

Supporting Information

Table S1. Electronic transition data in terms of band wavelength ( $\lambda$ /nm), oscillator strength ( $f$ ), and electronic configurations obtained by CAM-B3LYP/6-31G(d) level for each molecule in THF.

Dyes	$\lambda$ /nm	$E$ /eV	$f$	Main configuration
TSA1	496	2.50	1.9997	H-1->LUMO (37%), HOMO->LUMO (50%)
	337	3.68	0.3080	H-1->L+1 (15%), HOMO->LUMO (28%), HOMO->L+1 (41%)
	304	4.08	0.1884	H-4->LUMO (13%), H-2->LUMO (30%), H-1->L+1 (19%), HOMO->L+2 (14%)
TSA2	428	2.90	2.1520	H-1->LUMO (30%), HOMO->LUMO (58%)
	283	4.38	0.3277	H-2->LUMO (22%), H-1->L+1 (15%), HOMO->L+2 (27%)
TSA3	503	2.47	2.1583	H-1->LUMO (40%), HOMO->LUMO (44%)
	381	3.25	0.2222	H-2->LUMO (19%), H-1->LUMO (29%), HOMO->LUMO (14%), HOMO->L+1 (25%)
	345	3.59	0.2752	H-1->L+1 (16%), HOMO->LUMO (36%), HOMO->L+1 (29%)
	319	3.89	0.1835	H-4->LUMO (15%), H-2->LUMO (32%), H-1->L+1 (18%), HOMO->L+2 (11%)
TSA4	504	2.46	2.4025	H-1->LUMO (38%), HOMO->LUMO (44%)
	348	3.56	0.2702	H-1->L+1 (16%), HOMO->LUMO (39%), HOMO->L+1 (25%)
	319	3.89	0.4387	H-4->LUMO (16%), H-2->LUMO (29%), H-1->L+1 (19%), HOMO->L+2 (11%)
TBA1	517	2.40	1.8388	H-1->LUMO (31%), HOMO->LUMO (52%), HOMO->L+1 (10%)
	415	2.99	0.1621	H-1->LUMO (36%), HOMO->L+1 (37%)
	297	4.18	0.2157	H-2->LUMO (20%), HOMO->L+2 (19%), HOMO->L+3 (16%), H-1->L+1 (9%)
TBA2	488	2.54	1.3816	H-1->LUMO (20%), HOMO->LUMO (71%)
	379	3.27	0.2597	H-1->LUMO (57%), HOMO->LUMO (15%), HOMO->L+1 (10%)
	348	3.56	0.4485	H-1->LUMO (14%), H-1->L+1 (42%), HOMO->L+1 (25%)
	294	4.22	0.1981	H-2->LUMO (15%), HOMO->L+1 (10%), HOMO->L+2 (29%), HOMO->L+3 (16%)
TBA3	522	2.38	2.0998	H-1->LUMO (33%), HOMO->LUMO (47%), HOMO->L+1 (11%)
	428	2.90	0.1121	H-2->LUMO (10%), H-1->LUMO (32%), HOMO->L+1 (41%)
	338	3.67	0.1493	H-2->LUMO (24%), H-1->L+1 (21%), HOMO->L+1 (25%)
	310	4.00	0.2027	H-1->L+2 (23%), HOMO->L+2 (15%), H-1->L+1 (8%), HOMO->LUMO (9%), HOMO->L+1 (8%), HOMO->L+3 (7%)
	289	4.29	0.4715	H-8->LUMO (10%), HOMO->L+3 (17%), HOMO->L+4 (22%)
TBA4	520	2.38	2.116	H-1->LUMO (33%), HOMO->LUMO (44%), HOMO->L+1 (14%)
	427	2.90	0.3296	H-2->LUMO (11%), H-1->LUMO (32%), HOMO->L+1 (41%)
	312	3.97	0.1685	H-1->L+2 (25%), HOMO->L+2 (16%), HOMO->LUMO (7%), HOMO->L+1 (8%), HOMO->L+3 (8%)
	289	4.29	0.3830	HOMO->L+3 (14%), HOMO->L+5 (26%), H-2->L+1 (8%), HOMO->L+6 (8%)
	283	4.38	0.2614	H-10->L+1 (17%), H-9->LUMO (17%), H-9->L+1 (10%), H-4->LUMO (10%), H-4->LUMO (7%)

