Benzil-imidazole blue fluorophores and their applications in blue/white light-emitting diodes, sensing and anticounterfeiting

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Contents:

SI1. Experimental section

All the reactions are carried out under a nitrogen atmosphere. Commercially available reagents (Sigma Aldrich) were used as purchased without any further purification. All the reactions were monitored by thin-layer chromatography (TLC) with silica gel 60 F254 Aluminium plates (Merck). Column chromatography was carried out using silica gel (Sigma-Aldrich).

SI1.1 General information and measurements

^{1}H and ^{13}C NMR spectra were recorded using an AV 400 Avance-III FT-NMR Spectrometer (Bruker Biospin International, Switzerland) with spectrometer frequencies 400 MHz and 100 MHz, respectively, and Mass spectra of fluorophore were recorded on High Resolution Mass Spectrometer (HRMS) Waters, USA, XEVO G2-XS QTOF model. The FT-IR spectra were recorded on a Perkin–Elmer RX-I FTIR spectrophotometer. Thermogravimetric analysis (TGA) was performed using the TA Instrument TGAQ50 thermal analysis system. UV-vis absorption was measured using a UV-vis spectrophotometer (Shimadzu Corporation, japan/UV-2450 Pekin Elmer, USA/Lamda 25), and photoluminescence (PL) spectra were recorded using an Edinburgh instrument FLS980 spectrofluorometer. The absolute PL Quantum yields (PLQY) were measured using an Edinburgh instrument spectrofluorometer, integrating sphere SC-30 model. The fluorophores' quantum yield is calculated using equation (1).

$$\Phi = \frac{L_n(\lambda) - L_i(\lambda)}{L_0(\lambda)} \qquad (1)$$

$$\eta = \frac{E_i(\lambda) - (1 - \Phi)_0(\lambda)}{E_0(\lambda)\Phi} \qquad (2)$$

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 solid caused by direct excitation and $E_i(\lambda)$ is indirect illumination from the sphere, respectively. Photoluminescence lifetime of the dyes was measured at 298 K with an Edinburgh Instrument FLS 980 luminescence spectrometer based on the time correlated single photon counting technology for all the dyes. Cyclic voltammetry (CV) of the fluorophores were carried out by using AUTOLAB 302 Modular Potentiostat electrochemical analyzer at 298 ± 1 K. The tests were carried out in dimethylformamide (DMF) containing 0.1 M tetrabutylammonium perchlorate (Bu_4NClO_4) as a supporting electrolyte,

and the scan rate were maintained at 100 mVs^{-1} with three conventional electrode configurations viz, a glassy carbon working electrode, a platinum plate auxiliary electrode, and an Ag/AgCl reference electrode.

SI1.2 Detection Measurement of Nitroaromatic Compound:

For quantitative measurement, the emission measurements were performed by increasing the different concentrations of PA in THF(1 $x10^{-5}$ M). Subsequent addition of 0µL to 120µL in the respective fluorophores (1 $x10^{-6}$ M) of the solution. By subsequent addition of picric acid, the absolute decrease of the intensity was observed as compared to other nitroaromatics compounds. We also check the response time within 10 sec adding the concentration of PA, and the quenching of emission happens, which results that even with the low concentration of PA, the fluorophores occur perfectly. The fluorescence quenching efficiency (η) for each analyte was calculated by the following equation:

$$\eta = \frac{I_0 - I}{I_0} \times 100$$

in which I_0 and I were the fluorescence intensities in the absence and presence of analyte, respectively.

SI1.3 Synthetic rout

Synthesis of 5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine (1): A mixture of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (10 mmol) and ammonium acetate (15 mmol) was taken in a 100ml conical flask containing 10ml absolute ethanol at room temperature, sealed and warmed using water bath 15 min until the dissolution of the solid contents. After bringing the reaction mixture to room temperature, 2-teralone (20 mmol) was add and sealed, the mixture was warm for 5 min, and the reaction mixture was kept aside for 24 h in open air. After the completion of the reaction as monitored by TLC, the resulting crude product was further purify by column chromatography over silica gel (60-120 mesh) using n-hexnae and ethyl acetate mixture (9:1) as eluent to give the compound **(1)**. Thus obtained solid was further purified by recrystallizing in 1:1 ethanol and tetrahydrofuran mixture to afford compound **(1)** 65% as a yellow solid

2-(4-bromophenyl)-1,4,5-triphenyl-1H-imidazole and their derivatives:

A mixture of Benzil (10.0 mmol), aniline derivatives (10.0 mmol), 4-bromobenzaldehyde (10.0 mmol), ammonium acetate (15.0 mmol), and acetic acid (15 mL) was refluxed for 24 hrs. After

that, the mixture was cooled to room temperature, then the crude product was extract with Ethyl acetate (3x30 mL and finaly dried with sodium sulfate. It was then purified by chromatography using Hexane/Ethyl acetate (9:1) as an eluent to obtain the product as white powder. Yield: 75 - 90%.

SI2. NMR (^{1}H and ^{13}C) spectra, FTIR and HRMS spectra of fluorophores.

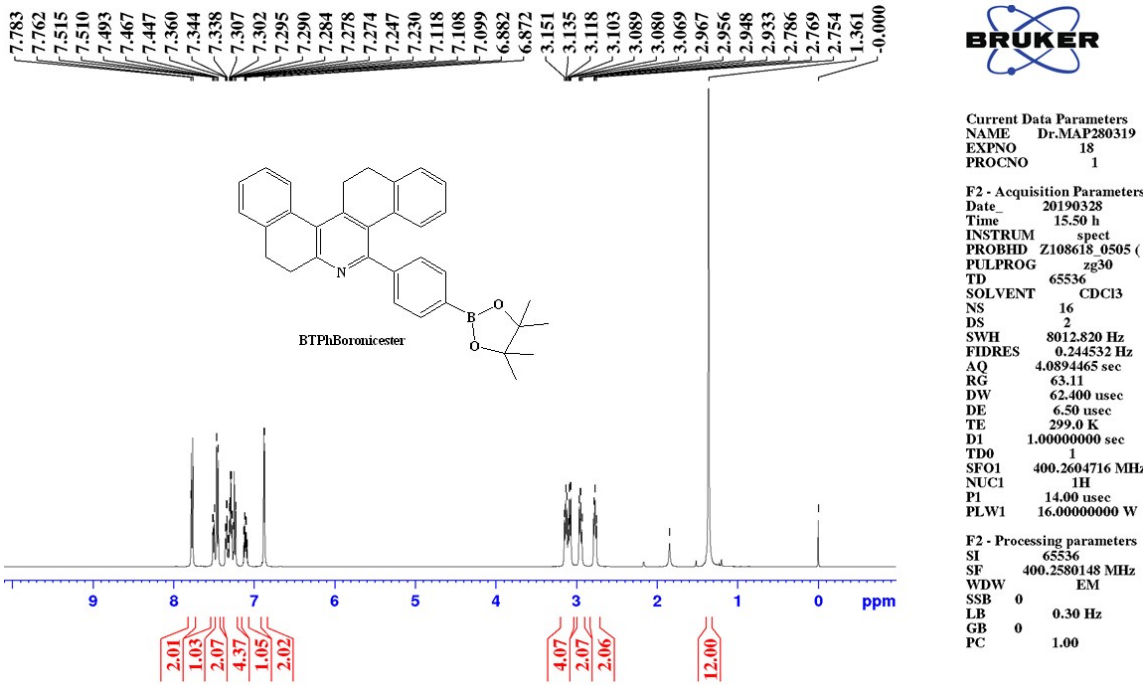

Fig. S1.1. ^{1}H NMR spectra of 5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine

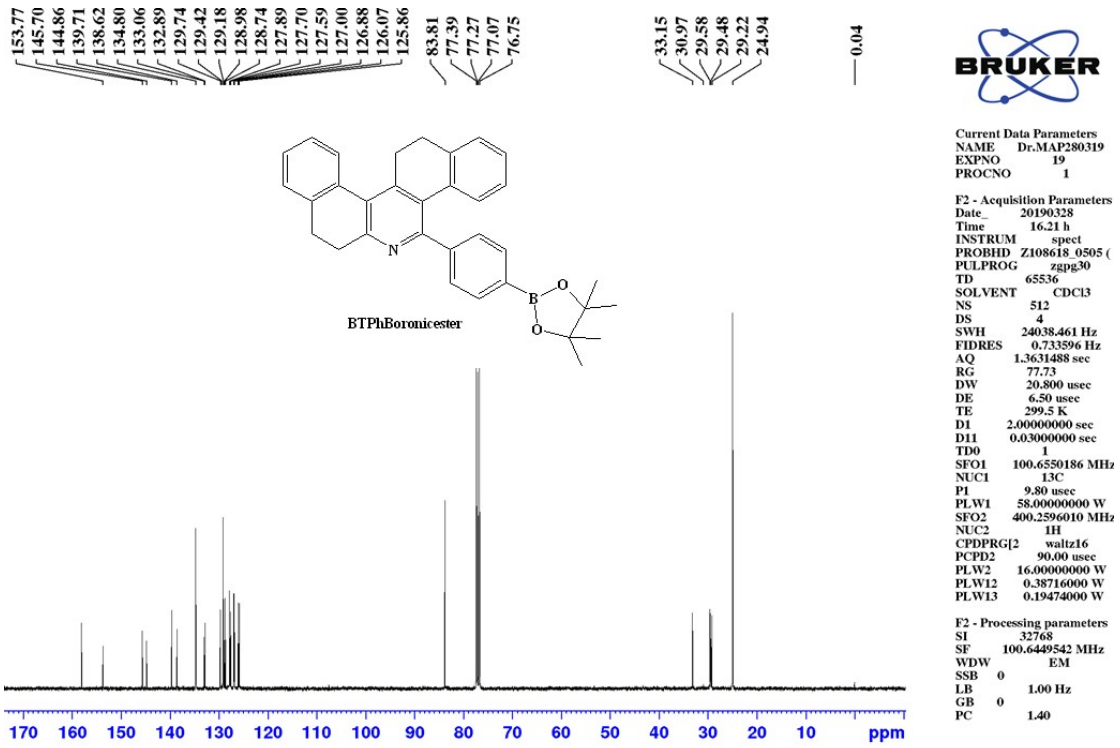

Fig. S1.2. ^{13}C-NMR of 5-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine

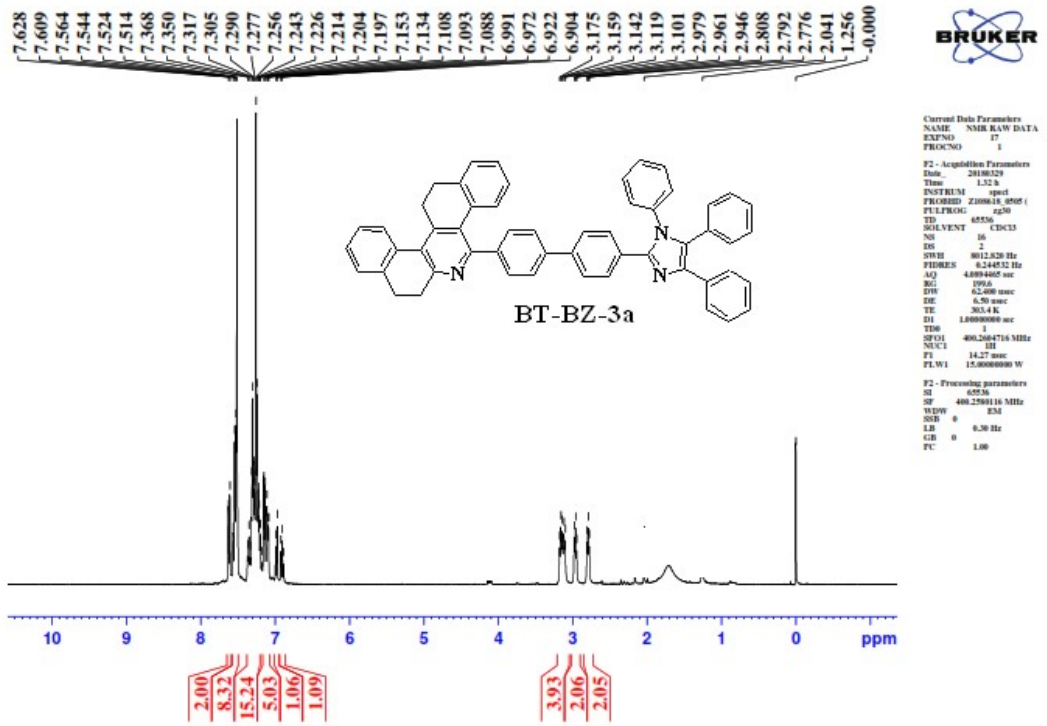

Fig.S1.3. ^{1}H-NMR 5-(4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3a)

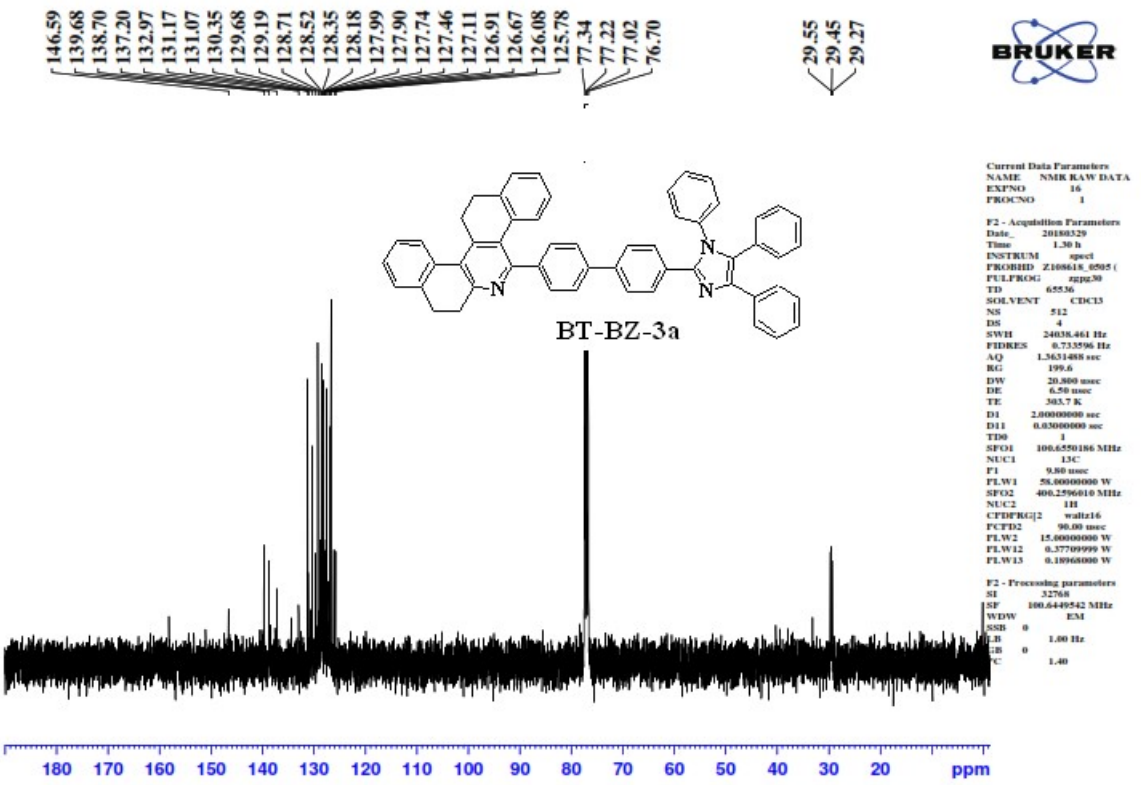

Fig.S1.4. ^{13}C-NMR 5-(4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3a)

