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Efficient near ultraviolet emissive (CIEy < 0.06) Organic Light-Emitting Diodes based on Phenanthroimidazole-Alkyl spacer-Carbazole fluorophores: Experimental and Theoretical investigation

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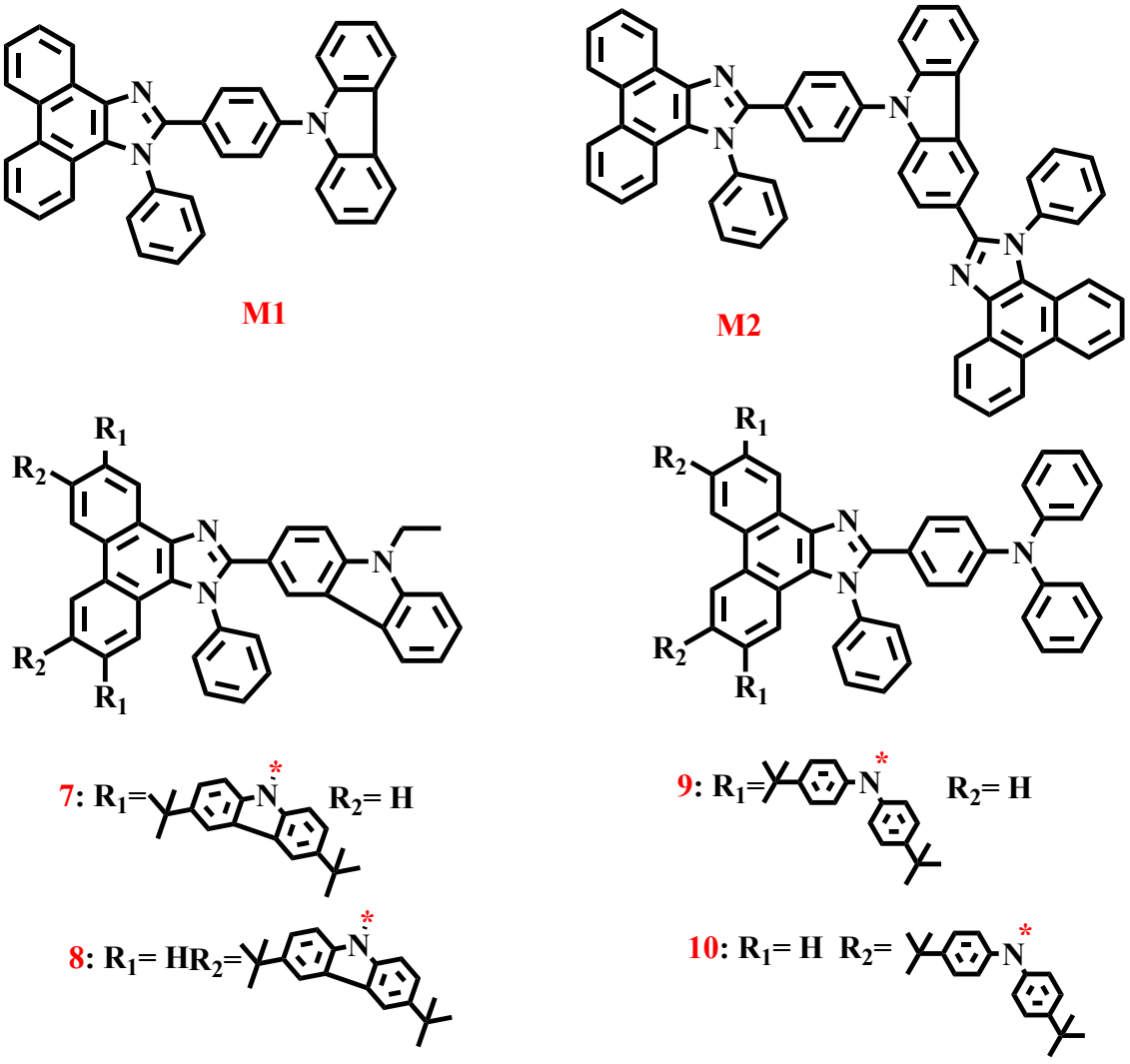

Fig. S1. Reported purely organic small-molecules for blue-OLED.

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, ^{13}C-NMR,

and ^{19}F-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 FTIR spectra were recorded on a Shimadzu IR Affinity-1S spectrophotometer. Elemental analysis was obtained using Elementary Analysis System, Germany/Vario EL spectrometer. The mass spectra were recorded by LC–MS (Perkin–Elmer, USA/Flexer SQ 300 M). The absorption spectrum of the target fluorophores 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 quantum yield of the fluorophores was calculated by using equation (SI1)

$$\Phi = \frac{L_0(\lambda) - L_i(\lambda)}{L_0(\lambda)} \qquad \text{(SI1)}$$

$$\eta = \frac{E_i(\lambda) - (1 - \Phi)E_0(\lambda)}{E_0(\lambda)\Phi}$$

Where, $L_0(\lambda)$ is the integrated excitation profile (sample is directly excited by the incident beam) and $L_i(\lambda)$ are the integrated excitation profile attained from the empty integrated sphere. $E_0(\lambda)$ is the integrated luminescence of thin film and powder caused by direct excitation and $E_i(\lambda)$ is indirect illumination from the sphere, respectively. The CIE color coordinates were calculated by using PL emission data (MATLAB software). The electrochemical properties of the fluorophores 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

Bu4NClO4 was used as the supporting electrolyte, and the scan rate was maintained as 100 mV s^{-1}. The optimize structures and HOMO-LUMO energy levels of the fluorophores were calculated by using DFT calculation with B3LYP/6-31G (d, p) basis set. After confirming the ground state geometry of the fluorophores, we were vertically excited the fluorophores to get the first excited state using time-dependent density functional theory (TD-DFT).

SI1.2. Device fabrication and measurement:

The device fabrication involved both spin coating and thermal evaporation (under less than 10^{-5} Torr). First, spin coating of an aqueous solution of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS) at 4,000 rpm for 20 s to form a thin film of hole injection layer on pre-treated Indium tin oxide (ITO) anode. The emissive layer (EML) solution was prepared by dissolving the 4,4′-Bis(N-carbazolyl)-1,1′-biphenyl (CBP) host and guest dopants in tetrahydrofuran (THF) at 50 ^{0}C for 30 min under stirring. The EML solution was spin coated at 2,500 rpm for 20s under a nitrogen atmosphere. The electron transporting layer TPBi, the electron injection layer LiF, and the cathode Al by thermal evaporation.

The device characteristics; luminance, color coordinates (CIE coordinates), and electroluminescence (EL) spectrum were measured by Photo Research PR-655 spectra scan. The current-voltage (I-V) characteristics were measured by Keithley 2,400. The device area was 0.9 mm^2 and all the devices measured in the forward bias.

Synthesis of 4-(4-bromobutoxy) benzaldehyde (Intermediate-1): In the two necks round bottom flask 4-hydroxybenzaldehyde (2.5 gr, 1 eq) and acetonitrile 30 ml were taken. To this reaction mixture potassium carbonate (5.69 gr, 2 eq) was added. Then after 10 minutes, 1,4-dibromo butane (4.42 gr, 1 eq) was added to the reaction mixture. The resulting reaction mixture was stirred for 48 hr at 85 ^{0}C under a nitrogen atmosphere. The reaction was monitored by thin

layer chromatography (ethyl-acetate (EtOAc) in pet ether 1:9) for the completion of the reaction. After completion of the reaction, the reaction mixture poured in a minimum amount of water and extracted with an ethyl acetate solvent. The solvent was evaporated to get the yellow color crude compound. The obtained crude compound was purified by column chromatography by using silica gel (100-200 mesh), eluent ethyl-acetate in pet ether (1:9). Yield 80 %, the semisolid compound obtained. ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 9.85 (s, 1H), 7.82-7.79 (m, 2H), 6.95 (t, 2H), 4.06 (t, 2H), 3.47 (t, 2H), 2.04-2.00 (m, 2H), 1.99-1.88 (m, 2H), ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm): 190.82, 163.90, 132.01, 129.92, 114.74, 114.72, 68.02, 33.29, 29.29, 27.69.

Synthesis of 4-(4-(9H-carbazol-9-yl)butoxy) benzaldehyde (Intermediate-2): The mixture of 4-(4-bromobutoxy) benzaldehyde (3 gr, 1 eq), 9H-carbazole (1.94 gr, 1 eq) and tetrahydrofuran (THF) (25 ml) was taken in 100 ml two neck round bottom flask. Than potassium hydroxide (1.96 gr, 3 eq) base was added. Followed by added tetrabutylammonium bromide (0.15 gr, 0.04 eq) water (5 ml) solution to the reaction mixture. The resulting reaction mixture was refluxed 18 hr. The completion of the reaction was monitored by thin layer chromatography (ethyl-acetate (EtOAc) in pet-ether 1:9). After completion of the reaction, the reaction mixture poured in a minimum amount of water and extracted with an ethyl acetate solvent. The solvent was evaporated to get the yellow color crude compound. The obtained crude compound was purified by column chromatography by using silica gel (100-200 mesh), eluent ethyl-acetate in pet-ether (1:9). Yield 50 %, the pale yellow color compound obtained. ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 9.86 (s, 1H), 8.12 (d, 2H), 7.79 (t, 2H), 7.50-7.41 (m, 4H), 7.25 (t, 2H), 6.92 (d, 2H), 4.41 (t, 2H), 3.98 (t, 2H), 2.13-2.06 (m, 2H), 1.90-1.83 (m, 2H), ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm): 190.89, 163.89, 140.34, 132.03, 129.89, 125.72, 122.90, 120.48, 114.67, 108.61, 67.84, 42. 64, 26.86, 25.79.

General procedure for the synthesis of PI derivatives: A mixture of intermediate-2 (0.50 gr, 1 eq), 9,10-phenanthrenequinine (0.30 gr, 1 eq), amine (0.17 gr, 1.3 eq) and ammonium acetate (1.16 gr, 10 eq) and acetic acid (30 ml) were refluxed for 12 hr, under nitrogen in an oil bath. After completion of reaction, the mixture was cooled and poured minimum amount of water. The corresponding reaction mixture was neutralize with dilute ammonium hydroxide solution. The resultant mixture was extracted with dichloromethane (DCM) followed by purification by column chromatography on silica gel (100-200 mesh) with ethyl acetate/petroleum ether (2:8) as the eluent.

2-(4-(4-(9H-carbazol-9-yl)butoxy)phenyl)-1-phenyl-1H-phenanthro[9,10-d]imidazole (PIPOCz): Yield: 65%, pale yellow color, ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 8.88 (d, J=7.2 Hz, 1H), 8.78 (d, J=8 Hz, 1H), 8.72 (d, J=8.4 Hz, 1H), 8.13 (d, J=7.6 Hz, 2H)7.77-7.66 (m, 1H), 7.66-7.59 (m, 4H), 7.53-7.42 (m, 8H), 7.29-7.24 (m, 4H), 7.18 (d, J=7.6 Hz, 1H), 6.78 (d, J=8.8 Hz, 2H), 4.42 (t, J=6.8 Hz, 2H), 3.94 (t, J=6.0 Hz, 2H), 2.13-2.06 (m, 2H), 1.89-1.82 (m, 2H), ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm): 159.29, 140.34, 130.83, 130.14, 129.72, 129.16, 127.24, 126.22, 125.68, 125.51, 124.71, 124.09, 123.10, 122.85, 122.71, 120.77, 120.42, 118.86, 114.13, 108.62, 67.42, 42.71, 26.92, 25.86. FTIR (KBr, υ/cm^{-1}): 3429, 3060, 2944, 1611, 1450, 1381, 1328, 1251, 1182, 1029, 830, 745, 722,531. CHNS Elemental Analysis: Anal. Calc. for $C_{43}H_{33}N_3O$: C, 84.98; H, 5.47; N, 6.91; Found: C, 85.07; H, 5.68; N, 6.99 %. EI-MS: m/z exp. (calc.). 607.74 found 626.97 $[M+H_2O]^+$

2-(4-(4-(9H-carbazol-9-yl)butoxy)phenyl)-1-p-tolyl-1H-phenanthro[9,10-d]imidazole (PIPTOCz): Yield: 68%, pale brown color, ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 8.88 (d, J=7.2 Hz, 1H), 8.78 (d, J=8.4 Hz, 1H), 8.72 (d, J=8.4 Hz, 1H), 8.13 (d, J=7.6 Hz, 2H), 7.75 (t, J=7.2 Hz, 1H), 7.66 (t, J=7.2 Hz, 1H), 7.53-7.39 (m, 11H), 7.31-7.23 (m, 4H), 6.79 (d, J=8.8 Hz,

2H), 4.41 (t, J=6.8 Hz, 2H), 3.94 (t, J=6.0 Hz, 2H), 2.55 (s, 3H), 2.09-2.07 (m, 2H), 1.87-1.83 (m, 2H), ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm): 159.29, 140.35, 139.80, 136.08, 133.94, 130.84, 130.77, 129.47, 129.08, 128.79, 128.19, 127.97, 127.26, 127.16, 126.24, 125.69, 125.48, 124.71, 124.05, 123.13, 122.99, 122.86, 122.67, 120.83, 120.43, 120.04, 118.87, 114.12, 108.65, 67.41, 42.70, 26.92, 25.85, 24.51. FTIR (KBr, υ/cm^{-1}): 3442, 3051, 2944, 1611, 1512, 1466, 1381, 1328, 1251, 1190, 1024, 837, 753, 715, 534. CHNS Elemental Analysis: Anal. Calc. for $C_{44}H_{35}N_3O$: C, 84.99; H, 5.67; N, 6.76; Found: C, 85.23; H, 5.89; N, 6.92 %. EI-MS: m/z exp. (calc.). 621.77 found 641.21 $[M+H_2O]^+$.

