Electronic Supplementary Material (ESI) for Materials Advances.

Triphenylamine-Imidazole based Luminophores for Deep-blue Organic Light Emitting Diodes: Experimental and Theoretical Investigations

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Contents:

SI4. Photophysical properties of the luminophores

Fig. S11. Molar extinction coefficient vs. wavelength graphs of synthesized molecules in solution (a) and solid (b) states.

SI5. Quantum yield studies of luminophores in solution and solid states

Fig. S12. The PLQY of BIPTPA luminophore in solution and solid states.

Fig. S13. The PLQY of DBIPTPA luminophore in solution and solid states.

Fig. S14. The PLQY of TBIPTPA luminophore in solution and solid states.

SI6. The computed vertical transitions and their oscillator strengths (f) and configuration and atom coordinates of the luminophores.

SI1. Experimental section

SI1.1. General Information and Measurements:

All the reactions were performed under nitrogen atmosphere. Solvents were carefully dried and distilled from appropriate drying agents prior to use. Commercially available reagents (Sigma Aldrich) were used without further purification unless otherwise stated. All the reactions were monitored by thin-layer chromatography (TLC) with silica gel 60 F_{254} Aluminium plates (Merck). Column chromatography was carried out using silica gel (Sigma-Aldrich). ^{1}H-NMR and ^{13}C-NMR spectra were recorded using an AV 400 Avance-III 400MHz FT-NMR Spectrometer (Bruker Biospin International, Switzerland) with tetramethylsilane (TMS) as a standard reference. The mass spectra were recorded by LC–MS (Perkin–Elmer, USA/Flexer SQ 300 M). The FTIR spectra were recorded on a Shimadzu IR Affinity-1S spectrophotometer. The thermal properties of the luminophores were collected on a thermogravimetric analyser (TGA) under a nitrogen atmosphere at a heating rate of 10 °C/min. The absorption spectrum of the target luminophores in solution phase and solid (DRS) were measured by using UV-visible spectrometer (Shimadzu Corporation,

Japan/UV-2450 Perkin Elmer, USA/Lamda 25). The photoluminescence excitation and emission spectra were recorded by Horiba Jobin Yvon, USA/Fluoromax 4P spectrophotometer. The absolute quantum yields were determined by using Edinburgh Instruments, spectrofluorometer, FS5, Integrating Sphere SC-30. The CIE color coordinates were calculated by using PL emission data (MATLAB software). The electrochemical properties of the luminophores were measured by using cyclic voltammetry (CV), AUTOLAB 302N Modular potentiostat, at RT in dimethylformamide (DMF). The working (glass-carbon rod), auxiliary (counter, Pt wire), and reference (Ag/Agcl wire) electrodes were used for CV analysis. The DMF which contains 0.1 M Bu_4NClO_4 was used as the supporting electrolyte, and the scan rate was maintained as 100 mV s^{-1}.

SI1.2. Device fabrication and measurement

For wet-processing, the fabrication process included first spin coating an aqueous solution of PEDOT: PSS at 4000 rpm for 20 s to form a hole-injection layer on a pre-cleaned ITO anode. Before depositing the following emissive layer (EML), the solution was prepared by dissolving the host and guest molecules in tetrahydrofuran at 50 C for 0.25 h with stirring. The resulting solution was then spin-coated at 2500 rpm for 20s under nitrogen, followed by deposition of the electron-transporting layer TPBi, the electron injection layer LiF, and the cathode Al, by thermal evaporation under less than 10^{-5} Torr.

The luminance, CIE chromatic coordinates, and electroluminescence spectrum of the resulting ultra-deep blue OELDs were measured by using Photo Research PR-655 spectra scan. A Keithley 2400 electrometer was used to measure the current-voltage (I–V) characteristics. The emission area of the devices was 2.5 mm^{-2}, and only the luminance in the forward direction was measured.

SI1.3. Computational details:

The molecules under study were first optimized in the gas phase using density functional theory and the Becke three parameter Lee–Yang–Parr (B3LYP) [1] form for the exchange–correlation potential and the 6-31G(d,p) basis set. All the structures were found to be in the minima of the potential energy surface as the normal mode of frequencies were all positive. After that we performed the UV-vis spectra calculations using time dependent density functional theory (TD-DFT) [2] with gas phase optimized geometries. Singlet and triplet energy calculations were performed by using the TD-SCF and B3LYP/6-31G(P) approach.