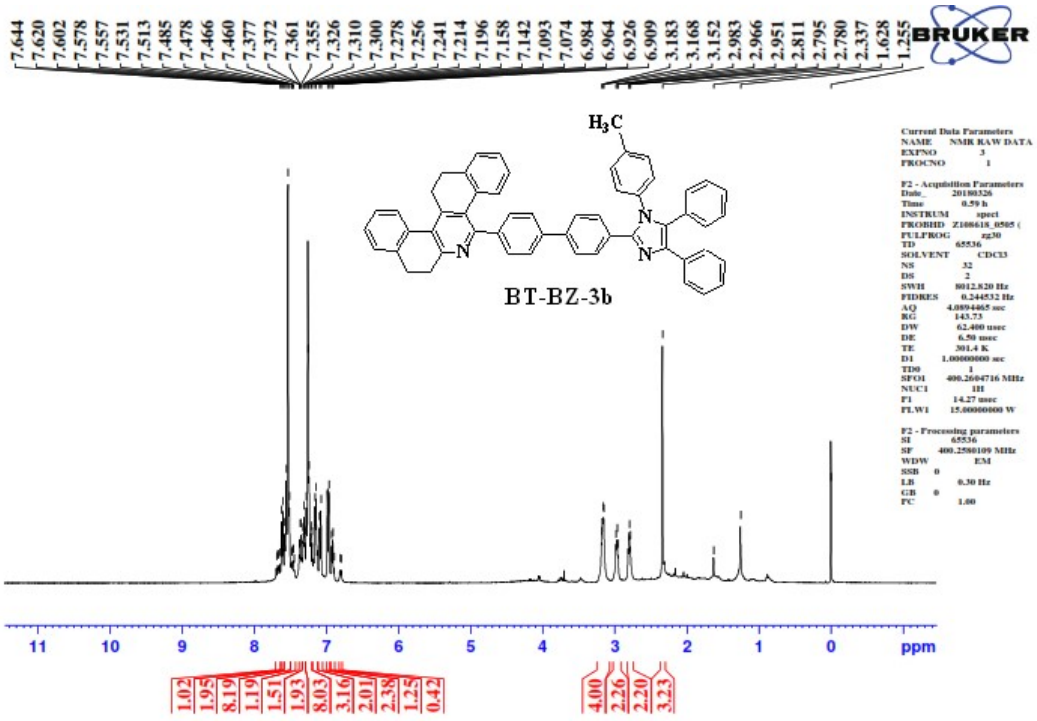

Fig.S1.5. ^{1}H-NMR 5-(4'-(4,5-diphenyl-1-(p-tolyl)-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3b)

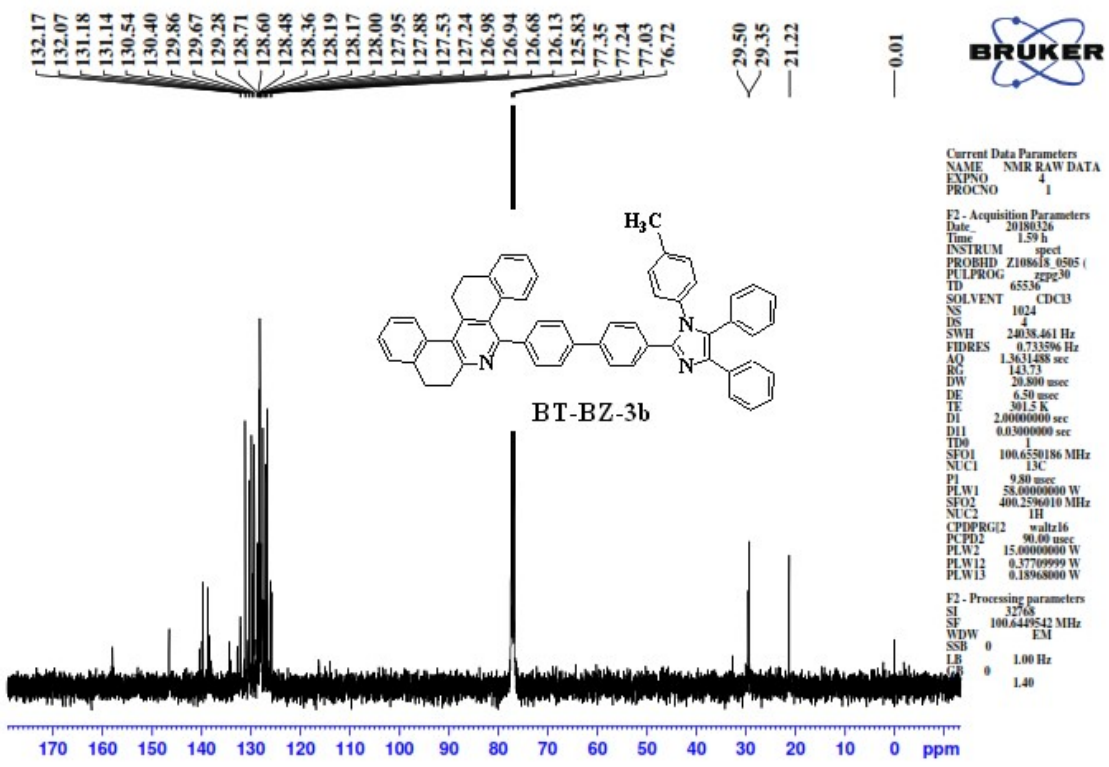

Fig.S1.6. ^{13}C-NMR 5-(4'-(4,5-diphenyl-1-(p-tolyl)-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3b)

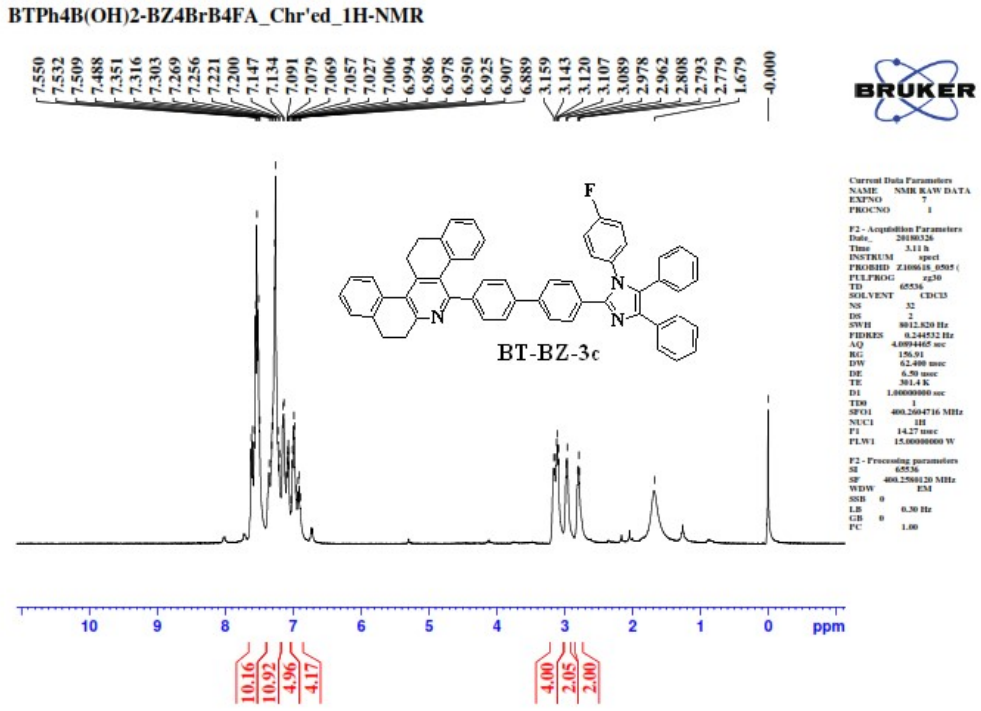

Fig.S1.7. ^{1}H-NMR 5-(4'-(1-(4-fluorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3c)

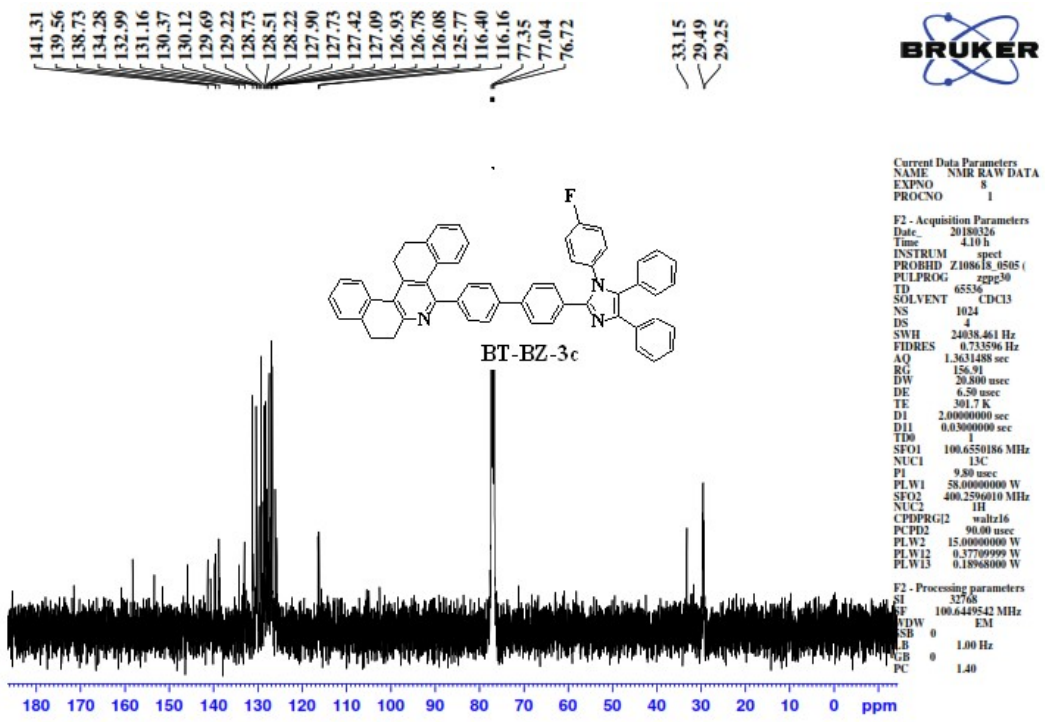

Fig.S1.8. ^{13}C-NMR 5-(4'-(1-(4-fluorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3c)

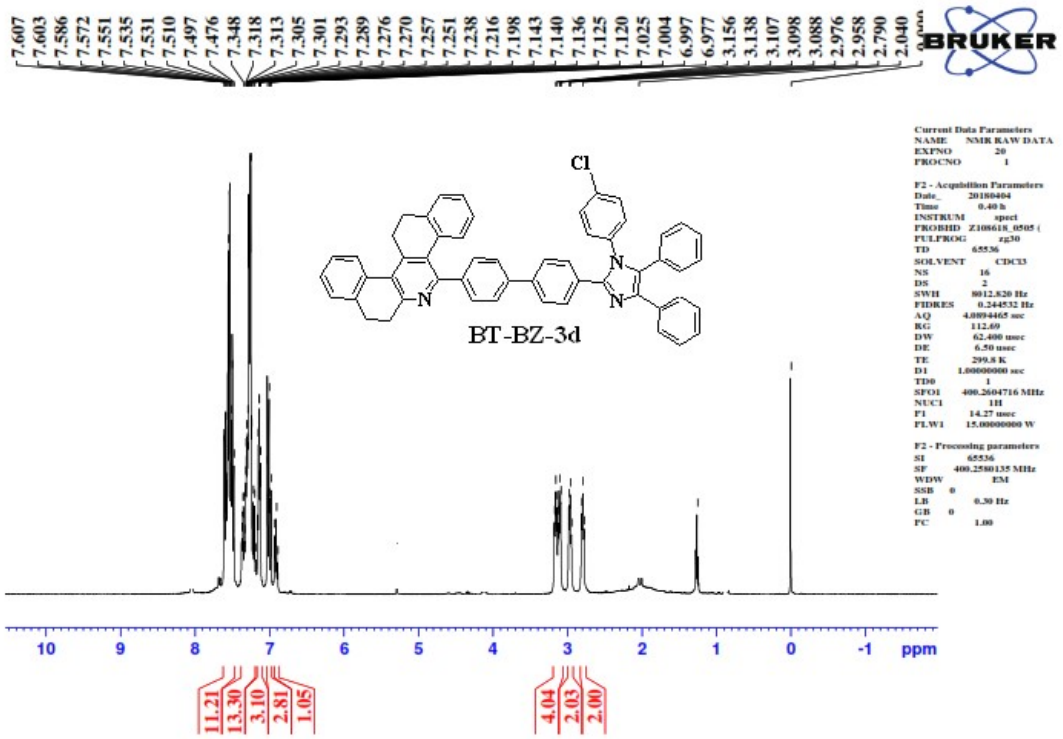

Fig.S1.9. ^{1}H-NMR 5-(4'-(1-(4-chlorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3d)

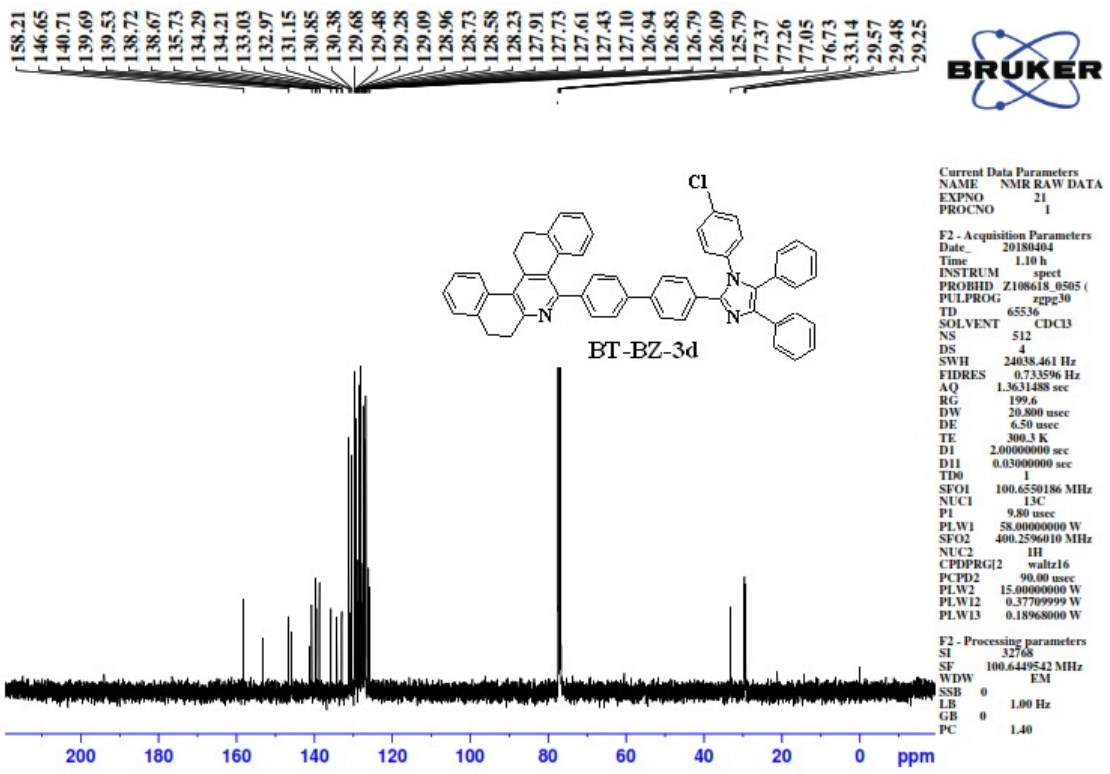

Fig.S1.10 ^{13}C-NMR 5-(4'-(1-(4-chlorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3d)

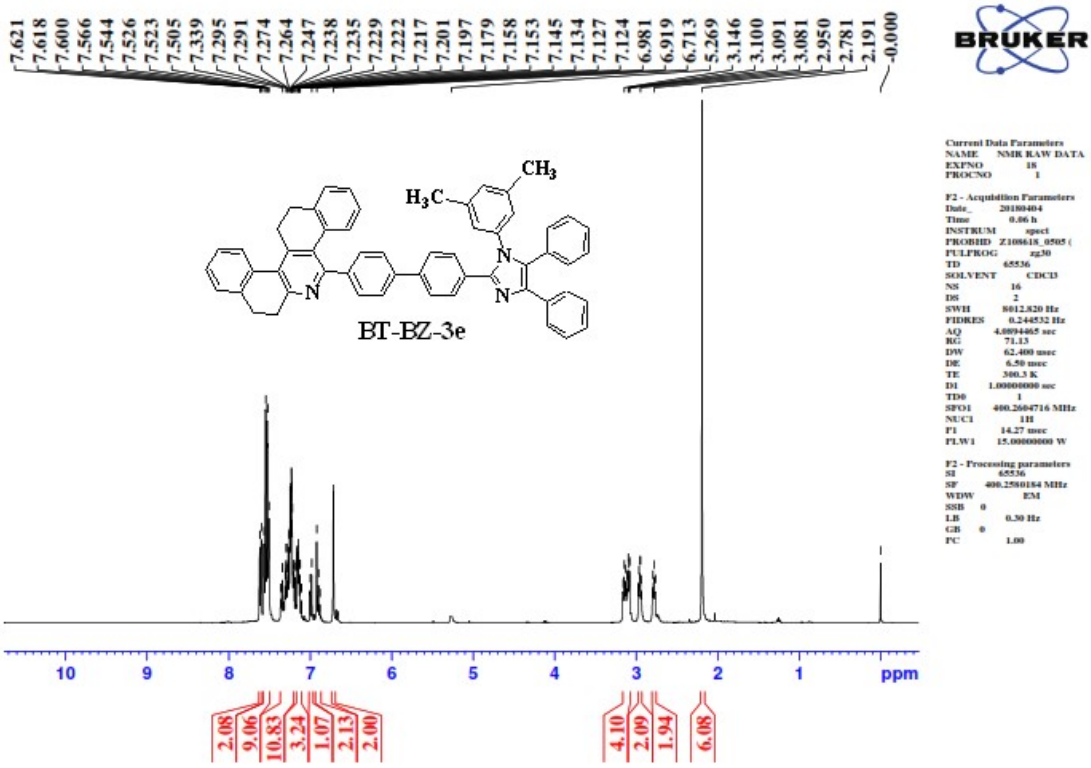

Fig.S1.11 ^{1}H-NMR (4'-(1-(3,5-dimethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3e)