2-(4-(4-(9H-carbazol-9-yl)butoxy)phenyl)-1-(4-tert-butylphenyl)-1H-phenanthro[9,10-d]imidazole (PITBOCz): Yield: 70%, brown color, ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 8.91 (d, J=8 Hz, 1H), 8.78 (d, J=8.4 Hz, 1H), 8.72 (d, J=8.0 Hz, 1H), 8.14 (d, J=8.0 Hz, 2H), 7.77 (t, J=7.2 Hz, 1H), 7.68 (t, J=7.2 Hz, 1H), 7.65-7.59 (m, 2H), 7.53-7.41 (m, 9H), 7.30-7.20 (m, 4H), 6.77 (d, J=9.2 Hz, 2H), 4.40 (t, J=7.2 Hz, 2H), 3.92 (t, J=6.0 Hz, 2H), 2.12-2.05 (m, 2H), 1.87-1.83 (m, 2H), 1.48 (s, 9H), ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm): 159.25,153.12, 151.04, 140.36, 137.21, 136.08, 130.80, 129.07, 128.57, 128.18, 128.06, 127.22, 127.01, 126.22, 125.70, 125.45, 124.64, 124.05, 123.16, 123.12, 122.88, 122.72, 120.84, 120.44, 118.88, 114.07, 108.65, 67.41, 42.70, 35.03, 31.44, 26.95, 25.87. FTIR (KBr, υ/cm^{-1}): 3435, 3044, 2952, 1611, 1466, 1381, 1328, 1251, 1182, 1029, 830, 753, 722, 523. CHNS Elemental Analysis: Anal. Calc. for $C_{47}H_{41}N_3O$: C, 85.03; H, 6.23; N, 6.33; Found: C, 85.29; H, 6.47; N, 6.43 %. EI-MS: m/z exp. (calc.). 663.85 found 683.20 $[M+H_2O]^+$.

2-(4-(4-(9H-carbazol-9-yl)butoxy)phenyl)-1-(9,9-diethyl-9H-fluoren-2-yl)-1H-phenanthro [9,10-d]imidazole (PIFOCz): Yield: 72% , white color, ^{1}H-NMR (400 MHz, $CDCl_3$, TMS, δ ppm): 8.88 (d, J=7.2 Hz, 1H), 8.77 (d, J=8.4 Hz, 1H), 8.71 (d, J=8.0 Hz, 1H), 8.09 (d, J=8.0 Hz,

2H), 7.86 (d, J=8.0 Hz, 1H), 7.82-7.80 (m, 1H), 7. 75 (t, J=7.2 Hz, 1H), 7.67-7.63 (m, 1H), 7.56 (d, J=8.8 Hz, 2H), 7.50-7.49 (m, 1H), 7.47-7.34 (m, 11H), 7.23-7.16 (m, 3H), 6.72 (d, J=8.8 Hz, 2H), 4.33 (t, J=7.2 Hz, 2H), 3.86 (d, J=3.6 Hz, 2H), 2.08-1.99 (m, 6H), 1.80 (d, J=8.8 Hz, 2H), 0.43 (t, J=7.2 Hz, 3H), 0.27 (t, J=7.2 Hz, 3H). ^{13}C-NMR (100 MHz, $CDCl_3$, TMS, δ ppm):159.29, 151.93, 150.22, 143.07, 140.32, 140.22, 137.46, 137.23, 130.83, 129.09, 128.17, 127.74, 127.28, 127.25, 126.08, 125.66, 125.47, 124.73, 124.09, 123.80, 123.13, 123.05, 122.74, 121.08, 120.99, 120.40, 120.32, 118.84, 114.07, 108.60, 67.41, 56.66, 42.67, 32.97, 32.79, 26.89, 25.82, 8.41, 8.29. FTIR (KBr, υ/cm^{-1}): 3435, 3044, 2960, 2868, 1611, 1466, 1381, 1320, 1251, 1190, 1036, 837, 753, 722, 561. CHNS Elemental Analysis: Anal. Calc. for $C_{54}H_{45}N_3O$: C, 86.25; H, 6.03; N, 5.59; Found: C, 87.62; H, 6.34; N, 5.71 %. EI-MS: m/z exp. (calc.). 751.95 found 771.79 $[M+H_2O]^+$.

SI2. Fourier transform infrared (FTIR) Spectroscopy:

The room temperature FTIR spectra of the fluorophores were recorded at the spectral window of 400 to 4000 cm^{-1} and the same is shown in Fig. S2, the corresponding observed major frequency of functional group is summarised in Table S1. The frequency at 1611 cm^{-1} corresponds to the C=N functional group of the imidazole moiety. The peak around 3400 cm^{-1} corresponds to ≥ C–H in all the fluorophores.[1] The frequency around 3050 cm^{-1} corresponds to the aromatic C-H stretch. The stretching frequency around 2900 cm^{-1} corresponds to the alkyl C-H functional group. The frequency around 1250 cm^{-1} is corresponding to the C-N function of the imidazole. The frequency in the range of 500 to 900 cm^{-1} corresponds to the aromatic C-H bending frequency.

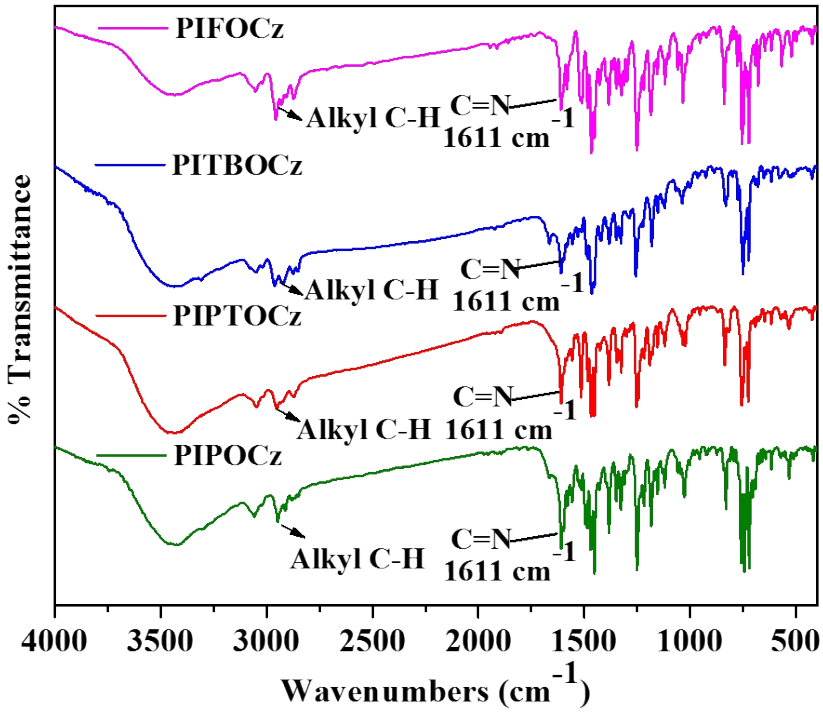

Fig. S2. Fourier transform infrared spectra of the PI derivatives.

Table S1. The major FTIR bands [cm^{-1}] for all the fluorophores.

Bonding	PIPOCz	PIPTOCz	PITBOCz	PIFOCz
C=N stretch	1611	1611	1611	1611
NH–CH	3429	3442	3435	3435
Aromatic C-H, C-C, C=C, stretching frequency	3060, 1450, 1381, 1328, 1182	3051, 1512, 1466, 1381, 1328, 1190	3044, 1466, 1381, 1328, 1182	3044,1466, 1381, 1320, 1190
Alkyl C-H stretch	2944	2944	2952	2960, 2868
C-N stretch	1251	1251	1251	1251
C-O stretch	1029	1024	1029	1036
C–H bending frequency	830, 745, 722, 531	837, 753, 715, 534	830, 753, 722, 523	837, 753, 722, 561

SI3. NMR spectra (^{1}H, ^{13}C, and ^{19}F) spectra of PI derivatives

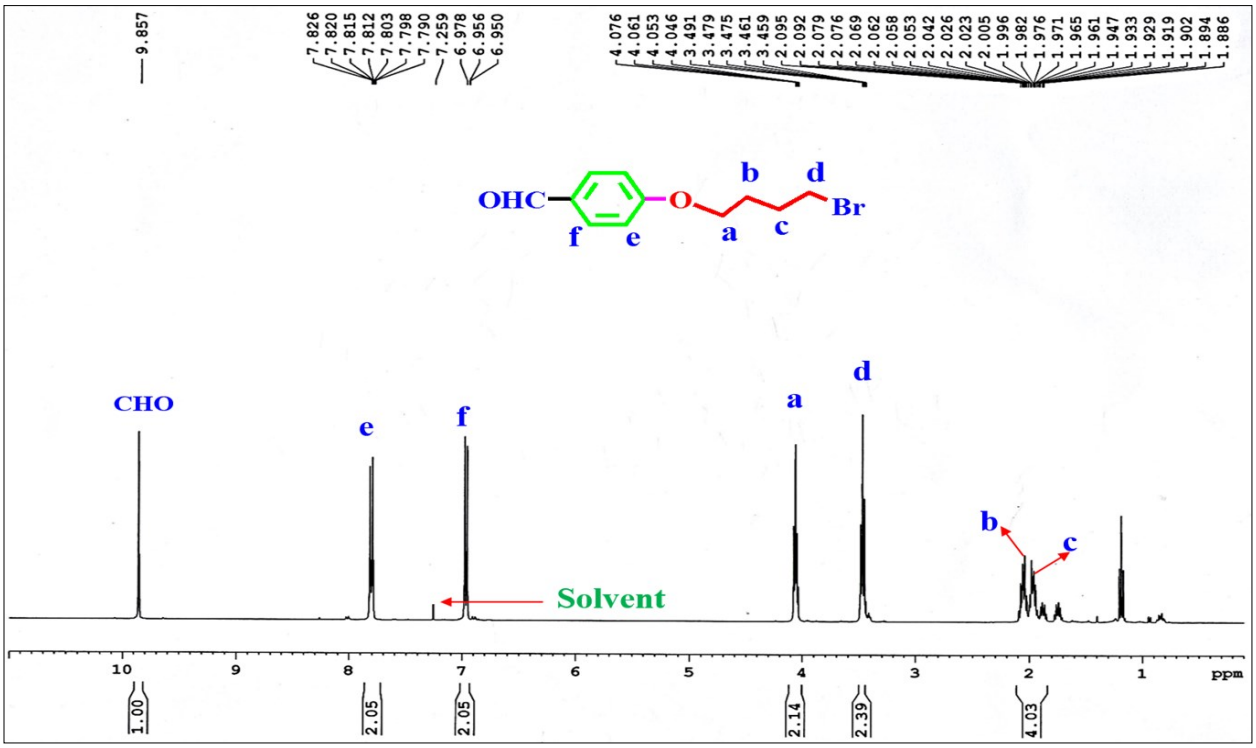

Fig. S3. The ^{1}H NMR spectra of the Intermediate-1.

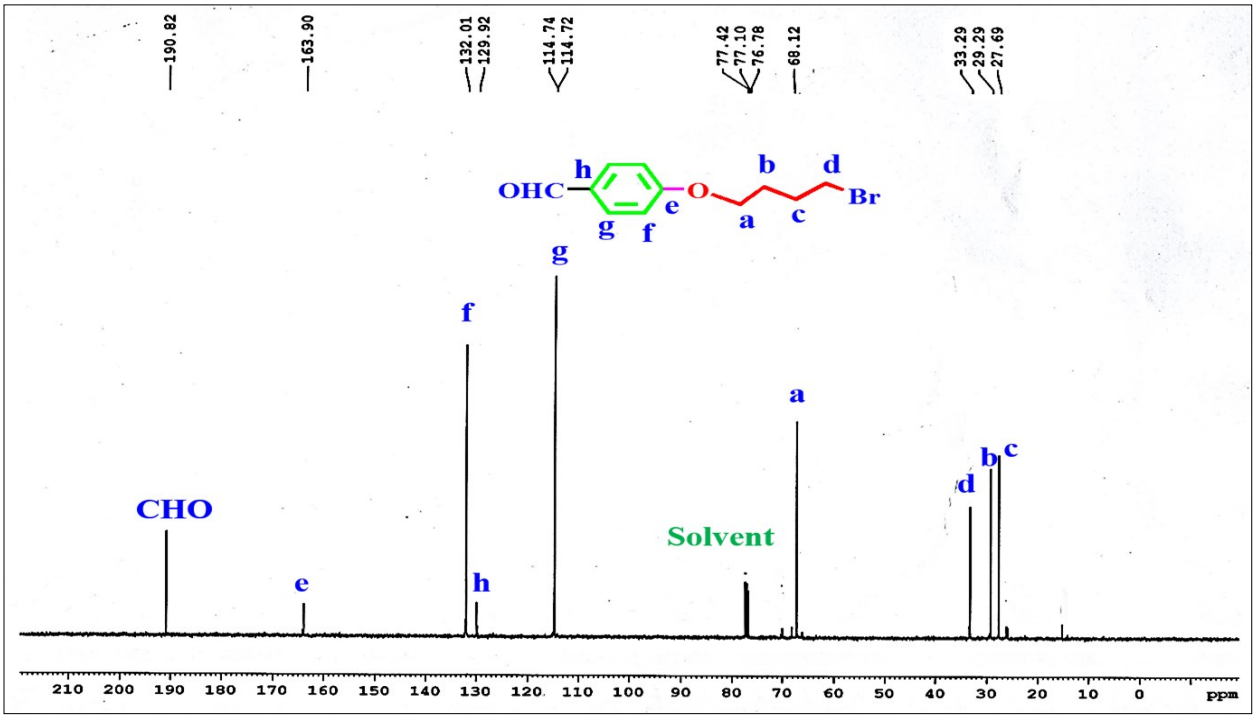

Fig. S4. The ^{13}C NMR spectra of the Intermediate-1.