SI2 NMR spectra (^{1}H and ^{13}C) and mass spectra of the molecules

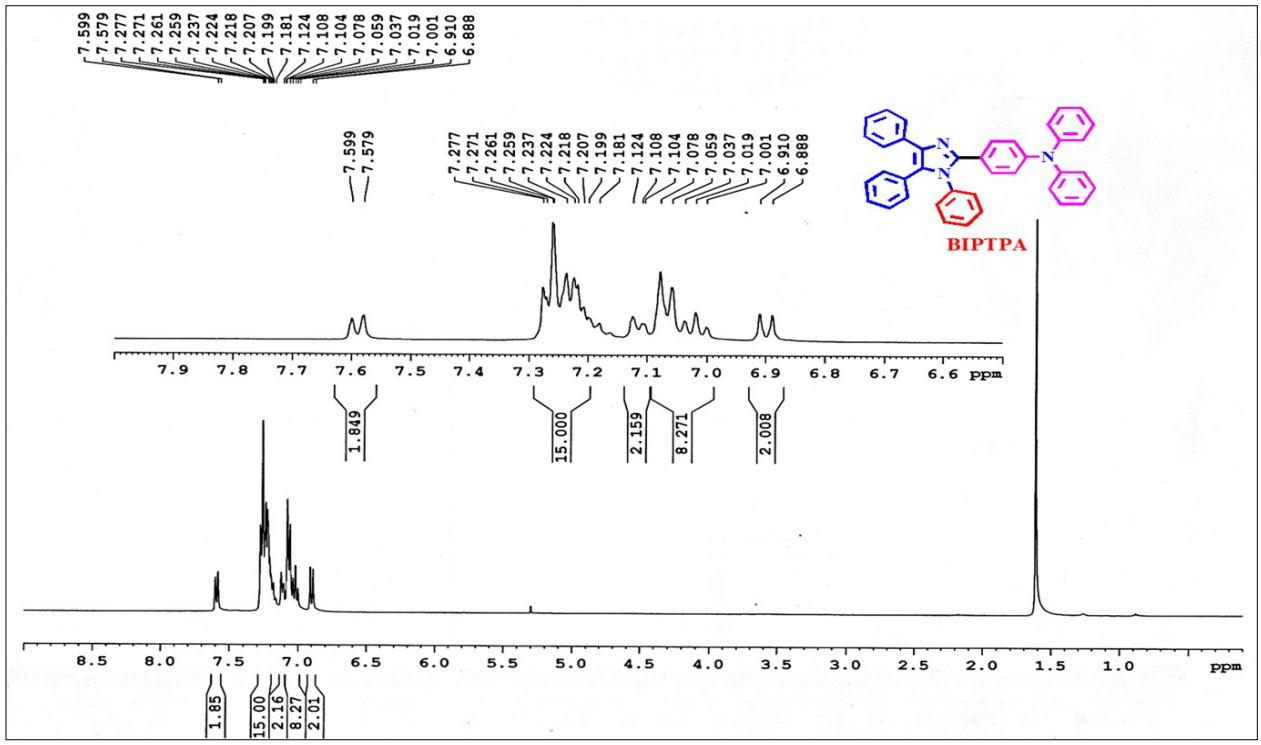

Fig. S1. The ^{1}H NMR spectra of the BIPTPA

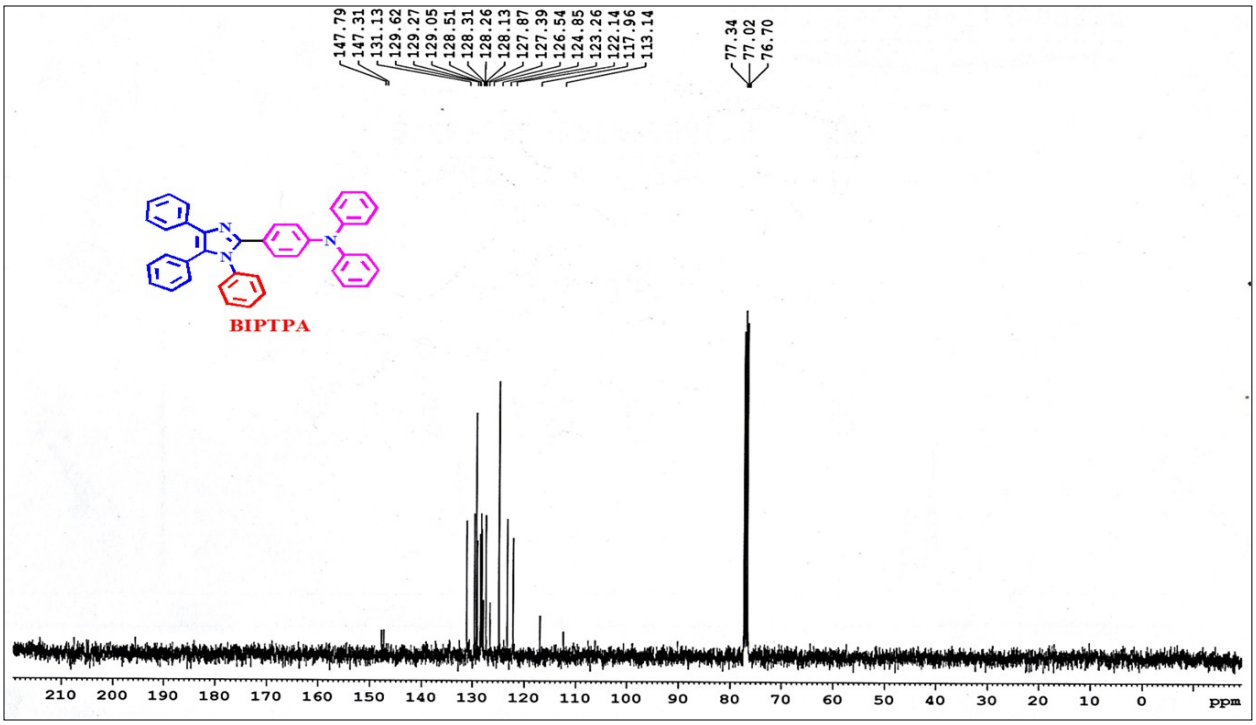

Fig. S2. The ^{13}C NMR spectra of the BIPTPA

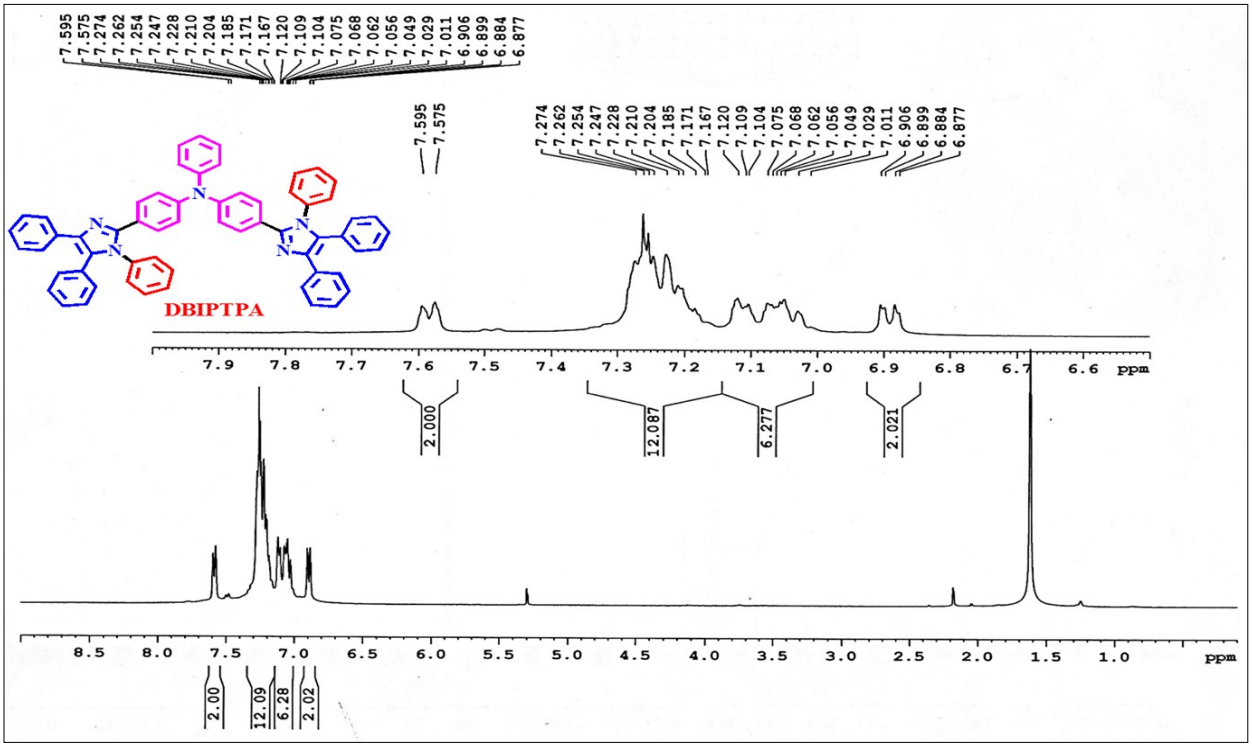

Fig. S3. The ^{1}H NMR spectra of the DBIPTPA.

