SUPPLEMENTARY INFORMATION

Triphenylamine based yellowish-orange emitting Donor – π – Acceptor organic dyes for hybrid WLEDs: synthesis, characterization and theoretical studies.

Aravind Babu Kajjam[a], P. Shyam Vinod Kumar[b], V. Subramanian[b] and V. Sivakumar[a]*

[a] Department of Chemistry, National Institute of Technology, Rourkela 769 008, India.

[b]CSIR-Central Leather Research Institute, Adyar, Chennai – 600 020

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1. NMR Spectroscopy:

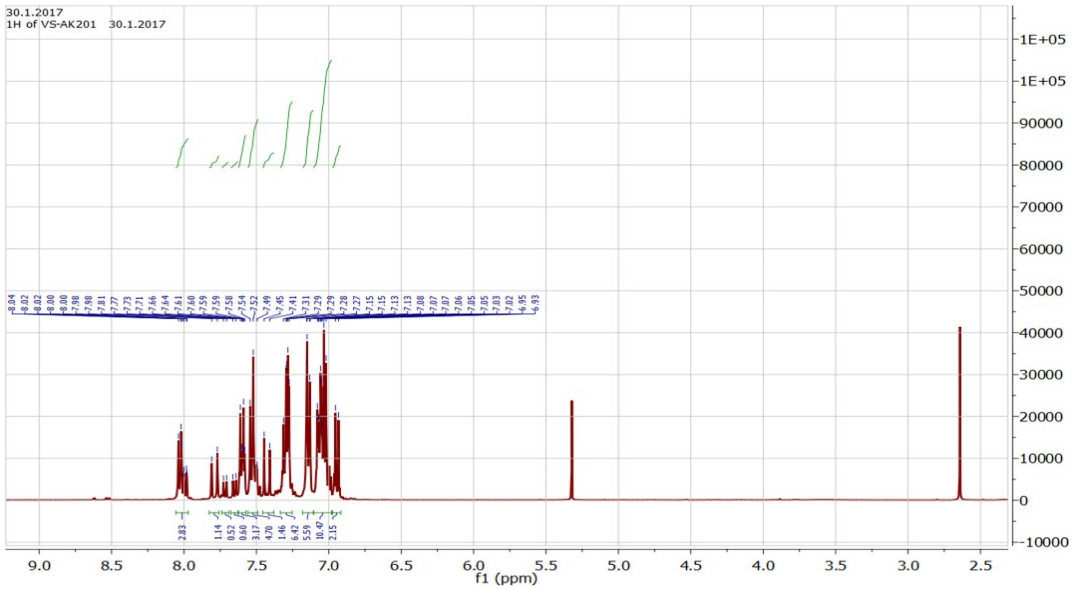


Fig. S1. ^{1}H-NMR spectra of TPA-1.

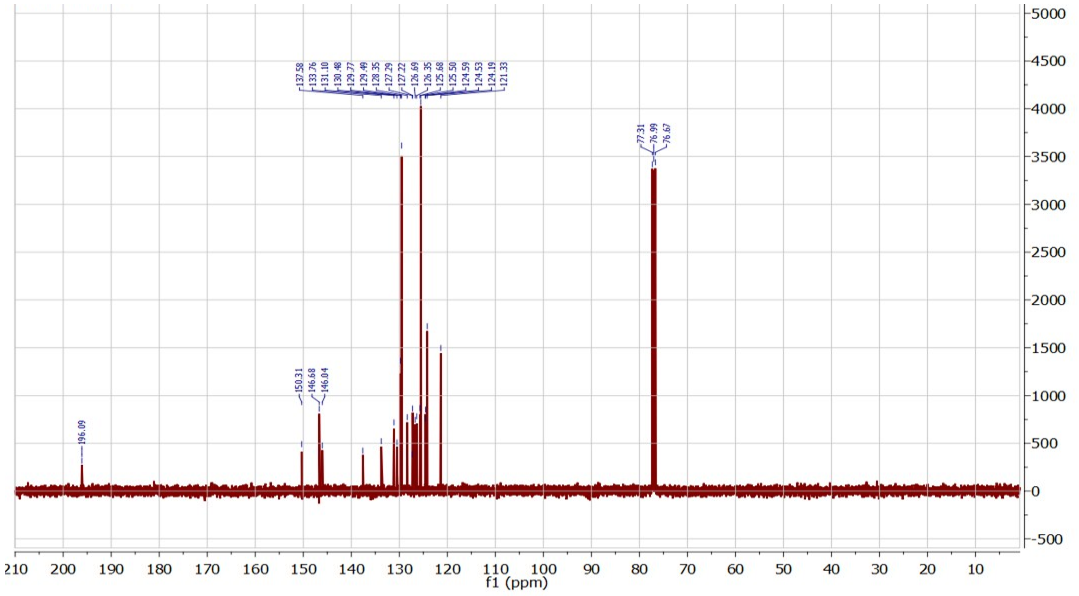


Fig. S2. ^{13}C-NMR spectra of TPA-1.

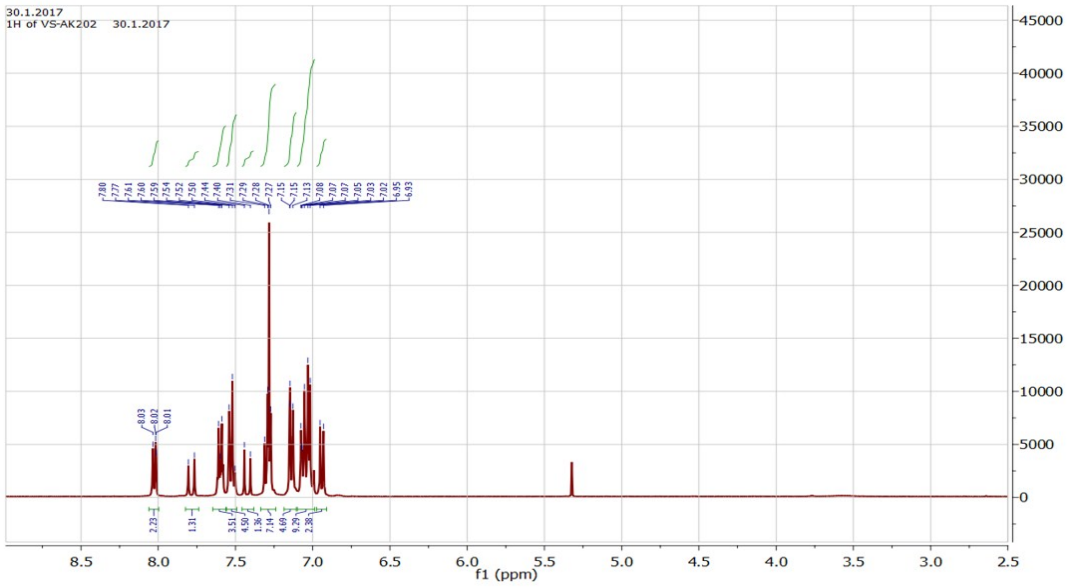


Fig. S3. ^{1}H-NMR spectra of TPA-2.

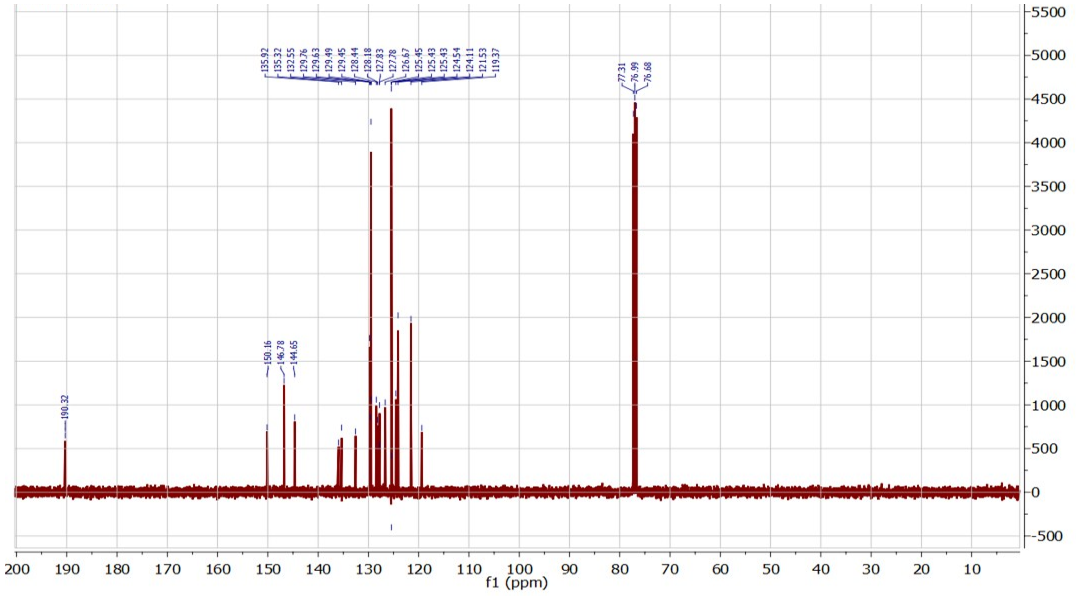


Fig. S4. ^{13}C-NMR spectra of TPA-2.

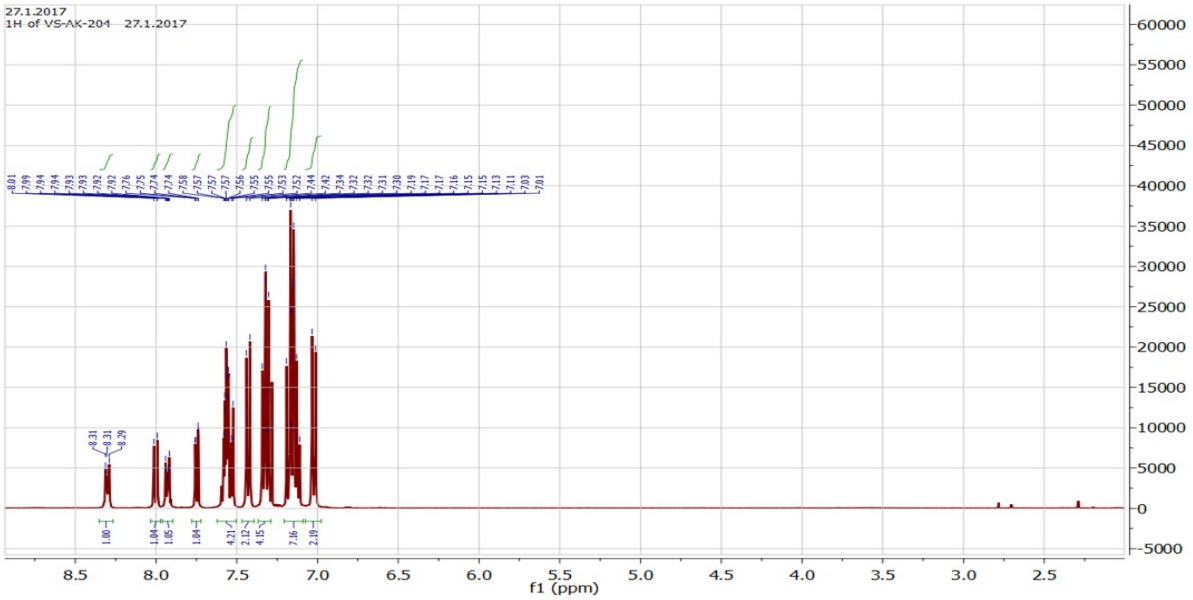


Fig. S5. ^{1}H-NMR spectra of TPA-3.

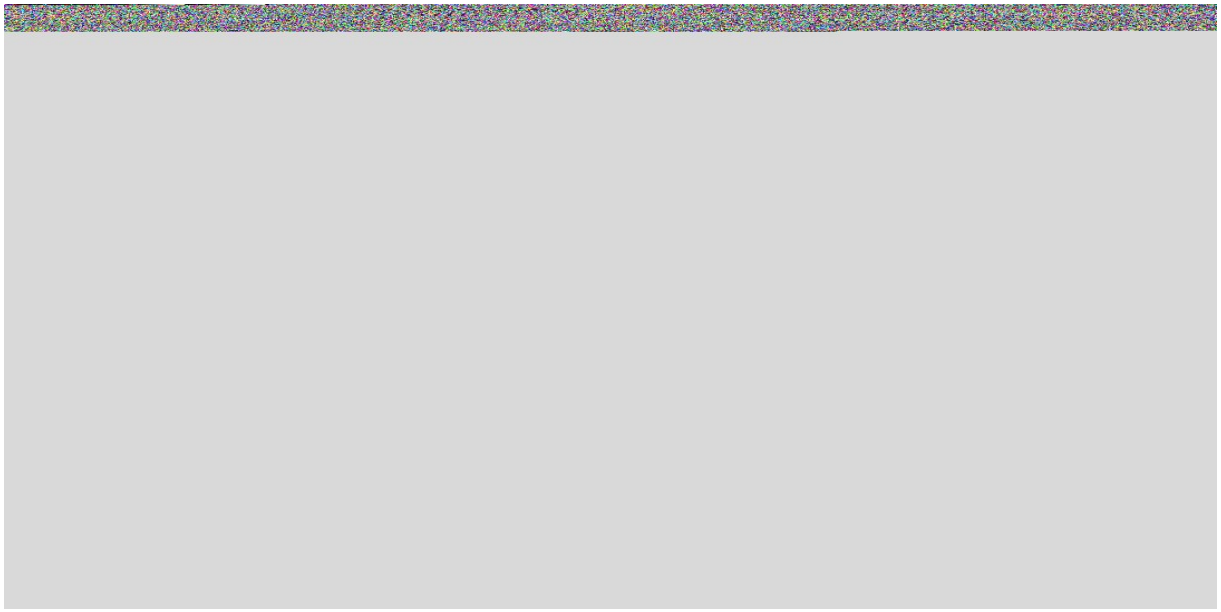


Fig. S6. ^{13}C-NMR spectra of TPA-3.

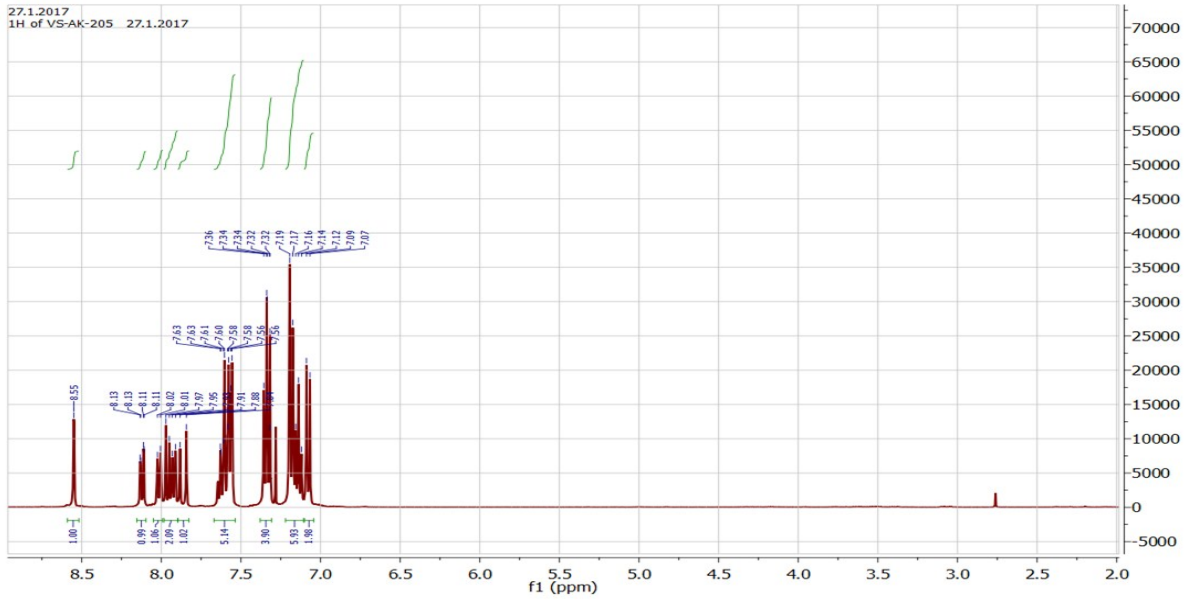


Fig. S7. 1H-NMR spectra of TPA-4.