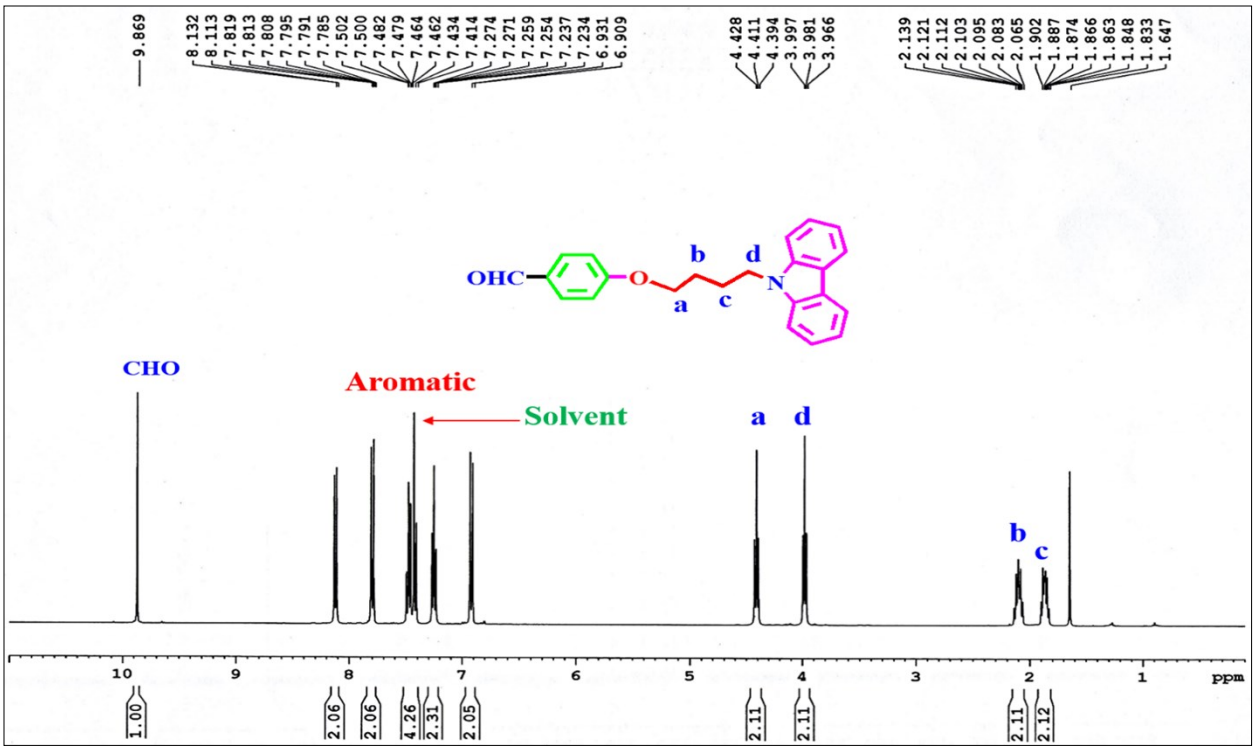

Fig. S5. The [1]H NMR spectra of the Intermediate-2.

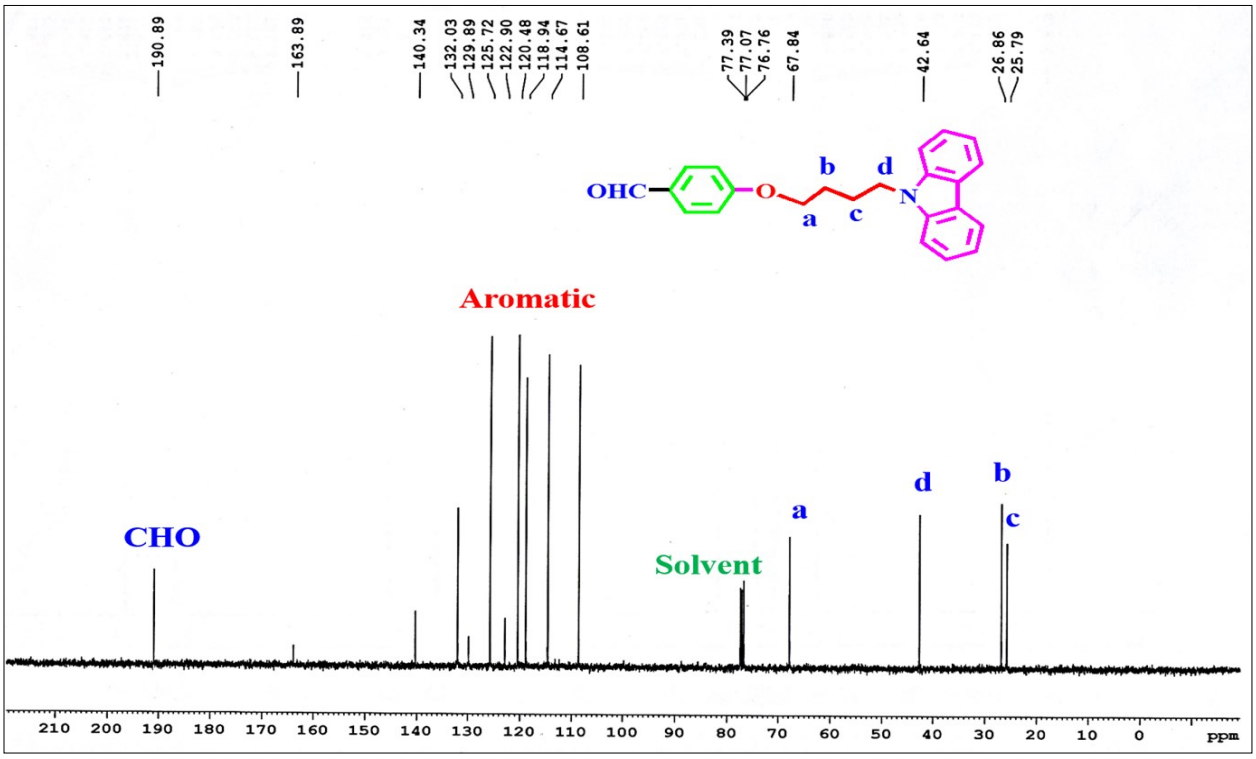

Fig. S6. The [13]C NMR spectra of the Intermediate-2.

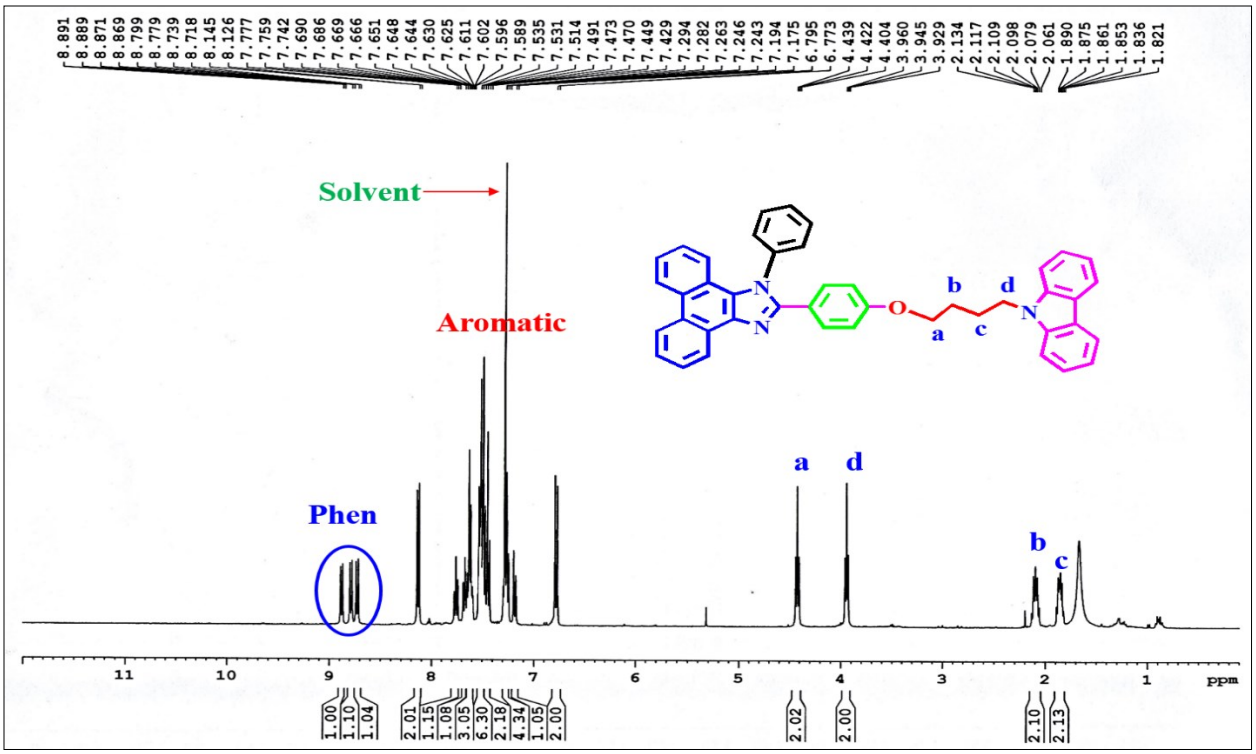

Fig. S7. The ^{1}H NMR spectra of the PIPOCz.