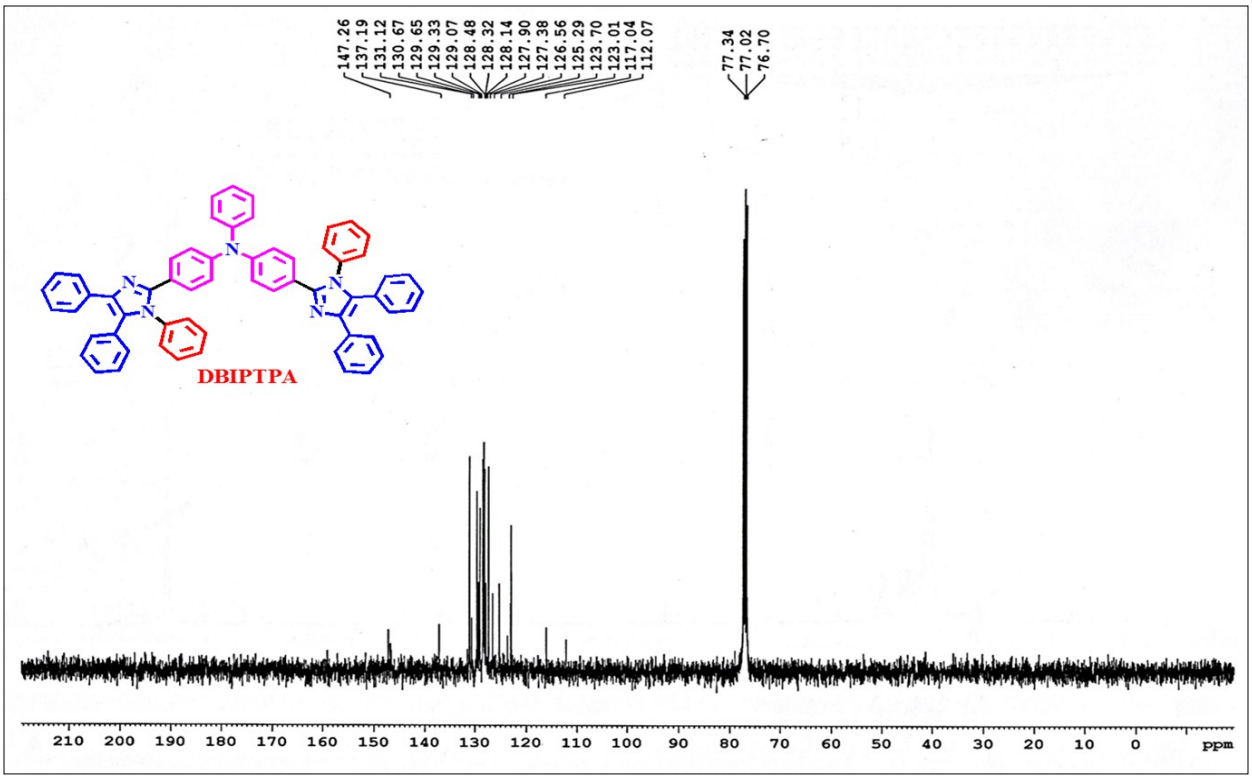

Fig. S4. The ^{13}C NMR spectra of the DBIPTPA

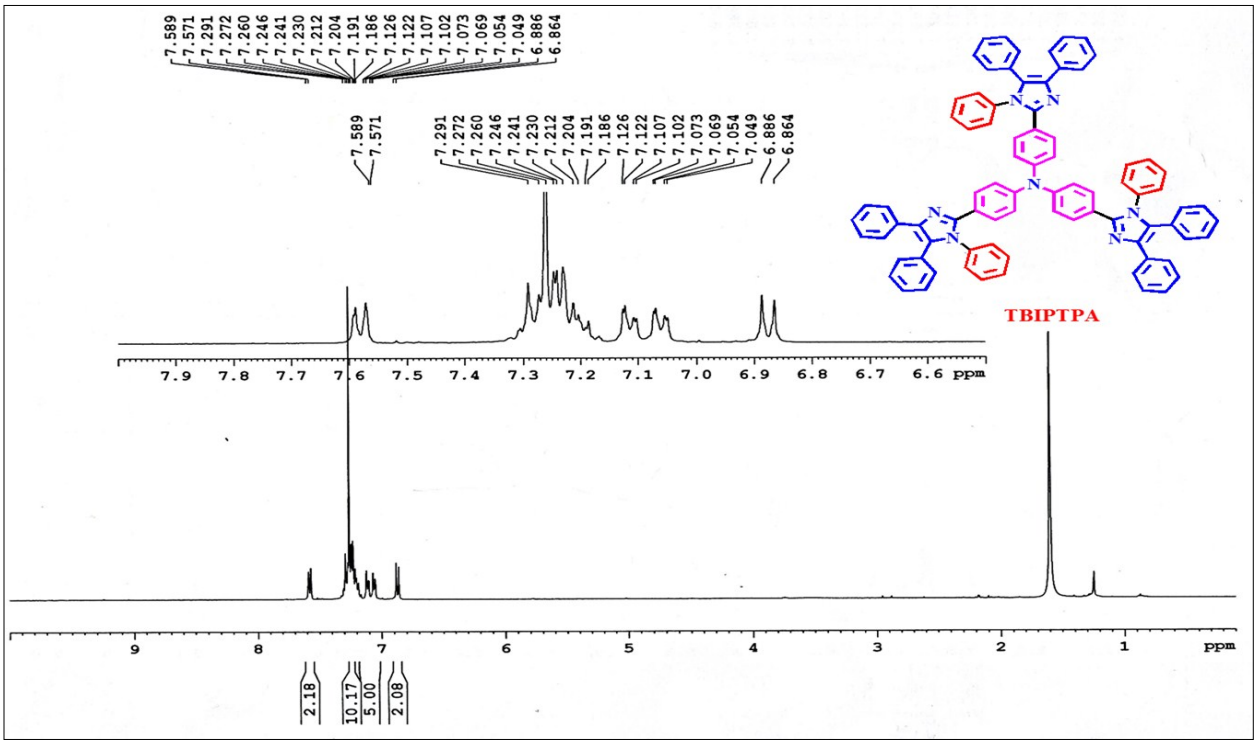

Fig. S5. The ^{1}H NMR spectra of the TBIPTPA.