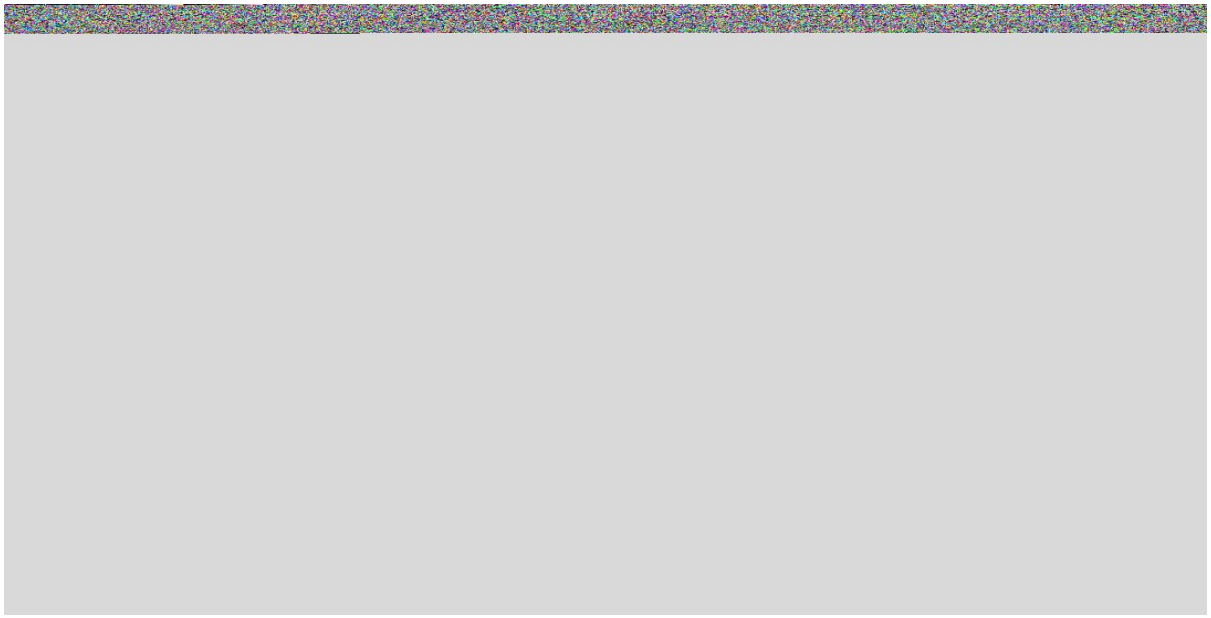


Fig. S8. ^{13}C-NMR spectra of TPA-4.

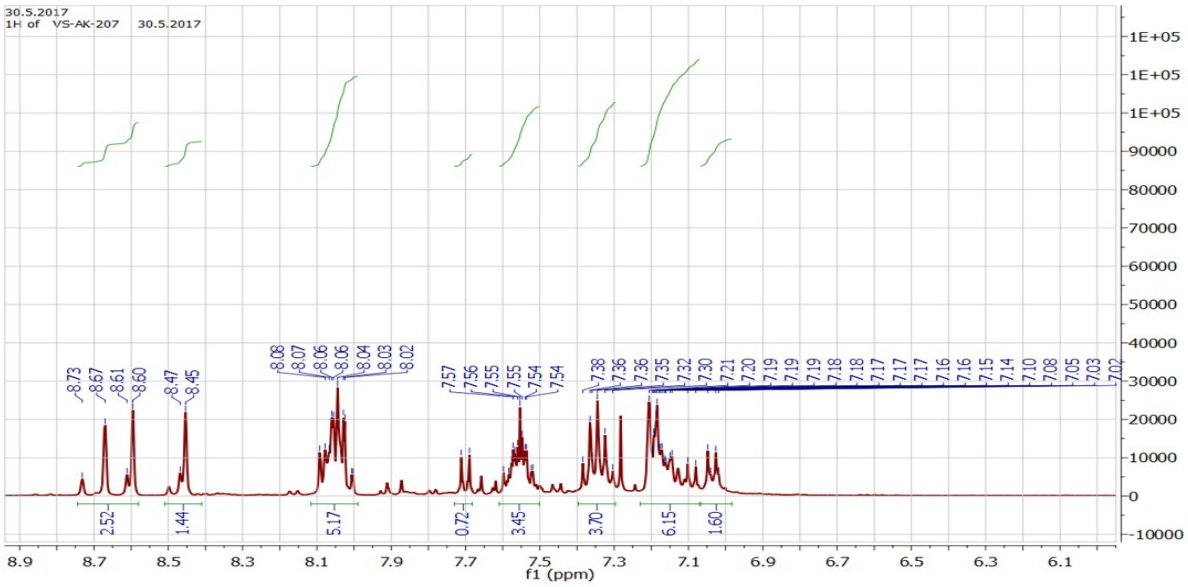


Fig. S9. 1H-NMR spectra of TPA-5.

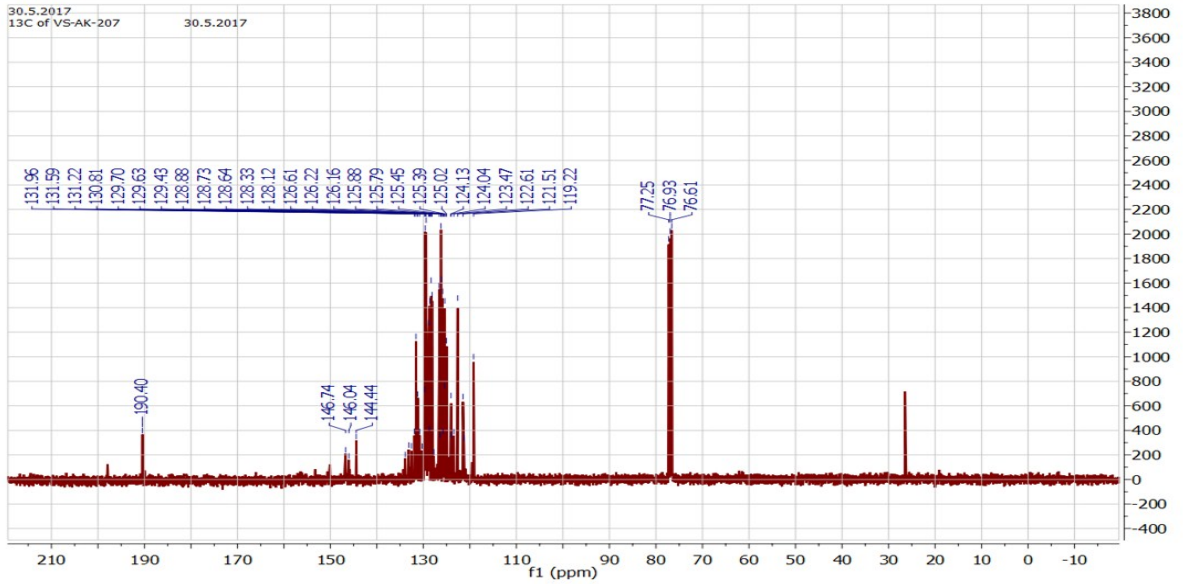


Fig. S10. ^{13}C-NMR spectra of TPA-5.

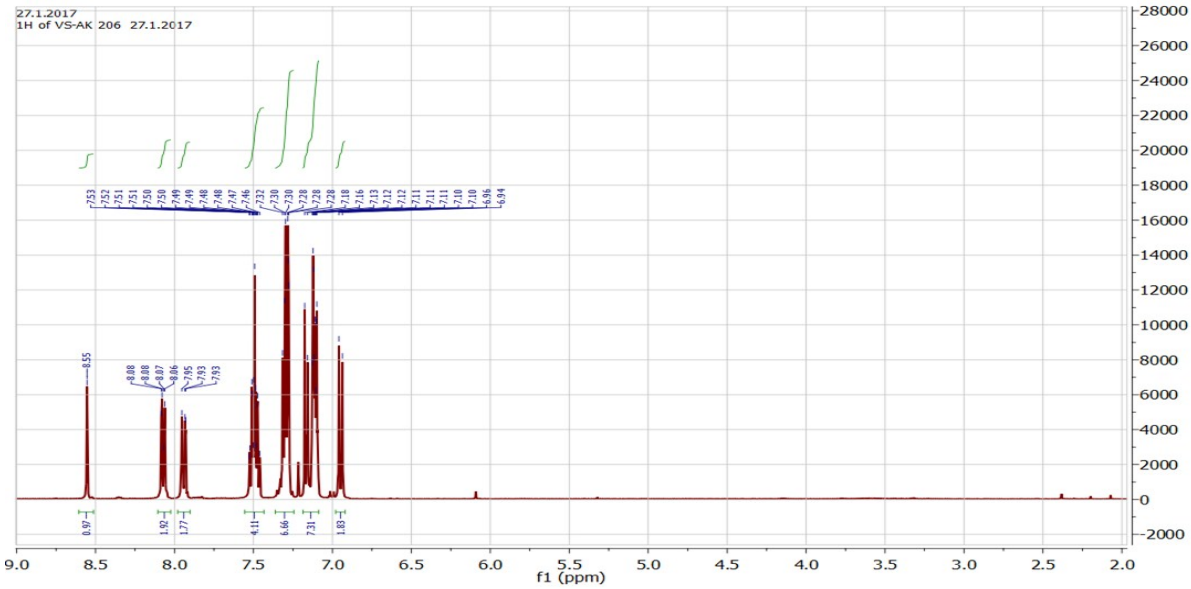


Fig. S11. 1H-NMR spectra of TPA-6.

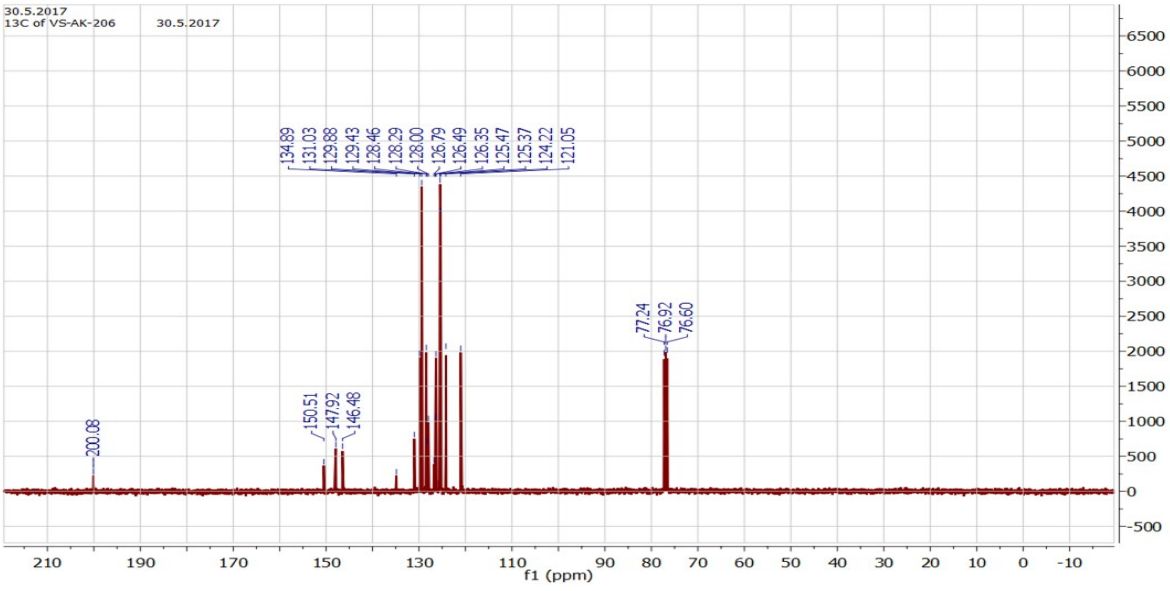


Fig. S12. ^{13}C-NMR spectra of TPA-6.

2. Mass spectra:

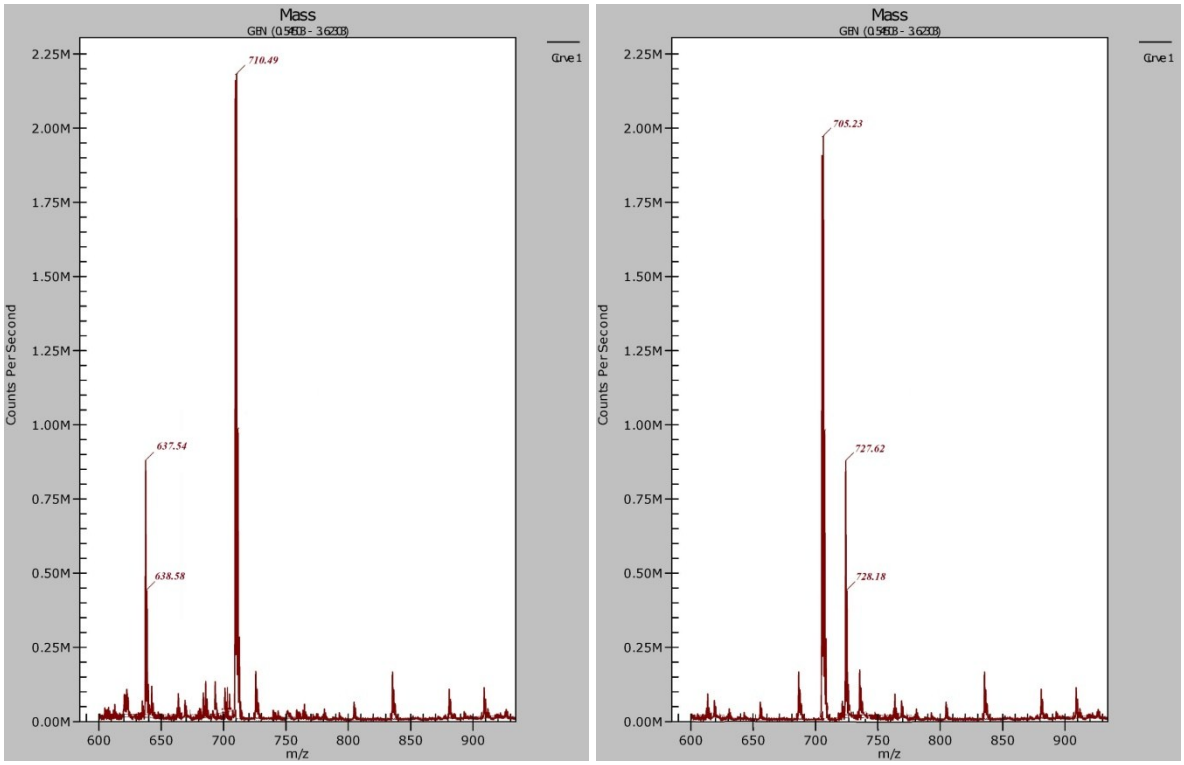


Fig S13. Mass spectra of TPA-1 and TPA-2.

