Supporting Information

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In this supporting information, we show the excited state calculation results obtained from B3LYP, HandH, the dielectric-dependent method using eqs. (3) and (4) in the absorption and emission cases of Bu2N-TTz-Py, Ph2N-TTz-Py, and Ph2-TTz-CHO dyes.

Table S1a Excited state calculation results obtained from the B3LYP method in the absorption case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.6069	475.61	1.1993
	2	3.5966	344.73	0.3760
	3	3.8427	322.65	0.0204
DCM	1	2.5531	485.62	1.1565
	2	3.5404	350.20	0.4136
	3	3.8175	324.78	0.0272
methanol	1	2.5483	486.54	1.1215
	2	3.5272	351.51	0.4293
	3	3.8205	324.52	0.0272

Table S1b Excited state calculation results obtained from the HandH method in the absorption case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	3.3000	375.71	1.5251
	2	4.3845	282.78	0.0238
	3	4.6507	266.59	0.0496
DCM	1	3.2714	378.99	1.5129
	2	4.3529	284.83	0.0271
	3	4.6347	267.51	0.0474
methanol	1	3.2757	378.49	1.4895
	2	4.3530	284.82	0.0296
	3	4.6312	267.72	0.0444

Table S1c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the absorption case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	3.0162	411.06	1.4258
	2	4.1146	301.33	0.1051
	3	4.3347	286.02	0.0944
DCM	1	2.9772	416.45	1.3992
	2	4.0665	304.89	0.1299
	3	4.3034	288.10	0.0967
methanol	1	2.9781	416.32	1.3709
	2	4.0582	305.51	0.1437
	3	4.3020	288.20	0.0917

Table S1d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the absorption case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.9793	416.15	1.4077
	2	4.0416	306.77	0.0985
	3	4.2621	290.90	0.0754
DCM	1	2.9406	421.63	1.3837
	2	3.9945	310.39	0.1215
	3	4.2284	293.22	0.0786
methanol	1	2.9413	421.53	1.3567
	2	3.9864	311.02	0.1344
	3	4.2259	293.39	0.0743

Table S2a Excited state calculation results obtained from the B3LYP method in the emission case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.3978	517.07	1.3507
	2	3.4379	360.64	0.3143
	3	3.6802	336.89	0.0035
DCM	1	2.2268	556.78	1.5177
	2	3.3502	370.08	0.3045
	3	3.5380	350.44	0.0001
methanol	1	2.1692	571.57	1.5716
	2	3.3195	373.50	0.2957
	3	3.4885	355.41	0.0007

Table S2b Excited state calculation results obtained from the HandH method in the emission case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.7554	449.96	1.6984
	2	4.0464	306.41	0.0230
	3	4.4660	277.62	0.0084
DCM	1	2.5739	481.70	1.8540
	2	3.8956	318.27	0.0213
	3	4.3788	283.15	0.0063
methanol	1	2.5125	493.46	1.9011
	2	3.8412	322.77	0.0205
	3	4.3498	285.04	0.0062

Table S2c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the emission case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.6389	469.83	1.6304
	2	3.8785	319.67	0.0757
	3	4.0713	304.54	0.0146
DCM	1	2.4598	504.04	1.7846
	2	3.7459	330.99	0.0589
	3	3.9682	312.45	0.0303
methanol	1	2.3996	516.70	1.8318
	2	3.6959	335.46	0.0530
	3	3.9362	314.99	0.0343

Table S2d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the emission case of Bu2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.5565	484.98	1.6235
	2	3.7786	328.12	0.0651
	3	3.9802	311.50	0.0043
DCM	1	2.3735	522.37	1.7786
	2	3.6440	340.24	0.0544
	3	3.8749	319.97	0.0127
methanol	1	2.3109	536.51	1.8266
	2	3.5925	345.12	0.0502
	3	3.8419	322.72	0.0150

Table S3a Excited state calculation results obtained from the B3LYP method in the absorption case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.5013	495.67	1.1308
	2	3.3966	365.03	0.4371
	3	3.5051	353.73	0.1109
CHCl3	1	2.4845	499.03	1.1091
	2	3.3786	366.97	0.4391
	3	3.5027	353.97	0.1264
DCM	1	2.4768	500.57	1.1009
	2	3.3701	367.89	0.4407
	3	3.5024	353.99	0.132
Acetone	1	2.4787	500.2	1.0817
	2	3.3677	368.16	0.4456
	3	3.5097	353.26	0.1323