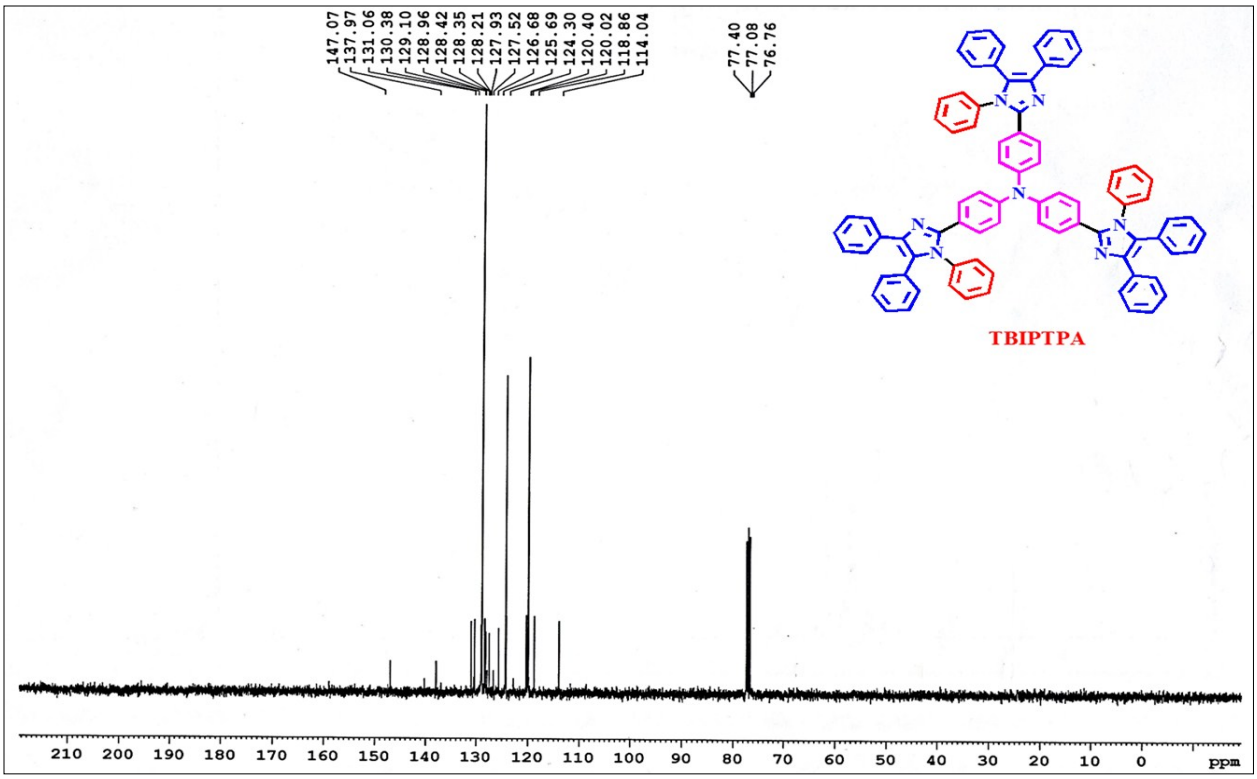

Fig. S6. The ^{13}C NMR spectra of the TBIPTPA

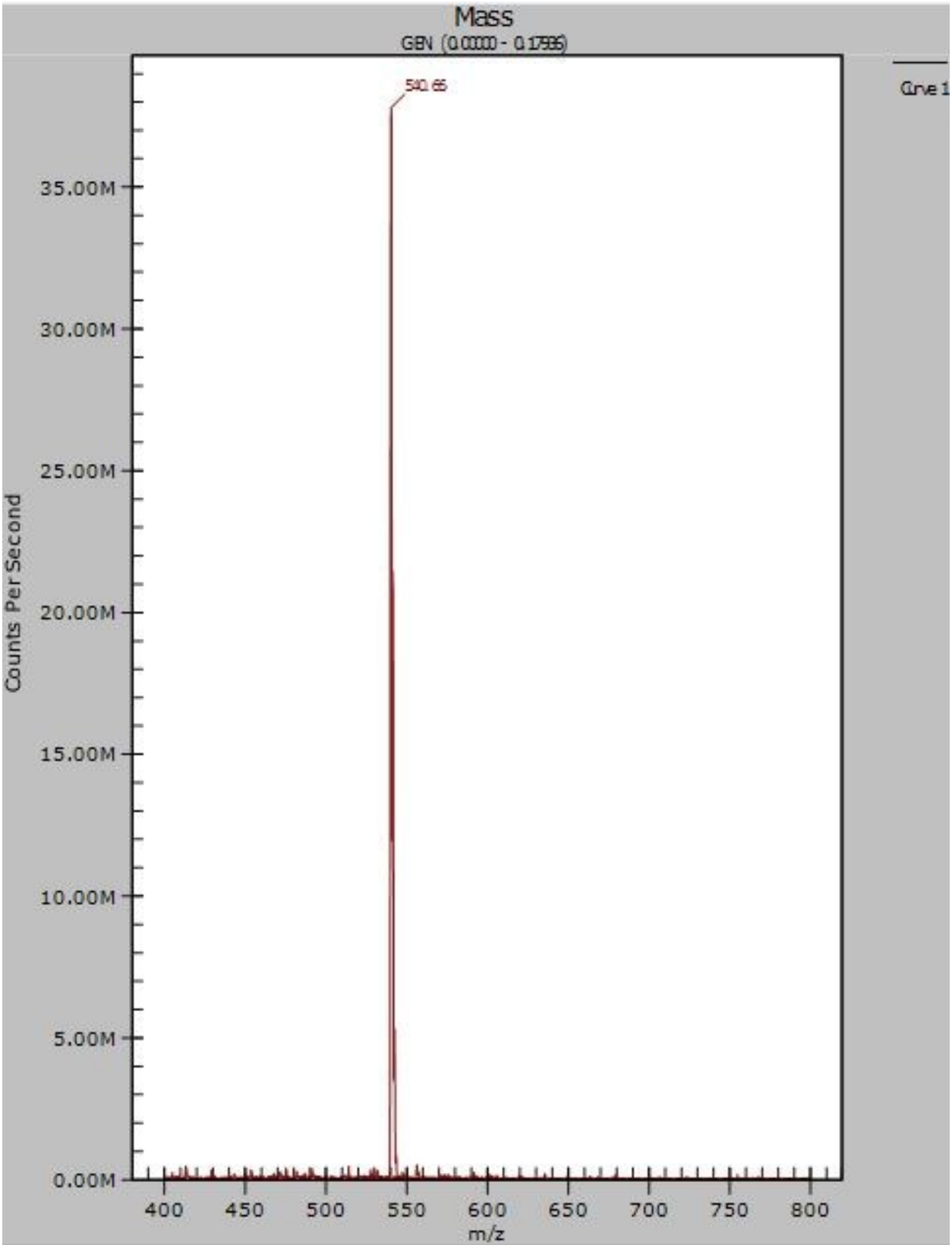

Fig. S7. The mass spectra of the BIPTPA.