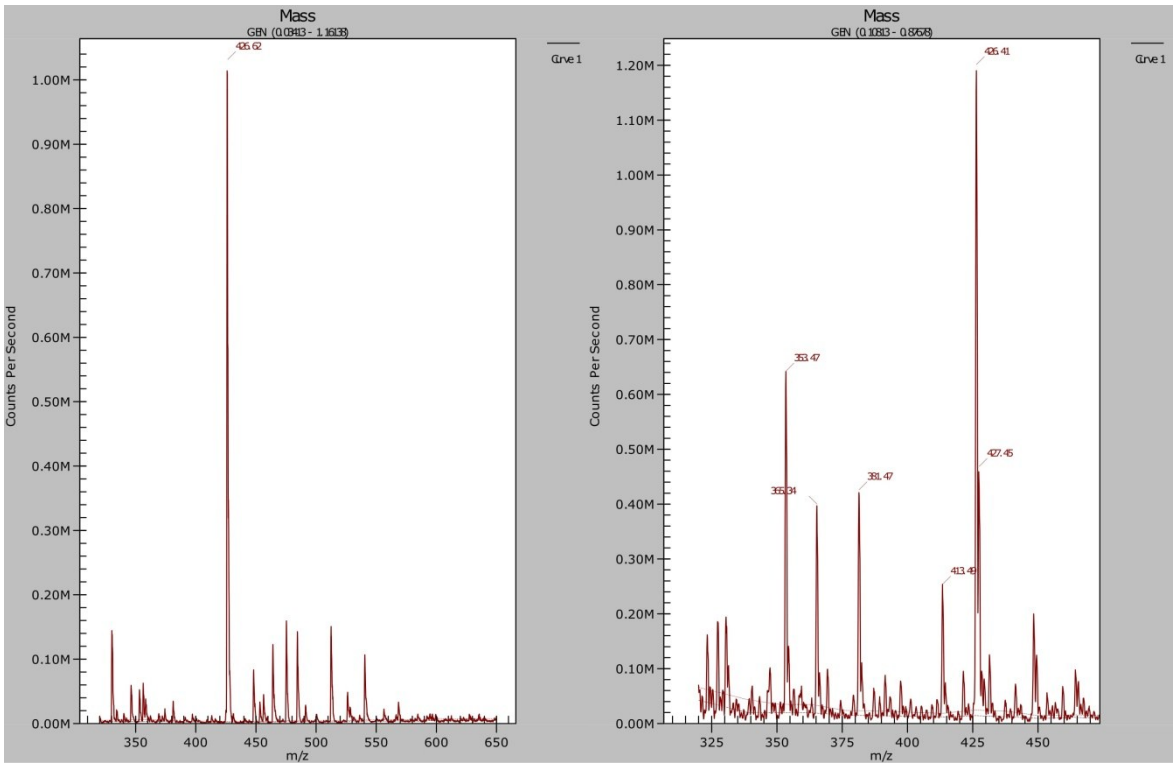


Fig. S14. Mass spectroscopy of TPA-3 and TPA-4.

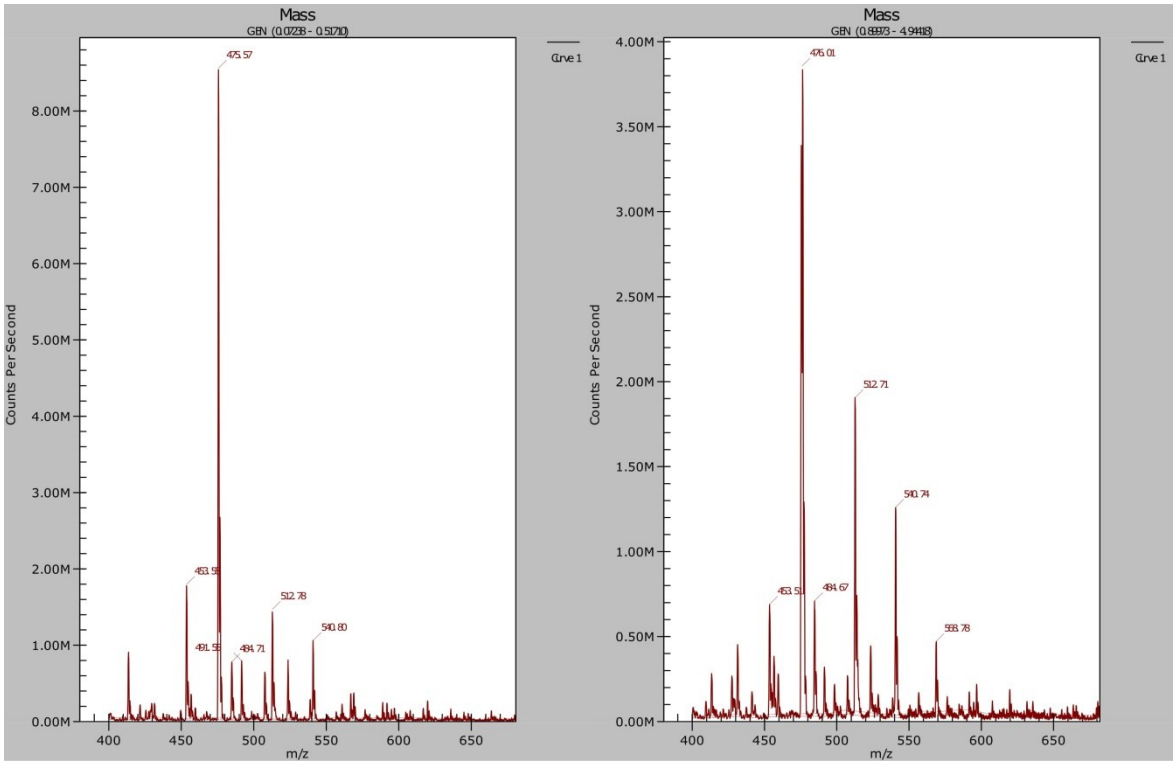


Fig. S15. Mass spectroscopy of TPA-5 and TPA-6.

Fluorescence Lifetime Decay Studies:

PL decays and PL lifetime were recorded on a time–resolved (Micro-Time 200, PicoQuant) confocal fluorescence lifetime imaging microscopy (FLIM) setup, which was equipped with an inverted microscope (Olympus IX 71). Measurements were performed at room temperature. The samples were excited (λ_{ex} = 405 nm) by ps diode pulse laser (power ~ 5μw) with a stable repetition rate of 20 MHz (FWHM: 176 ps) through a water immersion objective (Olympus UPlansApo; 60×; NA 1.2). Signal from the samples were collected by the same objective and passed through the dichroic mirror, filtered by using a 430 nm long-pass filter to cut off any exciting light. The signal was then focused onto a 50 μm diameter pinhole to remove the out-of focus signal, recollimated, and directed onto a (50/50) beam splitter prior to entering two single photon avalanche photodiodes (SPADs). The data acquisition was carried out with a SymPhoTime software controlled PicoHarp 300 time-correlated single-photon counting

(TCSPC) module in a time tagged time-resolved mode. The overall resolution of the setup was 4 ps.

The luminescence lifetime values (t) of the TPA derivatives were found to be in the range of 3.88 – 10.52 ns. The detailed information is tabulated in table 1. It suggests that, the fluorescence lifetime could be modulated by the different electron-donating and electron withdrawing abilities of donor and acceptor groups.

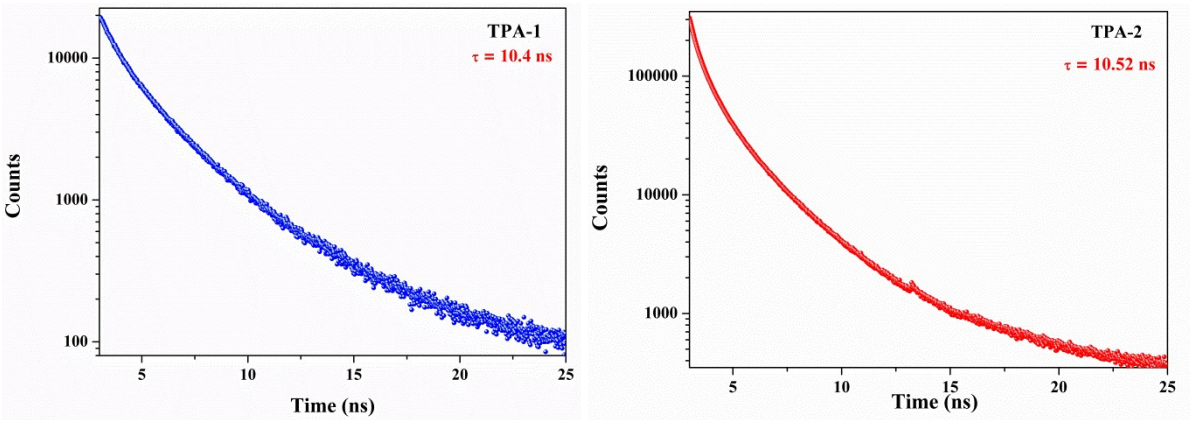


Fig. S16. Lifetime measurements of the TPA based organic dyes.

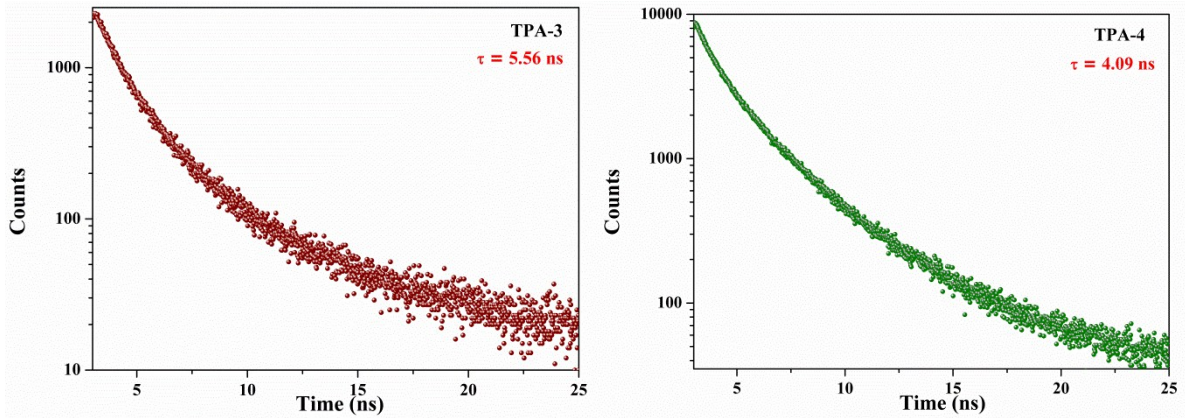


Fig. S17. Lifetime measurements of the TPA based organic dyes.

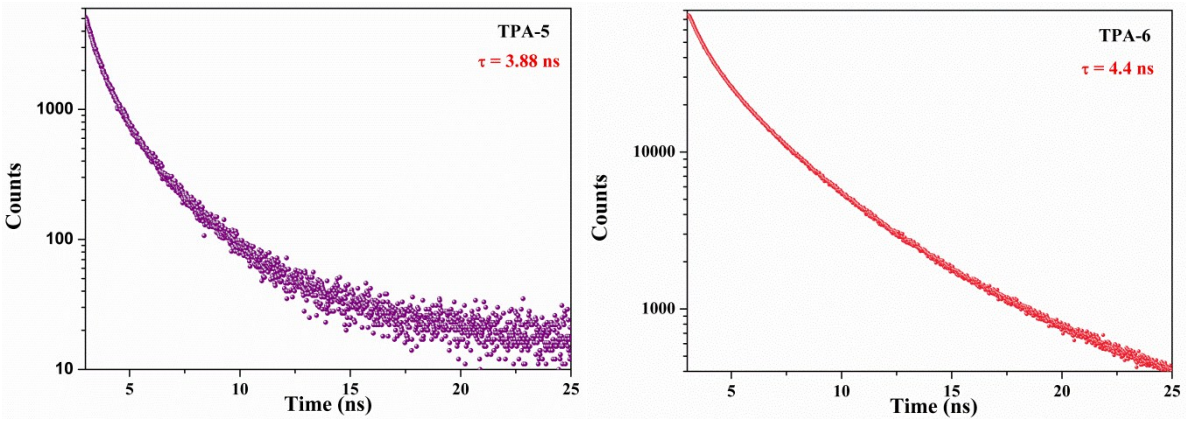
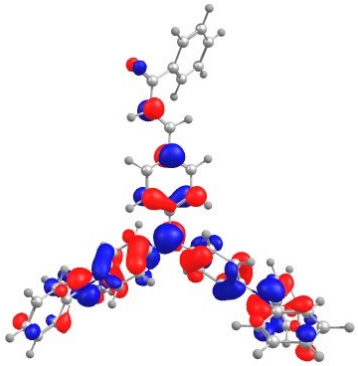
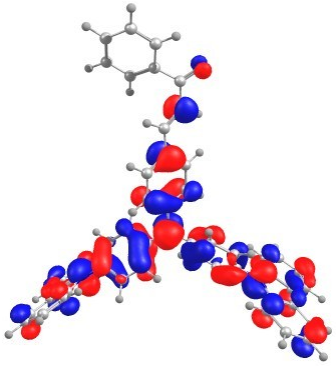
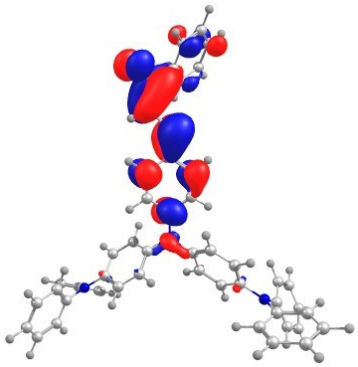
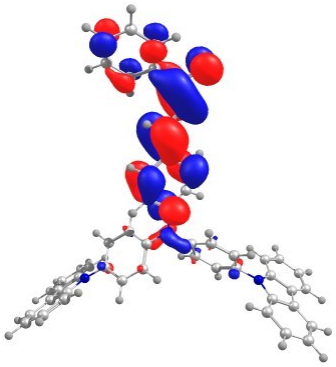


Fig. S18. Lifetime measurements of the TPA based organic dyes.