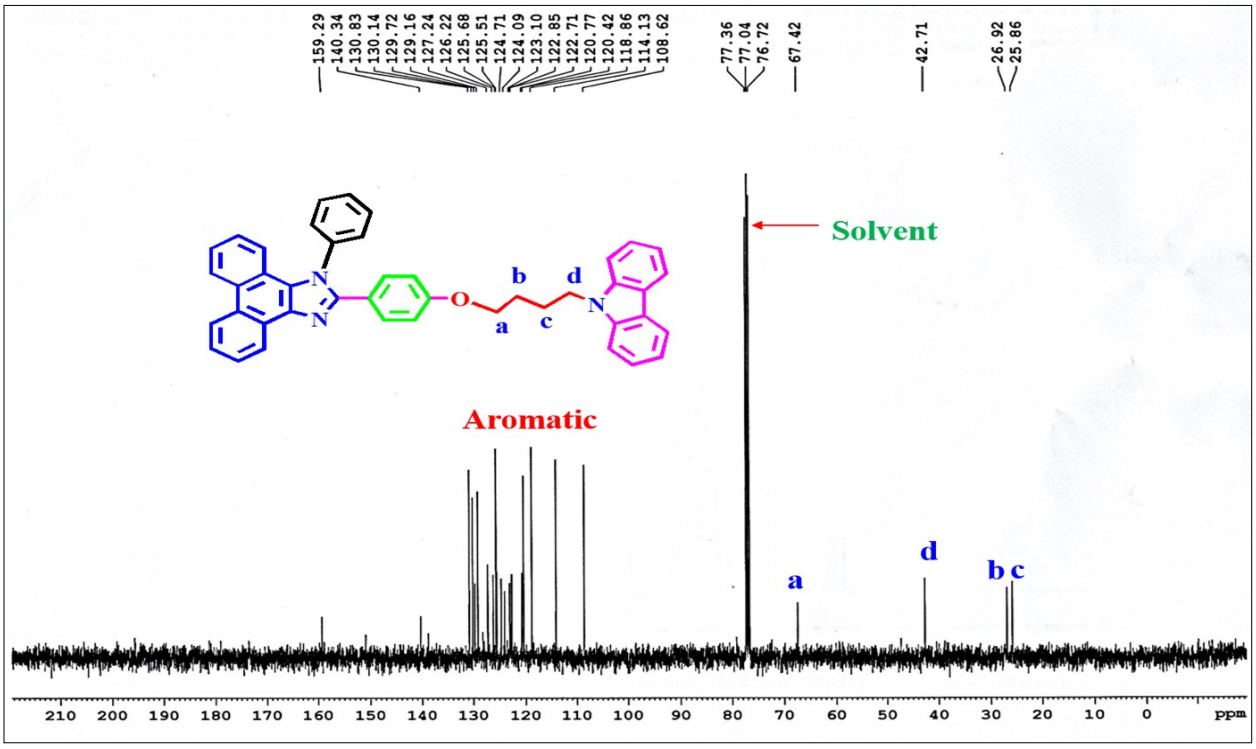

Fig. S8. The ^{13}C NMR spectra of the PIPOCz

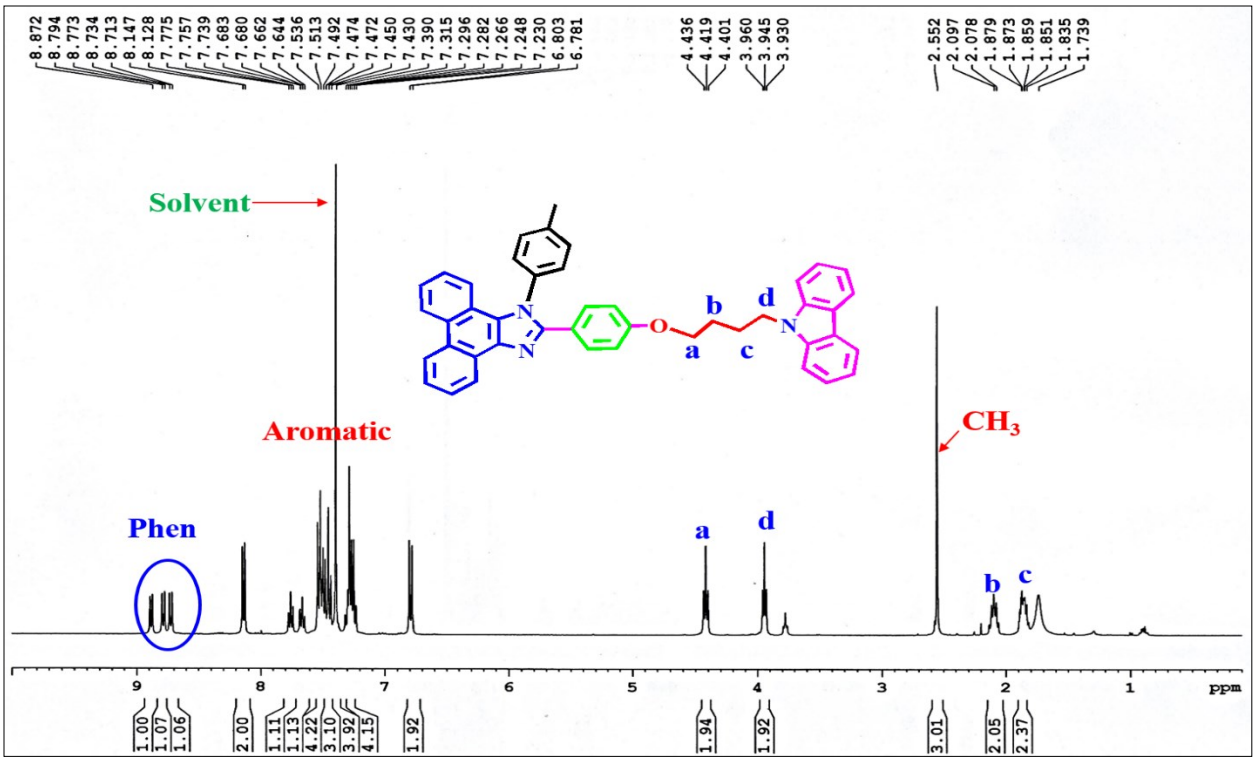

Fig. S9. The ^{1}H NMR spectra of the PIPTOCz.

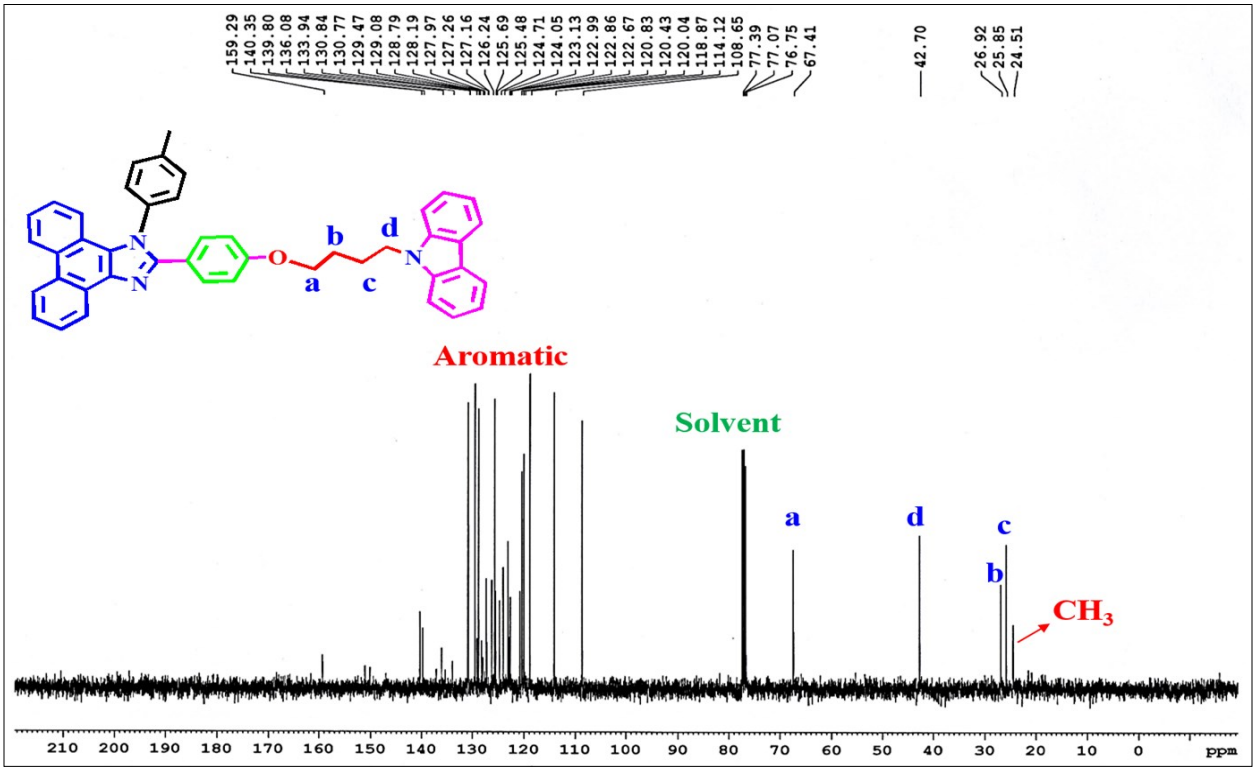

Fig. S10. The ^{13}C NMR spectra of the PIPTOCz

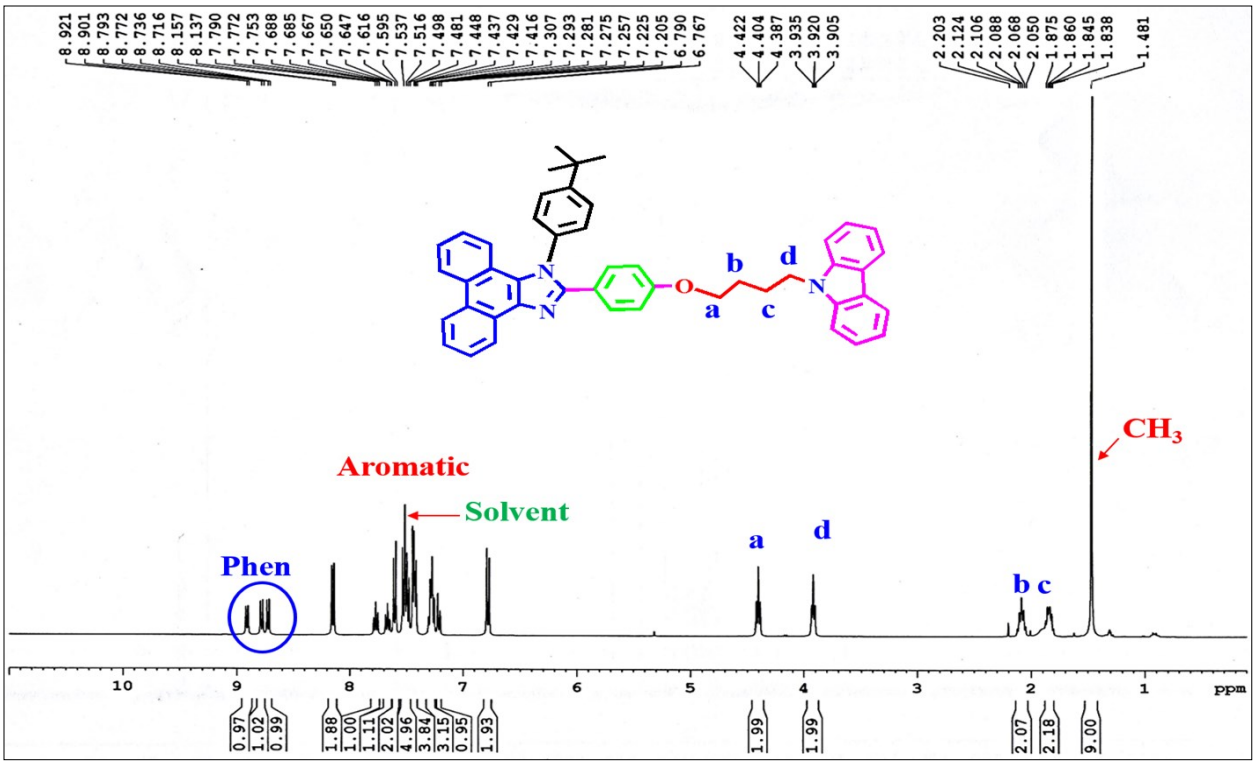

Fig. S11. The ^{1}H NMR spectra of the PITBOCz.