TDA1	588	2.11	1.9805	H-1->LUMO (11%), HOMO->LUMO (76%)
	356	3.48	0.5915	H-2->LUMO (63%), HOMO->L+1 (12%)
TDA2	547	2.27	1.8376	HOMO->LUMO (87%)
	349	3.55	0.4823	H-2->LUMO (29%), H-1->LUMO (21%), H-1->L+1 (18%), HOMO->L+1 (21%)
	332	3.73	0.2053	H-2->LUMO (42%), HOMO->L+1 (35%)
	290	4.28	0.1466	H-2->L+1 (14%), HOMO->L+2 (44%)
TDA3	586	2.12	2.1488	HOMO->LUMO (75%), HOMO->L+1 (11%)
	425	2.92	0.2073	H-2->LUMO (27%), H-1->LUMO (22%), HOMO->L+1 (41%)
	361	3.43	0.5813	H-2->LUMO (48%), H-1->LUMO (12%), H-1->L+1 (12%), HOMO->L+1 (8%)
TDA4	588	2.11	2.3235	H-1->LUMO (10%), HOMO->LUMO (71%), HOMO->L+1 (13%)
	425	2.92	0.1413	H-2->LUMO (26%), H-1->LUMO (19%), HOMO->L+1 (42%)
	363	3.42	0.6195	H-2->LUMO (51%), HOMO->L+1 (11%)
	299	4.15	0.1843	H-5->LUMO (25%), H-2->L+1 (11%), H-1->LUMO (12%), H-1->L+1 (12%)
TNA1	492	2.52	2.1372	H-1->LUMO (41%), HOMO->LUMO (45%)
	343	3.62	0.1683	H-1->L+1 (22%), HOMO->LUMO (32%), HOMO->L+1 (33%)
	310	4.00	0.2018	H-4->LUMO (12%), H-2->LUMO (32%), H-1->L+1 (22%), HOMO->L+1 (10%)
TNA2	436	2.84	2.1493	H-1->LUMO (30%), HOMO->LUMO (60%)
	283	4.38	0.2339	H-2->LUMO (32%), HOMO->L+1 (19%), HOMO->L+4 (10%)
TNA3	501	2.48	2.3392	H-1->LUMO (44%), HOMO->LUMO (40%)
	349	3.55	0.1435	H-1->L+1 (22%), HOMO->LUMO (39%), HOMO->L+1 (23%)
	324	3.83	0.3233	H-4->LUMO (13%), H-2->LUMO (34%), H-1->L+1 (20%), HOMO->L+1 (10%)
TNA4	501	2.48	2.4557	H-1->LUMO (42%), HOMO->LUMO (39%)
	391	3.17	0.1748	H-2->LUMO (16%), H-1->LUMO (26%), HOMO->LUMO (11%), HOMO->L+1 (35%)
	352	3.52	0.1634	H-1->L+1 (21%), HOMO->LUMO (42%), HOMO->L+1 (21%)
	325	3.82	0.2102	H-4->LUMO (14%), H-2->LUMO (30%), H-1->L+1 (23%)
TQA1	470	2.64	1.9656	H-1->LUMO (54%), HOMO->LUMO (32%)
	312	3.97	0.1134	H-1->L+1 (40%), HOMO->L+1 (22%)
	293	4.23	0.1916	H-3->LUMO (10%), H-1->L+2 (11%), HOMO->L+2 (16%), HOMO->L+4 (22%)
	285	4.35	0.2276	H-3->LUMO (21%), H-1->L+1 (12%), HOMO->L+2 (12%), HOMO->L+4 (16%)
TQA2	426	2.91	1.6827	H-1->LUMO (35%), HOMO->LUMO (54%)
	358	3.46	0.2065	H-1->LUMO (38%), H-1->L+1 (12%), HOMO->LUMO (19%), HOMO->L+1 (18%)
	323	3.84	0.1532	H-1->LUMO (17%), H-1->L+1 (37%), HOMO->LUMO (10%), HOMO->L+1 (10%)
	285	4.35	0.2539	HOMO->L+2 (32%), HOMO->L+5 (27%)
TQA3	481	2.58	2.1728	H-1->LUMO (59%), HOMO->LUMO (26%)
	326	3.80	0.2160	H-4->LUMO (12%), H-2->LUMO (20%), H-1->L+1 (28%), HOMO->L+1

---

			(19%)
	295	4.20	0.1502 H-2->LUMO (17%), H-1->L+2 (19%), HOMO->L+2 (12%)
	282	4.40	0.3765 H-1->L+2 (16%), HOMO->L+3 (16%), HOMO->L+5 (16%)
TQA4	480	2.58	2.2924 H-1->LUMO (56%), HOMO->LUMO (26%)
	396	3.13	0.1678 H-1->LUMO (20%), HOMO->LUMO (12%), HOMO->L+1 (45%)
	305	4.07	0.1404 H-2->LUMO (10%), H-1->L+1 (15%), H-1->L+2 (20%)
	295	4.20	0.1920 H-2->LUMO (22%), H-1->L+2 (11%), HOMO->L+2 (10%)
	282	4.40	0.3286 H-1->L+2 (15%), HOMO->L+3 (13%), HOMO->L+6 (32%)

---