DFT Analysis:

ST1: MO orbitals of TPA based organic dyes:

Orbital	TPA-1	TPA-2
HOMO		
LUMO		

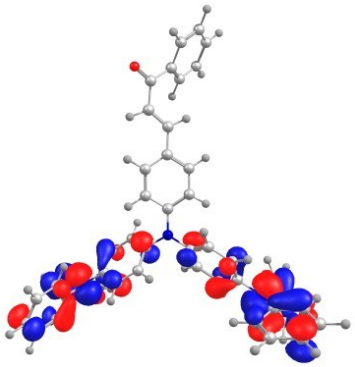
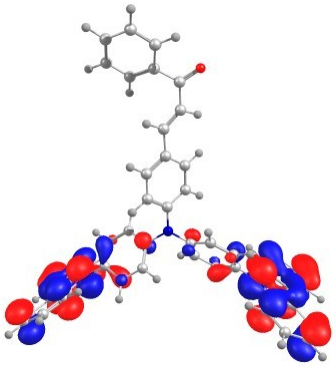
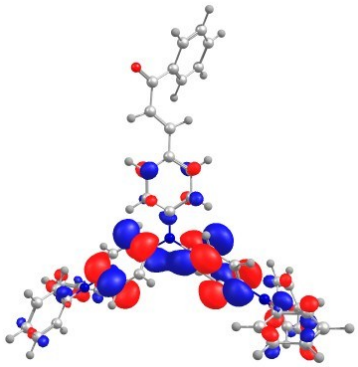
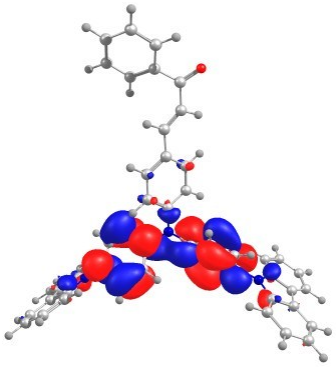
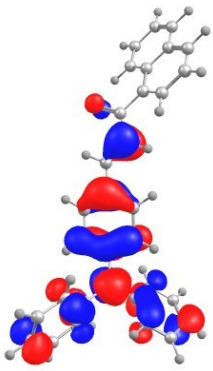
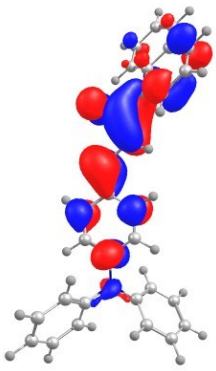
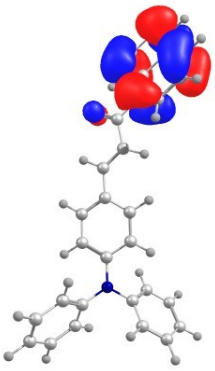
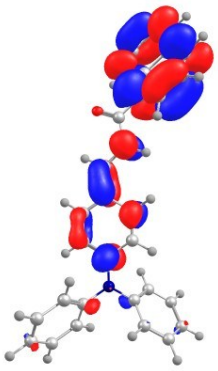
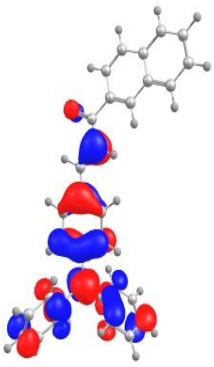
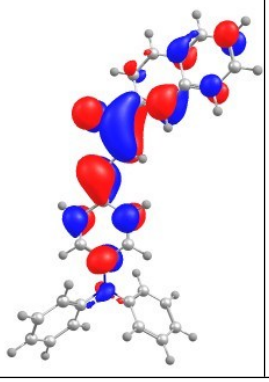
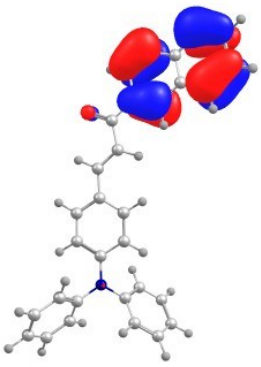
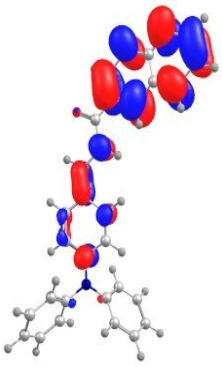
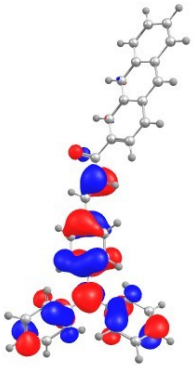
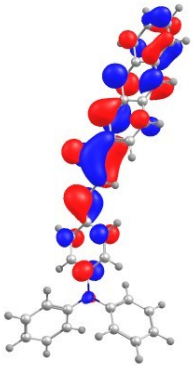
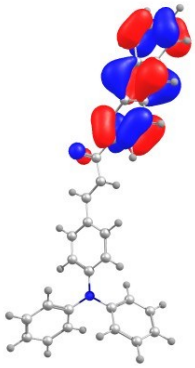
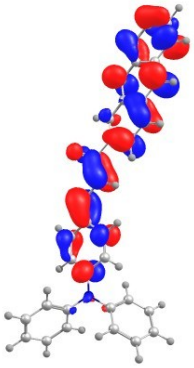
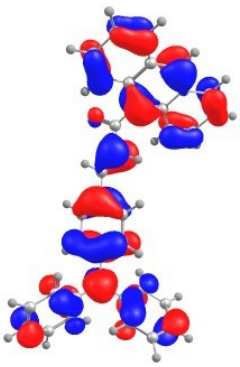
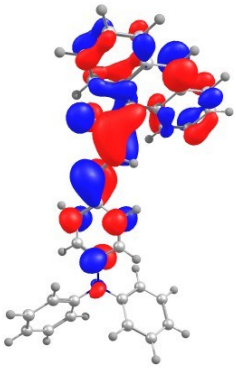
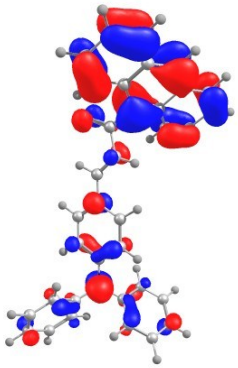
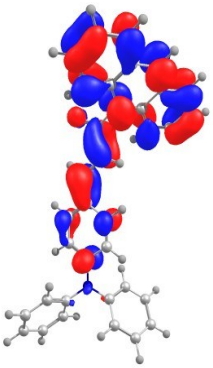
HOMO-1		
LUMO+1		

Table ST2: **MO orbitals of the TPA based organic dyes.**

Dye	HOMO	LUMO	HOMO-1	LUMO+1
TPA-3				
TPA-4				

TPA-5				
TPA-6				

ST3: Computed Vertical Transitions and Their Oscillator Strengths and Configurations[a]

Compound	State	λ_{max} (nm)	*f*	Configuration
TPA-1	DMSO	514.2	0.5041	HOMO → LUMO (70.4%)
		372.39	0.5461	HOMO-2 → LUMO (68.99%)
		366.03	0.6042	HOMO → LUMO+2 (66.78%)
		348.73	0.1635	HOMO → LUMO+1 (26.59%) HOMO → LUMO+3 (63.84%)
		316.52	0.3121	HOMO-2 → LUMO+5 (21.40%) HOMO → LUMO+4 (49.39%) HOMO → LUMO+5 (44.64%)
	Methanol	512.39	0.5401	HOMO → LUMO (70.41%)
		371.49	0.5441	HOMO-2 → LUMO (68.94%)
		355.62	0.5769	HOMO → LUMO+2 (66.62%)
		348.56	0.1785	HOMO → LUMO+1 (24.58%) HOMO → LUMO+3 (64.18%)
		316.11	0.2959	HOMO-2 → LUMO+5 (20.53%)

				HOMO → LUMO+4 (44.63%) HOMO → LUMO+5 (49.58%)
	THF	508.55	0.5556	HOMO → LUMO (70.39%)
		369.72	0.5443	HOMO-2 → LUMO (68.75%)
		356.40	0.6003	HOMO → LUMO+2 (66.07%)
		349	0.1638	HOMO → LUMO+1 (22.89%) HOMO → LOMO+3 (64.89%)
		316.34	0.2758	HOMO-2 → LUMO+5 (20.83%) HOMO → LUMO+4 (26.89%) HOMO → LUMO+5 (60.89%)
	Toluene	497.49	0.5806	HOMO → LUMO (70.33%)
		365.13	0.4455	HOMO-9 → LUMO (12.84%) HOMO-3 → LUMO (23.63%) HOMO-2 → LUMO (62.94%)
		360.12	0.1134	HOMO-9 → LUMO (17.36%) HOMO-4 → LUMO (19.68%) HOMO-3 → LUMO (56.94%)
		357.69	0.6280	HOMO → LUMO+2 (58.63%)
		349.84	0.1144	HOMO → LUMO+1 (20.47%) HOMO → LUMO+3 (65.25%)
		317.37	0.1071	HOMO → LUMO+5 (64.36%)
		316.76	0.2484	HOMO-1 → LUMO+5 (21.48%) HOMO → LUMO+4 (16.95%) HOMO → LUMO+5 (64.29%)
	Chloroform	500.57	0.5645	HOMO → LUMO (0.7037%)
		368.36	0.5406	HOMO-2 → LUMO (68.46%)
		351.85	0.6107	HOMO → LUMO+2 (65.21%)
		349.28	0.1562	HOMO → LUMO+2 (22.05%)

				HOMO → LUMO+4 (65.19%)
		316.49	0.2652	HOMO-1 → LUMO+5 (21.20%) HOMO → LUMO+4 (22.25%) HOMO → LUMO+5 (62.67%)
	Acetonitrile	512.77	0.5426	HOMO → LUMO (70.41%)
		371.68	0.5443	HOMO-2 → LUMO (69.96%)
		355.69	0.5821	HOMO → LUMO+2 (66.66%)
		348.58	0.1756	HOMO → LUMO+2 (24.79%) HOMO → LUMO+4 (64.68%)
		316.18	0.2991	HOMO-1 → LUMO+5 (20.71%) HOMO → LUMO+4 (45.80%) HOMO → LUMO+5 (48.48%)
	Acetone	511.98	0.5456	HOMO → LUMO (70.41%)
		371.31	0.5447	HOMO-2 → LUMO (68.93%)
		355.85	0.5868	HOMO → LUMO+2 (66.58%)
		348.67	0.1728	HOMO → LUMO+1 (24.36%) HOMO → LUMO+3 (64.28%)
		316.22	0.2942	HOMO-1 → LUMO+6 (20.43%) HOMO → LUMO+5 (38.23%) HOMO → LUMO+5 (54.60%)
	DCM	509.89	0.5577	HOMO → LUMO (70.39%)
		370.35	0.5450	HOMO-1 → LUMO (68.82%)
		356.41	0.6061	HOMO → LUMO+2 (66.27%)
		348.98	0.1615	HOMO → LUMO+1 (23.45%) HOMO → LUMO+3 (64.71%)
		316.44	0.2836	HOMO-1 → LUMO+6 (20.80%) HOMO → LUMO+5 (28.51%) HOMO → LUMO+6 (60.12%)

	Gas	470.50	0.5027	HOMO → LUMO (70.35%)
		355.79	0.4308	HOMO → LUMO+1 (68.46%)
		350.55	0.5358	HOMO-2 → LUMO (65.40%)
		349.31	0.2568	HOMO-2 → LUMO (13.80%) HOMO → LUMO+2 (44.90%) HOMO → LUMO+3 (50.32%)
		314.78	0.1648	HOMO-1 → LUMO+6 (17.67%) HOMO → LUMO+5 (17.67%) HOMO → LUMO+6 (65.19%)
TPA-2	DCM	469	0.6277	HOMO → LUMO (70.54%)
		376	0.2696	HOMO-2 → LUMO (69.17%)
		334	0.704	HOMO → LUMO+2 (54.42%) HOMO → LUMO+3 (13.96%)
		319	0.1026	HOMO-1 → LUMO+2 (17.10%) HOMO-1 → LUMO+4 (10.50%) HOMO → LUMO+1 (40.70%) HOMO → LUMO+3 (50.07%) HOMO → LUMO+5 (13.66%)
	Acetone	470.41	0.623	HOMO → LUMO (70.20%)
		376.35	0.2675	HOMO-2 → LUMO (69.77%)
		333	0.6969	HOMO → LUMO+1 (13.3%) HOMO → LUMO+4 (51.84%)
	Acetonitrile	470.98	0.622	HOMO → LUMO (70.21%)
		376.39	0.2656	HOMO-2 → LUMO (69.87%)
		333.23	0.6949	HOMO → LUMO+1 (12.40%) HOMO → LUMO+4 (54.60%)

	Chloroform	466.13	0.622	HOMO → LUMO (70.13%)
		376.07	0.2236	HOMO-2 → LUMO (62.48%)
		335	0.703	HOMO → LUMO+1 (30.10%) HOMO → LUMO+2 (60.11%) HOMO → LUMO+4 (13.13%)
		318.71	0.1312	HOMO-1 → LUMO+4 (11.30%) HOMO → LUMO+1 (42.73%) HOMO → LUMO-3 (43.12%) HOMO → LUMO+4 (12.9%) HOMO → LUMO+5 (15.8%)
	DMSO	472.27	0.6358	HOMO → LUMO (70.19%)
		376.76	0.2642	HOMO-3 → LUMO (69.88%)
		333.55	0.7068	HOMO → LUMO+1 (11.97%) HOMO → LUMO+4 (55.53%)
	Methanol	470.65	0.1696	HOMO → LUMO (70.72%)
		376.30	0.2660	HOMO-2 → LUMO (69.86%)
		333.17	0.6922	HOMO → LUMO+1 (12.61%) HOMO → LUMO+4 (54.29%)
	THF	468.05	0.6225	HOMO → LUMO (70.17%)
		376.09	0.268	HOMO-2 → LUMO (68.60%)
		314.35	0.7010	HOMO → LUMO+1 (19.19%) HOMO → LUMO+2 (57.70%) HOMO → LUMO+4 (30.21%)
		319.50	0.1077	HOMO-1 → LUMO+4 (11.55%) HOMO → LUMO+1 (41.25%) HOMO → LUMO+3 (49.44%) HOMO → LUMO+5 (13.90%)

	Toluene	461.17	0.6154	HOMO → LUMO (70.07%)
		373.72	0.3006	HOMO-5 → LUMO (16.70%) HOMO-3 → LUMO (67.76%)
		336.84	0.7002	HOMO → LUMO+1 (65.53%) HOMO → LUMO+2 (22.70%)
	Gas	442.98	0.4768	HOMO → LUMO (70.22%)
		366.47	0.3596	HOMO-2 → LUMO (69.47%) HOMO → LUMO+1 (69.15%)
		336.82	0.5633	HOMO → LUMO+1 (23.5 %)
		313.24	0.1597	HOMO → LUMO+2 (23.5 %) HOMO → LUMO+3 (56.33 %) HOMO → LUMO+4 (14.31 %)
TPA-3	Acetone	466	0.869	HOMO → LUMO (70.04%)
		374	0.1062	HOMO-4 → LUMO (32.62%) HOMO-3 → LUMO (53.7%) HOMO-2 → LUMO (18.4%)
		366	0.128	HOMO-4 → LUMO (16.5%) HOMO-3 → LUMO (19.7%) HOMO-2 → LUMO (65.08%)
	Acetonitrile	467	0.865	HOMO → LUMO (70.04%)
		374	0.107	HOMO-4 → LUMO (33.6%) HOMO-3 → LUMO (52.8%) HOMO-2 → LUMO (17.3%)
		366	0.129	HOMO-4 → LUMO (11.7%) HOMO-3 → LUMO (20.6%) HOMO-2 → LUMO (64.5%)