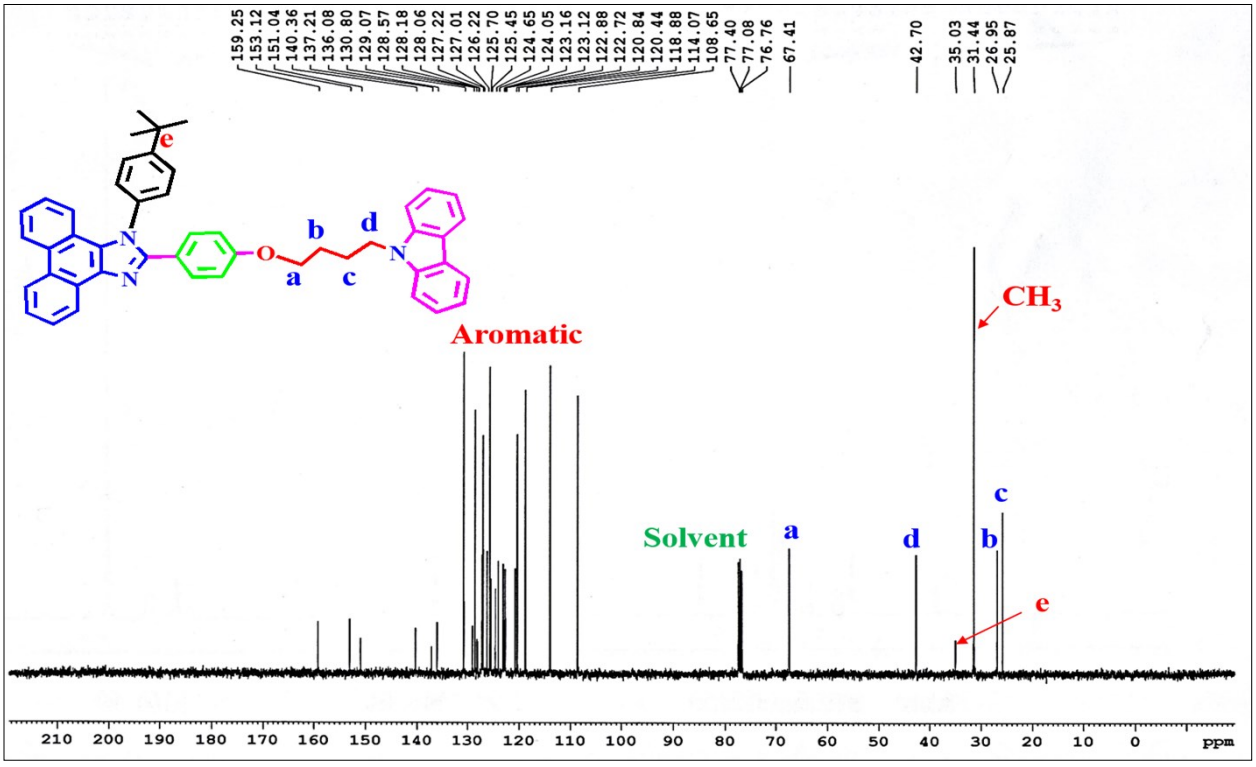

Fig. S12. The ^{13}C NMR spectra of the PITBOCz

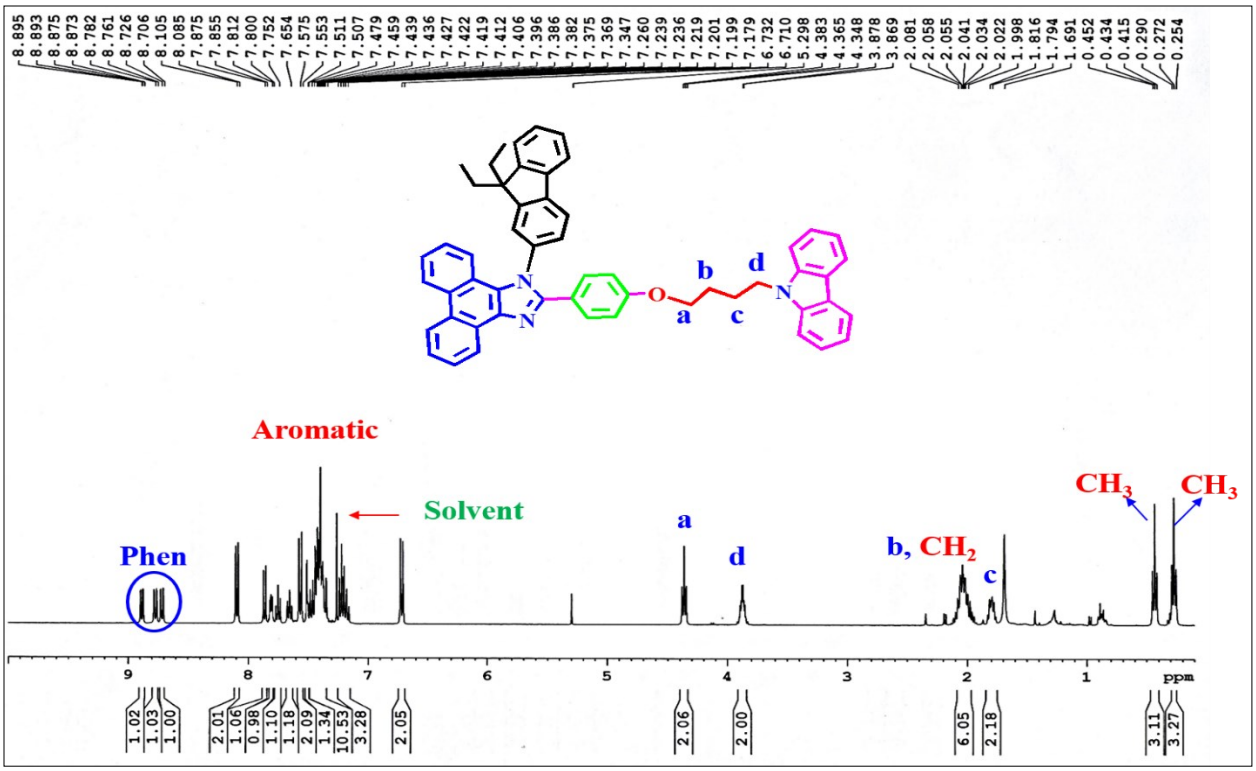

Fig. S13. The ^{1}H NMR spectra of the PIFOCz

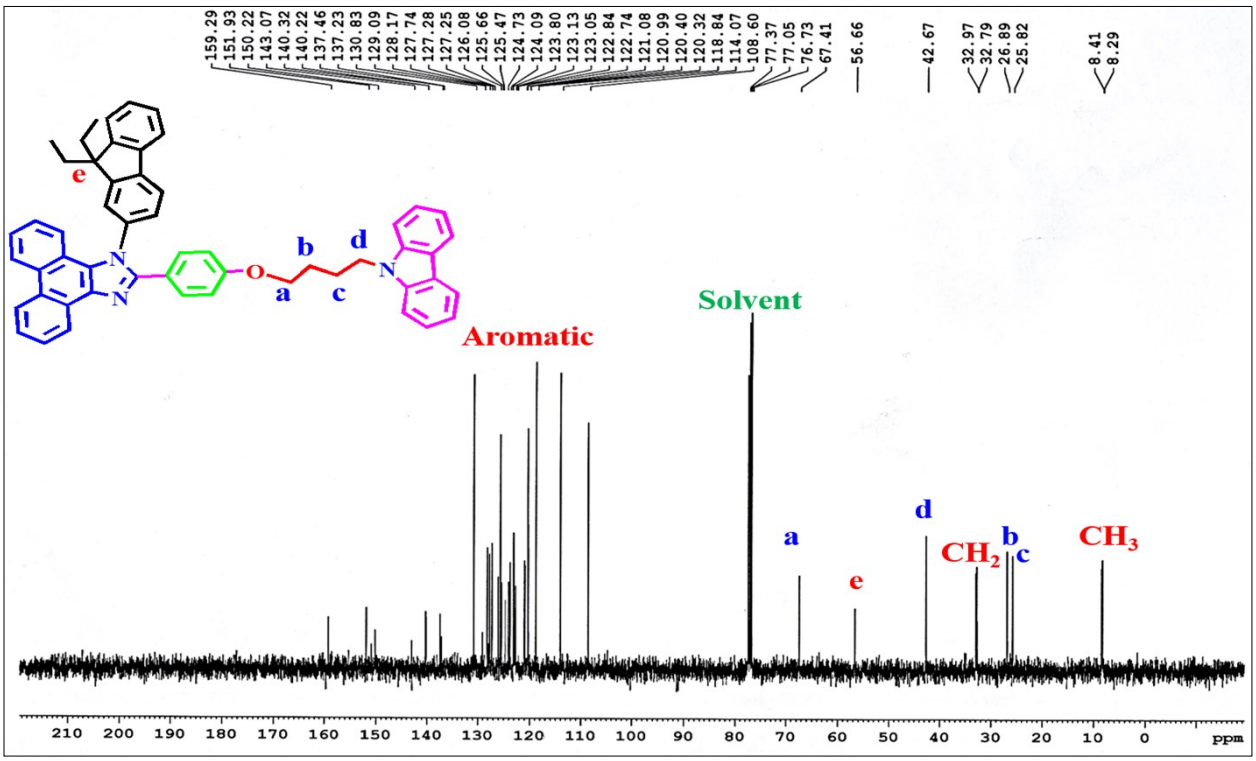

Fig. S14. The ^{13}C NMR spectra of the PIFOCz

SI4. Mass spectra of PI derivatives.

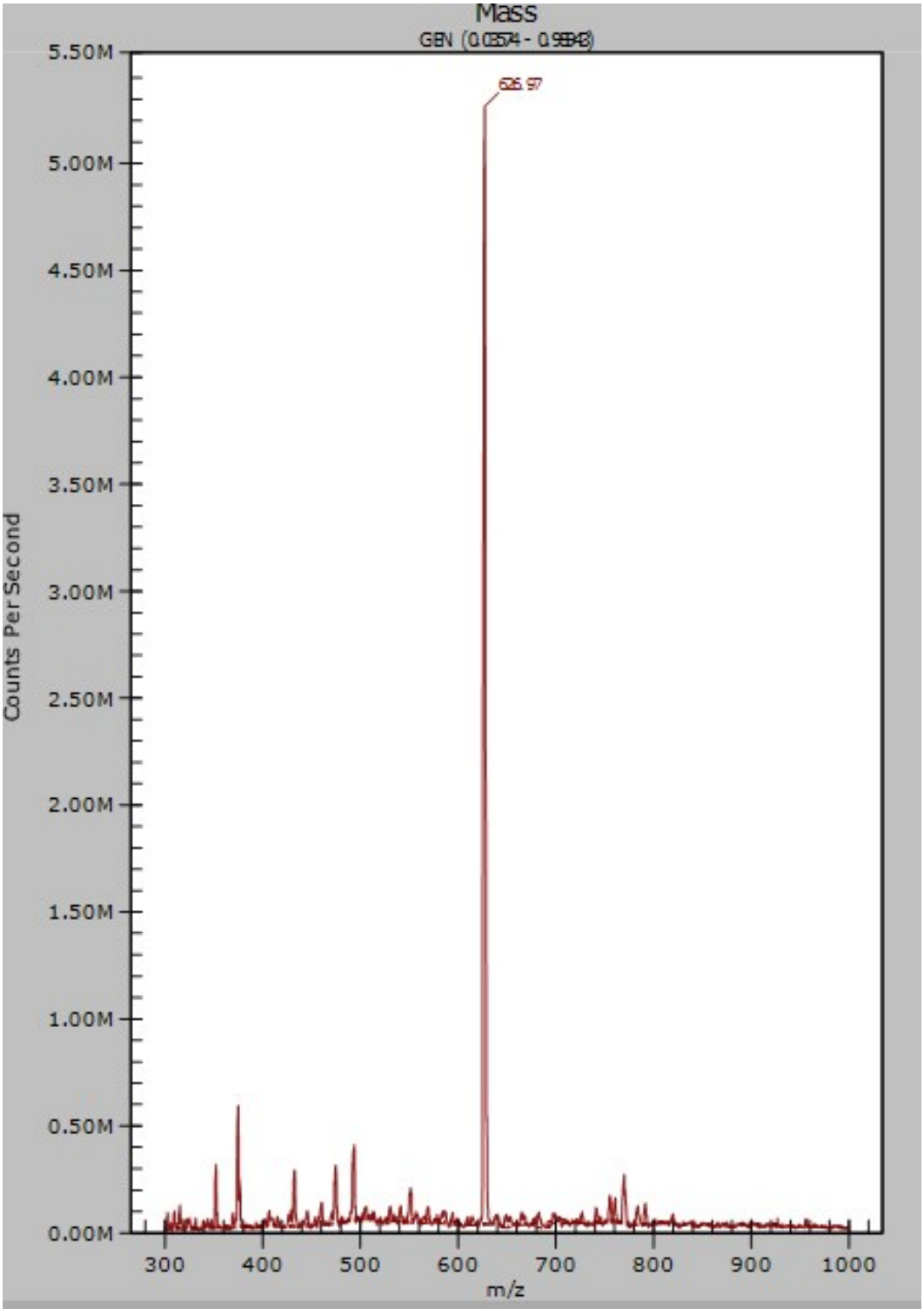

Fig. S15. Mass spectra of the PIPOCz.

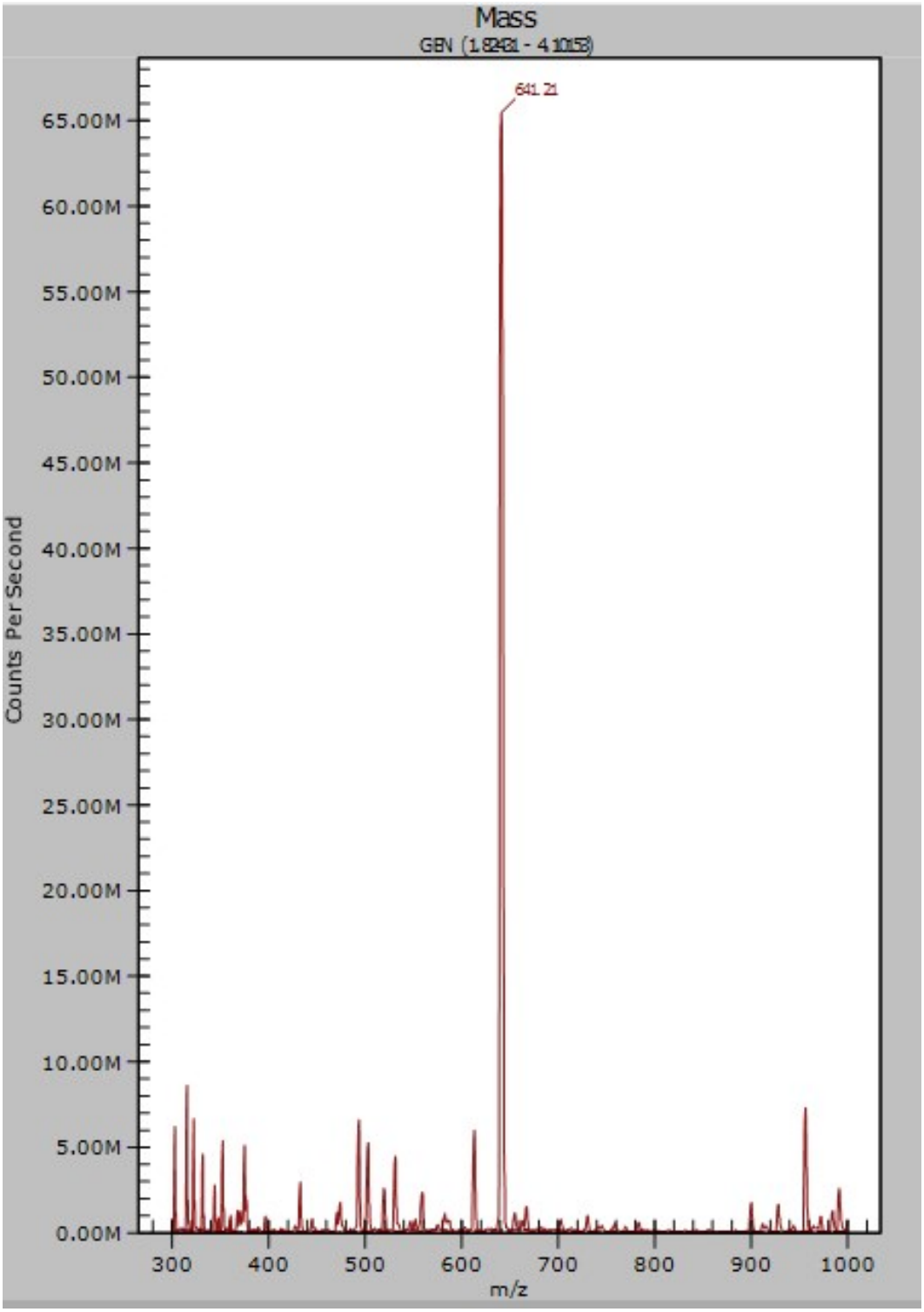

Fig. S16. Mass spectra of the PIPTOCz.