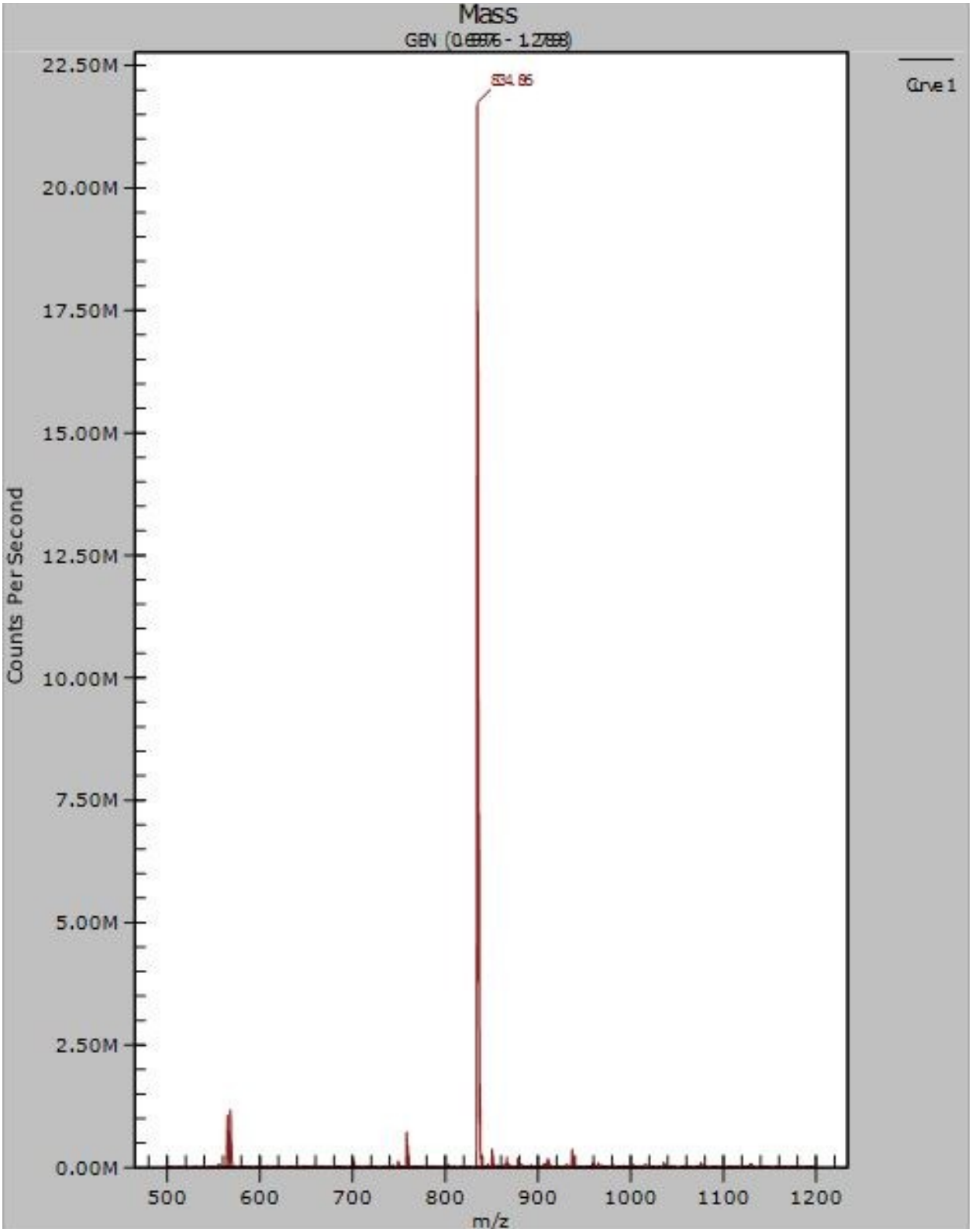

Fig. S8. The mass spectra of the DBIPTPA.

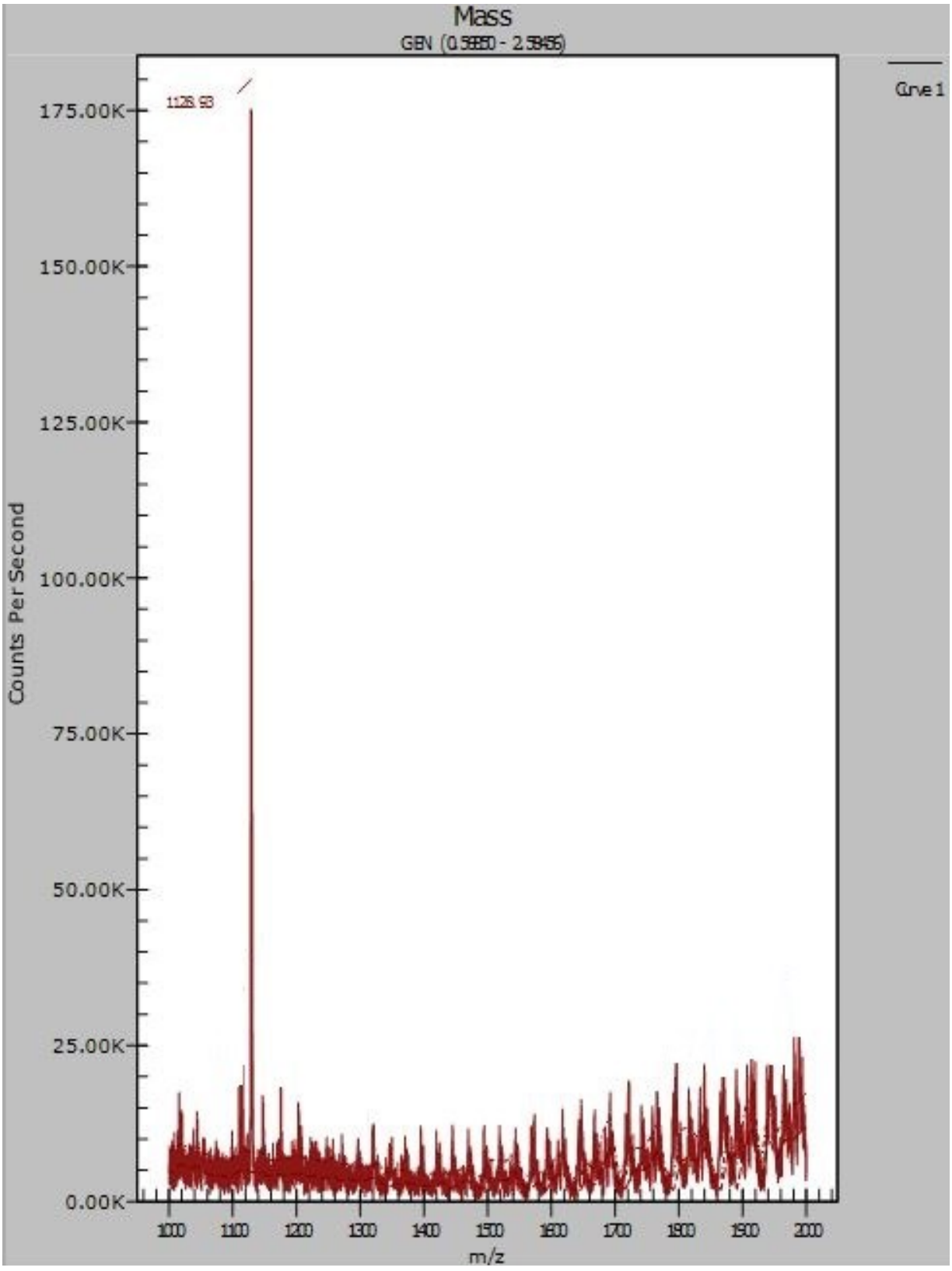

Fig. S9. The mass spectra of the TBIPTPA.