	$CHCl_3$	462	0.895	HOMO → LUMO (69.96%)
		378	0.13	HOMO-4 → LUMO (25.5%) HOMO-3 → LUMO (54.9%) HOMO-2 → LUMO (29.9%)
		367	0.117	HOMO-3 → LUMO (14.5%) HOMO-1 → LUMO (67.3%)
	DCM	465.5	0.885	HOMO → LUMO (70%)
		376.5	0.35	HOMO-4 → LUMO (29.5%) HOMO-3 → LUMO (55.4%) HOMO-2 → LUMO (22.18%)
		366.9	0.125	HOMO-3 → LUMO (17.5%) HOMO-1 → LUMO (66.2%)
	DMSO	469.1	0.879	HOMO → LUMO (70%)
		374	0.100	HOMO-4 → LUMO (33.8%) HOMO-3 → LUMO (52.2%) HOMO-2 → LUMO (11.9%)
		366	0.129	HOMO-4 → LUMO (12.5%) HOMO-3 → LUMO (21.6%) HOMO-2 → LUMO (64.1%)
	Gas	431	0.812	HOMO → LUMO (69.9%)
		390.4	0.100	HOMO-4 → LUMO (13.6%) HOMO-2 → LUMO (65.2%)
		366	0.59	HOMO → LUMO (68.7%)

	MeOH	466	0.862	HOMO → LUMO (70.04%)
		324.5	0.107	HOMO-4 → LUMO (33.5%) HOMO-3 → LUMO (53.03%) HOMO-2 → LUMO (17.4%)
		366.3	0.1289	HOMO-4 → LUMO (11.5%) HOMO-3 → LUMO (20.4%) HOMO-2 → LUMO (64.6%)
	THF	464.2	0.883	HOMO → LUMO (70.0%)
		377.02	0.1027	HOMO-4 → LUMO (28.5%) HOMO-3 → LUMO (55.6%) HOMO-2 → LUMO (23.7%)
		366.8	0.123	HOMO-3 → LUMO (16.6%) HOMO-2 → LUMO (66.6%)
	Toluene	456.45	0.915	HOMO → LUMO (69.8%)
		382.7	0.102	HOMO-4 → LUMO (20.01%) HOMO-3 → LUMO (42.69%) HOMO-2 → LUMO (49.5%)
		367.66	0.103	HOMO-3 → LUMO (10.06%) HOMO-1 → LUMO (68.3%)
TPA-4	Acetone	467.9	0.825	HOMO → LUMO (70.2%)
		366.7	0.104	HOMO-4 → LUMO (50.1%) HOMO-3 → LUMO (41.17%)
		362.5	0.164	HOMO-4 → LUMO (20.7%)

				HOMO-1 → LUMO (64.6%)
	Acetonitrile	468.56	0.822	HOMO → LUMO (70.23%)
		366.2	0.107	HOMO-6 → LUMO (13.1%) HOMO-4 → LUMO (47.8%) HOMO-1 → LUMO (39.5%)
		362.7	0.193	HOMO-4 → LUMO (23.6%) HOMO-1 → LUMO (62.8%)
	$CHCl_3$	463.2	0.844	HOMO → LUMO (70.19%)
		370.56	0.100	HOMO-4 → LUMO (46.8%) HOMO-3 → LUMO (49.7%)
		360.96	0.197	HOMO-4 → LUMO (11.3%) HOMO-1 → LUMO (67.5%)
	DCM	466.66	0.838	HOMO → LUMO (70.2%)
		368.24	0.108	HOMO-4 → LUMO (50.4%) HOMO-3 → LUMO (44.9%)
		362.0	0.198	HOMO-4 → LUMO (14.9%) HOMO-1 → LUMO (66.69%)
	DMSO	470.3	0.835	HOMO → LUMO (70.22%)
		366.13	0.105	HOMO-6 → LUMO (14.7%) HOMO-4 → LUMO (45.95%) HOMO-3 → LUMO (38.59%)
		362.98	0.192	HOMO-4 → LUMO (25.6%)

				HOMO-3 → LUMO (11.35%) HOMO-1 → LUMO (61.54%)
	Gas	432.63	0.7481	HOMO → LUMO (70.1%)
		382.86	0.103	HOMO-4 → LUMO (24.5%) HOMO-2 → LUMO (60.93%)
		354.54	0.158	HOMO-1 → LUMO (67.79%)
	Methanol	468.1	0.819	HOMO → LUMO (70.23%)
		366.28	0.164	HOMO-6 → LUMO (12.5%) HOMO-4 → LUMO (48.4%) HOMO-3 → LUMO (39.7%)
		362.62	0.193	HOMO-4 → LUMO (23.12%) HOMO-1 → LUMO (63.24%)
	THF	465.3	0.835	HOMO → LUMO (70.21%)
		368.7	0.104	HOMO-4 → LUMO (49.8%) HOMO-3 → LUMO (46.1%)
		361.69	0.198	HOMO-4 → LUMO (13.7%) HOMO-1 → LUMO (66.9%)
	Toluene	457.3	0.858	HOMO → LUMO (70.1%)
		374.7	0.102	HOMO-4 → LUMO (38.1%) HOMO-3 → LUMO (55.2%) HOMO-2 → LUMO (16.8%)
		359.1	0.192	HOMO-1 → LUMO (68.06%)

TPA-5	Gas	458.2	0.786	HOMO-1 → LUMO (20.68%) HOMO → LUMO (67.15%)
		441.03	0.191	HOMO-1 → LUMO (66.45%)
		394.84	0.103	HOMO-4 → LUMO (15.5%) HOMO-2 → LUMO (65.03%) HOMO-2 → LUMO+1 (15.27%)
	Acetone	495.0	0.9168	HOMO-1 → LUMO (10.21%) HOMO → LUMO (69.65%)
		456.2	0.120	HOMO-1 → LUMO (69.18%)
		383.21	0.2908	HOMO → LUMO+1 (69.24%)
	Acetonitrile	495.8	0.9132	HOMO-1 → LUMO (10.09%) HOMO → LUMO (69.58%)
		456.6	0.120	HOMO-1 → LUMO (69.2%)
		383.46	0.290	HOMO → LUMO+1 (69.28%)
	Chloroform	489.08	0.9368	HOMO-1 → LUMO (11.17%) HOMO → LUMO (69.32%)
		453.38	0.159	HOMO-1 → LUMO (69.32%)
		381.78	0.172	HOMO-4 → LUMO (50.31%) HOMO-4 → LUMO+1 (11.77%) HOMO-3 → LUMO (30.17%) HOMO → LUMO+1 (34.06%)
	DCM	493.2	0.9317	HOMO-1 → LUMO (10.56%)

				HOMO → LUMO (69.45%)
		455.21	0.186	HOMO-1 → LUMO (69.16%)
		382.59	0.292	HOMO → LUMO+1 (69.04%)
	DMSO	497.55	0.9294	HOMO-1 → LUMO (10.00%) HOMO → LUMO (69.57%)
		457.25	0.121	HOMO-1 → LUMO (69.24%)
		383.94	0.288	HOMO → LUMO+1 (69.29%)
	THF	491.33	0.9279	HOMO-1 → LUMO (10.72%) HOMO → LUMO (69.43%)
		454.61	0.178	HOMO-1 → LUMO (69.12%)
		382.18	0.292	HOMO → LUMO+1 (6885%)
	Toluene	482.25	0.948	HOMO-1 → LUMO (12.48%) HOMO → LUMO (69.03%)
		450.44	0.110	HOMO-1 → LUMO (68.84%)
		386.1	0.1060	HOMO-4 → LUMO (41.03%) HOMO-3 → LUMO(53.42%) HOMO-3 → LUMO+1 (11.6%)
TPA-6	Acetone	491.2	0.722	HOMO-1 → LUMO (24.85%) HOMO → LUMO (65.76%)
		447.9	0.383	HOMO-1 → LUMO (63.3%) HOMO → LUMO (25.32%)
		392.31	0.238	HOMO-1 → LUMO (13.06%)

				HOMO → LUMO+1 (68.70%)
	Acetonitrile	491.77	0.721	HOMO-1 → LUMO (24.57%) HOMO → LUMO (65.88%)
		448.11	0.135	HOMO-1 → LUMO (63.38%)
		392.76	0.2392	HOMO-1 → LUMO (13.20%) HOMO → LUMO+1 (68.67%)
	$CHCl_3$	497.54	0.7208	HOMO-1 → LUMO (26.74%) HOMO → LUMO (64.89%)
		446.18	0.1618	HOMO-1 → LUMO (62.76%)
		388.96	0.2313	HOMO-1 → LUMO (12.30%) HOMO → LUMO+1 (68.90%)
	DCM	490.18	0.729	HOMO-1 → LUMO (25.53%) HOMO → LUMO (65.44%)
		447.41	0.147	HOMO-1 → LUMO (63.18%)
		391.15	0.2357	HOMO-1 → LUMO (12.59%) HOMO → LUMO+1 (68.63%)
	DMSO	492.17	0.7201	HOMO-1 → LUMO (24.36%) HOMO → LUMO (65.97%)
		448.27	0.134	HOMO-1 → LUMO (63.43%)
		393.11	0.2396	HOMO-1 → LUMO (13.32%) HOMO → LUMO (68.64%)
	Gas	469.67	0.4415	HOMO → LUMO (63.03%)

		431.5	0.2216	HOMO-1 → LUMO (60.5%) HOMO → LUMO (31.3%) HOMO → LUMO+1 (15.2%)
	Methanol	491.38	0.7176	HOMO-1 → LUMO (24.67%) HOMO → LUMO (65.84%)
		447.97	0.135	HOMO-1 → LUMO (63.31%)
		392.57	0.2396	HOMO-1 → LUMO (13.26%) HOMO → LUMO+1 (68.64%)
	THF	489.15	0.7229	HOMO-1 → LUMO (25.93%) HOMO → LUMO (65.28%)
		446.97	0.1495	HOMO-1 → LUMO (63.01%)
		390.46	0.2356	HOMO-1 → LUMO (12.60%) HOMO → LUMO+1 (68.82%)
	Toluene	483.64	0.6955	HOMO-1 → LUMO (28.33%) HOMO → LUMO (64.09%)
		443.81	0.1024	HOMO-1 → LUMO (62.20%)
		385.22	0.2114	HOMO-1 → LUMO (12.24%) HOMO → LUMO+1 (68.80%)

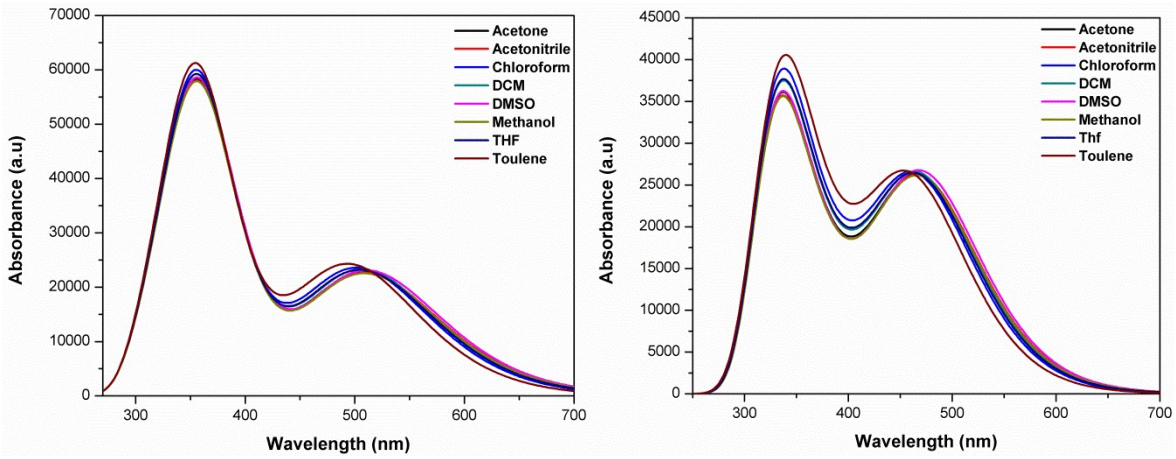


Fig. S19. Theoretical UV-Vis spectra of TPA-1 (left) and TPA-2 (right).