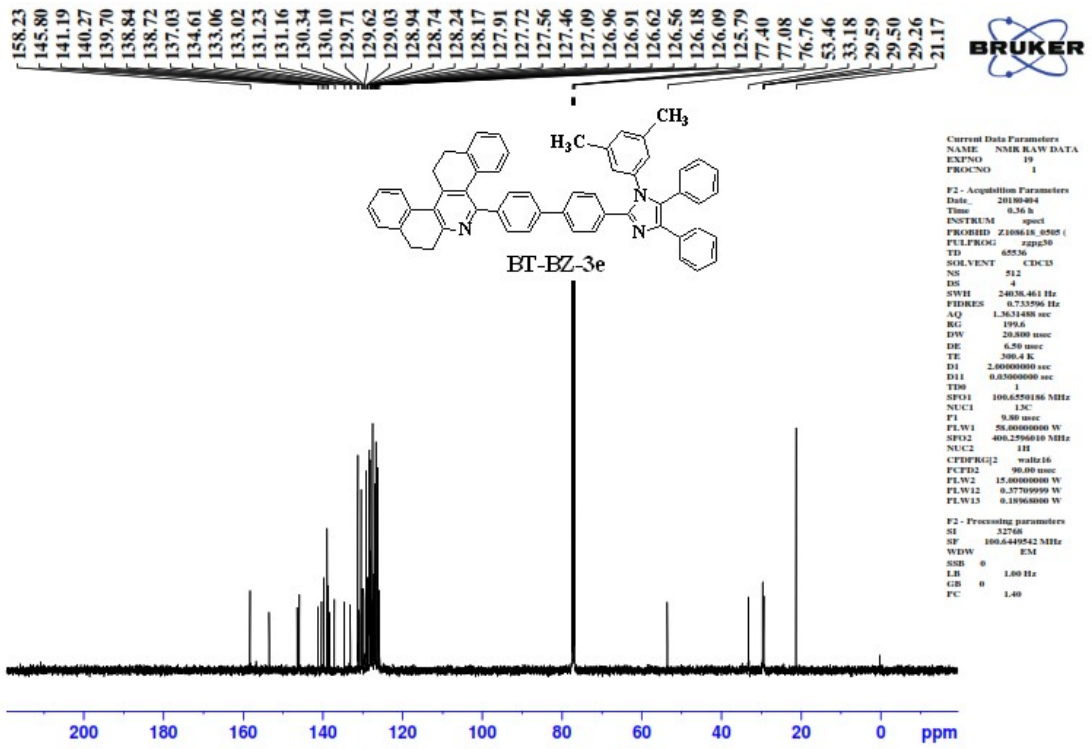

Fig.S1.12 ^{13}C-NMR 5-(4'-(1-(3,5-dimethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3e)

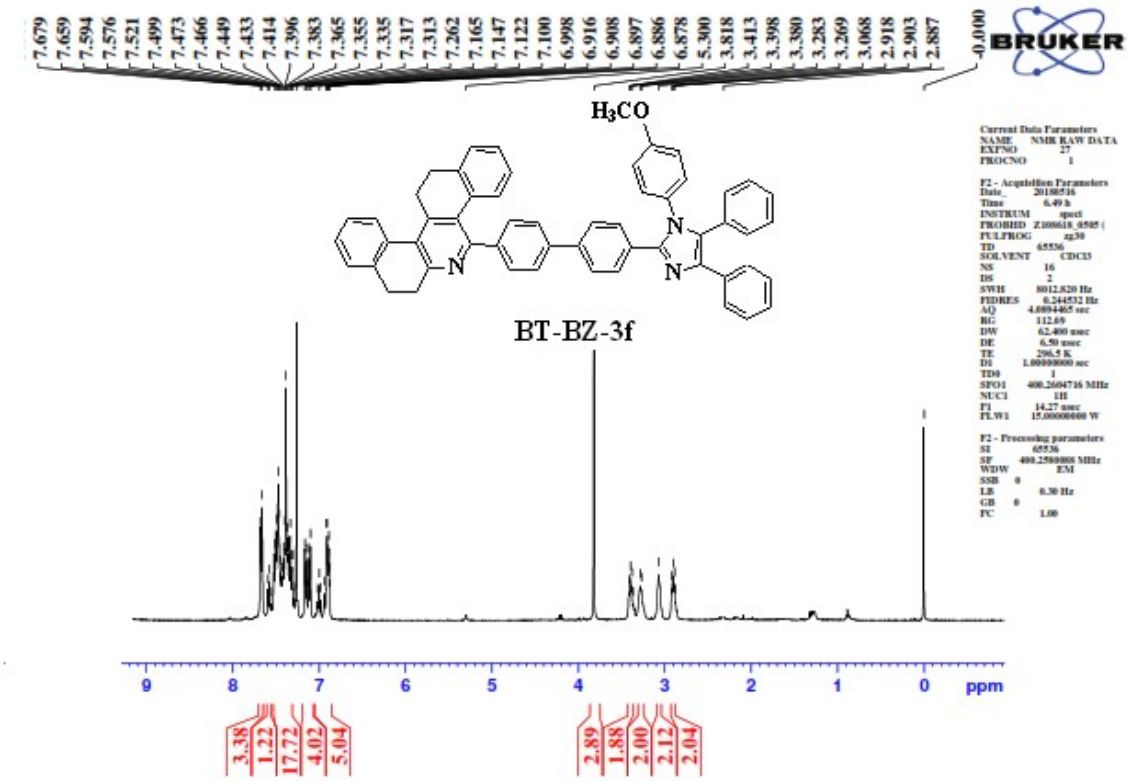

Fig.S1.13 ^{1}H-NMR 5-(4'-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3f)

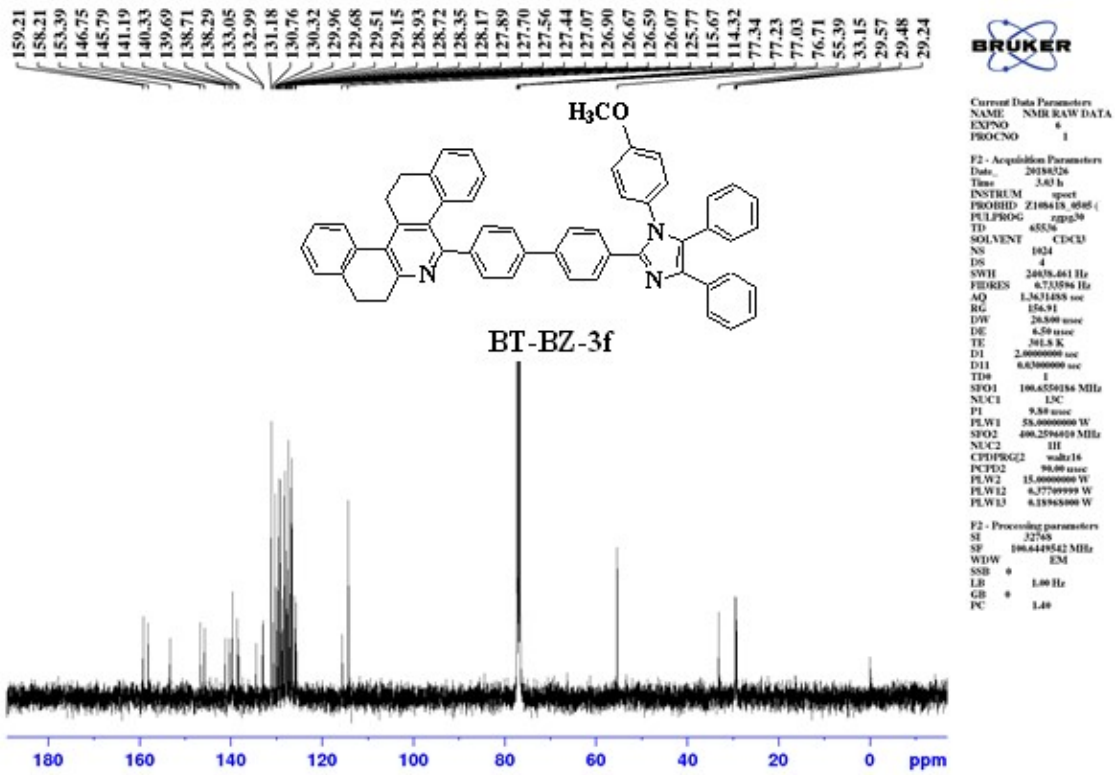

Fig.S1.14 5-(4'-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3f)-^{13}C-NMR

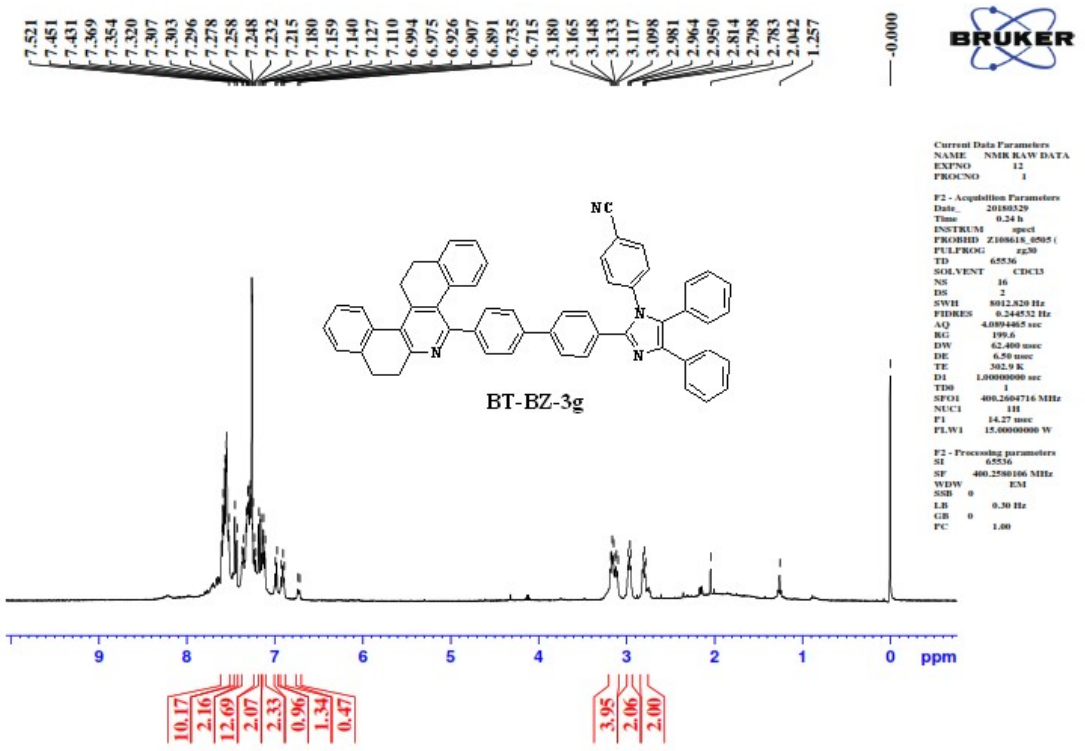

Fig.S1.15 ^{1}H-NMR 4-(4,5-diphenyl-2-(4'-(7,8,13,14-tetrahydrodibenzo[a,i]phenanthridin-5-yl)-[1,1'-biphenyl]-4-yl)-1H-imidazol-1-yl)benzonitrile(3g) ^{1}H-NMR

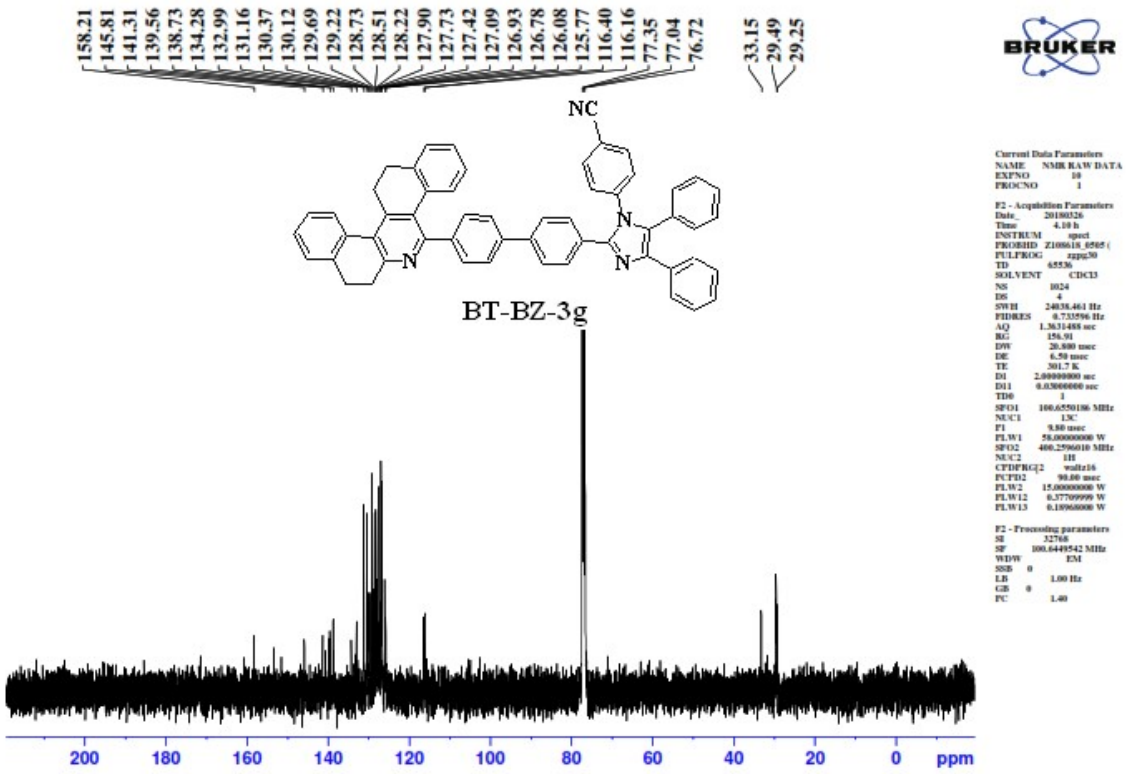

Fig.S1.16 ^{13}C-NMR 4-(4,5-diphenyl-2-(4'-(7,8,13,14-tetrahydrodibenzo[a,i]phenanthridin-5-yl)-[1,1'-biphenyl]-4-yl)-1H-imidazol-1-yl)benzonitrile(3g)

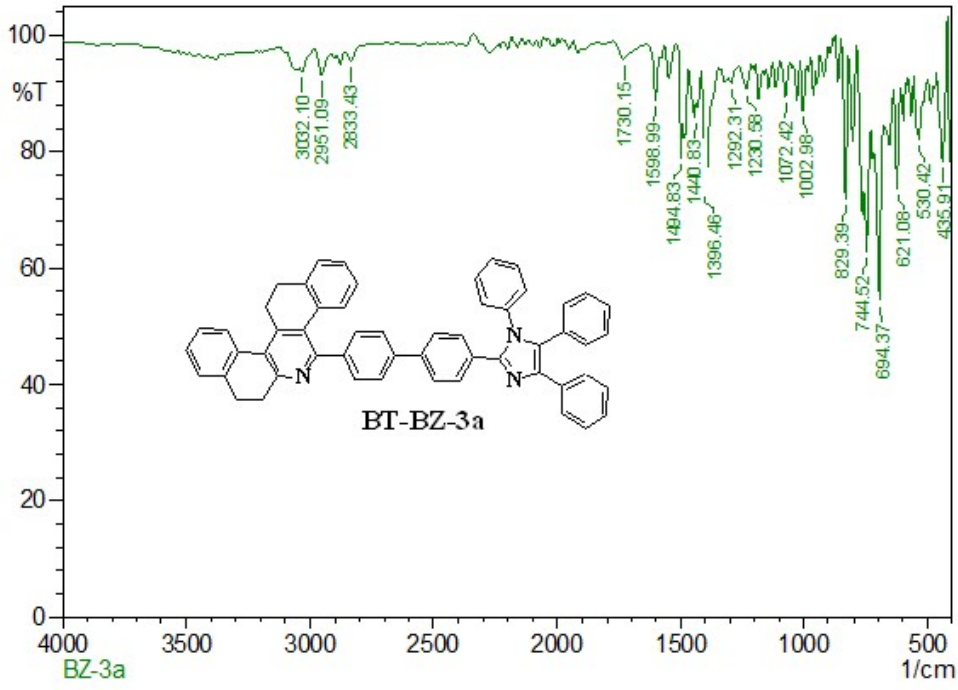

Fig. S2.1. IR Spectra of 5-(4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3a)

