902
27	6	0	-2.136693	-1.506195	-0.843077
28	1	0	-0.208817	-2.196811	-1.501653
29	6	0	-2.832199	-0.635289	0.007759
30	1	0	-2.642138	0.859620	1.543735

31	1	0	-2.691695	-2.156119	-1.511141
32	6	0	-5.083333	-1.725947	0.211419
33	6	0	-5.055524	0.516089	-0.159067
34	6	0	-4.745319	-3.058322	0.463877
35	6	0	-6.434764	-1.299441	0.161334
36	6	0	-4.685223	1.837953	-0.421333
37	6	0	-6.417037	0.128779	-0.077291
38	6	0	-5.785388	-3.967427	0.644949
39	1	0	-3.710447	-3.376297	0.523846
40	6	0	-7.460158	-2.233790	0.346635
41	6	0	-5.702320	2.776703	-0.579712
42	1	0	-3.643615	2.126181	-0.508346
43	6	0	-7.419129	1.092333	-0.239649
44	6	0	-7.130148	-3.564749	0.583625
45	1	0	-5.547726	-5.008870	0.840741
46	1	0	-8.499966	-1.921574	0.310662
47	6	0	-7.056341	2.412997	-0.485953
48	1	0	-5.438846	3.810009	-0.784921
49	1	0	-8.466427	0.810270	-0.179631
50	1	0	-7.916680	-4.299083	0.727488
51	1	0	-7.824407	3.169566	-0.613345
52	7	0	-4.249347	-0.616797	0.016696
53	6	0	2.068859	1.683121	0.452571
54	6	0	1.361525	2.411025	-0.505127
55	6	0	2.540826	2.310352	1.611170
56	6	0	1.111968	3.773859	-0.287216
57	1	0	1.008657	1.926138	-1.407392
58	6	0	2.302340	3.670301	1.812763
59	1	0	3.084126	1.726599	2.346827
60	6	0	1.585985	4.407329	0.873877
61	1	0	2.669258	4.153272	2.712482
62	1	0	1.390227	5.462631	1.027245
63	6	0	0.375611	4.526487	-1.262283
64	7	0	-0.223461	5.140864	-2.047181

The Comparison of our luminophores with other reported PA sensors.

Table ST23: The Comparison of our luminophores with other reported PA sensors.

S. No	Sensor	Solvent	Quenching constant (M-1)	Detection limit (M)	Ref.
1	hexaphenylsilole	THF/Water	-	4.81 ppb	1
2	tetraphenylethene	Water	2.7×10^5	0.4 ppm	2
3	Polymers based on di (naphthalen-2-yl)-1,2-diphenylethene	H_2O/THF (9/1)	4.70×10^4	1.81×10^{-6}	3
4	Triazine-COF	THF	8.71×10^4	10.7 ppm	4
5	poly(silylenevinylene)	THF	8.491×10^3	1.0 ppm	5
6	Diphenylfumaronitriles	H_2O/THF (8/2)	5.60×10^4	1.80×10^{-10}	6
7	Imidazole derivatives	H_2O/DMF (9/1)	1.30×10^4	3.55×10^{-6}	7
8	Thiophene aromatic amine derivatives	THF	-	5.70×10^{-6}	8
9	3-(Benzyloxy)-2-(4-(di-p-tolylamino)phenyl)-4H-chromen-4-one	Water	1.93×10^4	3.70×10^{-9}	9
10	[P(dimethylacrylamide*co*-Benzophenone acrylamide-*co*-glycidyl methacrylate]	Water	7.75×10^4	5.60×10^{-7}	10
11	9,14-diphenylpyreno [4,5-g]isoquinoline	MeCN	-	2.42×10^{-6}	11
12	7,10-bis(4-bromophenyl)-8,9-bis(4-(2-(2-(2-methoxyethoxy) ethoxy)ethoxy)- phenyl)-fluoranthene	EtOH	5.60×10^5	2.6 ppb	12
13	Fluorescein derivatives	EtOH	2.50×10^5	1.10×10^{-7}	13
14	1,3-Bis(benzo[d]thiazol-2-yl)benzene derivatives	H_2O/THF (9/1)	1.54×10^5	29.1 ppb	14
15	1,3,5-tri(1H-benzo[d]imidazol-2-yl)benzene derivative	THF	1.15×10^5	50 ppb	15
16	tetraphenylethylene	THF	5.7×10^4	1.45 ppb	16
17	terthiophene	THF/water	5.7×10^3	70 ppb	17
18	AC-2	THF	2.5×10^3	450 ppb	this work

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