SI3. Fourier transform infrared (FTIR) Spectroscopy:

The FTIR spectrum of the BIPTPA, DBIPTPA, and TBIPTPA luminophores was measured from 500– 4000 cm^{-1} (Fig. S13) and the vibrational frequencies are provided in Table 1. The peak approximately 3040 cm^{-1} corresponds to Aromatic C–C, C=C stretching frequency [3, 4]. The frequency around 1600 cm^{-1} corresponds to the C=N function of imidazole. The peak at ~700 cm^{-1} is likely due to the aromatic C–H bending frequencies.

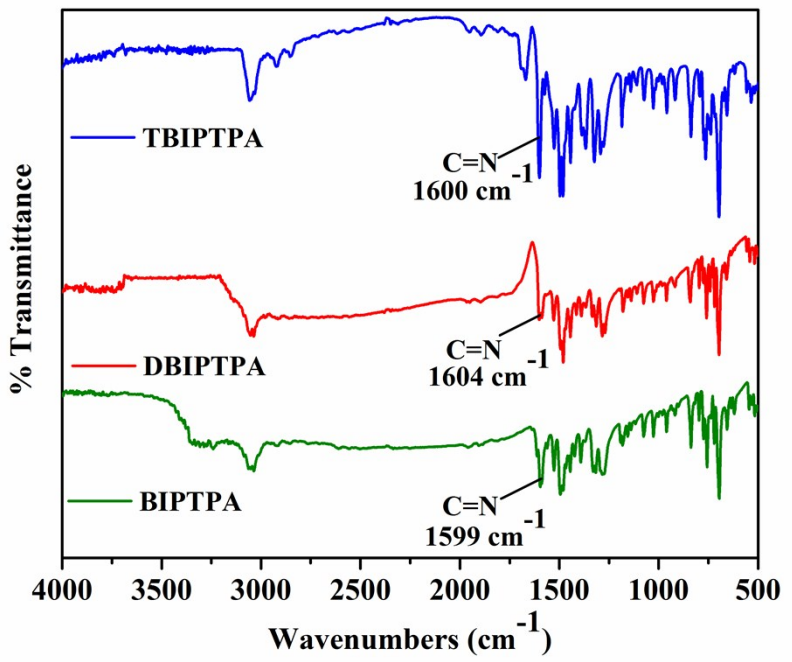

Fig. S10. FTIR spectra of the BIPTPA, DBIPTPA and TBIPTPA luminophores.

Table S1. The major FTIR bands [cm^{-1}] for BIPTPA, DBIPTPA, and TBIPTPA luminophores.

Bonding	BIPTPA	DBIPTPA	TBIPTPA
C=N	1599	1604	1600
Aromatic C-H, C–C, C=C stretching frequency.	3043, 1491, 1283, 1077	3046, 1481, 1441, 1281, 1071	3059, 1490, 1440, 1370, 1290,1180
C–H bending frequency	1017, 957, 756, 696	1021, 961, 842, 762, 701	1031, 961, 841, 771, 691

SI4 Photophysical properties of the luminophores

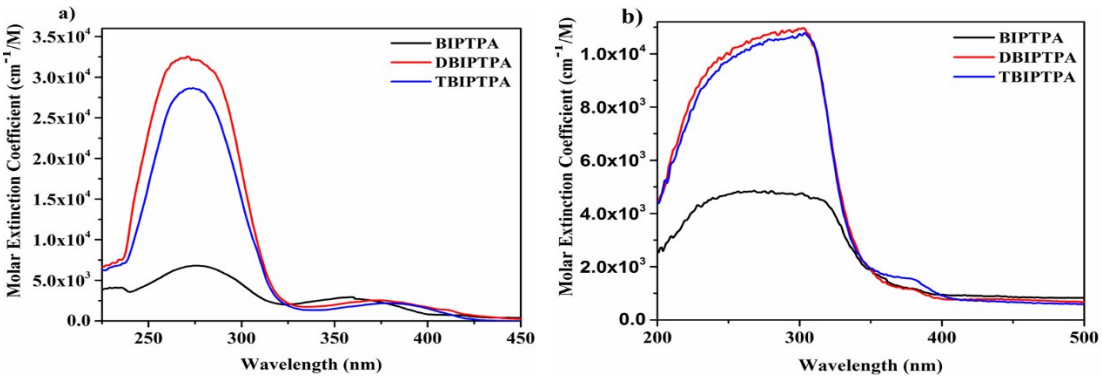

Fig. S11. Molar extinction coefficient vs. wavelength graphs of synthesized molecules in solution (a) and solid (b) states.

Table S2. Molar extinction coefficient (ε) data for all the luminophores.

Compounds	**Solution**		**Solid**	
	λ_{max} (nm)	**Molar extinction Coefficient (ε) cm^{-1}/M**	**λ_{max} (nm)**	**Molar extinction Coefficient (ε) cm^{-1}/M**
BIPTPA	276	6835.31	290	4815.78
	360	3024.46	381	1157.89
DBIPTPA	270	32495.82	290	10844.55
	370	2475.38	380	1117.43
TBIPTPA	273	28482.17	290	10605.35
	375	2230.71	382	1571.39

Table S3. The CIE chromaticity coordinates data for the luminophores.