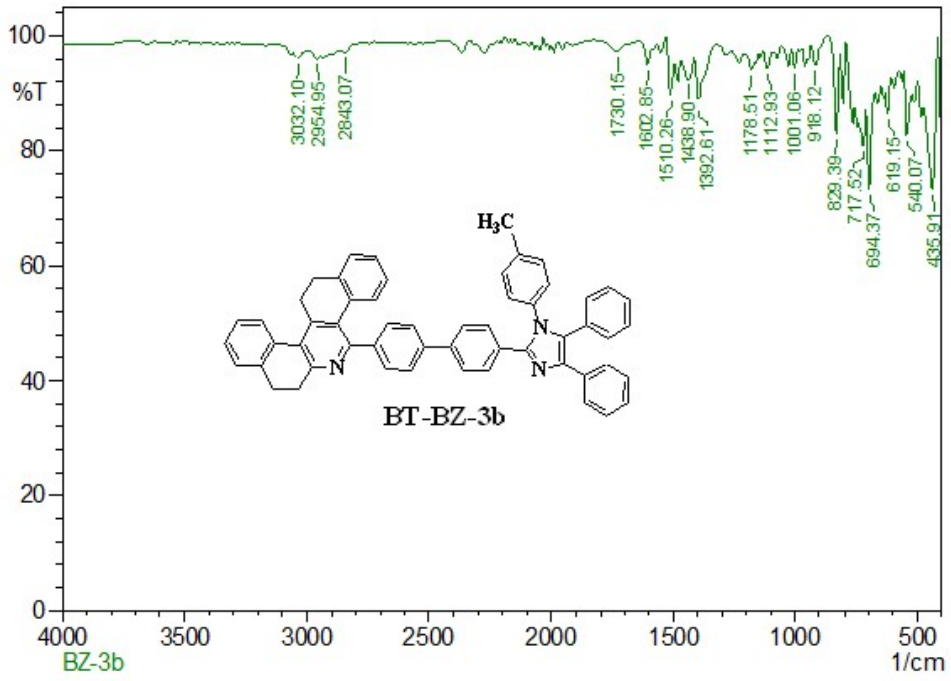

Fig. S2.2. 5-(4'- IR Spectra of (4,5-diphenyl-1-(p-tolyl)-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3b)

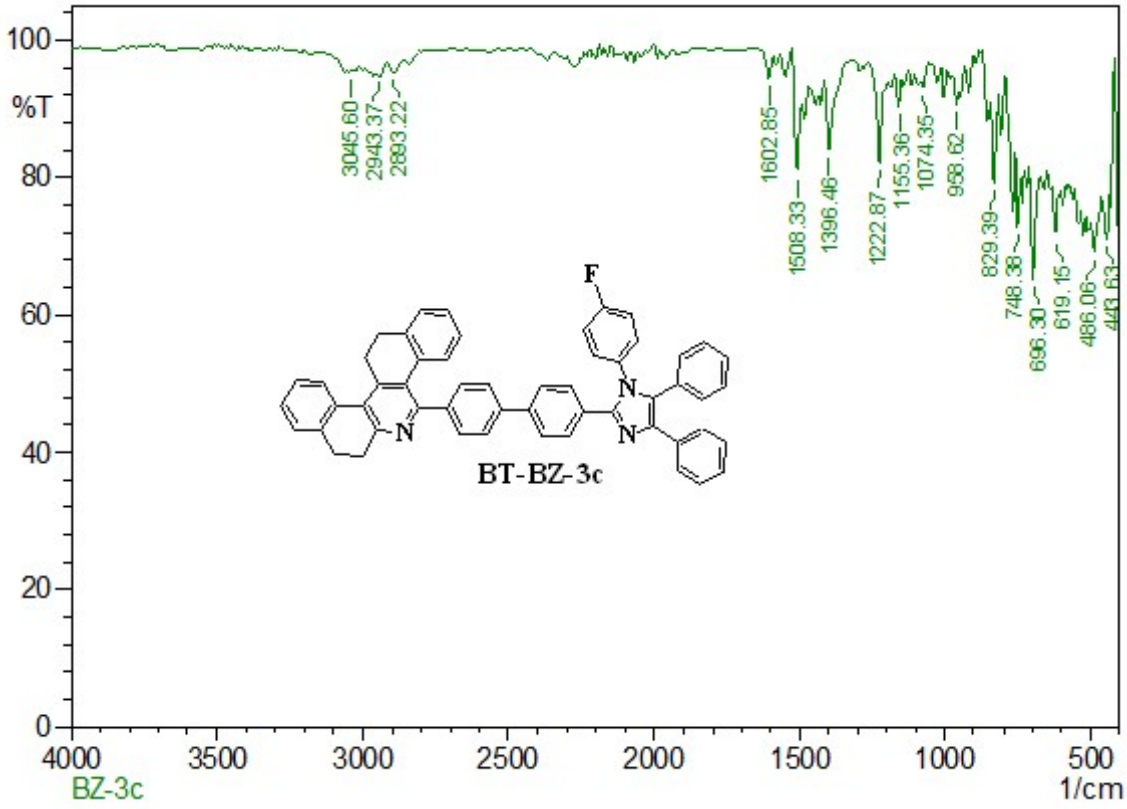

Fig. S2.3. IR Spectra of 5-(4'-(1-(4-fluorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3c)

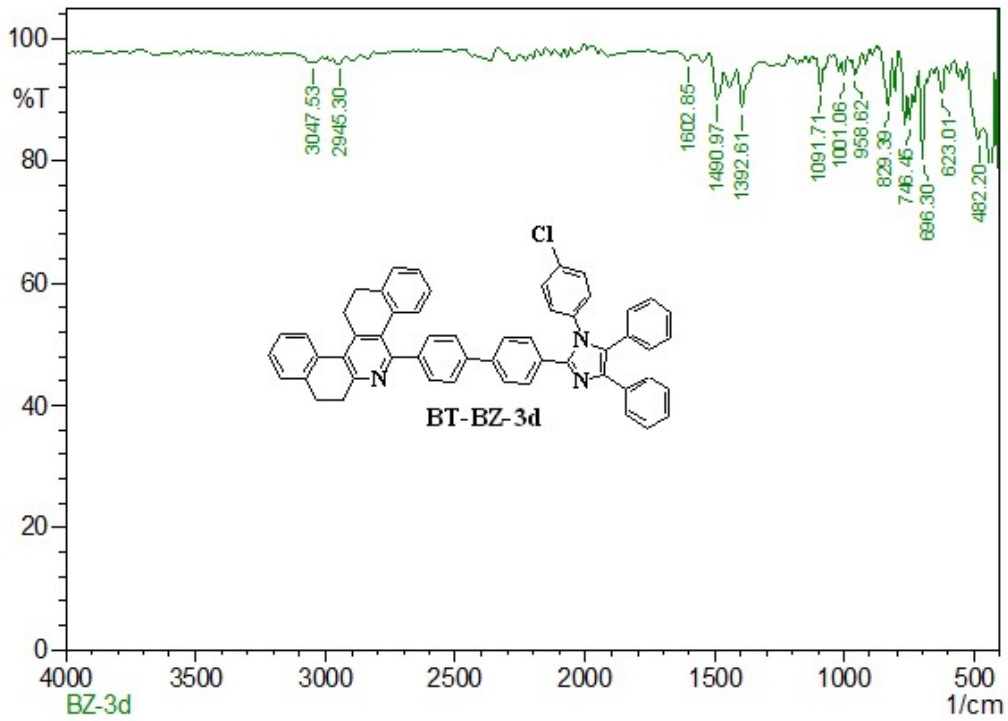

Fig. S2.4. IR Spectra of 5-(4'-(1-(4-chlorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3d)

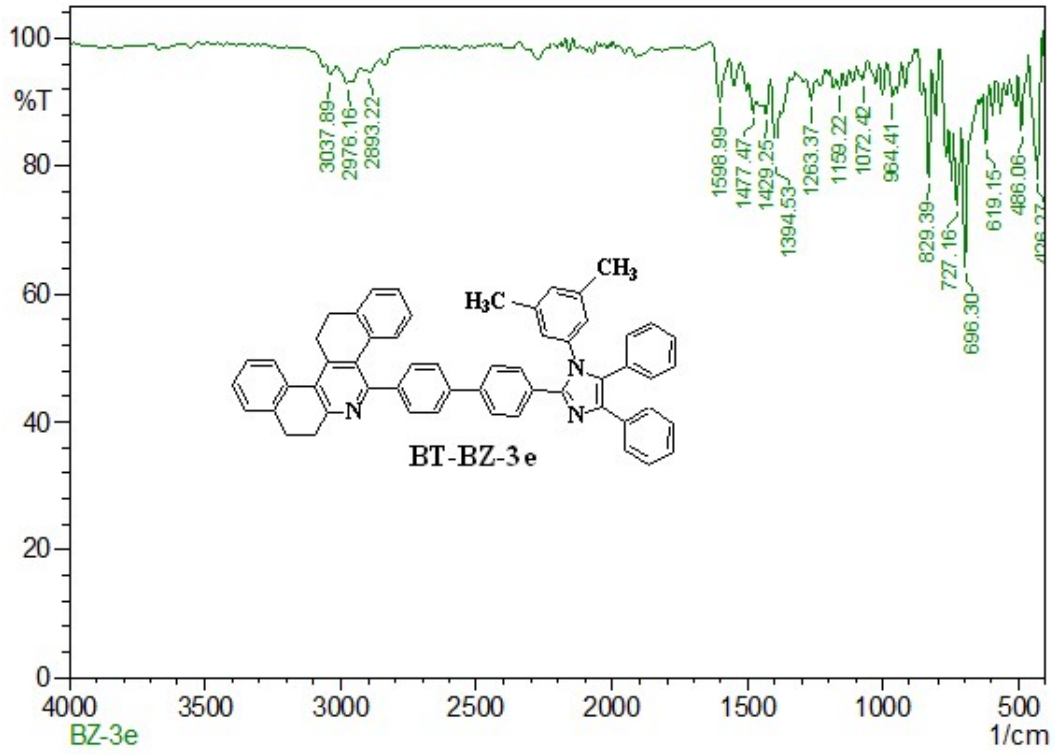

Fig. S2.5. IR Spectra of 5-(4'-(1-(3,5-dimethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3e)

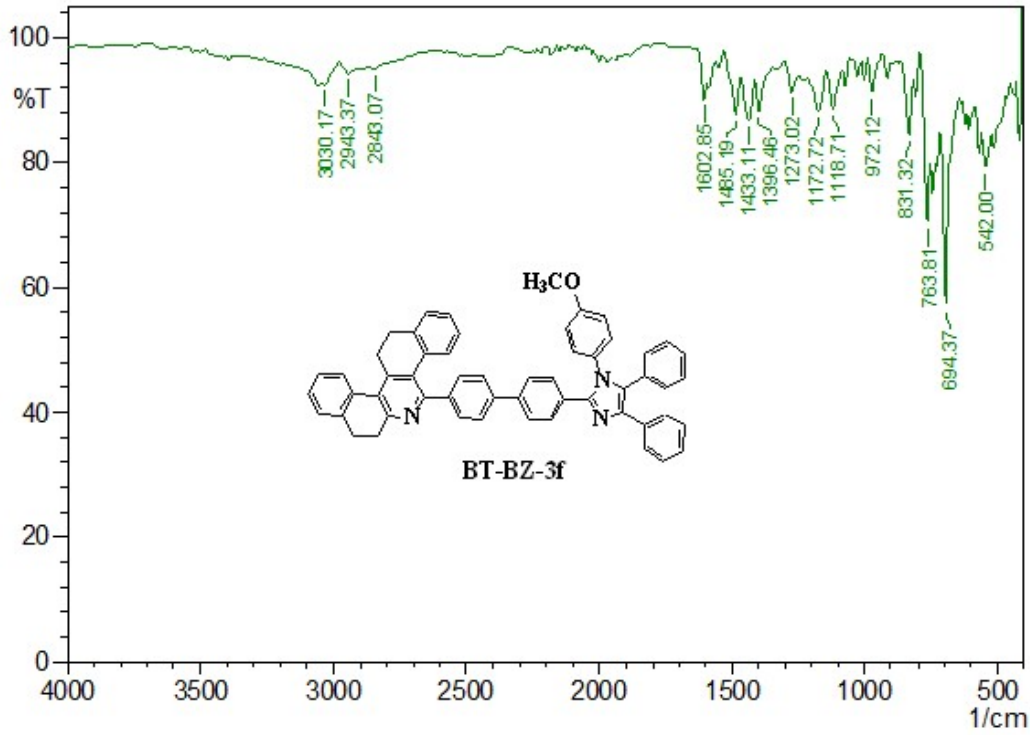

Fig. S2.6. IR Spectra of 5-(4'-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3f)

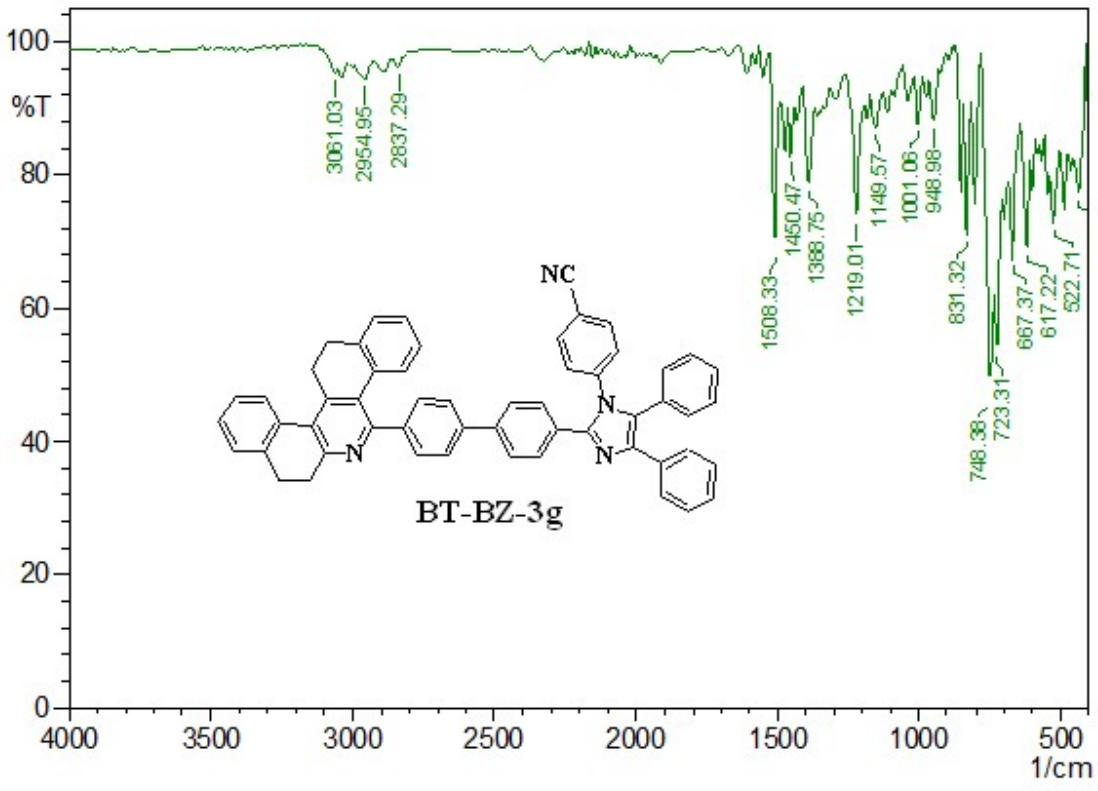

Fig. S2.7. IR Spectra of 4-(4,5-diphenyl-2-(4'-(7,8,13,14-tetrahydrodibenzo[a,i]phenanthridin-5-yl)-[1,1'-biphenyl]-4-yl)-1H-imidazol-1-yl)benzonitrile(3g)