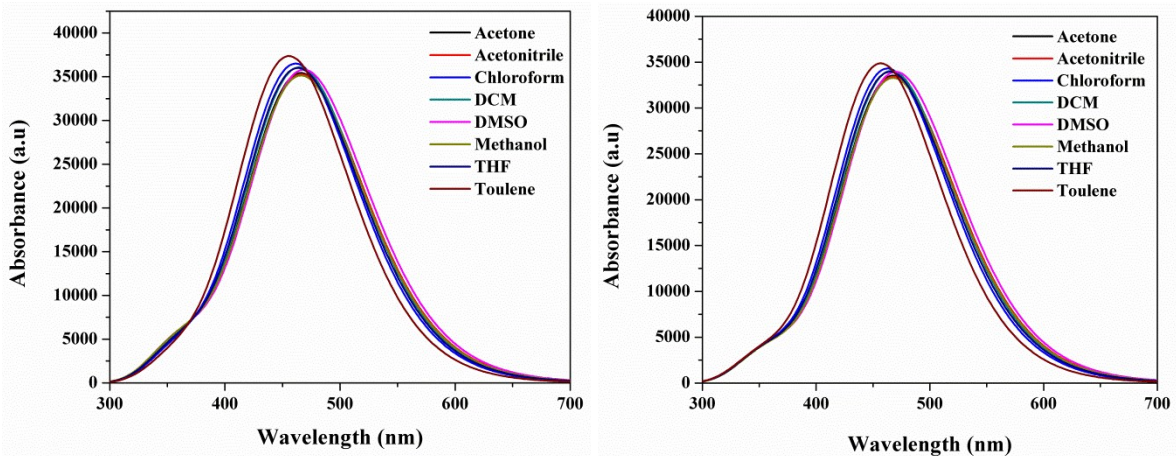


Fig. S20. Theoretical UV-Visible spectra of TPA-1-NP and TPA-2-NP

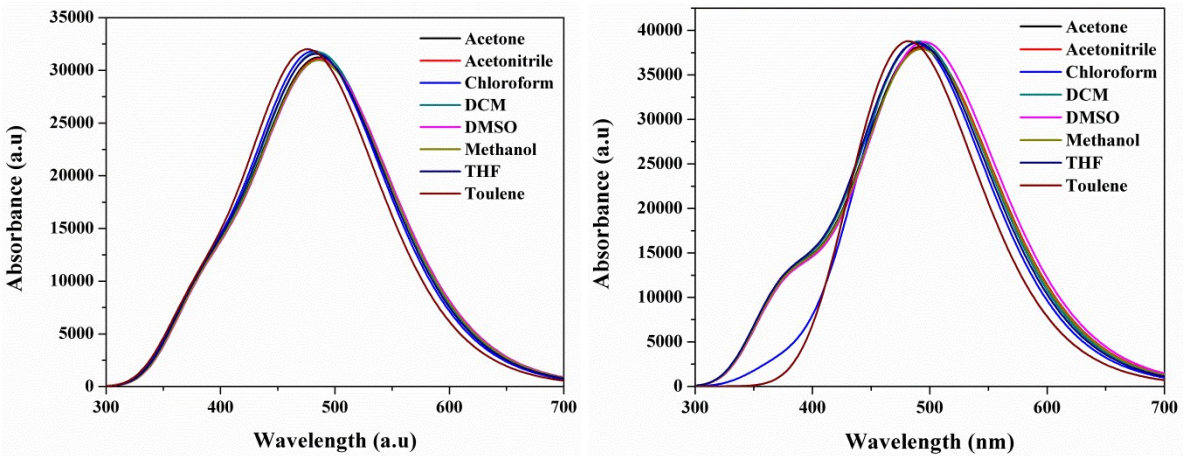


Fig. S21. Theoretical UV-Visible spectra of TPA-9-AP and TPA-2-AP

3. Solvatorchromism studies:

The fluorescence excitation and emission spectra of organic dyes in different polar and non-polar solvents are given in Fig. S19 - S24, respectively. It is clearly demonstrates that the significant solvent dependent shifts was observed in the emission maxima. Table ST4 and ST, summarizes the absorption maxima and Stoke's shift of all the yellowish – Orange dyes. However, solvent polarity exerts a great effect on their PL emission. With the increase of the solvent polarity gradually, the PL spectrum of each compound is progressively shifted to a longer wavelength. The excitation peaks of TPA-1 and TPA-2 are 375 and 383 nm in toluene and 429, 433 nm in DMF. Compared with the emission peak in a toluene solution, the peak positions in DMF are red-shifted by 50 nm in both TPA-1 and TPA-2, respectively. Solvent-dependent spectral shifts are often interpreted in terms of the Lippert−Mataga equation (eq-1), which describes the solvatochromic Stokes shift Δf (expressed in wavenumbers) as a function of the change of the dipole moment $\Delta\mu_{ge} = \mu_e - \mu_g$ of the dye material upon excitation. The validity of equation-1 can be checked by using various solvents with different dielectric constants (ε) and refractive indices (n) and by plotting stokes shift verses Δf for the 7 solvents. [1,2]

$$\Delta V = \frac{2\Delta f}{4\pi\epsilon_0 hca^3}(\mu_e - \mu_g) + \text{Constant} \quad \text{..... eq.1}$$

$$f(\epsilon) = \frac{f(\epsilon - 1)}{f(2\epsilon + 1)} \quad \text{and} \quad f(n^2) = \frac{(n^2 - 1)}{(2n^2 + 1)} \quad \text{..... eq.2}$$

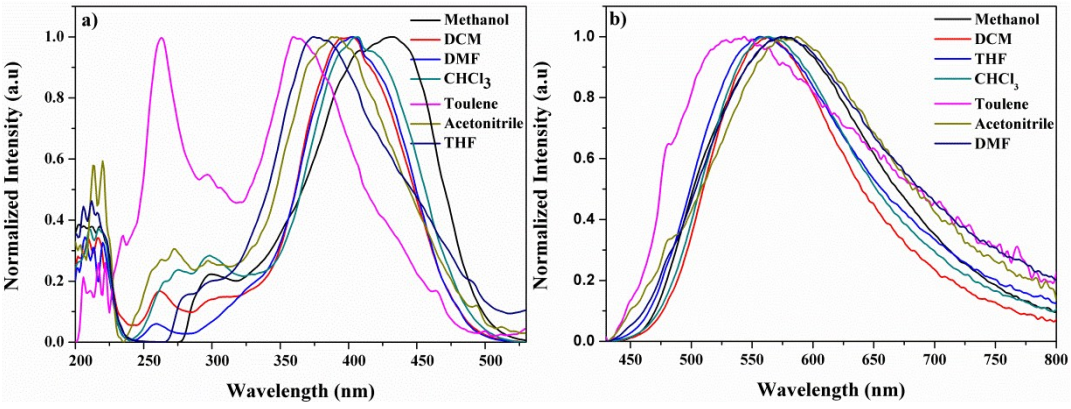


Fig. S22. Normalized excitation (a) and emission spectra (b) of TPA-1 in solvents of different polarity.

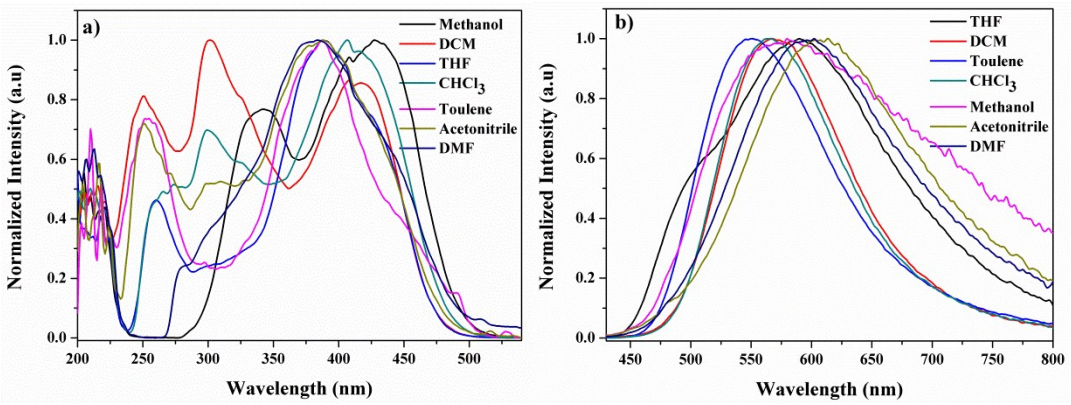


Fig. S23. Normalized excitation (a) and emission spectra (b) of TPA-2 in solvents of different polarity.

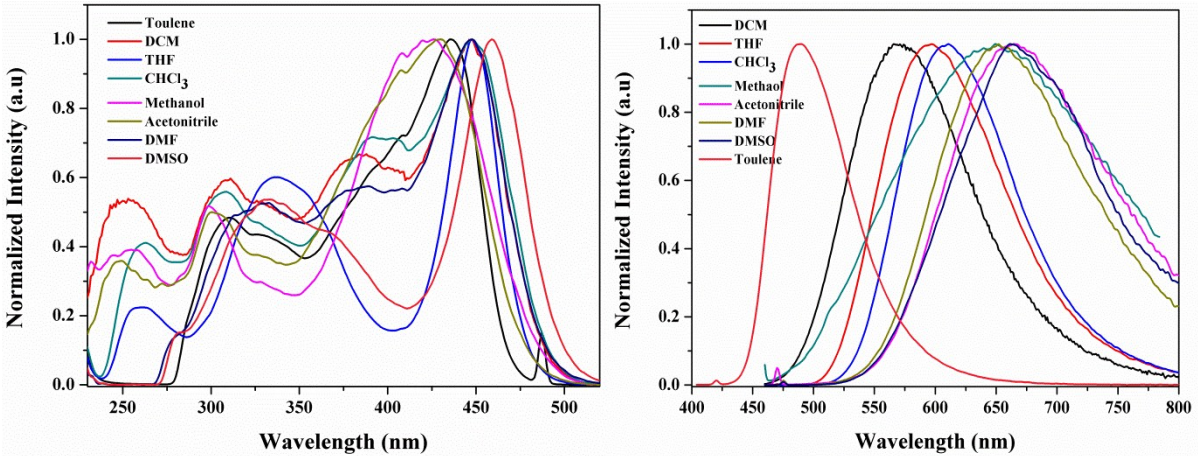


Fig. S24. Excitation and emission spectra of TPA-3 in different solvents.

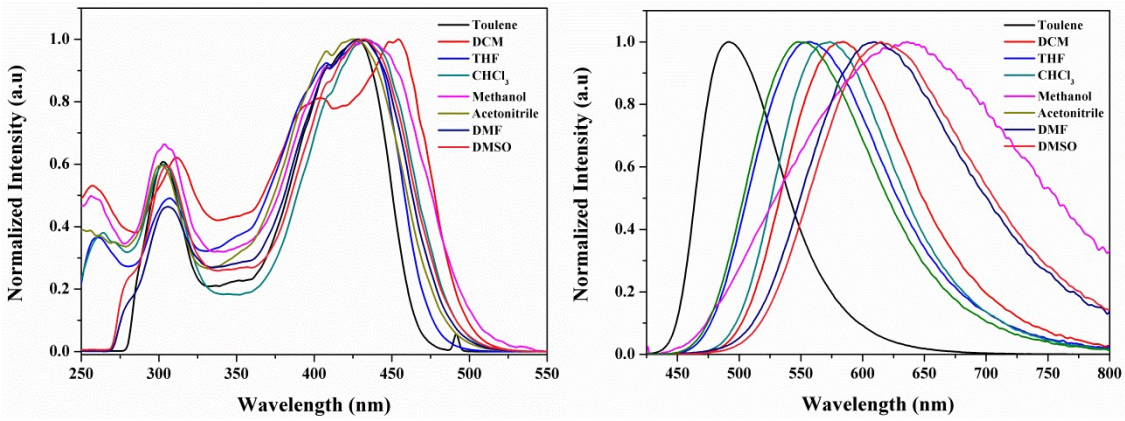


Fig. S25. Excitation and emission spectra of TPA-4 in different solvents.

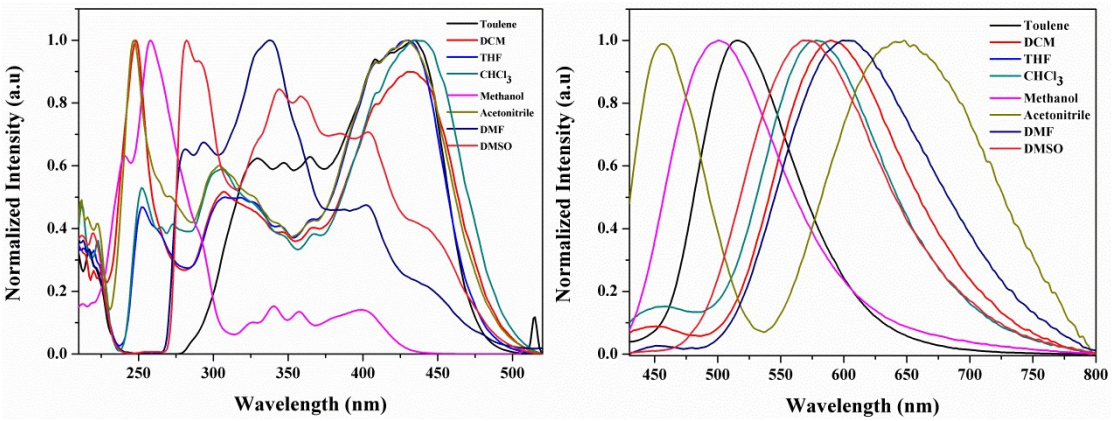


Fig. S23. Excitation and emission spectra of TPA-5 in different solvents.

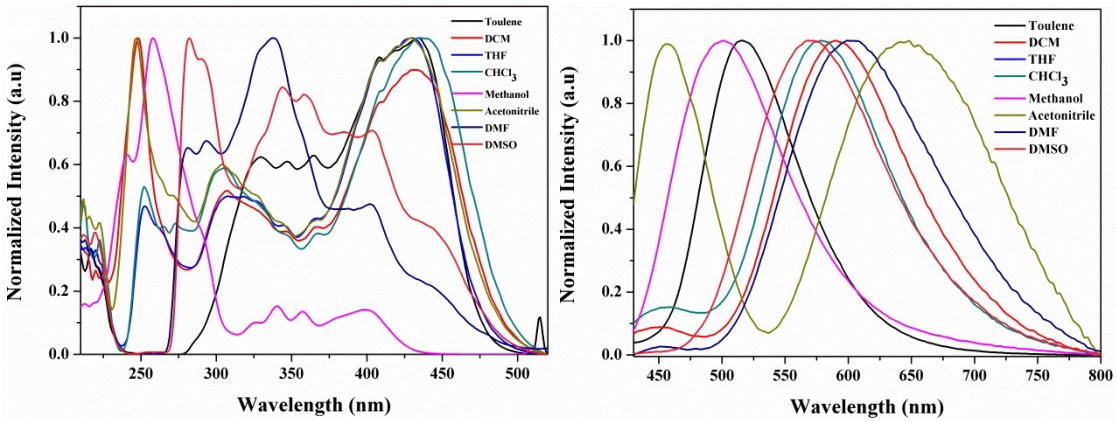


Fig. S26. Excitation and emission spectra of TPA-6 in different solvents.

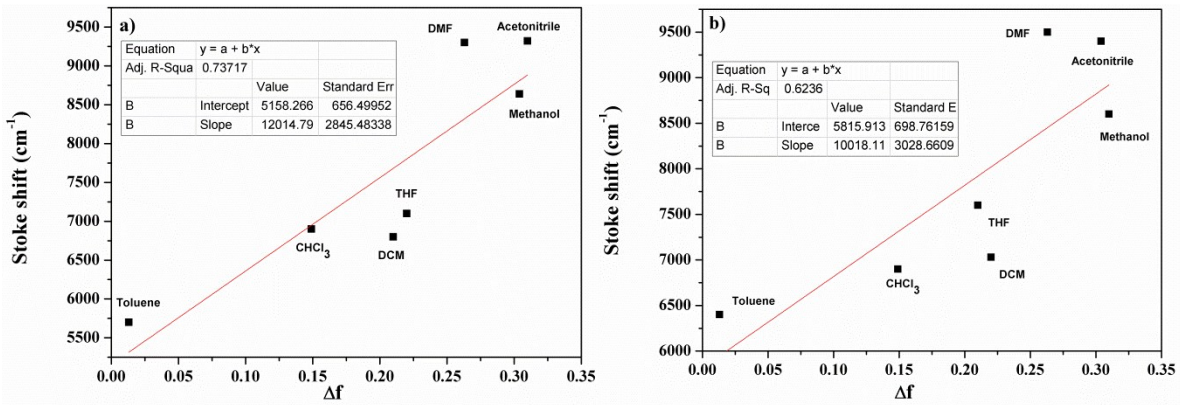


Fig. S27. Lippert-Mataga plots of TPA-1 (a) and TPA-2 (b).