Table S3b Excited state calculation results obtained from the HandH method in the absorption case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	3.2356	383.19	1.5599
	2	4.1697	297.34	0.0190
	3	4.2295	293.14	0.0390
CHCl3	1	3.2321	383.60	1.5514
	2	4.1705	297.29	0.0170
	3	4.2355	292.72	0.0374
DCM	1	3.2310	383.74	1.5489
	2	4.1711	297.25	0.0157
	3	4.2390	292.48	0.0366
Acetone	1	3.2372	383.00	1.5350
	2	4.1785	296.72	0.0142
	3	4.2435	292.18	0.0356

Table S3c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the absorption case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.8319	437.82	1.3508
	2	3.8153	324.97	0.0009
	3	3.8731	320.12	0.3529
CHCl3	1	2.8217	439.4	1.3344
	2	3.8058	325.78	0.0155
	3	3.8672	320.6	0.3605
DCM	1	2.8173	440.08	1.3283
	2	3.8003	326.25	0.029
	3	3.8658	320.72	0.354
acetone	1	2.8216	439.41	1.3105
	2	3.8013	326.16	0.0493
	3	3.8698	320.39	0.3381

Table S3d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the absorption case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
toluene	1	2.8405	436.48	1.3705
	2	3.7832	327.73	0.0141
	3	3.8455	322.41	0.2863
CHCl3	1	2.8307	438	1.3553
	2	3.7809	327.93	0.0008
	3	3.8327	323.49	0.3124
DCM	1	2.8268	438.6	1.3505
	2	3.7794	328.05	0.0017
	3	3.8293	323.78	0.3162
acetone	1	2.8314	437.88	1.3346
	2	3.7844	327.62	0.0131
	3	3.8312	323.62	0.3077

Table S4a Excited state calculation results obtained from the B3LYP method in the emission case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.1241	583.71	0.7056
	2	3.0004	413.23	0.9214
	3	3.1784	390.08	0.0012
CHCl3	1	2.1122	586.98	1.0602
	2	2.9996	413.33	0.6964
	3	3.1734	390.7	0.0133
DCM	1	2.0884	593.69	1.24
	2	2.9989	413.43	0.5789
	3	3.1581	392.59	0.0259
acetone	1	2.0662	600.05	1.3474
	2	2.9957	413.87	0.5065
	3	3.1431	394.46	0.038

Table S4b Excited state calculation results obtained from the HandH method in the emission case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.6982	459.50	1.7631
	2	3.8315	323.60	0.0133
	3	4.0988	302.49	0.0321
CHCl3	1	2.6027	476.37	1.8678
	2	3.7580	329.92	0.0077
	3	4.0816	303.76	0.0285
DCM	1	2.5487	486.45	1.9218
	2	3.7135	333.87	0.0054
	3	4.0667	304.87	0.0234
acetone	1	2.5106	493.84	1.9579
	2	3.6811	336.81	0.0040
	3	4.0547	305.78	0.0200

Table S4c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the emission case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.4796	500.01	1.4595
	2	3.4603	358.30	0.2663
	3	3.6270	341.83	0.0537
CHCl3	1	2.3973	517.18	1.6211
	2	3.4263	361.86	0.1779
	3	3.5774	346.58	0.0858
DCM	1	2.3489	527.85	1.6997
	2	3.3990	364.77	0.1339
	3	3.5511	349.15	0.1039
acetone	1	2.3145	535.68	1.7500
	2	3.3765	367.20	0.1073
	3	3.5337	350.86	0.1140

Table S4d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the emission case of Ph2N-TTz-Py.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Toluene	1	2.4389	508.37	1.5566
	2	3.3934	365.37	0.1476
	3	3.5826	346.08	0.0502
CHCl3	1	2.3479	528.06	1.6973
	2	3.3588	369.13	0.0899
	3	3.5271	351.52	0.0696
DCM	1	2.2949	540.27	1.7664
	2	3.3309	372.22	0.0627
	3	3.4973	354.52	0.0792
acetone	1	2.2572	549.27	1.8114
	2	3.3084	374.75	0.0464
	3	3.4774	356.54	0.0840