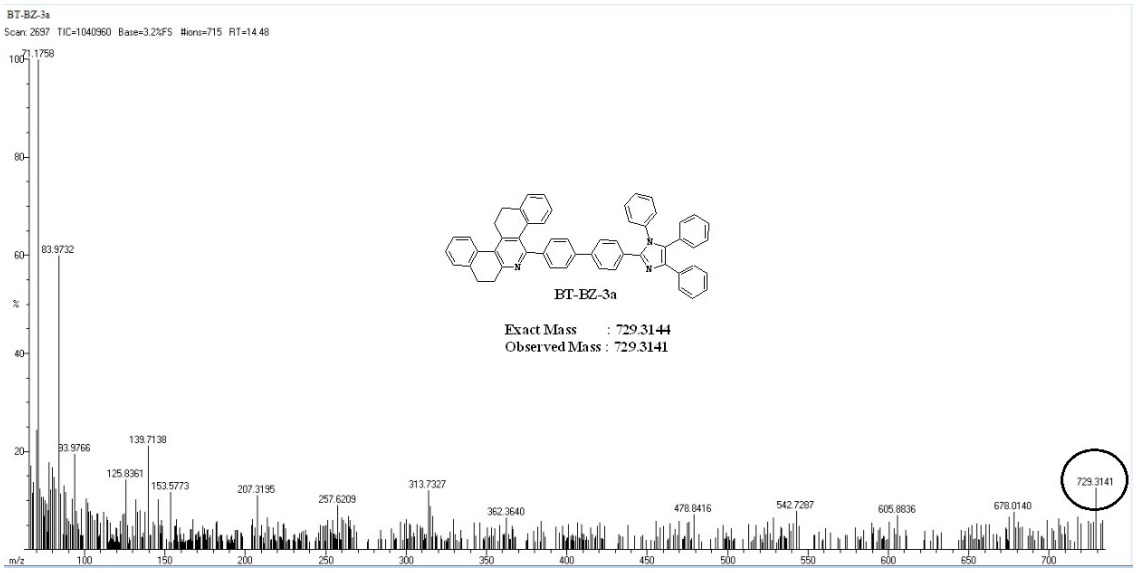

Fig. S3.1. HRMS Spectra of 5-(4'-(1,4,5-triphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3a)

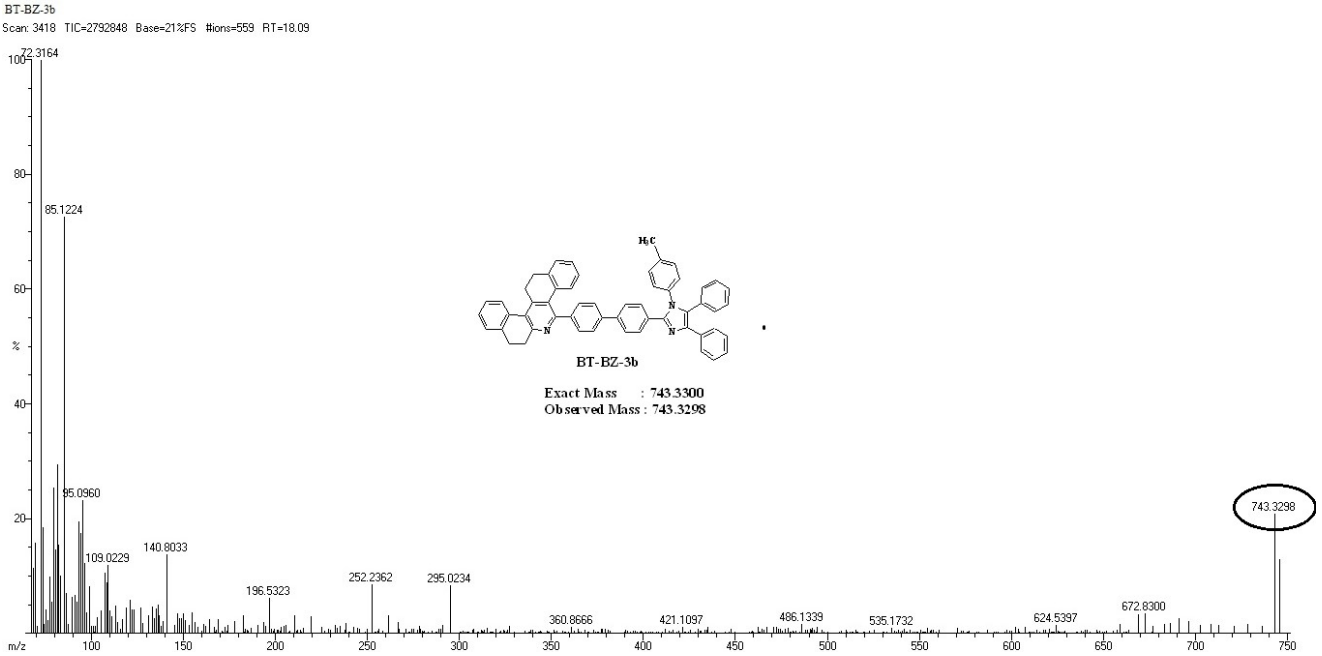

Fig. S3.2. HRMS Spectra of (4,5-diphenyl-1-(p-tolyl)-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3b)

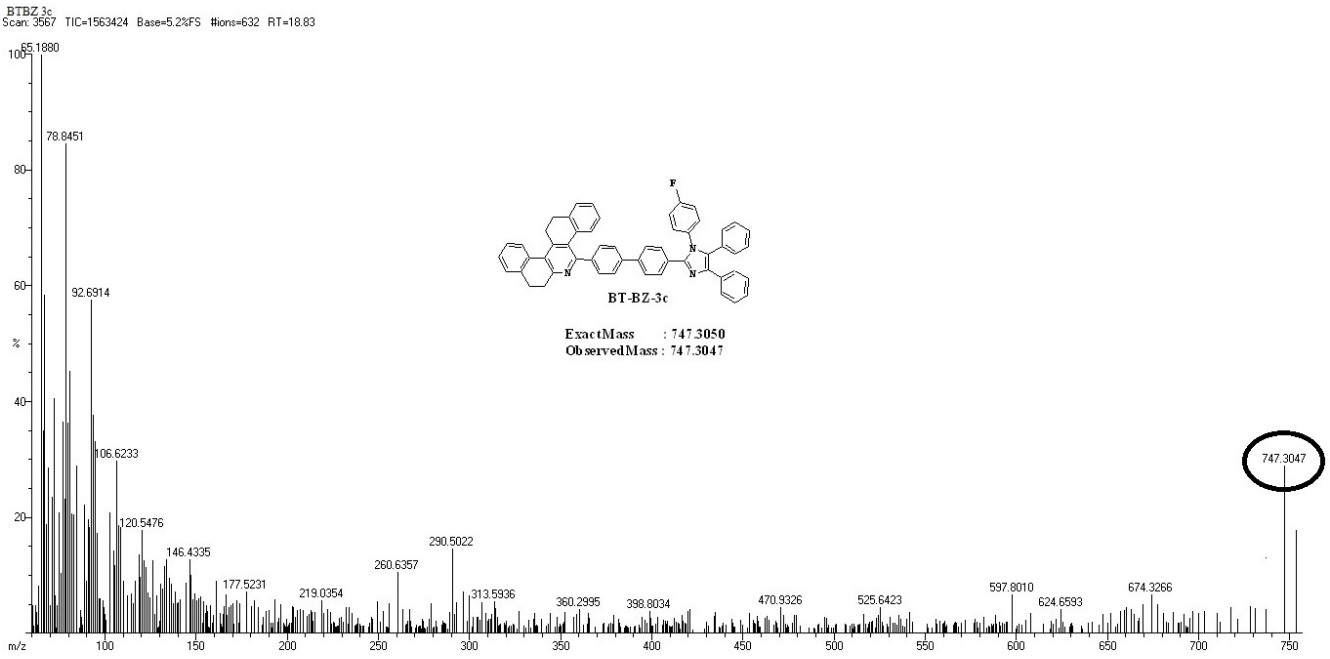

Fig. S3.3. HRMS Spectra of 5-(4'-(1-(4-fluorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3c)

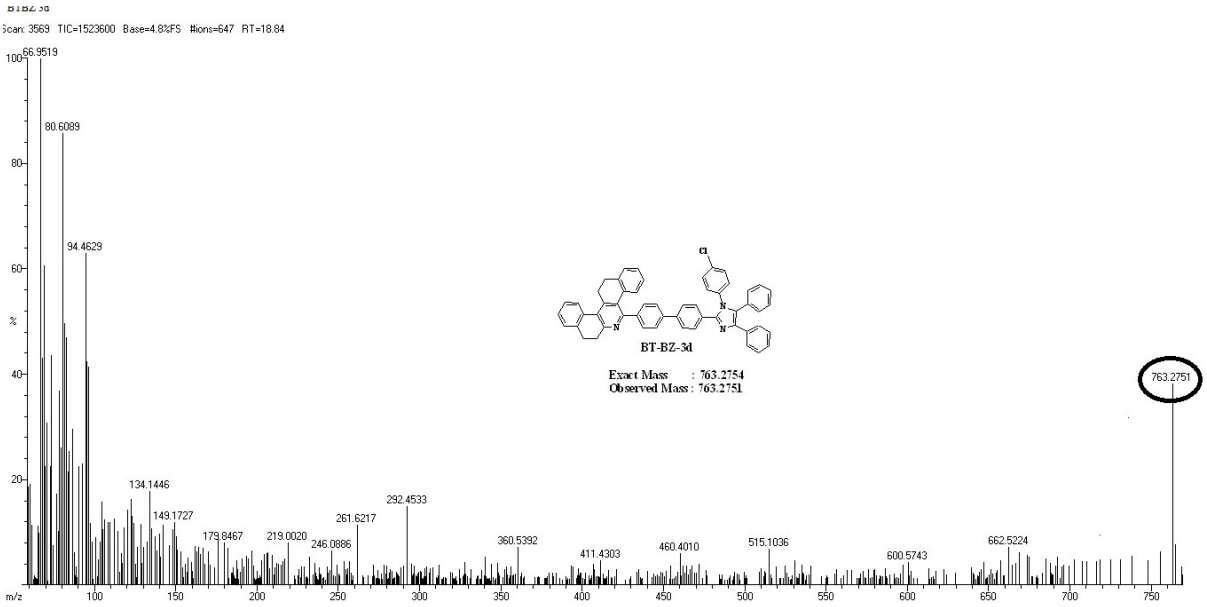

Fig. S3.4. HRMS Spectra of 5-(4'-(1-(4-chlorophenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3d)

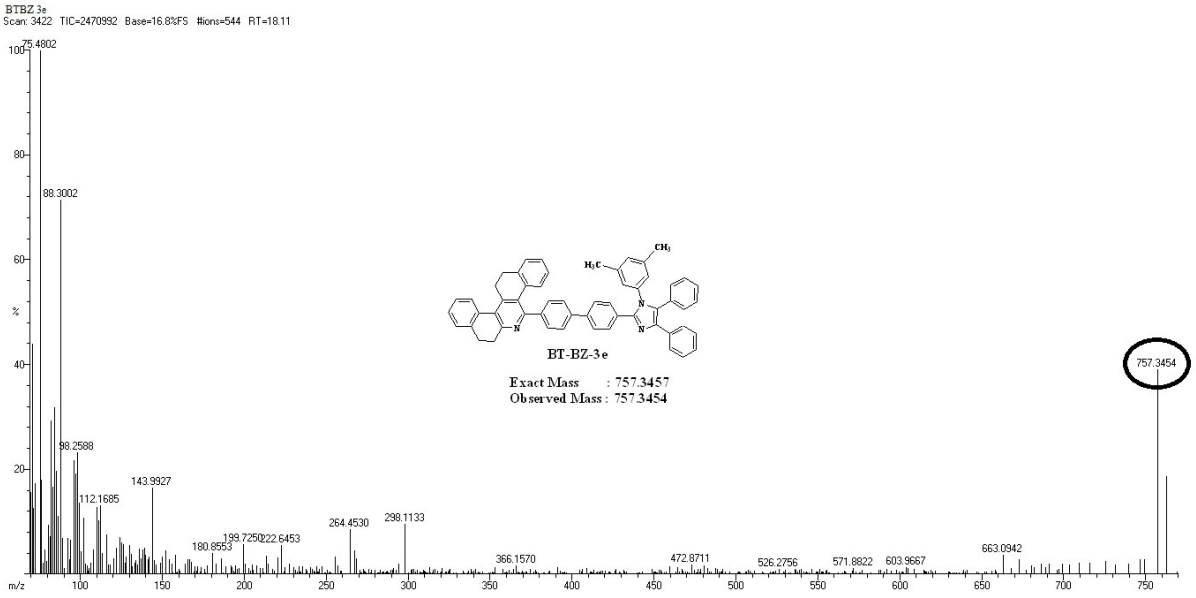

Fig. S3.5. HRMS Spectra of 5-(4'-(1-(3,5-dimethylphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3e)

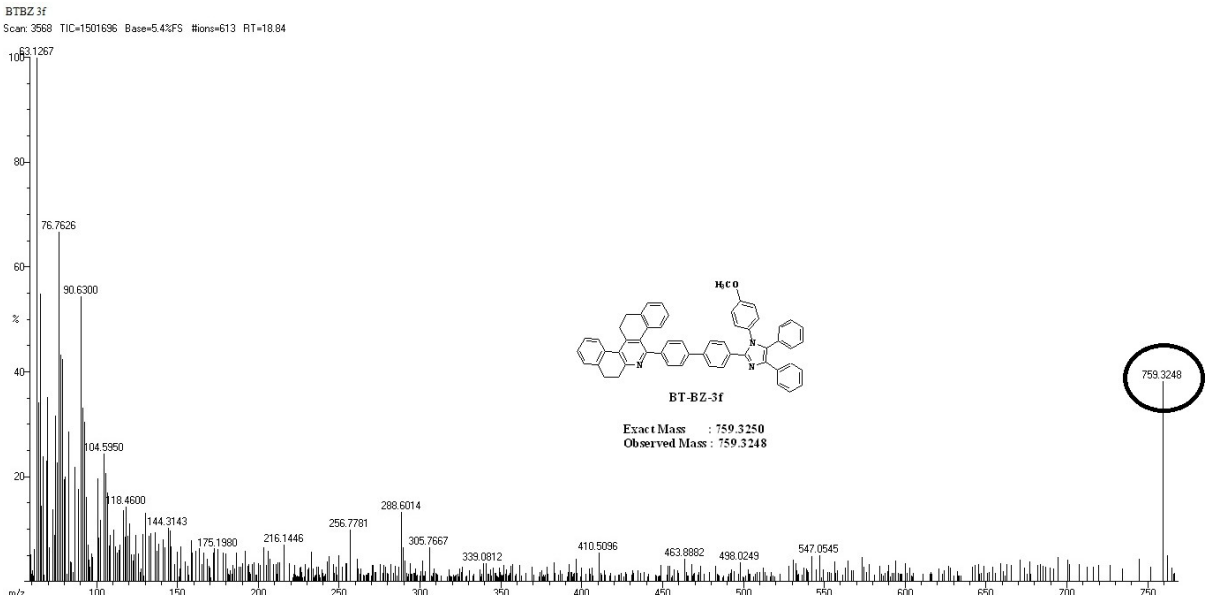

Fig. S3.6. HRMS Spectra of 5-(4'-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)-[1,1'-biphenyl]-4-yl)-7,8,13,14-tetrahydrodibenzo[a,i]phenanthridine(3f)

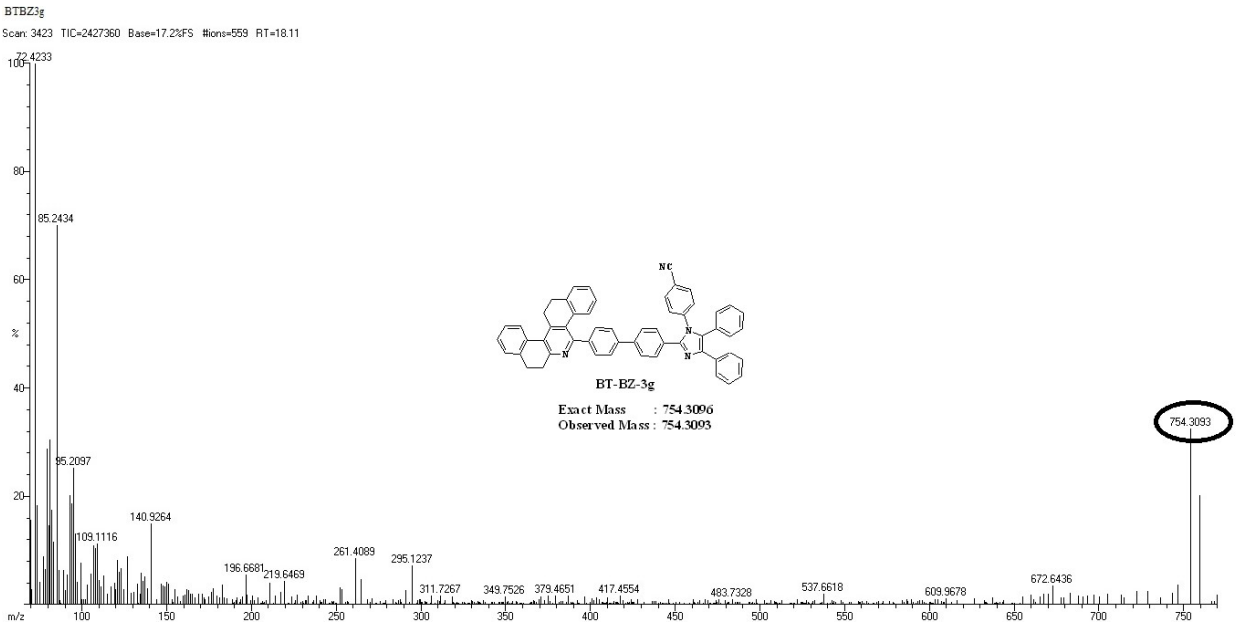

Fig.S3.7. HRMS Spectra of 4-(4,5-diphenyl-2-(4'-(7,8,13,14-tetrahydrodibenzo[a,i]phenanthridin-5-yl)-[1,1'-biphenyl]-4-yl)-1H-imidazol-1-yl)benzonitrile(3g)