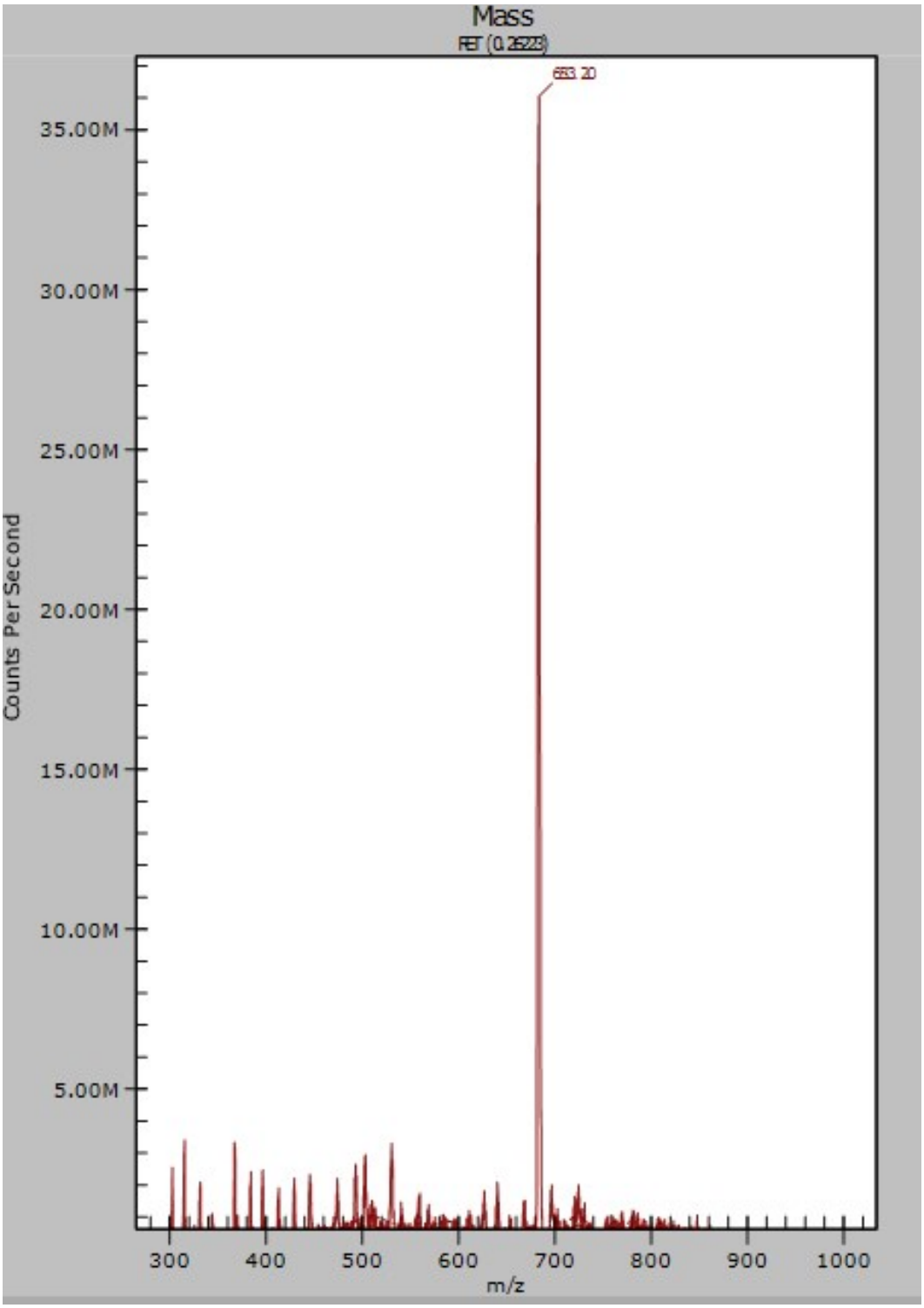

Fig. S17. Mass spectra of the PITBOCz.

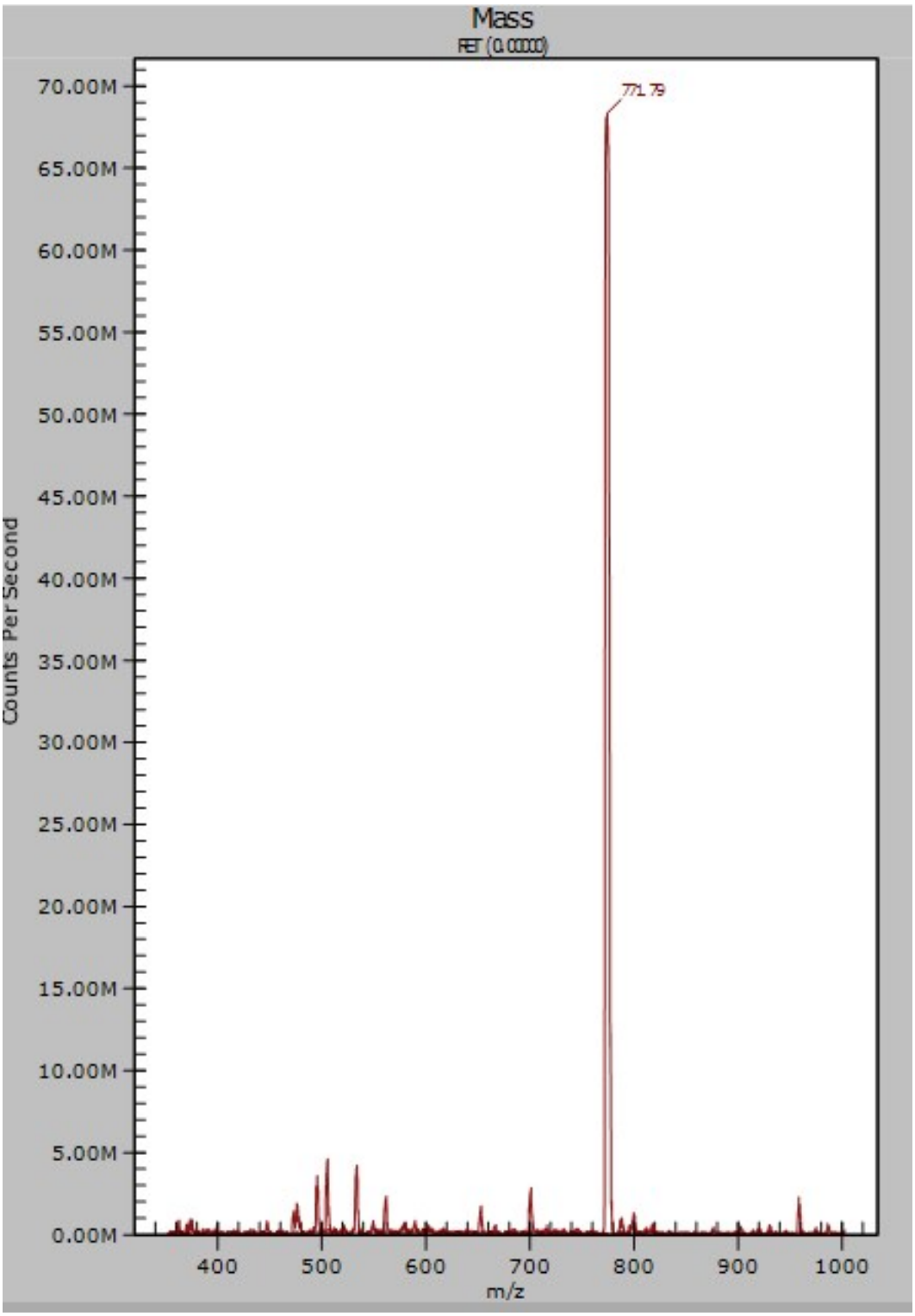

Fig. S18. Mass spectra of the PIFOCz.

SI5. Photophysical properties of PI derivatives

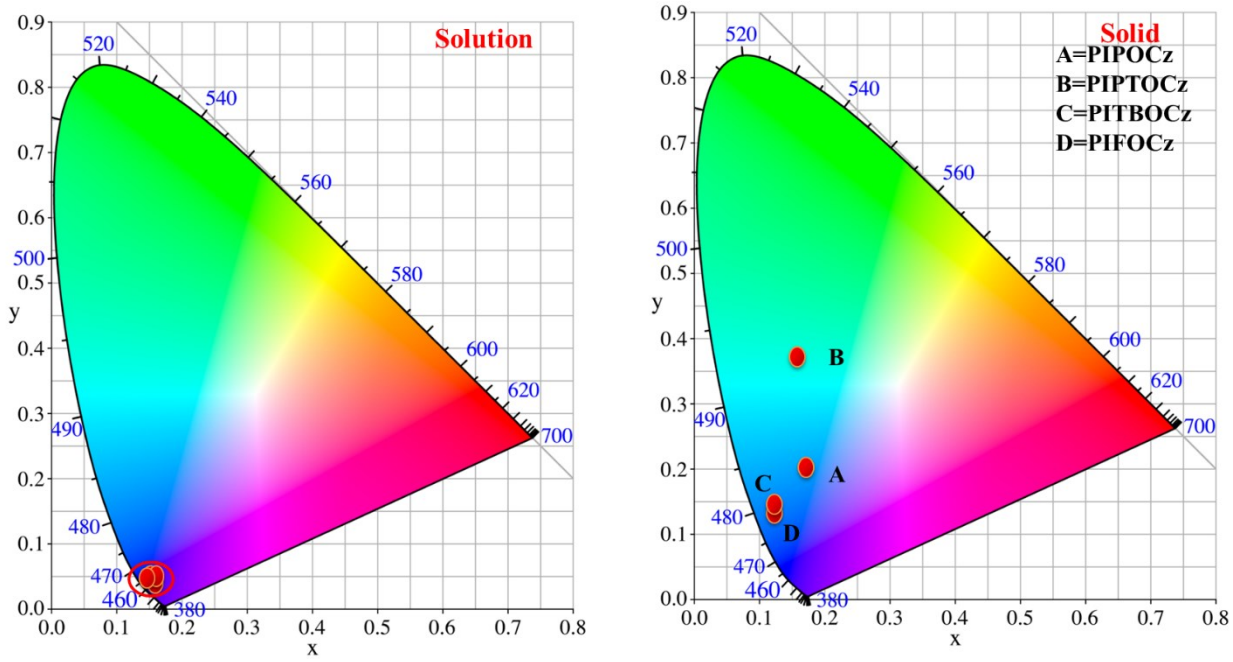

Fig. S19. The CIE chromaticity diagram of the fluorophores in solutions and solid phase.

Table S2. The CIE chromaticity coordinates data for the fluorophores.

Fluorophores	CIE color coordinates			
	Solution		Solid	
	x	y	x	y
PIPOCz	0.158	0.059	0.200	0.224
PIPTOCz	0.157	0.058	0.268	0.390
PITBOCz	0.158	0.061	0.169	0.127
PIFOCz	0.158	0.050	0.166	0.128

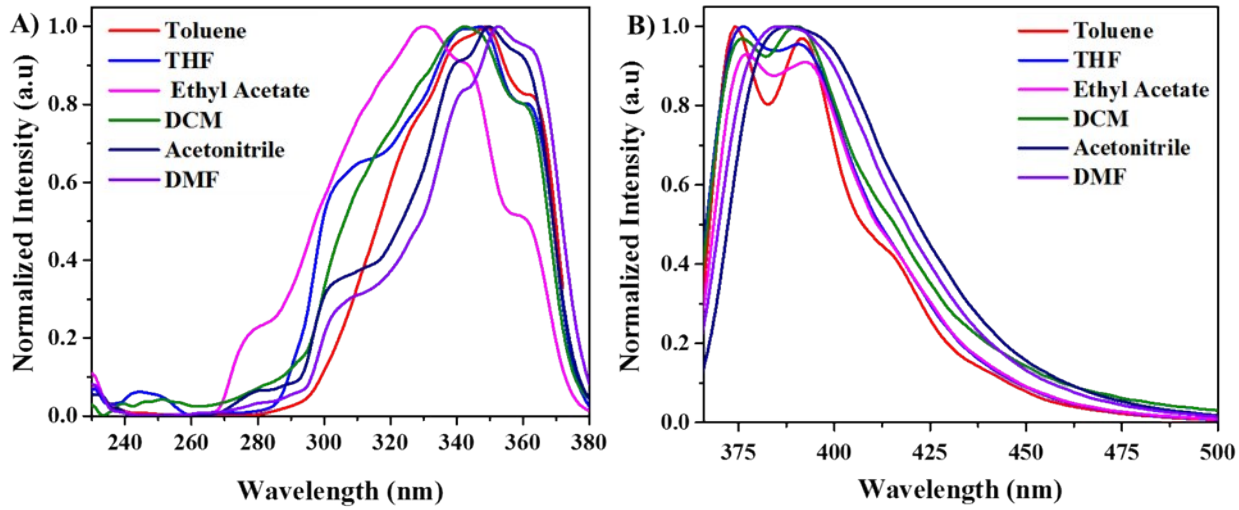

Fig. S20. (A) Excitation and (B) emission spectra of PIPOCz in different solvents.

SI6. Quantum yield studies of PI derivatives in solution and solid state

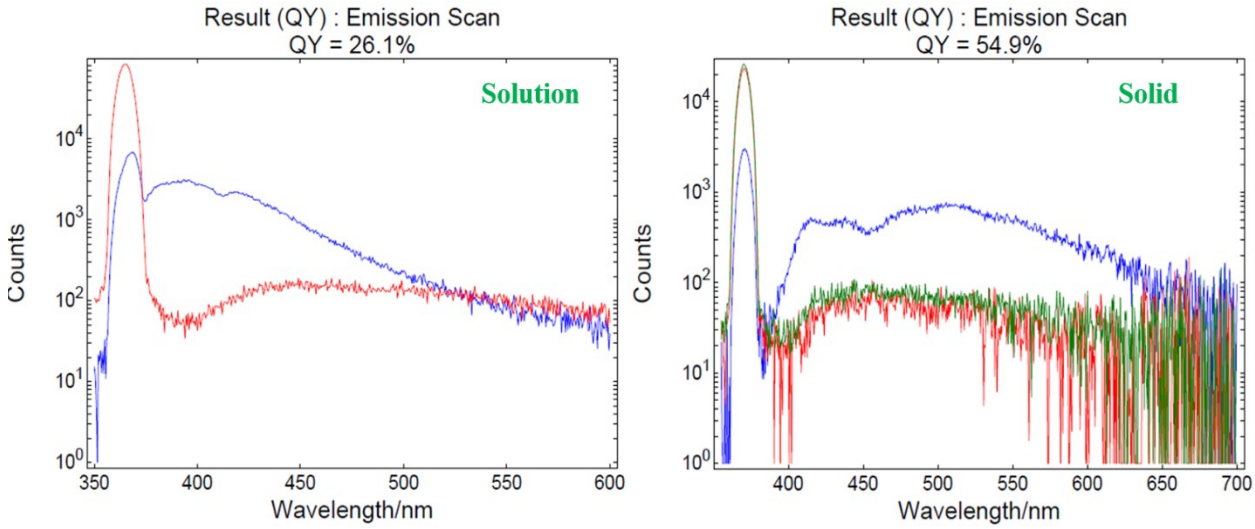

Fig. S21. The PLQY of the PIPOCz in solution and solid.