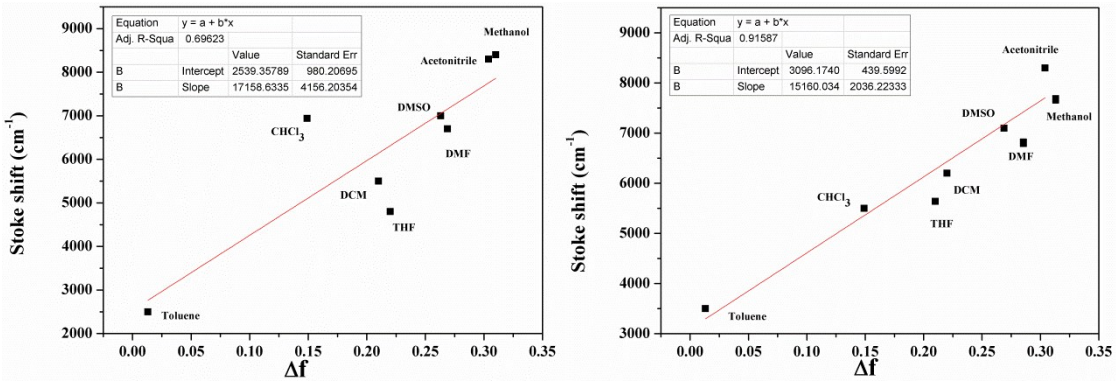


Fig. S28. Lippert−Mataga plots of TPA-3 (left) and TPA-4 (right) in different solvents.

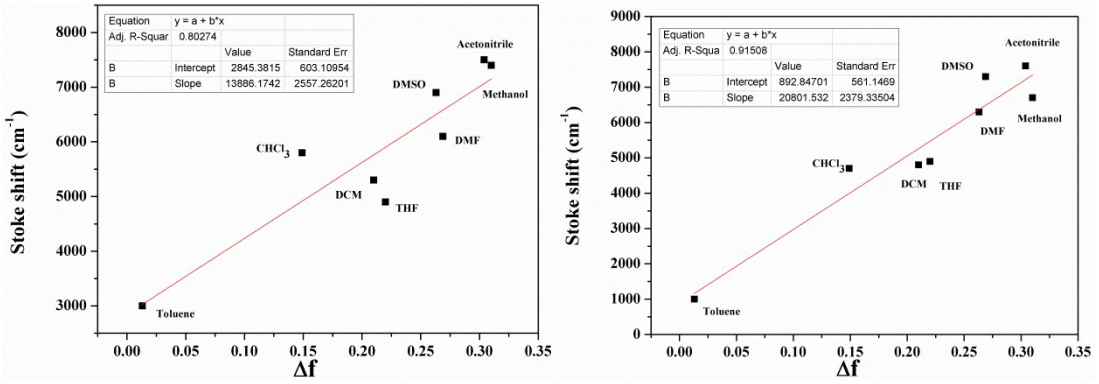


Fig. S29. Lippert−Mataga plots of TPA-5 (left) and TPA-6 (right) in different solvents.

Fig S25 – S27 represents the Lippert−Mataga plot for TPA-1 - TPA-6 in different solvents which are mentioned in the supplementary information (ST4 and ST5). All the organic dyes are showing good linear ship relation.

ST 4: Photoluminescence spectral data of various solvents of TPA based organic dyes.

Solvent	λ_{em} (max) (nm)		Stoke's shift (Δv) (cm^{-1})	
	TPA-1	TPA-2	TPA-1	TPA-2
Toulene	375	383	6400	5700
$CHCl_3$	406	406	6900	6900
THF	403	389	7600	6800
DCM	403	406	7030	7100
DMF	433	429	9500	9300
Acetonitrile	389	389	9400	8640
Methanol	358	387	8600	9320

ST 5: Photoluminescence spectral data of various solvents of TPA based organic dyes.

Solvent	λ_{em} (max) (nm)				Stoke's shift ($\Delta\nu$) (cm^{-1})			
	TPA-3	**TPA-4**	**TPA-5**	**TPA-6**	**TPA-3**	**TPA-4**	**TPA-5**	**TPA-6**
Toulene	475	476	515	505	2450	3000	3600	1900
$CHCl_3$	611	574	564	578	6940	5500	5500	4700
THF	595	561	540	574	5500	5300	5640	4800
DCM	572	582	582	590	4800	4900	6200	4900
DMF	653	609	606	606	7000	6900	6200	6300
Acetonitrile	671	625	628	666	8300	7500	8300	7600
Methanol	665	636	602	628	8400	7400	7600	6700
DMSO	662	617	632	624	6700	6900	7500	7300

4. CIE Color Coordinates

The Commission International del'Eclairage (CIE) chromaticity coordinates of the synthesized dyes and the corresponding emission intensities are tabulated below.

ST6. CIE color coordinates of hybrid LEDs at different concentrations of TPA based organic dyes.

TPA-Acetophenone			**TPA-1**		**TPA-2**	
Connc.	**x**	**y**	**x**	**y**	**x**	**y**
0.01	0.23	0.32	0.31	0.37	0.22	0.25
0.02	0.23	0.34	0.34	0.40	0.24	0.28
0.04	**0.24**	**0.46**	0.33	0.39	0.36	0.39
0.06	0.20	0.30	**0.31**	**0.36**	**0.32**	**0.33**
0.08	0.26	0.40	0.33	0.38	0.37	0.42
0.1	0.28	0.43	0.32	0.38	0.30	0.31

ST7. CIE color coordinates of hybrid LEDs at different concentrations of TPA based organic dyes.

TPA-3			TPA-4		TPA-5		TPA-6	
Conc.	**x**	**y**	**x**	**y**	x	y	**x**	**y**
0.01	0.21	0.32	0.24	0.43	0.27	0.33	0.23	0.30
0.02	0.21	0.33	0.25	0.44	0.26	0.32	0.24	0.34
0.04	0.21	0.34	0.29	0.44	**0.28**	**0.33**	**0.26**	**0.34**
0.06	0.23	0.37	0.28	0.45	0.25	0.34	0.27	0.39
0.08	0.23	0.37	0.28	0.50	0.27	0.34	0.27	0.40
0.10	0.23	0.38	0.28	0.51	0.28	0.38	0.28	0.41

ST 8: CIE color coordinates of all TPA based organic dyes in different solvents.

Solvent	TPA-1		TPA-2		TPA-3		TPA-4		TPA-5		TPA-6	
	x	**y**	**x**	**y**	**x**	**y**	**x**	**y**	**x**	**y**	**x**	**y**
Toulene	0.42	0.47	0.43	0.50	0.17	0.39	0.18	0.41	0.42	0.47	0.21	0.41
DCM	0.44	0.51	0.42	0.51	0.45	0.52	0.48	0.50	0.46	0.43	0.46	0.50
THF	0.40	0.54	0.40	0.50	0.38	0.54	0.41	0.53	0.40	0.54	0.40	0.49
$CHCl_3$	0.44	0.52	0.42	0.50	0.42	0.54	0.41	0.52	0.44	0.52	0.43	0.52
Methanol	0.43	0.47	0.43	0.46	0.45	0.45	0.47	0.45	0.43	0.47	0.48	0.46
Acetonitrile	0.48	0.45	0.39	0.42	0.51	0.44	0.55	0.43	0.48	0.45	0.51	0.45
DMF	0.47	0.47	0.41	0.46	0.51	0.46	0.53	0.45	0.47	0.47	0.48	0.47
DMSO	0.42	0.47	0.43	0.50	0.53	0.45	0.54	0.44	0.48	0.44	0.50	0.46

xyz coordinates of TPA based organic dyes by DFT analysis:

TPA-1:

6 -3.947955000 -4.905596000 1.353740000

6 -4.058494000 -6.298044000 1.495497000

6 -4.407117000 -6.853229000 2.724931000

6	-4.632550000	-6.036930000	3.835104000
6	-4.514074000	-4.652409000	3.699191000
6	-4.184206000	-4.086624000	2.469365000
7	-3.601045000	-4.333647000	0.098039000
6	-2.665031000	-3.269576000	0.038365000
6	-4.196237000	-4.829891000	-1.094641000
6	-3.426731000	-5.011168000	-2.255100000
6	-4.017575000	-5.490101000	-3.422518000
6	-5.375438000	-5.813764000	-3.450659000
6	-6.140852000	-5.643720000	-2.295396000
6	-5.563516000	-5.147806000	-1.128382000
6	-2.861572000	-2.184392000	-0.832421000
6	-1.934400000	-1.151054000	-0.902546000
6	-0.798607000	-1.148456000	-0.079616000
6	-0.611623000	-2.220044000	0.806457000
6	-1.518420000	-3.272921000	0.850690000
7	0.130553000	-0.067812000	-0.131153000
6	1.513832000	-0.313822000	-0.199929000
6	-0.373361000	1.265366000	-0.092348000
6	0.083224000	2.236851000	-0.996187000
6	-0.410127000	3.535827000	-0.952943000
6	-1.406194000	3.897138000	-0.029979000
6	-1.877908000	2.916934000	0.859063000
6	-1.356835000	1.628310000	0.839376000

7	-1.923631000	5.217673000	0.002625000
6	-2.190223000	5.848067000	1.249431000
6	-2.173932000	5.914896000	-1.211776000
6	-3.359400000	6.604801000	1.428648000
6	-3.611920000	7.229326000	2.648209000
6	-2.718561000	7.096975000	3.713072000
6	-1.559615000	6.337689000	3.540581000
6	-1.289026000	5.724354000	2.319137000
6	-1.823819000	7.268541000	-1.340380000
6	-2.078182000	7.949921000	-2.528741000
6	-2.666005000	7.294228000	-3.612268000
6	-3.007261000	5.945902000	-3.490097000
6	-2.774191000	5.260661000	-2.299494000
6	2.441306000	0.578303000	0.370962000
6	3.802812000	0.323678000	0.289892000
6	4.310939000	-0.824623000	-0.346756000
6	3.372147000	-1.711033000	-0.913778000
6	2.011249000	-1.464891000	-0.848348000
6	5.752947000	-1.037758000	-0.385877000
6	6.414935000	-2.070410000	-0.954582000
6	7.881252000	-2.198244000	-1.077013000
6	8.812651000	-1.474431000	-0.143104000
8	8.348342000	-2.901063000	-1.972386000
6	8.516693000	-1.239760000	1.207950000

6	9.451677000	-0.618643000	2.037468000
6	10.685513000	-0.217541000	1.524508000
6	10.992496000	-0.457392000	0.181845000
6	10.068141000	-1.093374000	-0.641274000
1	-3.870592000	-6.936975000	0.639163000
1	-4.488194000	-7.932518000	2.817107000
1	-4.896761000	-6.473849000	4.793072000
1	-4.693862000	-4.004038000	4.552005000
1	-4.107576000	-3.009546000	2.364679000
1	-2.367985000	-4.775954000	-2.234283000
1	-3.406994000	-5.624587000	-4.310819000
1	-5.830572000	-6.193679000	-4.360011000
1	-7.199982000	-5.884897000	-2.303501000
1	-6.165386000	-5.005374000	-0.237267000
1	-3.740756000	-2.162083000	-1.467123000
1	-2.097587000	-0.325331000	-1.587283000
1	0.260894000	-2.234282000	1.451387000
1	-1.349026000	-4.099744000	1.531861000
1	0.842525000	1.973719000	-1.725276000
1	-0.035647000	4.276762000	-1.650853000
1	-2.647559000	3.175181000	1.578356000
1	-1.726581000	0.886292000	1.539277000
1	-4.062873000	6.699732000	0.608429000
1	-4.521101000	7.811298000	2.769302000

1	-2.922489000	7.579177000	4.664037000
1	-0.851164000	6.232079000	4.357260000
1	-0.380236000	5.147358000	2.185493000
1	-1.354340000	7.778753000	-0.506105000
1	-1.800711000	8.996909000	-2.611114000
1	-2.855610000	7.826683000	-4.539059000
1	-3.472504000	5.424329000	-4.321663000
1	-3.054823000	4.217065000	-2.204176000
1	2.086224000	1.465847000	0.881857000
1	4.497405000	1.025733000	0.744452000
1	3.714216000	-2.602199000	-1.430360000
1	1.316158000	-2.158797000	-1.307017000
1	6.340126000	-0.252331000	0.085497000
1	5.881534000	-2.849043000	-1.493893000
1	7.568275000	-1.570539000	1.617538000
1	9.217765000	-0.453934000	3.085300000
1	11.409564000	0.272130000	2.169455000
1	11.955837000	-0.154384000	-0.218065000
1	10.297388000	-1.310672000	-1.679128000

TPA-2:

7	0.075468000	-0.173434000	-0.004860000
6	1.291936000	-0.908765000	-0.008033000
6	-1.181062000	-0.856624000	0.010521000
6	0.096896000	1.256612000	-0.010895000

6	-2.240394000	-0.420775000	-0.806170000
6	-3.474527000	-1.069276000	-0.771696000
6	-3.667409000	-2.189609000	0.053319000
6	-2.605583000	-2.637619000	0.856376000
6	-1.382217000	-1.968250000	0.849346000
6	2.417021000	-0.445540000	0.701760000
6	3.604896000	-1.170408000	0.684996000
6	3.724617000	-2.385168000	-0.024506000
6	2.587329000	-2.839291000	-0.730262000
6	1.399052000	-2.119153000	-0.727179000
6	-0.770572000	1.987700000	0.820842000
6	-0.768424000	3.382137000	0.795946000
6	0.125160000	4.078301000	-0.034458000
6	1.004123000	3.350377000	-0.853593000
6	0.977804000	1.956246000	-0.856011000
6	4.999626000	-3.099086000	-0.000254000
7	-4.922277000	-2.861257000	0.076544000
7	0.139762000	5.501706000	-0.047137000
6	-5.699682000	-3.116707000	1.224828000
6	-6.880338000	-3.808166000	0.833294000
6	-6.815233000	-3.980360000	-0.607202000
6	-5.598567000	-3.385344000	-1.044287000
6	-0.001754000	6.317875000	-1.188345000
6	0.067867000	7.681455000	-0.786811000

6	0.261030000	7.692467000	0.652347000
6	0.299738000	6.335250000	1.078896000
6	0.412888000	8.717683000	1.595634000
6	0.605684000	8.383930000	2.937569000
6	0.654860000	7.035158000	3.341022000
6	0.505942000	5.994485000	2.420161000
6	-0.216299000	5.957278000	-2.523108000
6	-0.341785000	6.983947000	-3.462969000
6	-0.261713000	8.338443000	-3.084390000
6	-0.060981000	8.692361000	-1.748811000
6	-5.465349000	-2.763512000	2.558168000
6	-6.423901000	-3.129735000	3.506918000
6	-7.591484000	-3.826388000	3.138340000
6	-7.826139000	-4.164397000	1.804129000
6	-7.663210000	-4.586781000	-1.543778000
6	-7.291385000	-4.599334000	-2.889524000
6	-6.077191000	-4.017203000	-3.303438000
6	-5.214473000	-3.406091000	-2.389457000
6	5.280280000	-4.288436000	-0.586126000
6	6.543083000	-5.037218000	-0.472854000
6	7.831950000	-4.368079000	-0.112025000
6	8.147598000	-3.051855000	-0.498119000
6	9.392757000	-2.500003000	-0.177997000
6	10.332825000	-3.252817000	0.534403000