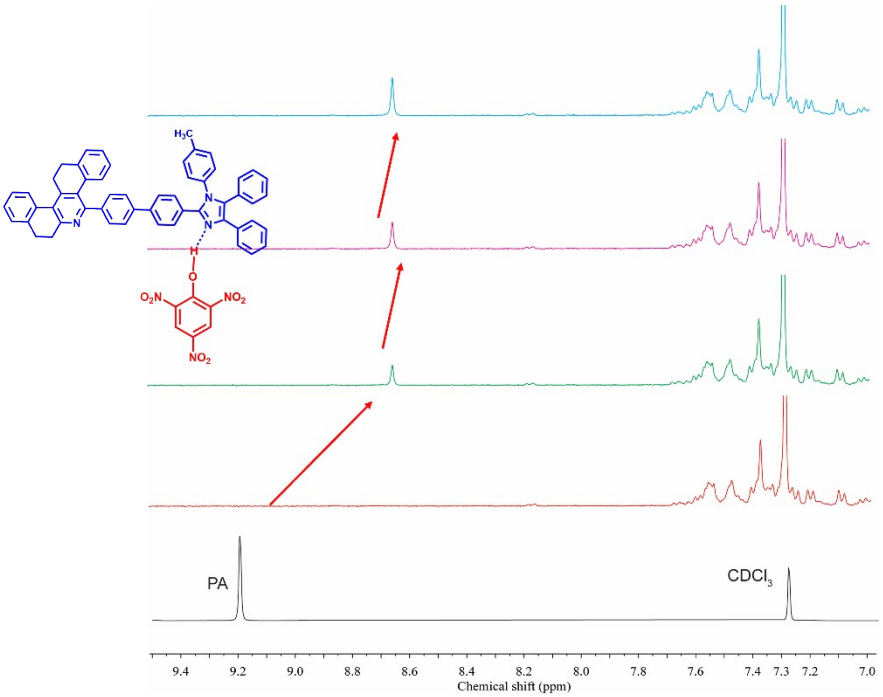

Fig. S4.1 ^{1}H NMR spectrum of BTBZ-3b with PA (0, 0.5, 1.0 equiv) in CDCl3.

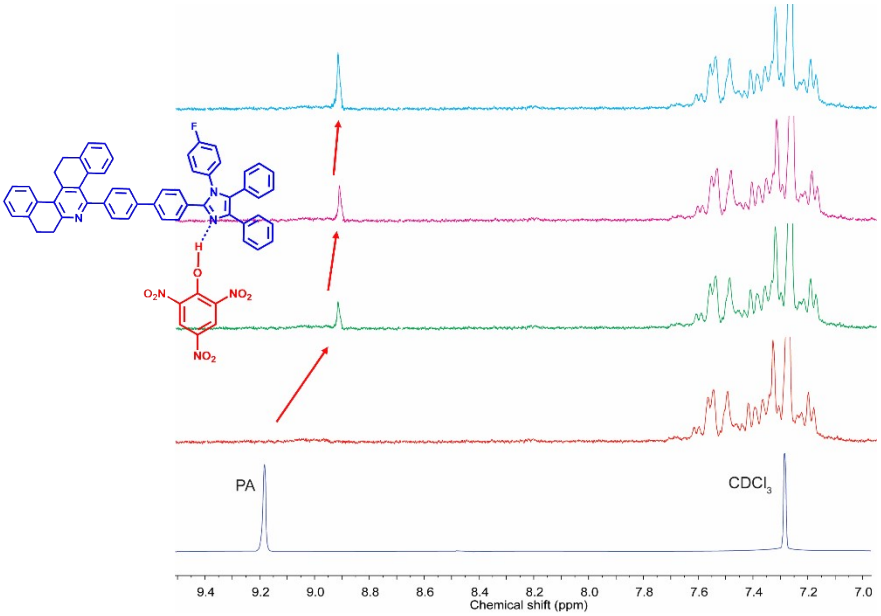

Fig. S4.2 [1]H NMR spectrum of BTBZ-3c with PA (0, 0.5, 1.0 equiv) in CDCl3.

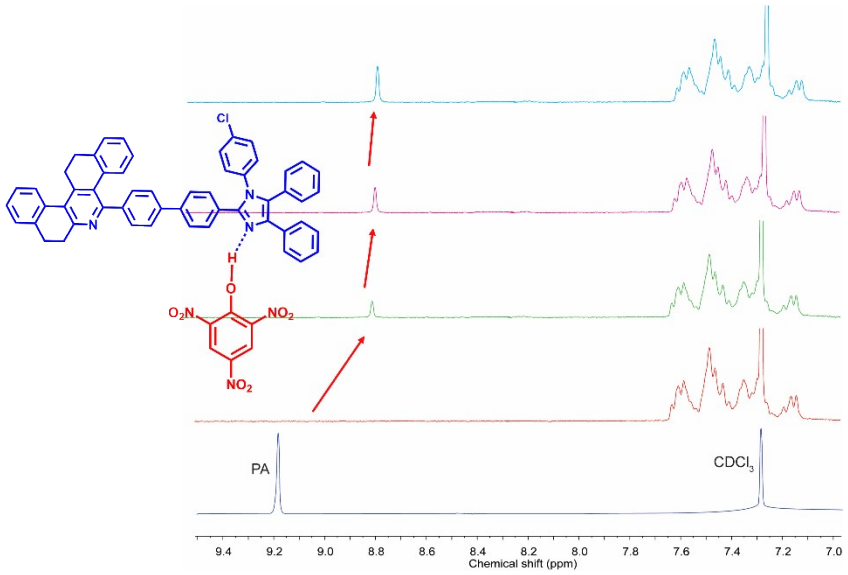

Fig. S4.3 [1]H NMR spectrum of BTBZ-3d with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

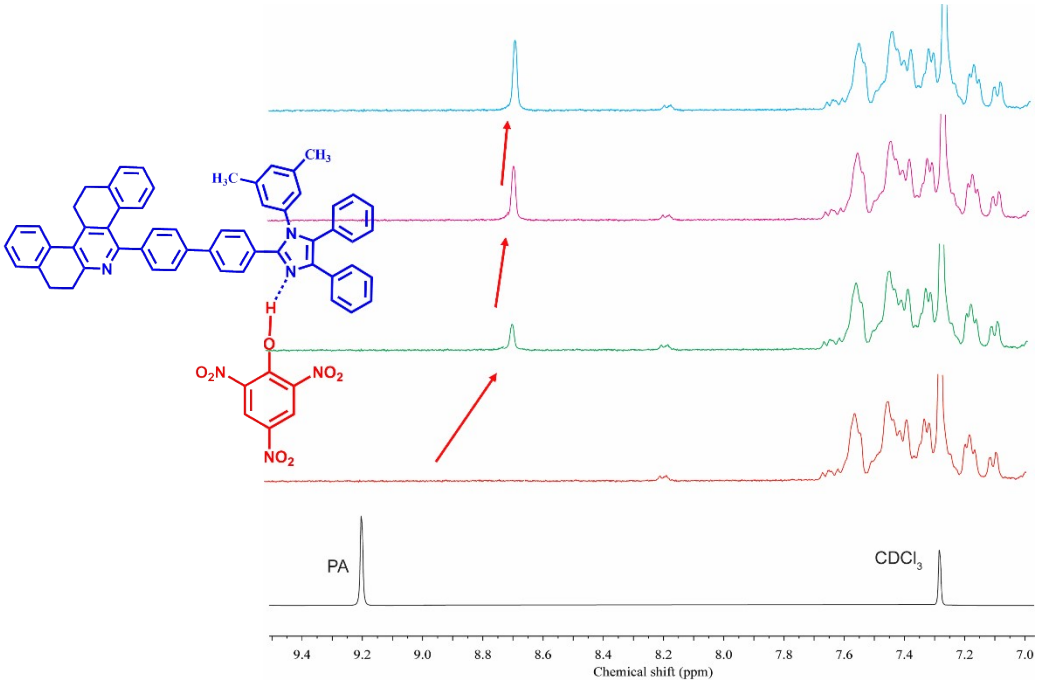

Fig. S4.4 ^{1}H NMR spectrum of BTBZ-3e with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

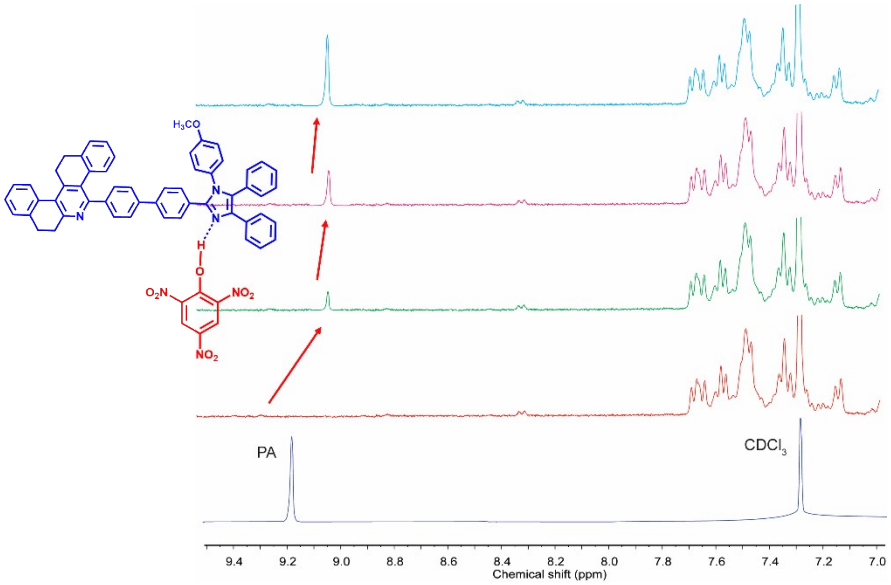

Fig. S4.5 ^{1}H NMR spectrum of BTBZ-3f with PA (0, 0.5, 1.0 equiv) in $CDCl_3$.

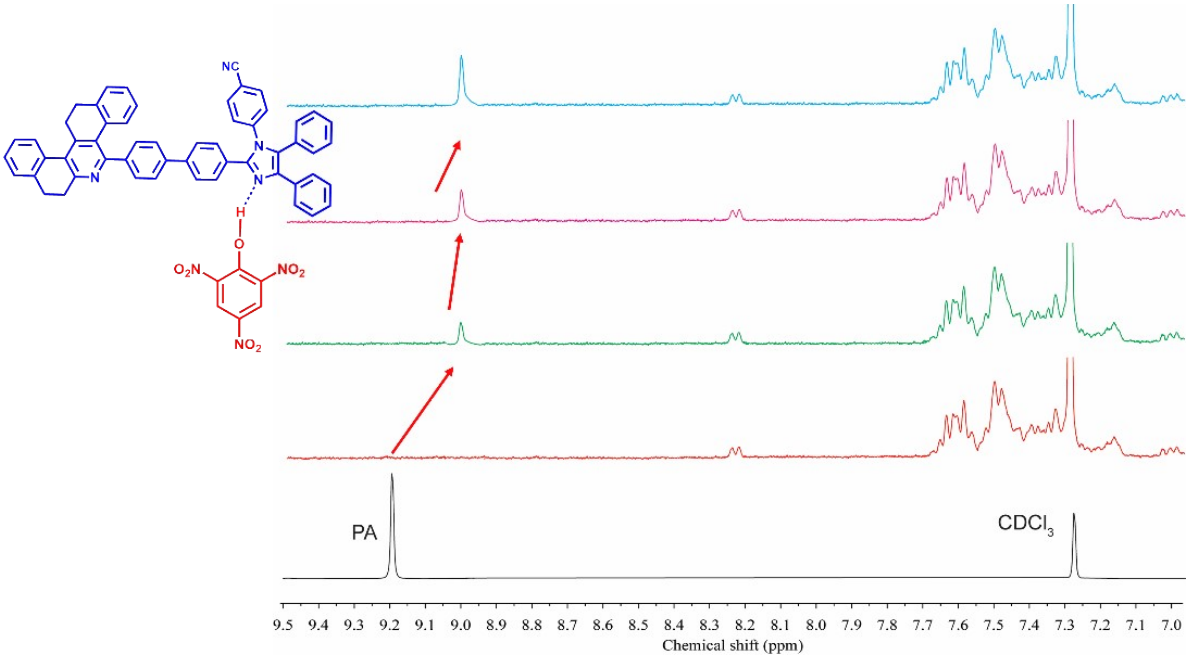

Fig. S4.6 ^{1}H NMR spectrum of BTBZ-3g with PA (0, 0.5, 1.0 equiv) in $CDCl_3$

SI3. Theoretical study of fluorophores

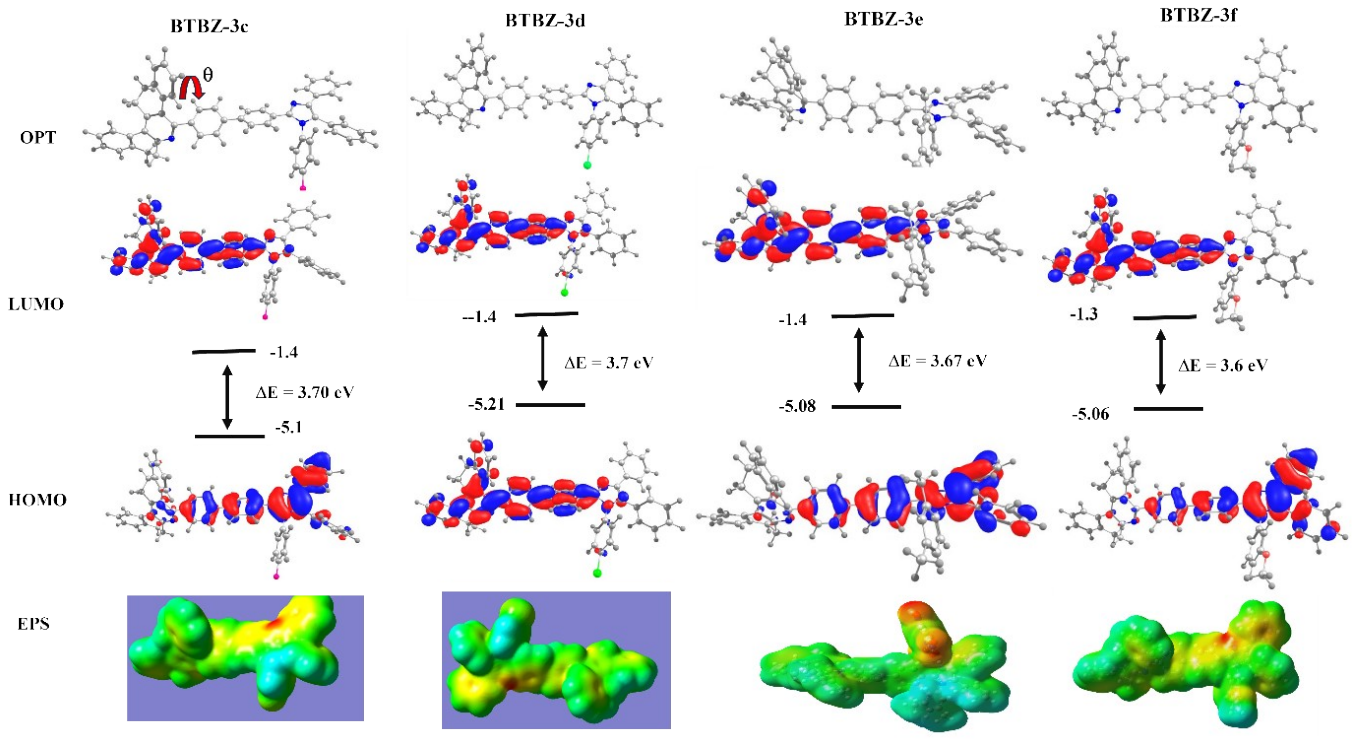

Fig. S5. Optimized geometries and calculated electron distributions of FMOs of the fluorophores

Table S1: Computed vertical transitions and their oscillator strengths and configurations of fluorophores.