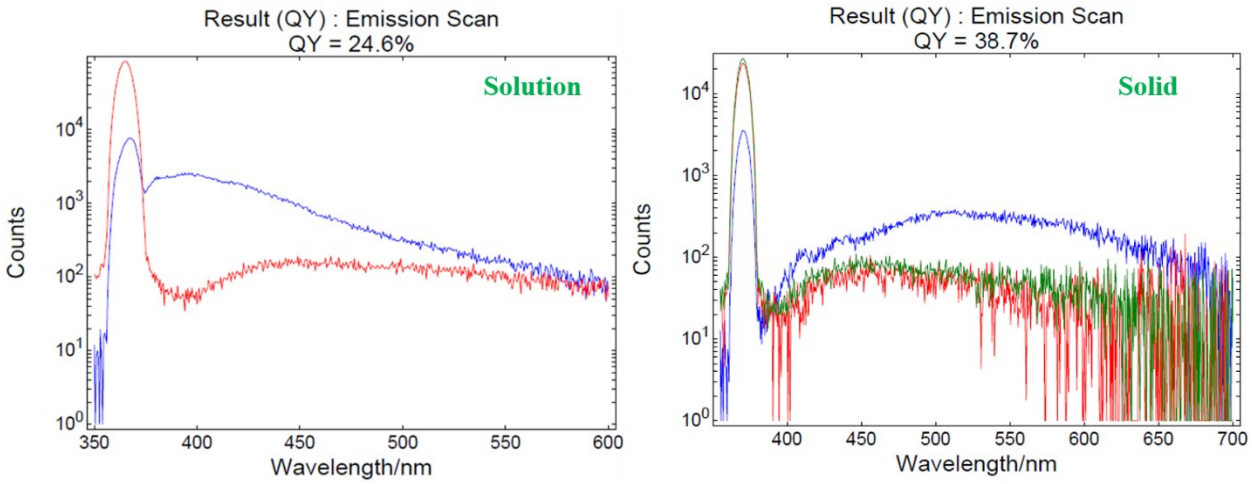

Fig. S22. The PLQY of the PIPTOCz in solution and solid.

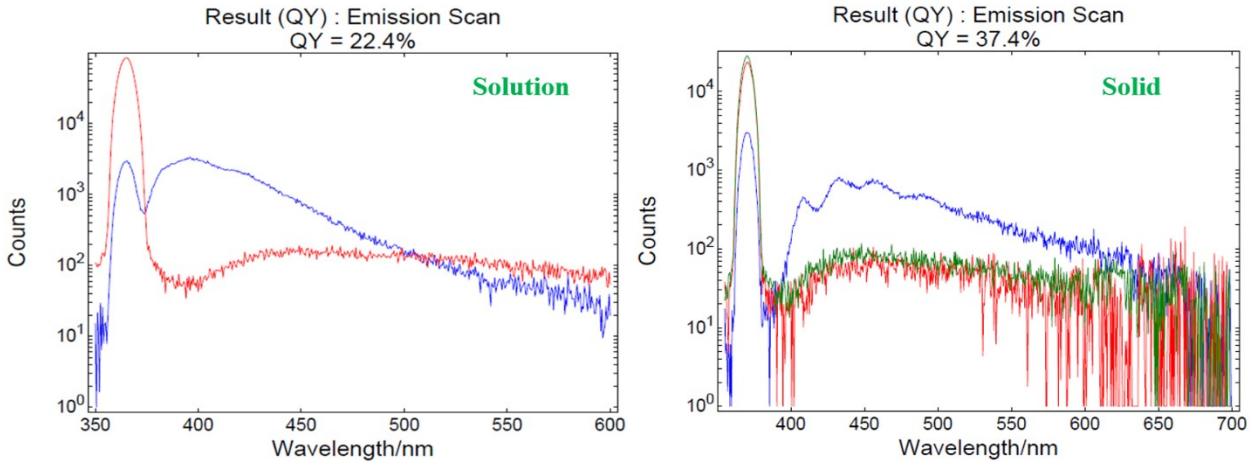

Fig. S23. The PLQY of the PITBOCz in solution and solid.

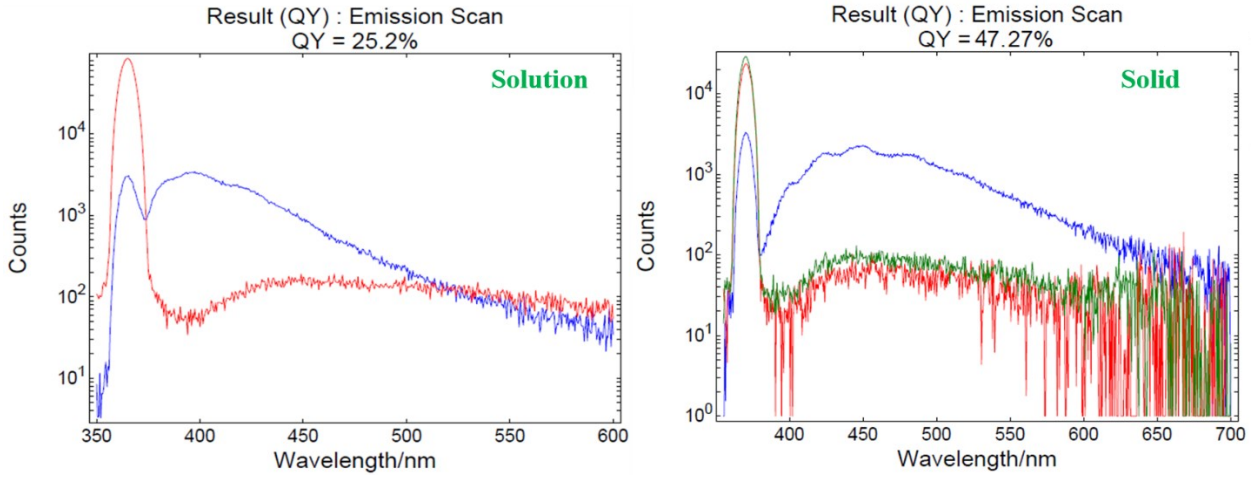

Fig. S24. The PLQY of the PIFOCz in solution and solid.

SI7. The calculated UV/Vis absorption spectra and vertical excitation wavelengths, orbital contribution and oscillator strength (f) of PI derivatives.

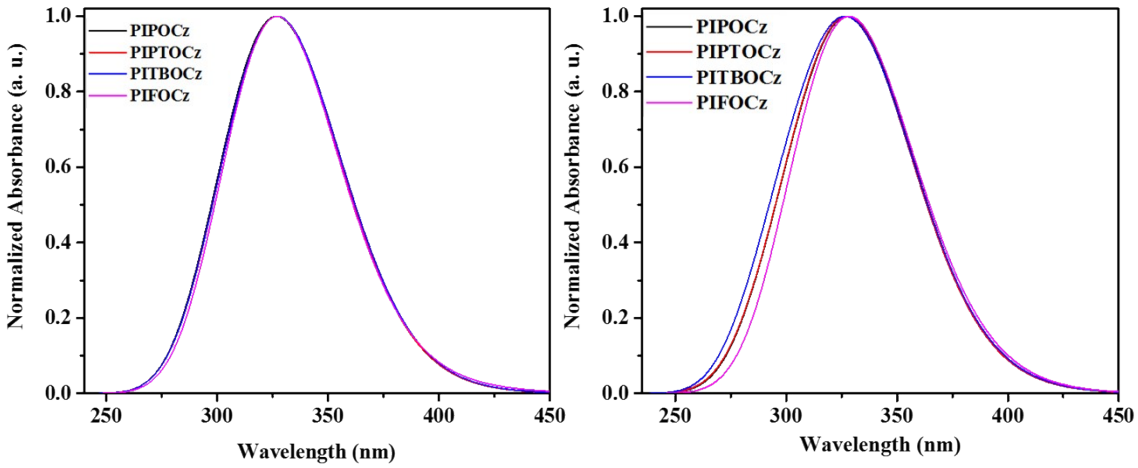

Fig. S24. Calculated UV/Vis absorption spectra of the fluorophores in gas (a) and DCM solution (b) phase.

Table S3. The computed vertical transitions and their oscillator strengths (*f*) and configuration of the PIPOCz fluorophore.

Fluorophore	State	Energy (eV)	λ_{max} nm	*f*	Configuration
PIPOCz Singlet	Gas	3.6604	338.7	0.0718	HOMO→ LUMO+1 (50.61%) HOMO→ LUMO+3 (13.83%)
		3.6845	336.50	0.2687	HOMO-3→ LUMO (13.78%) HOMO-3→ LUMO+4(10.88%) HOMO-3→ LUMO+5(10.06%) HOMO→ LUMO (45.05%) HOMO→ LUMO+1 (44.49%)
		3.8518	32.89	0.0906	HOMO→ LUMO (13.52%) HOMO→ LUMO+3 (67.90%)
		3.9445	314.32	0.2010	HOMO→ LUMO (22.41%) HOMO→LUMO+1(11.19%) HOMO→ LUMO+4 (60.35%)
Triplet	Gas	2.7173	456.28	-	HOMO-3→ LUMO+4 (13.62%) HOMO→ LUMO (56.15%) HOMO→ LUMO+4 (22.71%)
Singlet	DCM	3.6503	339.65	0.3976	HOMO→ LUMO (59.05%) HOMO→ LUMO+1 (33.48%)
		3.8009	326.20	0.3338	HOMO-3→ LUMO (16.29%) HOMO→ LUMO+1 (57.81%)
		4.111	301.58	0.1936	HOMO→ LUMO+4 (61.94%)
Triplet	DCM	2.7465	451.42	-	HOMO-4→ LUMO+4 (12.62%) HOMO→ LUMO (54.19%)

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

Fluorophore	State	Energy (eV)	λ_{max} nm	*f*	Configuration
PIPTOCz Singlet	Gas	3.6816	338.7	0.0718	HOMO→ LUMO+1 (53.97%)
		3.7176	336.50	0.2687	HOMO→ LUMO (52.89%) HOMO→ LUMO+1(40.11%) HOMO→ LUMO+3(13.39%) HOMO→ LUMO+4 (16.91%)
		3.9618	32.89	0.0906	HOMO-3→ LUMO (20.28%) HOMO→ LUMO+4 (62.26%)
Triplet	Gas	2.7207	455.70	-	HOMO-3→ LUMO+1 (19.52%) HOMO→ LUMO (56.88%)
Singlet	DCM	3.6481	339.86	0.3849	HOMO-3→ LUMO+3 (10.07%) HOMO→ LUMO (59.67%)
		3.8171	324.81	0.3728	HOMO→ LUMO (34.52%) HOMO→ LUMO+1 (58.25%)
		4.0890	303.21	0.0952	HOMO→ LUMO+3 (65.33%)
		4.1682	297.45	0.0919	HOMO→ LUMO+3 (10.84%) HOMO→ LUMO+4 (68.78%)
Triplet	DCM	2.7496	450.91	-	HOMO-3→ LUMO+1 (20.14%) HOMO→ LUMO (53.35%) HOMO→ LUMO+1 (26.22%) HOMO→ LUMO+3 (11.77%)

Table S5. The computed vertical transitions and their oscillator strengths (*f*) and configuration of the PITBOCz fluorophore.

Fluorophore	State	Energy (eV)	λ_{max} nm	*f*	Configuration
PITBOCz Singlet	Gas	3.6729	337.57	0.1172	HOMO→ LUMO+1 (61.94%)
		3.6975	335.32	0.2792	HOMO→ LUMO (59.91%) HOMO→ LUMO+1(27.89%) HOMO→ LUMO+3(20.49%)
		3.9374	314.89	0.2305	HOMO-3→ LUMO (14.00%) HOMO→ LUMO+3 (46.38%) HOMO→ LUMO+4 (43.88%)
Triplet	Gas	3.1273	396.46	-	HOMO-4→ LUMO+8 (11.21%) HOMO-3→ LUMO+1 (26.75%) HOMO→ LUMO+4 (14.67%) HOMO→ LUMO+5 (38.60%)
Singlet	DCM	3.6414	340.49	0.3966	HOMO-3→ LUMO+3 (10.29%) HOMO→ LUMO (59.87%)
		3.8080	325.58	0.3626	HOMO→ LUMO (34.15%) HOMO→ LUMO+1 (58.57%)
		4.1593	298.09	0.2243	HOMO→ LUMO+3 (13.89%) HOMO→ LUMO+4 (67.64%)
Triplet	DCM	2.7436	451.91	-	HOMO-3→ LUMO+1 (19.67%) HOMO→ LUMO (53.93%) HOMO→ LUMO+1 (25.51%) HOMO→ LUMO+3 (13.14%)

Table S6. The computed vertical transitions and their oscillator strengths (*f*) and configuration of the PIFOCz fluorophore.