Table S5a Excited state calculation results obtained from the B3LYP method in the absorption case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.1512	576.35	1.0539
	2	3.0251	409.85	0.7610
	3	3.1932	388.27	0.1195
DCM	1	2.2676	546.77	1.0562
	2	3.0961	400.45	0.7723
	3	3.2436	382.24	0.0785
Cl2-benz	1	2.2554	549.72	1.0902
	2	3.0888	401.40	0.7669
	3	3.2274	384.16	0.0799

Table S5b Excited state calculation results obtained from the HandH method in the absorption case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	3.0207	410.44	1.7268
	2	3.9560	313.41	0.0158
	3	4.1770	296.82	0.2778
DCM	1	3.1235	396.94	1.7506
	2	3.9747	311.93	0.0051
	3	4.2269	293.32	0.0512
Cl2-benz	1	3.1096	398.71	1.7812
	2	3.9569	313.33	0.0054
	3	4.2249	293.46	0.0536

Table S5c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the absorption case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.6326	470.96	1.3997
	2	3.5149	352.74	0.2934
	3	3.5858	345.77	0.3058
DCM	1	2.6379	470	1.3699
	2	3.515	352.73	0.339
	3	3.5955	344.83	0.2692
Cl2-benz	1	2.6248	472.35	1.4037
	2	3.507	353.53	0.2949
	3	3.5806	346.27	0.3092

Table S5d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the absorption case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.6477	468.27	1.4307
	2	3.5172	352.51	0.2873
	3	3.5533	348.93	0.2269
DCM	1	2.6535	467.25	1.4021
	2	3.5173	352.5	0.3526
	3	3.564	347.88	0.1708
Cl2-benz	1	2.6403	469.58	1.4353
	2	3.5097	353.26	0.2865
	3	3.5499	349.27	0.2324

Table 6a Excited state calculation results obtained from the B3LYP method in the emission case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	1.9505	635.67	1.2660
	2	2.8007	442.69	0.8059
	3	2.9560	419.44	0.0247
DCM	1	1.9248	644.14	1.3532
	2	2.7884	444.65	0.7499
	3	2.9368	422.17	0.0387
Cl2-benz	1	1.9195	645.94	1.3695
	2	2.7857	445.07	0.7389
	3	2.9327	422.76	0.0419

Table S6b Excited state calculation results obtained from the HandH method in the emission case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.4460	506.89	2.1478
	2	3.5418	350.06	0.0008
	3	3.8751	319.95	0.0469
DCM	1	2.4080	514.88	2.1826
	2	3.5078	353.46	0.0012
	3	3.8612	321.10	0.0436
Cl2-benz	1	2.4005	516.49	2.1893
	2	3.5010	354.14	0.0014
	3	3.8585	321.33	0.0429

Table S6c Excited state calculation results obtained from the dielectric-dependent method using eq. (3) in the emission case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.2187	558.82	1.8268
	2	3.2075	386.54	0.2048
	3	3.2802	377.98	0.1791
DCM	1	2.1841	567.66	1.8793
	2	3.1846	389.33	0.1463
	3	3.2605	380.26	0.2205
Cl2-benz	1	2.1772	569.45	1.8892
	2	3.1796	389.94	0.1360
	3	3.2568	380.69	0.2275

Table S6d Excited state calculation results obtained from the dielectric-dependent method using eq. (4) in the emission case of Ph2N-TTz-CHO.

	State	Energy [eV]	Energy [nm]	Oscillator Strength
Cl-benz	1	2.1731	570.55	1.9113
	2	3.1650	391.74	0.1047
	3	3.2491	381.59	0.1550
DCM	1	2.1354	580.61	1.9577
	2	3.1415	394.67	0.0695
	3	3.2277	384.12	0.1777
Cl2-benz	1	2.1279	582.65	1.9665
	2	3.1365	395.29	0.0634
	3	3.2237	384.60	0.1814