Compound	State	Energy (eV)	λ_{max} nm	*f*	Configuration
BT-BZ-3a Singlet	Gas	3.3283	372.52	1.0659	HOMO-1 → LUMO (14.11%). HOMO → LUMO (68.30%).
		3.7463	330.95	0.219	HOMO-1 → LUMO (67.28%).
		3.8712	320.27	0.0411	HOMO-1→ LUMO+2 (44.04%). HOMO-2 → LUMO+4 (41.23%).
		3.1921	316.92	0.0334	HOMO → LUMO (10.22%). HOMO-1→ LUMO+1(28.20%). HOMO → LUMO+1(54.83%). HOMO → LUMO+4 (11.10%).
		3.9285	315.60	0.0794	HOMO → LUMO+1 (13.76%). HOMO → LUMO+2 (31.32%). HOMO → LUMO+3 (56.32%). HOMO → LUMO+4 (13.41%).
		3.9609	313.02	0.1204	HOMO → LUMO+3 (15.43%). HOMO → LUMO+4 (50.69%).
	DCM	3.3303	372.30	1.3810	HOMO-1 → LUMO (15.62%). HOMO → LUMO (67.76%).
		3.7287	332.51	0.0642	HOMO-1 → LUMO (6769%).
		3.9605	313.05	0.1182	HOMO-2 → LUMO (21.73%). HOMO → LUMO+1 (51.76%).
Triplet	Gas	2.5945	417.88	0	HOMO-1→ LUMO (38.19%). HOMO → LUMO (46.84%). HOMO → LUMO+2 (18.48%).
	DCM	2.6045	476.03	0	HOMO-2→ LUMO+2 (11.66%). HOMO-1 → LUMO (34.95%). HOMO → LUMO (49.84%). HOMO → LUMO+1 (12.56%).

BT-BZ-3b Singlet	Gas	3.3165	373.85	01.0396	HOMO-1 → LUMO (13.70%). HOMO → LUMO (68.41%).
		3.7498	330.64	0.2432	HOMO-1 → LUMO (69.23%).
		3.8899	318.73	0.41067	HOMO → LUMO (43.66%).
	DCM	3.3242	372.98	1.3696	HOMO → LUMO (67.79%).
		3.7315	332.26	0.0811	HOMO-1 → LUMO (67.73 %).
					HOMO → LUMO (15.16%).
		3.9514	313.77	0.1717	HOMO-2 → LUMO (15.46%). HOMO-1 → LUMO+2 (20.34%). HOMO → LUMO+1 (60.32%).
Triplet	Gas	2.5956	477.66	0	HOMO-1 → LUMO (37.52%). HOMO → LUMO (46.64%). HOMO → LUMO+2 (21.10%).
	DCM	2.6068	475.63	0	HOMO-2 → LUMO+2 (11.36%). HOMO-1 → LUMO+1 (15.42%). HOMO → LUMO (18.37%). HOMO → LUMO+1 (39.33%).
BT-BZ-3c Singlet	Gas	3.3594	369.07	1.1222	HOMO-1 → LUMO (14.56%). HOMO → LUMO (64.16%).
		3.7368	331.87	0.0119	HOMO → LUMO (59.51%). HOMO → LUMO+3 (16.25%).
		3.7633	329.46	0.1517	HOMO-1 → LUMO (67.19%).
	DCM	3.3476	370.37	1.3985	HOMO → LUMO (67.73%).
		3.7413	331.39	0.0522	HOMO-1 → LUMO (67.64%). HOMO → LUMO (15.20%).
		3.9685	312.42	0.1315	HOMO-2 → LUMO (20.40%). HOMO-1 → LUMO+2 (24.71%). HOMO → LUMO+1 (52.78%).

Triplet	Gas	2.6061	475.75	0	HOMO-3 → LUMO+3 (11.19%). HOMO-2→ LUMO+2 (10.93%). HOMO-1→ LUMO (36.38%). HOMO → LUMO+2 (47.80%).
	DCM	2.6151	474.11	0	HOMO-2→ LUMO+2 (11.76%). HOMO-1 → LUMO+1 (16.66%). HOMO → LUMO (50.22%). HOMO → LUMO+1 (12.87%).
BT-BZ-3d Singlet	Gas	3.3688	368.04	1.0840	HOMO-1 → LUMO (14.19%). HOMO → LUMO+1 (67.05%).
		3.7097	334.21	0.0595	HOMO-1 → LUMO (31.85%). HOMO → LUMO+1 (56.41%). HOMO → LUMO+4 (25.30%).
		3.7515	330.49	0.1182	HOMO-1 → LUMO (58.63%).
	DCM	3.3558	369.46	1.3358	HOMO-1 → LUMO (15.77%). HOMO → LUMO (67.49%).
		3.7189	333.39	0.0582	HOMO-1 → LUMO (67.02%).
					HOMO → LUMO+1 (11.61%).
		3.8697	320.40	0.0772	HOMO → LUMO+1 (63.93%). HOMO → LUMO+3 (11.32%). HOMO → LUMO+4 (19.67%).
Triplet	Gas	2.6115	474.76	0	HOMO-2→ LUMO+3 (11.32%). HOMO-1 → LUMO (36.35%). HOMO-1 → LUMO+1 (14.68%). HOMO → LUMO (47.73%).
	DCM	2.6208	473.08	0	HOMO-2 → LUMO+2 (12.13%). HOMO-1 → LUMO (34.84%). HOMO-1 → LUMO+1 (17.74%). HOMO → LUMO (49.30%).
BT-BZ-3e Singlet	Gas	3.7373	331.75	0.2772	HOMO → LUMO (67.25%).

		3.8624	321.00	0.1836	HOMO → LUMO+2 (51.46%). HOMO → LUMO+3 (13.00%). HOMO → LUMO+4 (11.36%).
		3.9064	317.39	0.0236	HOMO-1 → LUMO+1 (26.10%). HOMO-1 → LUMO+2 (13.60%). HOMO → LUMO+1 (45.04%). HOMO → LUMO+2 (38.54%).
		3.9677	312.48	0.0403	HOMO → LUMO+3 (60.39%).
		4.1004	302.97	0.0357	HOMO → LUMO+3 (67.25%).
		4.23894	392.46	0.0357	HOMO → LUMO+5 (68.05%).
	DCM	3.3269	372.67	1.3221	HOMO → LUMO (67.60%).
		3.7192	333.36	0.1041	HOMO-1 → LUMO (67.68%). HOMO → LUMO (15.58%).
		3.9258	315.82	0.2337	HOMO → LUMO+1 (66.40%).
Triplet	Gas	2.6014	476.60	0	HOMO-1 → LUMO (39.43%). HOMO → LUMO (45.28%). HOMO → LUMO+2 (18.71%).
	DCM	2.6127	474.54	0	HOMO-2 → LUMO+2 (11.90%). HOMO-1 → LUMO+1 (15.73%). HOMO → LUMO (48.01%). HOMO → LUMO+1 (14.16%).
BT-BZ-3f Singlet	Gas	3.3056	375.08	0.9862	HOMO-1 → LUMO (13.74%). HOMO → LUMO (68.26%).
		3.7243	332.90	0.2776	HOMO-1 → LUMO (67.44%).
		3.8342	323.36	0.0896	HOMO → LUMO+1 (58.74%). HOMO → LUMO+1 (17.77%). HOMO → LUMO+4 (19.63%).
		3.9026	317.69	0.0252	HOMO-1 → LUMO+2 (27.16%). HOMO → LUMO+2 (52.21%).
		3.9167	316.56	0.1110	HOMO → LUMO+1 (19.69%). HOMO → LUMO+2 (23.93%).

					HOMO → LUMO+3 (61.04%).
		4.1102	301.65	0.1933	HOMO → LUMO+3 (12.39%). HOMO → LUMO+4 (64.91%).
		4.2416	292.31	0.0353	HOMO-7 → LUMO (26.77%). HOMO-3 → LUMO (22.02%). HOMO-1 → LUMO+2 (33.24%).
	DCM	3.3221	373.21	1.3200	HOMO → LUMO (67.58%).
		3.7080	334.37	0.0973	HOMO-1 → LUMO (67.68%). HOMO → LUMO (15.52%).
		3.9240	315.96	0.1861	HOMO → LUMO (67.16%).
Triplet	Gas	2.5930	478.16	0	HOMO-8 → LUMO (11.31%). HOMO-1 → LUMO (39.44%). HOMO → LUMO (45.26%). HOMO → LUMO+1 (17.62%).
	DCM	2.6051	475.92	0	HOMO-4 → LUMO+1 (11.18%). HOMO-3 → LUMO+2 (11.62%). HOMO → LUMO (48.31%).
BT-BZ-3g Singlet	Gas	3.0474	406.85	0.0084	HOMO-1 → LUMO (13.68%). HOMO → LUMO (69.17%).
		3.3874	366.01	1.0501	HOMO → LUMO (67.15%).
		3.6282	341.72	0.1317	HOMO → LUMO+2 (61.52%).
		3.7555	330.14	0.0540	HOMO-1 → LUMO+1 (64.38%). HOMO → LUMO+1 (15.91%). HOMO → LUMO+2 (18.66%).
		3.9788	311.61	0.0381	HOMO → LUMO+3 (39.67%). HOMO → LUMO+4 (32.85%).
		3.9934	310.48	0.1400	HOMO-2 → LUMO+1 (14.69%). HOMO-1 → LUMO+4 (14.57%). HOMO → LUMO+2 (19.90%). HOMO → LUMO+3 (46.34%).

					HOMO → LUMO+5 (17.82%).
		4.1474	298.94	0.0279	HOMO → LUMO+2 (38.46%). HOMO → LUMO+5 (4053%).
	DCM	3.2201	385.03	0.0317	HOMO-1 → LUMO (15.48%). HOMO → LUMO (68.65%).
		3.3785	366.98	1.3217	HOMO → LUMO (67.45%).
		3.7178	333.49	0.0341	HOMO-1 → LUMO (56.22%). HOMO → LUMO (12.23%).
Triplet	Gas	2.6154	474.05	0	HOMO-2 → LUMO+4 (11.13%). HOMO → LUMO+1 (48.62%).
	DCM	2.6270	471.97	0	HOMO-2 → LUMO+3 (12.13%). HOMO → LUMO+1 (48.62%).
Orbital contributions below 10% are omitted					

SI3.1: Optimized Cartesian coordinates

1) BT-BZ-3a

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6	9.121709000	2.244792000	-0.780477000

6	9.034596000	-1.329758000	-0.894954000
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1	-3.665241000	1.950285000	-0.536865000

2) BT-BZ-3b

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1	3.522482000	2.156293000	0.324471000
1	1.350393000	-2.233320000	-0.378111000
6	-5.663831000	2.143581000	1.885928000
6	-5.462557000	3.478573000	2.232227000
6	-5.127412000	4.436339000	1.265878000

6	-4.994289000	4.013854000	-0.063432000
6	-5.196730000	2.682770000	-0.422054000
6	-5.530170000	1.742877000	0.554978000
1	-5.563563000	3.779783000	3.271498000
1	-4.728788000	4.736338000	-0.830535000
6	12.101537000	1.649663000	-1.481054000
6	11.037139000	2.038447000	-2.294954000
6	9.721701000	1.700968000	-1.974587000
6	9.453781000	0.925301000	-0.819844000
6	10.532769000	0.587428000	0.015527000
6	11.841934000	0.937869000	-0.311638000
6	8.556928000	2.196470000	-2.800536000
6	8.041881000	0.572468000	-0.508675000
6	7.030934000	1.439354000	-0.987930000
6	7.413330000	2.608572000	-1.865118000
6	5.327348000	0.199464000	-0.029507000
6	6.248905000	-0.702367000	0.550860000
6	7.620778000	-0.558823000	0.218163000
1	8.869594000	3.035319000	-3.430379000
1	13.118712000	1.923855000	-1.744859000
1	11.226252000	2.628937000	-3.188007000
1	10.350575000	0.073858000	0.951222000
1	12.653878000	0.663218000	0.355296000
1	7.741899000	3.453693000	-1.242869000
7	5.733583000	1.245300000	-0.772606000
1	6.527011000	2.930874000	-2.416159000

1	8.201461000	1.405326000	-3.476747000
6	7.814055000	-3.035211000	0.598887000
6	6.641296000	-2.956480000	1.540979000
6	8.554407000	-1.689473000	0.611963000
6	5.877316000	-1.771035000	1.519392000
6	6.336629000	-3.967203000	2.454383000
6	5.294825000	-3.811322000	3.368389000
6	4.565731000	-2.621266000	3.383753000
1	5.067566000	-4.603287000	4.075985000
1	6.931366000	-4.877349000	2.456525000
1	8.491077000	-3.844895000	0.888850000
1	9.407068000	-1.719416000	-0.070236000
1	7.477421000	-3.248883000	-0.425679000
1	-5.905903000	1.406943000	2.644868000
1	8.959136000	-1.524439000	1.620911000
1	-5.090268000	2.364690000	-1.453982000
1	3.771758000	-2.475827000	4.110238000
6	-8.961808000	-2.577976000	-0.699336000
6	-8.968251000	0.935012000	-1.093774000
1	-8.573665000	0.689741000	-2.074788000
1	-9.368282000	-1.828492000	-0.030287000
6	4.857705000	-1.609716000	2.471652000
1	4.293226000	-0.685124000	2.501970000
1	3.797984000	-2.070103000	-0.348969000
6	-4.939952000	5.886697000	1.641774000
1	-5.883431000	6.440108000	1.557536000

1	-4.592500000	5.991570000	2.673605000
1	-4.215018000	6.379220000	0.987269000

3) BT-BZ-3c

6	7.943138000	4.525202000	-2.397691000
6	7.114525000	3.507654000	-1.932215000
6	7.618250000	2.492319000	-1.100162000
6	9.801710000	3.559259000	-1.206168000
6	9.292957000	4.555064000	-2.041100000
6	6.702383000	1.435586000	-0.633164000
6	8.244312000	-0.561808000	0.072160000
6	6.977661000	0.182502000	-0.103452000
6	8.777570000	-0.819180000	1.345386000
1	8.257848000	-0.451871000	2.224760000
6	9.976566000	-1.517302000	1.487556000
6	10.664983000	-1.964957000	0.358965000
6	10.149740000	-1.708570000	-0.912848000
1	7.533317000	5.298417000	-3.041731000
1	6.064114000	3.483511000	-2.199608000
1	10.846997000	3.578194000	-0.910402000
1	9.939360000	5.348610000	-2.404825000
1	10.376320000	-1.705172000	2.479806000
1	11.599666000	-2.506693000	0.470005000
1	10.681848000	-2.050769000	-1.795612000
6	4.769282000	0.544074000	-0.203055000
7	5.342183000	1.630423000	-0.684530000
7	5.728658000	-0.381057000	0.184790000

6	0.469951000	0.221240000	-0.055405000
6	1.264144000	-0.544815000	0.813032000
6	2.653400000	-0.466686000	0.788482000
6	3.309467000	0.382517000	-0.117869000
6	2.517245000	1.162673000	-0.980684000
6	1.132040000	1.082997000	-0.948676000
6	-1.008774000	0.125776000	-0.029236000
6	-1.653525000	-1.101116000	0.204224000
6	-3.041220000	-1.193174000	0.219052000
6	-3.842758000	-0.057771000	0.026068000
6	-3.203247000	1.167611000	-0.216805000
6	-1.815613000	1.255997000	-0.247183000
1	0.785980000	-1.188834000	1.544754000
1	3.220754000	-1.054873000	1.498682000
1	3.014332000	1.827574000	-1.677757000
1	0.551205000	1.674983000	-1.649436000
1	-1.059069000	-1.999515000	0.341096000
1	-3.523062000	-2.154248000	0.363119000
1	-1.348984000	2.220748000	-0.421344000
6	5.681439000	-2.148092000	1.890587000
6	5.483011000	-3.479506000	2.251823000
6	5.123768000	-4.392180000	1.266039000
6	4.958426000	-4.018405000	-0.062997000
6	5.164599000	-2.685794000	-0.413884000
6	5.521729000	-1.749003000	0.560391000
1	5.599321000	-3.814063000	3.276467000