Fluorophore	State	Energy (eV)	λ_{max} nm	*f*	Configuration
PIFOCz Singlet	Gas	3.2619	380.10	0.0108	HOMO→ LUMO (70.35%)
		3.6789	337.01	0.1933	HOMO-3→ LUMO+1 (12.94%) HOMO-3→ LUMO+5(11.19%) HOMO→ LUMO+1(46.74%) HOMO→ LUMO+4 (21.60%) HOMO→ LUMO+3 (42.69%)
		3.7891	327.21	0.2516	HOMO→ LUMO+3 (53.52%)
Triplet	Gas	2.7173	456.59	-	HOMO→ LUMO (19.12%) HOMO→ LUMO+1 (53.25%) HOMO→ LUMO+5 (11.18%)
Singlet	DCM	3.5323	351.00	0.0509	HOMO→ LUMO (70.02%)
		3.6494	339.74	0.3421	HOMO→ LUMO+1 (61.45%)
		3.8565	321.49	0.3738	HOMO→ LUMO+1 (30.59%) HOMO→ LUMO+2 (60.26%)
Triplet	DCM	2.7446	451.73	-	HOMO-5→ LUMO+5 (11.50%) HOMO-4→ LUMO+2 (54.19%) HOMO-3→ LUMO+2 (12.62%) HOMO→ LUMO+1 (44.70%) HOMO→ LUMO+2 (28.87%)

SI8. Electroluminescence characteristics:

Table S7. Summary of performance of reported purely organic small molecules based solution-processed blue OLEDs so far.-effect of doping concentration on the operating voltage (OV), power efficiency (PE), current efficiency (CE), external quantum efficiency (EQE), CIE coordinates, and

maximum luminance of the solution-processed devices with CBP host. [PE, CE, and EQE at 100 cdm^{-2} and maximum].

Solution-processed EML		Operation voltage (V)	$PE_{max}/CE_{max}/EQE_{max}$ $lmW^{-1}/cdA^{-1}/\%$	$PE_{100}/CE_{100}/EQE_{100}$ $lmW^{-1}/cdA^{-1}/\%$	CIE_{xy} coordinates	Maximum Luminance (cdm^{-2})	Ref
Emitter (Dopant)	**Emitter Concentration (wt%)**						
2,7-CSF	-	3.4	-/0.67/1.71	-/-/-	0.156, 0.054	349	**2**
2,7-CSFX	-	2.8	-/0.89/2.07	-/-/-	0.157, 0.051	886	
3,6-CSFX	-	4.2	-/0.42/0.88	-/-/-	0.251, 0.233	248	
2,7-CSBF	-	3.2	-/1.23/2.49	-/-/-	0.155, 0.050	1332	
5,9-CSBF	-	3.4	-/4.42/4.10	-/-/-	0.150, 0.091	2304	
DPIPOBn	1	9.2	-/-/-	0.2/0.4/0.6	0.16, 0.09	475	**3**
	3	9.3	-/-/-	0.5/0.9/1.6	0.16, 0.10	725	
	5	9.4	-/-/-	0.2/0.6/0.8	0.16, 0.10	508	
	100	9.6	-/-/-	0.1/0.2/0.1	0.29, 0.30	198	
DPITBOBn	1	8.9	-/-/-	0.1/0.3/0.4	0.16, 0.10	549	
	3	9.1	-/-/-	0.5/1.2/1.9	0.16, 0.11	856	
	5	9.4	-/-/-	0.4/0.8/1.2	0.16, 0.11	460	
	100	9.6	-/-/-	0.1/0.2/0.1	0.26, 0.32	178	
PY-II	-	4.5	-/-/-	0.41/0.17/-	(0.16, 0.16)	202	**4**
BIPOCz	0.5	4.1	0.2/ 0.3/ 1.9	0.1/ 0.2/ 1.1	(0.17, 0.07)	434	**5**
	1	4.8	0.3/ 0.5/ 1.5	0.1/ 0.3/ 0.7	(0.18, 0.10)	311	
	3	5.4	0.2/ 0.4/ 1.1	0.1/ 0.2/ 0.5	(0.18, 0.10)	301	
	5	5.4	0.1/ 0.3/ 0.7	0.1/ 0.2/ 0.4	(0.17, 0.09)	349	
	100	4.1	- / - / -	- / - / -	-	67	
BIPTOCz	0.5	4.1	0.1/0.2/ 1.4	0.1/0.2/0.8	(0.17, 0.06)	485	
	1	4.5	0.2/ 0.2/ 1.4	0.1/ 0.2/ 0.9	(0.17, 0.06)	450	
	3	4.7	0.1/ 0.2/ 1.4	0.1/ 0.2/ 0.7	(0.17, 0.08)	381	
	5	4.7	0.1/ 0.2/ 0.8	0.1/ 0.2/ 0.3	(0.13, 0.07)	373	
	100	4.6	- / - / -	- / - / -	-	49	
BITBOCz	0.5	4.1	0.1/ 0.2/ 1.5	0.1/ 0.2/ 0.9	(0.17, 0.06)	474	
	1	4.2	0.2/ 0.3/ 1.3	0.1/ 0.2/ 1.0	(0.17, 0.06)	454	
	3	4.6	0.2/ 0.3/ 1.1	0.1/ 0.2/ 0.7	(0.17, 0.07)	408	
	5	4.7	0.1/ 0.3/ 1.0	0.1/ 0.2/ 0.5	(0.17, 0.08)	374	
	100	4.7	- / - / -	- / - / -	-	21	
BIFOCz	0.5	4.1	0.2/ 0.3/ 1.6	0.1/ 0.2/ 0.9	(0.17, 0.07)	437	
	1	4.6	0.2/ 0.2/ 1.4	0.1/ 0.2/ 0.6	(0.18, 0.08)	518	
	3	5.0	0.1/ 0.2/ 0.8	0.1/ 0.1/ 0.4	(0.18, 0.08)	576	
	5	6.5	0.1/ 0.3/ 1.0	0.1/ 0.2/ 0.4	(0.18, 0.09)	619	
	100	4.2	0.1/ 0.1/ 0.1	0.1/ 0.1/ 0.1	(0.25, 0.30)	125	

C3FLA-2		9.2	0.2/ 0.5/ 0.5	- / - / -	0.158, 0.136	645	**6**
C2FLA-1		7.6	0.1/ 0.2/ 0.1	- / - / -	0.199, 0.197	257	**6**
MDP3FL		6.0	0.1/ 0.07/ 0.1	- / - / -	0.159, 0.099	153	**6**
4a		4.9	0.1/ 0.2/ 0.1	- / - / -	0.23, 0.33	156	**7**
4b		4.8	0.2/ 0.4/ 0.1	- / - / -	0.24, 0.41	256	**7**
4c		4.8	0.1/ 0.2/ 0.1	- / - / -	0.26, 0.49	207	**7**
5a		4.5	0.1/ 0.1/ 0.1	- / - / -	0.24, 0.45	277	**7**
8a		-	- / - / -	- / - / -	-	10	**8**
9a		-	- / - / -	- / - / -	-	19	**8**
JV55		5.1	0.1/ 0.1/ 0.2	- / - / -	0.19, 0.16)	215	**9**
TPI-1		9.2	- / - / -	- / - / -	-	8	**10**
TPI-2		9.0	- / - / -	- / - / -	-	11	**10**

SI9. Atom coordinates of PI derivatives.

PIPOCZ:

6	-0.941950000	-0.073330000	0.701554000
6	-0.086146000	-1.029422000	1.265924000
6	-0.393989000	0.995716000	-0.019647000
6	1.289432000	-0.924534000	1.112215000
1	-0.522003000	-1.843796000	1.836297000
6	0.987150000	1.091103000	-0.168742000
1	-1.027918000	1.752708000	-0.466763000
6	1.858120000	0.137804000	0.383684000
1	1.919472000	-1.667509000	1.585358000
1	1.414034000	1.924271000	-0.716367000
6	5.507933000	0.050578000	-0.030229000
6	5.162129000	1.394721000	-0.096760000
7	4.295806000	-0.618268000	0.176959000
7	3.811473000	1.570554000	0.046784000
6	3.302393000	0.363155000	0.209960000
6	6.144765000	2.424682000	-0.274320000
6	5.781910000	3.785876000	-0.318289000
6	7.506795000	2.030051000	-0.394671000
6	6.746518000	4.763226000	-0.475356000

1	4.731011000	4.038994000	-0.220758000
6	8.465390000	3.058693000	-0.550413000
6	8.097879000	4.393089000	-0.590135000
1	6.463224000	5.811954000	-0.507062000
1	9.517894000	2.814250000	-0.641074000
1	8.862223000	5.156251000	-0.710442000
6	6.861871000	-0.409878000	-0.191701000
6	7.864063000	0.605792000	-0.363813000
6	7.250546000	-1.770084000	-0.208082000
6	9.203034000	0.182620000	-0.516012000
6	8.574317000	-2.138740000	-0.364321000
1	6.500397000	-2.542166000	-0.104328000
6	9.561115000	-1.154117000	-0.513640000
1	9.984909000	0.921986000	-0.645779000
1	8.843222000	-3.191622000	-0.373907000
1	10.603629000	-1.435241000	-0.635012000
6	4.094598000	-2.033920000	0.269640000
6	4.402567000	-2.703842000	1.458681000
6	3.584967000	-2.736109000	-0.824956000
6	4.202064000	-4.081306000	1.547196000
1	4.800081000	-2.141572000	2.298265000
1	3.352414000	-2.200487000	-1.739929000
6	3.689716000	-4.787311000	0.455449000
1	4.444027000	-4.601965000	2.469423000
1	3.532143000	-5.859774000	0.527385000
6	3.380914000	-4.113348000	-0.727525000
6	-3.200504000	0.700918000	0.414970000
1	-2.961938000	1.690671000	0.828090000
1	-3.122131000	0.761388000	-0.680653000
6	-4.600369000	0.272145000	0.832915000
1	-4.633978000	0.217100000	1.929070000

1	-5.297841000	1.063734000	0.532856000
6	-5.031576000	-1.068257000	0.225750000
1	-4.982369000	-1.005655000	-0.869556000
1	-4.324361000	-1.849608000	0.528599000
6	-6.442347000	-1.516534000	0.640121000
8	-2.275104000	-0.266048000	0.914567000
6	-9.822175000	2.278398000	2.049185000
6	-8.853212000	1.633612000	2.836934000
6	-8.024576000	0.646636000	2.307072000
6	-8.187717000	0.308573000	0.959440000
6	-9.164012000	0.951040000	0.150652000
6	-9.980757000	1.941472000	0.707936000
1	-10.450779000	3.045254000	2.492655000
1	-8.743510000	1.909929000	3.882209000
1	-7.277902000	0.163267000	2.929592000
1	-10.731407000	2.439706000	0.099727000
6	-8.034675000	-0.614797000	-1.098014000
6	-7.687028000	-1.389908000	-2.209426000
6	-8.385242000	-1.174633000	-3.396218000
6	-9.404242000	-0.210481000	-3.481834000
6	-9.748252000	0.557391000	-2.372466000
6	-9.065212000	0.360242000	-1.167150000
1	-6.900949000	-2.137305000	-2.158468000
1	-8.132944000	-1.765095000	-4.272963000
1	-9.927475000	-0.065471000	-4.422663000
1	-10.539402000	1.299734000	-2.440675000
1	2.983029000	-4.658777000	-1.578521000
1	-6.640664000	-2.519637000	0.242955000
1	-6.510410000	-1.594101000	1.729951000
7	-7.510155000	-0.635847000	0.190918000

PIPTOCz:

6	1.025732000	-0.059824000	0.696108000
6	0.155260000	0.893723000	1.242058000
6	0.494693000	-1.148120000	-0.008631000
6	-1.218403000	0.767117000	1.086920000
1	0.578453000	1.723634000	1.799483000
6	-0.884662000	-1.265693000	-0.158670000
1	1.140250000	-1.903144000	-0.442123000
6	-1.770224000	-0.315804000	0.375965000
1	-1.860658000	1.509499000	1.544415000
1	-1.298574000	-2.113977000	-0.692887000
6	-5.419449000	-0.289202000	-0.044277000
6	-5.054565000	-1.629412000	-0.084440000
7	-4.217699000	0.400985000	0.151392000
7	-3.701768000	-1.783062000	0.064024000
6	-3.210866000	-0.565102000	0.204596000
6	-6.022170000	-2.676502000	-0.243225000
6	-5.639898000	-4.032989000	-0.261236000
6	-7.389593000	-2.303749000	-0.372275000
6	-6.590223000	-5.026822000	-0.401022000
1	-4.585592000	-4.269014000	-0.157811000
6	-8.333167000	-3.348759000	-0.509708000

6	-7.946607000	-4.678272000	-0.524116000
1	-6.291950000	-6.071819000	-0.412835000
1	-9.388915000	-3.121059000	-0.606021000
1	-8.699810000	-5.454427000	-0.630938000
6	-6.779946000	0.148484000	-0.214046000
6	-7.767369000	-0.884459000	-0.368025000
6	-7.188446000	1.502443000	-0.253997000
6	-9.112275000	-0.483570000	-0.528243000
6	-8.517407000	1.848889000	-0.416973000
1	-6.449576000	2.286882000	-0.162788000
6	-9.489760000	0.847637000	-0.549640000
1	-9.883261000	-1.236439000	-0.645044000
1	-8.801696000	2.897434000	-0.444588000
1	-10.536193000	1.111374000	-0.676341000
6	-4.036109000	1.820987000	0.211394000
6	-4.350248000	2.519001000	1.381943000
6	-3.543598000	2.510752000	-0.897359000
6	-4.173370000	3.899928000	1.433880000
1	-4.740148000	1.976273000	2.237974000
1	-3.306623000	1.964167000	-1.804826000
6	-3.674229000	4.610286000	0.331712000

1	-4.426969000	4.435124000	2.345866000
6	-3.365095000	3.892414000	-0.830639000
6	3.295369000	-0.806442000	0.425463000
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