Luminophores	**Solution-CIE coordinates**		**Solid-CIE coordinates**	
	x	**y**	**x**	**y**
BITPA	0.179	0.150	0.160	0.117
DBITPA	0.161	0.115	0.167	0.137
TBITPA	0.162	0.120	0.224	0.297

SI5. Quantum yield studies of luminophores in solution and solid states

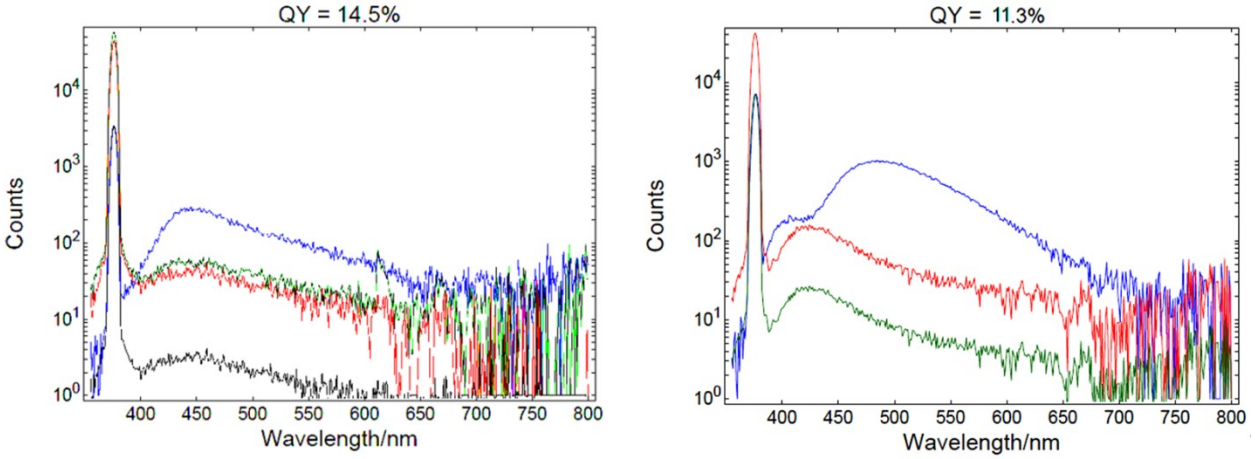

Fig. S12. The PLQY of BIPTPA luminophore in solution and solid states.

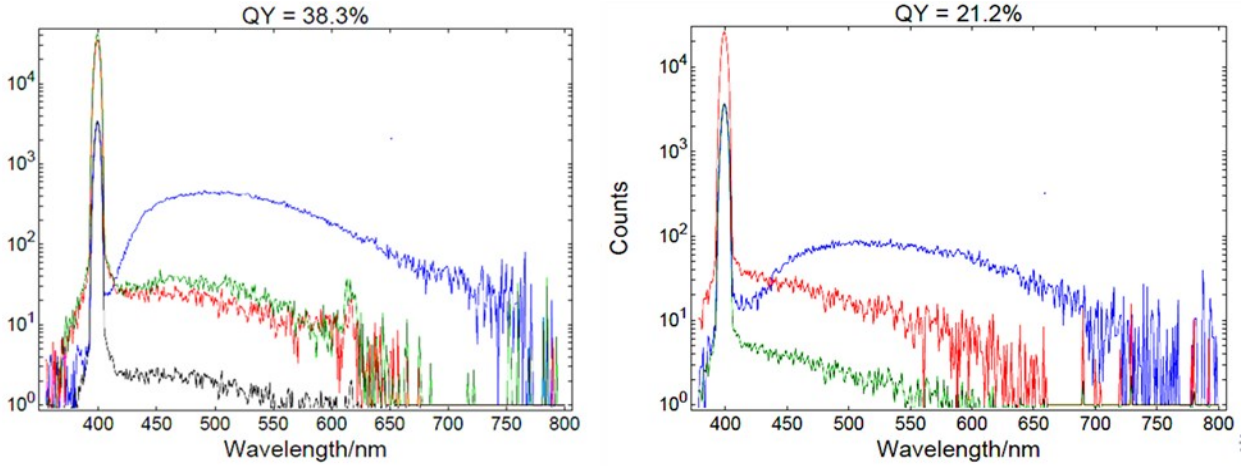

Fig. S13. The PLQY of DBIPTPA luminophore in solution and solid states.

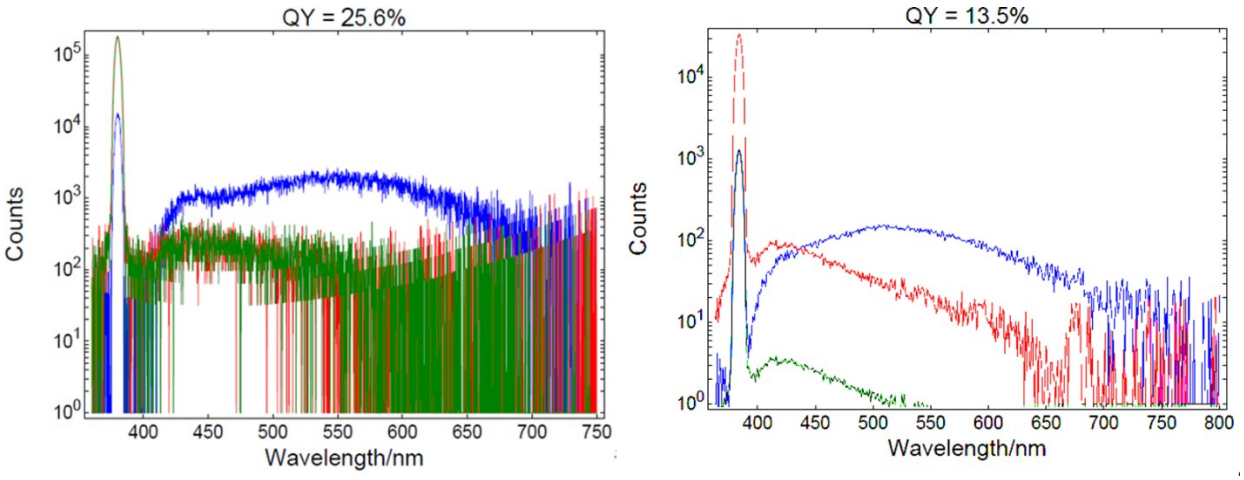

Fig. S14. The PLQY of TBIPTPA luminophore in solution and solid states.

SI6. The computed vertical transitions and their oscillator strengths (*f*) and configuration and atom coordinates of the luminophores.

Table S4. The computed vertical transitions and their oscillator strengths (*f*) and configuration of the luminophores.

Fluorophores	State	Energy (eV)	λ_{max} nm	*f*	Configuration
BIPTPA Singlet	Gas	3.5109	353.14	0.8196	HOMO→ LUMO (69.39%)
		3.6803	336.89	0.067	HOMO→ LUMO+1 (33.29%) HOMO→ LUMO+2 (60.71%)
Triplet	Gas	2.6916	460.63	-	HOMO-3→LUMO (10.21%) HOMO →LUMO (53.24%)
DBIPTPA Singlet	Gas	3.2779	378.25	1.0674	HOMO→ LUMO (69.53%)
		3.5662	347.66	0.0776	HOMO→ LUMO+1 (44.90%) HOMO→ LUMO+4 (24.98%)
		3.5791	346.41	0.1784	HOMO→ LUMO+1 (48.95%) HOMO→ LUMO+2 (36.77%) HOMO→ LUMO+5 (11.04%)
		3.668	337.94	0.1056	HOMO→ LUMO+3 (20.60%) HOMO→ LUMO+5 (63.78%)
		3.9421	314.51	0.1548	HOMO→ LUMO (66.66%)
Triplet	Gas	2.6006	476.74	-	HOMO → LUMO (61.92%)
TBIPTPA Singlet	Gas	3.2101	386.23	0.8042	HOMO→ LUMO (68.93%)
		3.5370	381.14	1.0082	HOMO→ LUMO+1 (69.13%)
		3.6507	339.61	0.0857	HOMO→ LUMO+5 (63.55%) HOMO→ LUMO+7 (14.02%)
Triplet	Gas	2.5919	478.35	-	HOMO-2→LUMO+1 (14.63%) HOMO→LUMO (46.33%) HOMO→LUMO+1 (38.36%)