6	10.032255000	-4.569562000	0.909938000
6	8.796616000	-5.126165000	0.578461000
8	6.524653000	-6.279830000	-0.667659000
1	-2.097539000	0.435070000	-1.455699000
1	-4.293585000	-0.711189000	-1.385048000
1	-2.744155000	-3.508653000	1.486760000
1	-0.574729000	-2.312628000	1.485145000
1	2.351944000	0.476246000	1.267658000
1	4.458684000	-0.799651000	1.245167000
1	2.637499000	-3.760204000	-1.300832000
1	0.546338000	-2.482730000	-1.288390000
1	-1.454813000	1.460201000	1.475341000
1	-1.458713000	3.937143000	1.421070000
1	1.703746000	3.881011000	-1.489434000
1	1.648947000	1.404420000	-1.504011000
1	5.781540000	-2.610495000	0.577098000
1	0.385652000	9.757979000	1.286522000
1	0.723096000	9.168582000	3.677648000
1	0.814588000	6.796464000	4.387731000
1	0.555054000	4.959794000	2.738623000
1	-0.289928000	4.918335000	-2.822370000
1	-0.507716000	6.729747000	-4.505047000
1	-0.361769000	9.111795000	-3.838772000
1	-0.010260000	9.737294000	-1.458904000

1	-4.574776000	-2.219175000	2.849642000
1	-6.264422000	-2.868279000	4.548215000
1	-8.315457000	-4.097925000	3.899465000
1	-8.731739000	-4.692388000	1.521981000
1	-8.594786000	-5.045094000	-1.226528000
1	-7.939618000	-5.064811000	-3.624569000
1	-5.802111000	-4.045392000	-4.353026000
1	-4.277705000	-2.969677000	-2.715628000
1	4.511460000	-4.847081000	-1.113082000
1	7.436232000	-2.473246000	-1.076565000
1	9.630576000	-1.488490000	-0.491732000
1	11.296384000	-2.821416000	0.786953000
1	10.763143000	-5.159739000	1.453450000
1	8.556071000	-6.150219000	0.841124000

TPA-3:

6	-3.864269000	-0.941673000	-0.050313000
8	-4.066987000	-1.999788000	-0.647294000
6	-2.489078000	-0.419270000	0.135602000
6	-1.424868000	-1.153869000	-0.256714000
1	-2.367918000	0.573444000	0.555285000
1	-1.656008000	-2.130575000	-0.680224000
6	-0.014845000	-0.804231000	-0.186312000
6	0.944822000	-1.725564000	-0.648762000
6	0.464418000	0.420063000	0.324773000
6	2.304083000	-1.449012000	-0.614569000
1	0.608526000	-2.674521000	-1.058009000
6	1.818486000	0.704789000	0.373703000

1	-0.235994000	1.157166000	0.704907000
6	2.768817000	-0.224937000	-0.099297000
1	3.014433000	-2.175562000	-0.992075000
1	2.156938000	1.648989000	0.785206000
7	4.146493000	0.067776000	-0.052227000
6	5.103646000	-0.970341000	0.147678000
6	4.913621000	-1.931823000	1.152003000
6	6.255576000	-1.031488000	-0.650392000
6	5.854952000	-2.941601000	1.341572000
1	4.028758000	-1.881664000	1.777778000
6	7.200051000	-2.034703000	-0.441690000
1	6.403974000	-0.291045000	-1.429279000
6	7.004143000	-2.997324000	0.550301000
1	5.694761000	-3.679204000	2.122564000
1	8.087163000	-2.069797000	-1.067346000
1	7.738770000	-3.781239000	0.706007000
6	4.609632000	1.405480000	-0.224563000
6	4.102825000	2.209056000	-1.257158000
6	5.590946000	1.927331000	0.631358000
6	4.563359000	3.514360000	-1.418780000
1	3.351310000	1.804979000	-1.927229000
6	6.057743000	3.227870000	0.451261000
1	5.982590000	1.308631000	1.431899000
6	5.544687000	4.030125000	-0.569842000
1	4.162379000	4.124870000	-2.222621000
1	6.817820000	3.618793000	1.121429000
1	5.906257000	5.044938000	-0.703488000
6	-4.997473000	-0.128586000	0.513512000
6	-6.296412000	-0.093747000	-0.107713000
6	-4.790265000	0.568536000	1.694162000

6	-6.607146000	-0.761085000	-1.325769000
6	-7.331155000	0.682812000	0.517213000
6	-5.820596000	1.305138000	2.315813000
1	-3.819365000	0.522934000	2.176633000
6	-7.861672000	-0.662465000	-1.886738000
1	-5.844305000	-1.365078000	-1.797116000
6	-8.614116000	0.757621000	-0.088664000
6	-7.063940000	1.364832000	1.733734000
1	-5.623291000	1.821550000	3.250290000
6	-8.878059000	0.099979000	-1.266730000
1	-8.073463000	-1.181309000	-2.817230000
1	-9.383953000	1.350162000	0.398867000
1	-7.864350000	1.935574000	2.197610000
1	-9.862053000	0.164195000	-1.721973000

TPA-4:

6	-3.667631000	-1.785277000	-0.666509000
8	-3.692821000	-2.942414000	-1.087913000
6	-2.389589000	-1.079407000	-0.430212000
6	-1.216660000	-1.727289000	-0.603408000
1	-2.413406000	-0.034122000	-0.143991000
1	-1.294625000	-2.770047000	-0.908312000
6	0.132093000	-1.208192000	-0.437604000
6	1.228485000	-2.055255000	-0.690523000
6	0.420853000	0.111693000	-0.032604000
6	2.539081000	-1.618846000	-0.559310000
1	1.040840000	-3.075913000	-1.013155000
6	1.723942000	0.556953000	0.112686000
1	-0.390437000	0.797974000	0.189484000
6	2.812982000	-0.300335000	-0.151672000
1	3.358955000	-2.293992000	-0.776065000

1	1.913870000	1.572770000	0.440362000
7	4.139273000	0.153704000	-0.005430000
6	5.168086000	-0.738181000	0.419117000
6	4.962127000	-1.596518000	1.509899000
6	6.404698000	-0.755756000	-0.242815000
6	5.973008000	-2.463906000	1.919032000
1	4.010468000	-1.578594000	2.030528000
6	7.415982000	-1.613876000	0.184945000
1	6.565575000	-0.095104000	-1.088190000
6	7.205736000	-2.475482000	1.263145000
1	5.799403000	-3.122904000	2.764734000
1	8.368369000	-1.616909000	-0.337175000
1	7.993437000	-3.147517000	1.589213000
6	4.476825000	1.510540000	-0.284556000
6	4.001590000	2.140029000	-1.445256000
6	5.301303000	2.227892000	0.595151000
6	4.336084000	3.466790000	-1.709273000
1	3.372929000	1.585083000	-2.133600000
6	5.644851000	3.548630000	0.313568000
1	5.668495000	1.744382000	1.494198000
6	5.161472000	4.177403000	-0.835536000
1	3.960986000	3.941125000	-2.611487000
1	6.283757000	4.091641000	1.003942000
1	5.425988000	5.208487000	-1.048478000
6	-4.961689000	-1.068562000	-0.404076000
6	-5.052739000	0.120844000	0.297183000
6	-6.154474000	-1.679096000	-0.888120000
6	-6.304607000	0.745750000	0.535158000
1	-4.166729000	0.598923000	0.702626000
6	-7.378163000	-1.094956000	-0.683593000

1	-6.055763000	-2.618190000	-1.420674000
6	-6.412940000	1.964887000	1.257418000
6	-7.495449000	0.130638000	0.029755000
1	-8.281041000	-1.565672000	-1.064088000
6	-7.639658000	2.552838000	1.467405000
1	-5.507434000	2.427672000	1.641484000
6	-8.744507000	0.762700000	0.262501000
6	-8.816095000	1.945865000	0.964224000
1	-7.710282000	3.485032000	2.019887000
1	-9.647037000	0.295399000	-0.122484000
1	-9.778637000	2.418737000	1.135842000

TPA-5:

6	-2.385049000	-1.400508000	-0.292201000
8	-2.485302000	-2.541092000	-0.746990000
6	-1.062806000	-0.766718000	-0.095804000
6	0.065973000	-1.456496000	-0.372462000
1	-1.018665000	0.262158000	0.242414000
1	-0.080500000	-2.475068000	-0.729534000
6	1.445262000	-1.009238000	-0.261046000
6	2.480316000	-1.870234000	-0.674659000
6	1.823780000	0.252287000	0.243921000
6	3.815484000	-1.498875000	-0.607593000
1	2.222922000	-2.847278000	-1.074881000
6	3.153068000	0.630283000	0.329195000
1	1.063906000	0.942812000	0.596582000
6	4.179373000	-0.237561000	-0.100979000
1	4.584581000	-2.181215000	-0.951015000
1	3.412764000	1.600257000	0.737919000
7	5.531692000	0.149796000	-0.018043000
6	6.551055000	-0.819437000	0.218355000

6	6.400256000	-1.780188000	1.229855000
6	7.723311000	-0.813241000	-0.551864000
6	7.400589000	-2.724073000	1.453511000
1	5.498945000	-1.781776000	1.833778000
6	8.726036000	-1.750101000	-0.309125000
1	7.841131000	-0.073088000	-1.336272000
6	8.569526000	-2.712885000	0.689708000
1	7.270185000	-3.462369000	2.239367000
1	9.628200000	-1.733726000	-0.913676000
1	9.349719000	-3.445411000	0.871784000
6	5.908020000	1.514669000	-0.187660000
6	5.373488000	2.278188000	-1.236626000
6	6.830783000	2.105214000	0.688631000
6	5.748184000	3.611179000	-1.393917000
1	4.667416000	1.821801000	-1.922294000
6	7.212531000	3.433759000	0.512925000
1	7.243924000	1.517492000	1.501574000
6	6.671152000	4.195656000	-0.524305000
1	5.326427000	4.190108000	-2.210393000
1	7.927806000	3.877792000	1.199143000
1	6.966012000	5.232273000	-0.654398000
6	-3.625517000	-0.621196000	0.047346000
6	-3.615267000	0.608531000	0.784403000
6	-4.832746000	-1.133251000	-0.377056000
6	-4.777855000	1.275868000	1.057982000
1	-2.679507000	1.012105000	1.154284000
6	-6.063687000	-0.466652000	-0.121311000
1	-4.828779000	-2.070904000	-0.924155000
6	-6.041643000	0.776751000	0.614259000
1	-4.756373000	2.202615000	1.625260000

6	-7.292193000	-0.978450000	-0.562648000
6	-7.246768000	1.440858000	0.866962000
6	-8.498068000	-0.314484000	-0.309839000
1	-7.305735000	-1.914339000	-1.115960000
6	-8.474709000	0.930886000	0.424454000
1	-7.231247000	2.376728000	1.420801000
6	-9.757742000	-0.824739000	-0.755068000
6	-9.713098000	1.600005000	0.673601000
6	-10.921579000	-0.151607000	-0.495055000
1	-9.771577000	-1.761011000	-1.306640000
6	-10.898374000	1.077016000	0.228540000
1	-9.694953000	2.535940000	1.225735000
1	-11.871308000	-0.550112000	-0.839185000
1	-11.831240000	1.597082000	0.425404000

TPA-6:

6	3.349951000	-0.951813000	1.050786000
8	3.483830000	-1.882133000	1.844463000
6	2.016236000	-0.481878000	0.612712000
6	0.894855000	-1.059471000	1.100509000
1	1.981710000	0.314033000	-0.124382000
1	1.053405000	-1.849425000	1.833929000
6	-0.488968000	-0.763011000	0.769334000
6	-1.516754000	-1.482276000	1.410176000
6	-0.878051000	0.214703000	-0.170453000
6	-2.856797000	-1.242250000	1.143356000
1	-1.251150000	-2.236828000	2.145857000
6	-2.211595000	0.457693000	-0.452642000
1	-0.121632000	0.783368000	-0.702297000
6	-3.231394000	-0.265072000	0.202541000
1	-3.622398000	-1.805199000	1.664873000

1	-2.479133000	1.205219000	-1.190875000
7	-4.588377000	-0.016348000	-0.083070000
6	-5.545875000	-1.072396000	-0.027701000
6	-5.280955000	-2.306941000	-0.639689000
6	-6.771383000	-0.880582000	0.626974000
6	-6.223110000	-3.332081000	-0.584329000
1	-4.338003000	-2.455313000	-1.155394000
6	-7.714785000	-1.905735000	0.661969000
1	-6.977036000	0.072472000	1.102797000
6	-7.445524000	-3.137260000	0.061978000
1	-6.004857000	-4.282586000	-1.062390000
1	-8.659644000	-1.743203000	1.172304000
1	-8.180030000	-3.935840000	0.096592000
6	-5.031015000	1.295185000	-0.424879000
6	-4.603369000	2.408358000	0.314741000
6	-5.913466000	1.484300000	-1.498958000
6	-5.041815000	3.686317000	-0.026469000
1	-3.930095000	2.264956000	1.153331000
6	-6.360122000	2.764154000	-1.821649000
1	-6.244514000	0.625698000	-2.073523000
6	-5.924499000	3.872154000	-1.092279000
1	-4.702385000	4.538606000	0.554976000
1	-7.042780000	2.895321000	-2.656168000
1	-6.269743000	4.868433000	-1.350411000
6	4.552577000	-0.289666000	0.420854000
6	4.727947000	1.112314000	0.510631000
6	5.493271000	-1.091763000	-0.273567000
6	3.863179000	1.961510000	1.276117000
6	5.850681000	1.732238000	-0.155747000
6	6.603170000	-0.453469000	-0.945335000

6	5.385715000	-2.517105000	-0.376896000
6	4.068981000	3.315240000	1.343334000
1	3.040835000	1.520056000	1.827774000
6	6.026834000	3.147923000	-0.062362000
6	6.746974000	0.934933000	-0.872446000
6	7.535569000	-1.254528000	-1.676092000
1	4.576360000	-3.018362000	0.137463000
6	6.302031000	-3.246848000	-1.087911000
6	5.160027000	3.922212000	0.659969000
1	3.399209000	3.932563000	1.934874000
1	6.874667000	3.595153000	-0.574646000
1	7.584521000	1.406980000	-1.381075000
6	7.392415000	-2.612922000	-1.748065000
1	8.362546000	-0.755280000	-2.174196000
1	6.199296000	-4.326547000	-1.145722000
1	5.306468000	4.996148000	0.726131000
1	8.106762000	-3.211932000	-2.305104000

Light harvesting efficiency (LHE):

The light harvesting efficiency (LHE) is a very important factor for organic dyes, considering the role of dyes in the optoelectronics. The LHE can be calculated using the oscillator strength obtained from TD-DFT calculations.[3] The LHE can be calculated using the following formula.[4]

$$LHE(\lambda) = 1\text{-}10^{-A} = 1\text{–}10^{-f}$$

where, f is the oscillator strength and A is absorbance of the organic molecule at a given wavelength. The calculated LHE of the dyes are tabulated in Table ST 9. From the table ST 9', it is clear that TPA-1, TPA-2 and TPA-6 dye molecules shows decreased LHE than the reference molecule TPA-Acetophenone. The lower HOMO–LUMO gap of TPA-6 results in

lower LHE with 0.63, while higher HOMO–LUMO gap molecule TPA-3 has a higher LHE with 0.84. This shows that TPA based organic dyes can be tuned through the proper substitution of (electron donating and electron withdrawing functional groups) for better LHE.

Compound	**TPA-Acetophenone**	**TPA-1**	**TPA-2**	**TPA-3**	**TPA-4**	**TPA-5**	**TPA-6**
LHE	0.827	0.685	0.666	0.845	0.821	0.836	0.638

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