Atom coordinates of the luminophores:

BIPTPA:

7	4.516276000	0.293748000	-0.094982000
6	5.250427000	-0.514727000	-1.006672000
6	4.873131000	-0.590556000	-2.357192000
6	6.366885000	-1.245747000	-0.569912000
6	5.593115000	-1.388507000	-3.244269000
1	4.016285000	-0.021553000	-2.703733000
6	7.091477000	-2.026538000	-1.468520000
1	6.661082000	-1.195776000	0.473660000
6	6.708241000	-2.107846000	-2.808900000
1	5.287286000	-1.434514000	-4.286290000
1	7.953368000	-2.585318000	-1.112957000
6	5.211315000	1.098681000	0.849872000
6	4.767647000	1.182649000	2.179533000
6	6.353931000	1.819635000	0.467218000
6	5.448257000	1.978657000	3.098900000
1	3.889055000	0.622876000	2.484163000
6	7.038545000	2.598224000	1.398362000
1	6.698961000	1.765200000	-0.560424000
6	6.589352000	2.687640000	2.717629000
1	5.090111000	2.032332000	4.123756000
1	7.920833000	3.149889000	1.084233000
6	3.098720000	0.298604000	-0.128427000
6	2.378513000	-0.883781000	-0.359152000

6	2.377118000	1.490257000	0.063305000
6	0.987657000	-0.877205000	-0.399005000
1	2.914330000	-1.814359000	-0.515608000
6	0.990194000	1.488581000	0.040315000
1	2.912968000	2.418897000	0.231182000
6	0.259953000	0.306142000	-0.187711000
1	0.474997000	-1.810444000	-0.597193000
1	0.442999000	2.414587000	0.178406000
6	-3.397304000	-0.050569000	-0.126663000
6	-3.183830000	1.289898000	-0.416568000
7	-2.119315000	-0.614701000	-0.022879000
7	-1.834459000	1.546225000	-0.472027000
6	-1.206694000	0.410738000	-0.229280000
6	-4.151771000	2.373724000	-0.665556000
6	-3.728714000	3.707616000	-0.527458000
6	-5.479464000	2.133131000	-1.058905000
6	-4.607899000	4.763076000	-0.756848000
1	-2.699165000	3.897807000	-0.243555000
6	-6.357614000	3.192133000	-1.285660000
1	-5.825068000	1.115263000	-1.202627000
6	-5.929291000	4.511950000	-1.133256000
1	-4.259539000	5.786536000	-0.641525000
1	-7.379458000	2.982694000	-1.592196000
1	-6.615554000	5.335609000	-1.312210000
6	-4.633262000	-0.814017000	0.148637000

6	-5.074340000	-1.842174000	-0.700328000
6	-5.406651000	-0.499931000	1.278851000
6	-6.248880000	-2.541609000	-0.422497000
1	-4.502547000	-2.079816000	-1.592276000
6	-6.583549000	-1.195137000	1.553082000
1	-5.077547000	0.297915000	1.938126000
6	-7.006423000	-2.220784000	0.705252000
1	-6.576049000	-3.332384000	-1.092448000
1	-7.168929000	-0.937432000	2.431709000
1	-7.922852000	-2.764055000	0.919749000
6	-1.852825000	-1.936897000	0.467633000
6	-1.896277000	-3.031592000	-0.399877000
6	-1.554233000	-2.121864000	1.819745000
6	-1.636773000	-4.312858000	0.087675000
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6	-1.292357000	-3.404648000	2.301235000
1	-1.526432000	-1.261584000	2.481222000
6	-1.333838000	-4.500918000	1.437687000
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1	7.121129000	3.301811000	3.438735000
1	7.271483000	-2.722775000	-3.505073000

DBIPTPA

7	0.099243000	3.136173000	-0.142313000

6	1.329553000	2.430610000	-0.162411000
6	1.492142000	1.289358000	-0.962358000
6	2.420775000	2.861350000	0.612753000
6	2.697650000	0.594874000	-0.979944000
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1	2.316429000	3.739744000	1.241539000
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6	-0.792829000	5.252778000	0.719673000
6	0.979774000	5.289549000	-0.927332000
6	-0.800386000	6.646221000	0.735581000
1	-1.473728000	4.693246000	1.353340000
6	0.977296000	6.682663000	-0.891000000
1	1.665245000	4.759785000	-1.581160000
6	0.086045000	7.370344000	-0.064548000
1	-1.495160000	7.167282000	1.389207000
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6	-1.309252000	1.265308000	0.594161000
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6	-2.514007000	0.570166000	0.563777000
1	-0.493262000	0.900621000	1.209702000

6	-3.405123000	2.188203000	-0.980599000
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6	4.480539000	-2.000823000	-0.825339000
6	3.821430000	-2.639766000	0.227397000
6	4.247404000	-2.395600000	-2.145480000
6	2.922014000	-3.671160000	-0.043853000
1	4.016285000	-2.322716000	1.247181000
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6	2.683792000	-4.066533000	-1.361412000
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1	3.164573000	-3.731648000	-3.437998000
1	1.982797000	-4.869730000	-1.570393000
7	5.405197000	-0.940464000	-0.540389000
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1	-8.921610000	1.270532000	-4.928445000
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6	-9.519750000	-3.252581000	2.341663000
1	-8.156026000	-4.900039000	2.061180000
1	-10.674647000	-1.433288000	2.441686000
1	-10.241566000	-3.839186000	2.903661000
6	8.612660000	0.521669000	0.481996000
6	8.786499000	1.639978000	1.316298000

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ТВІРТРА

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Reference:

[1] a) A. Becke, J. Chem. Phys. 98 (1993) 5648. b) C. Lee, W. Yang, R. G. Parr, Phys. Rev. B: Condens. Matter Mater.Phys. 37 (1998) 785–789.

[2] a) R. Bauernschmitt, R. Ahlrichs, Chem. Phys. Lett. 256 (1996) 454–464. b) G. Scalmani, M. J. Frisch, B. Mennucci, J. Tomasi, R. Cammi, V. Barone, J. Chem. Phys. 124 (2006) 094107.

[3] J. Jayabharathi, P. Ramanathan, V. Thanikachalam, C. Karunakaran, New J. Chem. 39 (2015) 3801.

[4] T. Jairam, H. Ulla, M.N. Satyanarayan, V. Sivakumar, Journal of Luminescence. 194 (2018) 600.