1	4.677818000	-4.762930000	-0.799373000
6	-12.103680000	-1.667557000	-1.447431000
6	-11.040657000	-2.067478000	-2.257720000
6	-9.724546000	-1.726994000	-1.943359000
6	-9.454686000	-0.936695000	-0.799032000
6	-10.532258000	-0.587398000	0.033410000
6	-11.842084000	-0.941126000	-0.287485000
6	-8.561151000	-2.234351000	-2.764042000
6	-8.042176000	-0.580551000	-0.494452000
6	-7.032419000	-1.454422000	-0.963562000
6	-7.416798000	-2.634953000	-1.824470000
6	-5.327082000	-0.202616000	-0.024452000
6	-6.246973000	0.707767000	0.544717000
6	-7.619512000	0.560307000	0.216324000
1	-8.875247000	-3.081267000	-3.382239000
1	-13.121384000	-1.944390000	-1.706367000
1	-11.231403000	-2.669258000	-3.142848000
1	-10.348335000	-0.061943000	0.962151000
1	-12.652959000	-0.657478000	0.376968000
1	-7.745404000	-3.471316000	-1.190547000
7	-5.734639000	-1.258293000	-0.752630000
1	-6.531434000	-2.965459000	-2.372164000
1	-8.205778000	-1.452587000	-3.451115000
6	-7.811362000	3.041794000	0.563800000
6	-6.636215000	2.975707000	1.503932000
6	-8.551976000	1.696516000	0.596636000

6	-5.872783000	1.789748000	1.497224000
6	-6.328567000	3.999307000	2.401881000
6	-5.284397000	3.856045000	3.315254000
6	-4.555877000	2.665933000	3.345790000
1	-5.054954000	4.657915000	4.010884000
1	-6.922902000	4.909657000	2.392554000
1	-8.487556000	3.855373000	0.844605000
1	-9.406100000	1.717424000	-0.084063000
1	-7.477273000	3.241770000	-0.464361000
1	5.947562000	-1.412334000	2.641403000
1	-8.954636000	1.545151000	1.608555000
1	5.045110000	-2.365135000	-1.443131000
1	-3.760249000	2.530429000	4.072389000
6	8.974882000	2.539993000	-0.736343000
6	8.949072000	-1.014488000	-1.055232000
1	8.548713000	-0.812216000	-2.043738000
1	9.384497000	1.786101000	-0.074311000
6	-4.850777000	1.641553000	2.449094000
1	-4.286907000	0.717069000	2.491614000
1	-3.797102000	2.059561000	-0.385767000
9	4.927972000	-5.679618000	1.610845000

4) BT-BZ-3d

6	-7.849145000	-5.133827000	-1.318691000
6	-7.033228000	-4.065715000	-0.953865000
6	-7.499769000	-2.742496000	-1.040313000
6	-9.615347000	-3.593920000	-1.884829000

6	-9.146469000	-4.904506000	-1.781579000
6	-6.595403000	-1.642104000	-0.657982000
6	-8.161058000	0.332983000	0.041941000
6	-6.882311000	-0.351353000	-0.233447000
6	-9.054803000	-0.211422000	0.980437000
1	-8.786142000	-1.129107000	1.493944000
6	-10.272950000	0.411107000	1.247329000
6	-10.617036000	1.592957000	0.588324000
6	-9.737332000	2.144780000	-0.344397000
1	-7.470707000	-6.149313000	-1.240881000
1	-6.021917000	-4.236590000	-0.601625000
1	-10.617071000	-3.401775000	-2.258972000
1	-9.782817000	-5.737776000	-2.065403000
1	-10.951463000	-0.025131000	1.974597000
1	-11.564784000	2.079607000	0.798824000
1	-9.999895000	3.060810000	-0.865477000
6	-4.670122000	-0.691241000	-0.350205000
7	-5.233657000	-1.825786000	-0.715476000
7	-5.634716000	0.259804000	-0.049638000
6	-0.378282000	-0.330389000	-0.161001000
6	-1.189307000	0.405860000	0.718614000
6	-2.577016000	0.317673000	0.672509000
6	-3.211992000	-0.512327000	-0.265895000
6	-2.405223000	-1.265422000	-1.137287000
6	-1.020499000	-1.173556000	-1.085839000
6	1.099355000	-0.224410000	-0.110593000

6	1.730485000	0.997861000	0.177815000
6	3.116915000	1.099493000	0.219115000
6	3.930675000	-0.021902000	-0.002569000
6	3.304913000	-1.241857000	-0.302173000
6	1.918686000	-1.339537000	-0.357660000
1	-0.725502000	1.031029000	1.475260000
1	-3.162510000	0.877058000	1.392699000
1	-2.887848000	-1.918883000	-1.855535000
1	-0.425182000	-1.741591000	-1.794092000
1	1.127323000	1.886503000	0.338137000
1	3.588681000	2.057961000	0.406862000
1	1.463177000	-2.300946000	-0.574362000
6	-5.849979000	2.117801000	1.535404000
6	-5.645950000	3.455466000	1.868837000
6	-5.005909000	4.295857000	0.958303000
6	-4.574394000	3.821687000	-0.280185000
6	-4.791915000	2.485895000	-0.611011000
6	-5.423247000	1.630440000	0.296759000
1	-5.975847000	3.840979000	2.826677000
1	-4.080982000	4.489030000	-0.977340000
6	12.199163000	1.718523000	-1.268654000
6	11.145553000	2.144150000	-2.078155000
6	9.827712000	1.780035000	-1.799661000
6	9.547135000	0.939120000	-0.694598000
6	10.614389000	0.563172000	0.139381000
6	11.925898000	0.941056000	-0.145002000

6	8.672693000	2.313101000	-2.615821000
6	8.133273000	0.558199000	-0.428790000
6	7.123308000	1.443420000	-0.875620000
6	7.510943000	2.663764000	-1.677436000
6	5.414398000	0.136644000	-0.021585000
6	6.333207000	-0.790197000	0.522180000
6	7.709567000	-0.616603000	0.223666000
1	8.988943000	3.188245000	-3.192127000
1	13.218328000	2.014452000	-1.499141000
1	11.344948000	2.784914000	-2.933515000
1	10.420177000	-0.003405000	1.041483000
1	12.728756000	0.635866000	0.519634000
1	7.823216000	3.473768000	-1.002420000
7	5.824200000	1.227108000	-0.695280000
1	6.631379000	3.011406000	-2.223853000
1	8.334086000	1.558709000	-3.340837000
6	7.918731000	-3.109503000	0.461091000
6	6.726747000	-3.096625000	1.382313000
6	8.646017000	-1.760832000	0.568634000
6	5.953707000	-1.917491000	1.418176000
6	6.412074000	-4.164040000	2.225198000
6	5.351535000	-4.071905000	3.126197000
6	4.613575000	-2.889605000	3.201032000
1	5.116757000	-4.907607000	3.778897000
1	7.013791000	-5.068575000	2.182893000
1	8.597418000	-3.929268000	0.716657000

1	9.512281000	-1.742867000	-0.096633000
1	7.604611000	-3.265077000	-0.580944000
1	-6.342830000	1.450847000	2.233883000
1	9.029138000	-1.652395000	1.593575000
1	-4.466583000	2.101709000	-1.571635000
1	3.805180000	-2.794304000	3.919881000
6	-8.800786000	-2.522122000	-1.523057000
6	-8.521587000	1.519679000	-0.618750000
1	-7.848986000	1.948308000	-1.354840000
1	-9.172288000	-1.509453000	-1.631492000
6	4.915344000	-1.821676000	2.359103000
1	4.343637000	-0.904252000	2.436281000
1	3.908317000	-2.122408000	-0.495046000
17	-4.741013000	5.980988000	1.377322000

5) BT-BZ-3e

6	-7.845668000	-5.173848000	1.321810000
6	-7.029583000	-4.132664000	0.886307000
6	-7.488271000	-2.803928000	0.903106000
6	-9.596936000	-3.594468000	1.821532000
6	-9.135735000	-4.911453000	1.787499000
6	-6.583691000	-1.731391000	0.449079000
6	-8.149953000	0.187701000	-0.389281000
6	-6.870316000	-0.466990000	-0.052591000
6	-8.519154000	1.427549000	0.158931000
1	-7.851775000	1.926319000	0.853964000

6	-9.737499000	2.018523000	-0.173611000
6	-10.612460000	1.379602000	-1.053466000
6	-10.259794000	0.144756000	-1.601383000
1	-7.473152000	-6.194245000	1.297044000
1	-6.023654000	-4.328548000	0.531575000
1	-10.593005000	-3.375853000	2.196410000
1	-9.772369000	-5.723688000	2.126454000
1	-10.005787000	2.976830000	0.261659000
1	-11.562468000	1.839621000	-1.309176000
1	-10.933611000	-0.359679000	-2.287860000
6	-4.661125000	-0.804100000	0.065901000
7	-5.223766000	-1.913952000	0.508089000
7	-5.624528000	0.128034000	-0.283096000
6	-0.363621000	-0.479681000	-0.111579000
6	-1.164194000	0.270114000	-0.988345000
6	-2.553667000	0.194919000	-0.950866000
6	-3.201765000	-0.635352000	-0.020944000
6	-2.403634000	-1.398245000	0.852183000
6	-1.018335000	-1.320004000	0.807230000
6	1.115424000	-0.392993000	-0.158306000
6	1.797277000	-0.247029000	-1.378724000
6	3.185298000	-0.172434000	-1.423009000
6	3.949723000	-0.216554000	-0.247105000
6	3.273789000	-0.373566000	0.972788000
6	1.886436000	-0.462766000	1.014922000
1	-0.692529000	0.937140000	-1.703566000

1	-3.128979000	0.779335000	-1.658040000
1	-2.896212000	-2.063398000	1.552554000
1	-0.430551000	-1.938457000	1.478640000
1	1.233644000	-0.227012000	-2.306601000
1	3.697846000	-0.097610000	-2.376013000
1	1.390873000	-0.567862000	1.975275000
6	-4.973612000	2.469123000	0.129244000
6	-4.794369000	3.757073000	-0.390612000
6	-5.056138000	4.077089000	-1.726987000
6	-5.515049000	3.059050000	-2.572701000
6	-5.698260000	1.767769000	-2.088550000
6	-5.423397000	1.470371000	-0.751442000
1	-4.441382000	4.538649000	0.278271000
1	-5.729675000	3.276729000	-3.615409000
6	12.323626000	-1.424164000	-1.441308000
6	11.313510000	-2.314628000	-1.806462000
6	9.972884000	-2.035826000	-1.538474000
6	9.622945000	-0.843280000	-0.858471000
6	10.648450000	0.065588000	-0.544903000
6	11.983651000	-0.221328000	-0.825450000
6	8.867101000	-2.951295000	-2.010530000
6	8.185676000	-0.577245000	-0.578814000
6	7.231752000	-1.165260000	-1.443685000
6	7.698611000	-2.104819000	-2.531037000
6	5.439191000	-0.206586000	-0.335933000
6	6.297864000	0.480131000	0.553023000

6	7.688091000	0.205567000	0.481693000
1	9.239704000	-3.625292000	-2.788304000
1	13.361550000	-1.656771000	-1.660455000
1	11.566061000	-3.237016000	-2.323541000
1	10.403599000	1.025158000	-0.106981000
1	12.753014000	0.502107000	-0.572074000
1	8.030889000	-1.530102000	-3.407734000
7	5.919472000	-1.000333000	-1.310859000
1	6.851502000	-2.719954000	-2.842568000
1	8.512867000	-3.583683000	-1.183446000
6	7.767768000	0.763823000	2.930303000
6	6.556022000	1.639747000	2.744586000
6	8.558184000	0.721490000	1.613899000
6	5.841606000	1.501159000	1.536458000
6	6.169581000	2.603275000	3.678010000
6	5.094009000	3.453057000	3.421117000
6	4.413715000	3.353524000	2.206459000
1	4.803351000	4.200676000	4.153368000
1	6.727281000	2.695700000	4.606786000
1	8.398798000	1.141190000	3.741126000
1	9.439482000	0.085158000	1.721472000
1	7.471115000	-0.259095000	3.202930000
1	8.921790000	1.735334000	1.392824000
1	-6.052156000	0.976716000	-2.741588000
1	3.594462000	4.030004000	1.981560000
6	-8.781970000	-2.549551000	1.388813000

6	-9.039238000	-0.443876000	-1.276291000
1	-8.764304000	-1.402172000	-1.705175000
1	-9.147016000	-1.530102000	1.442780000
6	4.787466000	2.390635000	1.271781000
1	4.260283000	2.331586000	0.326798000
1	3.838618000	-0.429110000	1.897227000
6	-4.879657000	5.487494000	-2.237180000
1	-5.836101000	6.024527000	-2.251487000
1	-4.192774000	6.059017000	-1.606925000
1	-4.489424000	5.496260000	-3.259539000
6	-4.677540000	2.178525000	1.579988000
1	-3.726111000	1.647144000	1.692226000
1	-4.612647000	3.106578000	2.153516000
1	-5.449401000	1.547659000	2.031322000

6) BT-BZ-3f

6	7.750579000	5.185312000	-1.100101000
6	6.947027000	4.086010000	-0.807787000
6	7.422127000	2.776668000	-0.998356000
6	9.521827000	3.707189000	-1.798851000
6	9.044458000	5.002456000	-1.592574000
6	6.529684000	1.643553000	-0.690266000
6	8.115021000	-0.372353000	-0.174316000
6	6.828690000	0.324059000	-0.372509000
6	9.029170000	0.108633000	0.778782000
1	8.768912000	0.984379000	1.364663000

6	10.256454000	-0.523319000	0.970432000
6	10.590033000	-1.652105000	0.219550000
6	9.689362000	-2.141564000	-0.727835000
1	7.365303000	6.188917000	-0.942102000
1	5.938482000	4.221102000	-0.432838000
1	10.520847000	3.551949000	-2.196783000
1	9.671354000	5.860002000	-1.819655000
1	10.950224000	-0.136456000	1.711172000
1	11.545303000	-2.146173000	0.370942000
1	9.942944000	-3.016417000	-1.319604000
6	4.615013000	0.657255000	-0.433490000
7	5.167369000	1.822117000	-0.715140000
7	5.588367000	-0.306547000	-0.221155000
6	0.325149000	0.274957000	-0.228436000
6	1.146766000	-0.562419000	0.544346000
6	2.534160000	-0.471148000	0.490561000
6	3.158515000	0.466684000	-0.348427000
6	2.340997000	1.317939000	-1.113448000
6	0.957197000	1.221549000	-1.054962000
6	-1.151925000	0.167011000	-0.169510000
6	-1.784402000	-1.078111000	-0.009793000
6	-3.170435000	-1.180633000	0.040555000
6	-3.983465000	-0.040078000	-0.044726000
6	-3.356809000	1.204034000	-0.216314000
6	-1.971146000	1.304182000	-0.279061000
1	0.691869000	-1.273937000	1.226727000

1	3.128051000	-1.115299000	1.127766000
1	2.815835000	2.051147000	-1.755744000
1	0.354437000	1.869893000	-1.683409000
1	-1.182244000	-1.980249000	0.041960000
1	-3.643179000	-2.152926000	0.128195000
1	-1.515681000	2.283038000	-0.393400000
6	5.791991000	-2.249585000	1.241482000
6	5.606795000	-3.618488000	1.484347000
6	5.009230000	-4.426901000	0.509469000
6	4.611084000	-3.856912000	-0.703054000
6	4.800088000	-2.503108000	-0.960544000
6	5.390345000	-1.703836000	0.026669000
1	4.149896000	-4.486945000	-1.457490000
6	-12.274201000	-1.616587000	-1.383172000
6	-11.230885000	-1.968400000	-2.240067000
6	-9.908481000	-1.637561000	-1.942307000
6	-9.612015000	-0.906752000	-0.765487000
6	-10.669172000	-0.606638000	0.111223000
6	-11.985499000	-0.949799000	-0.194213000
6	-8.765038000	-2.093235000	-2.819180000
6	-8.193345000	-0.560291000	-0.478986000
6	-7.192542000	-1.402299000	-1.020261000
6	-7.594642000	-2.537384000	-1.932981000
6	-5.467594000	-0.192423000	-0.060798000
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6	-7.756525000	0.542818000	0.280915000

1	-9.091450000	-2.907312000	-3.474062000
1	-13.297196000	-1.884816000	-1.630056000
1	-11.442085000	-2.524150000	-3.150290000
1	-10.463738000	-0.129352000	1.061208000
1	-12.780052000	-0.705042000	0.504546000
1	-7.903074000	-3.408230000	-1.336443000
7	-5.890589000	-1.209635000	-0.833975000
1	-6.722679000	-2.833122000	-2.520605000
1	-8.431354000	-1.273393000	-3.471881000
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6	-6.749957000	2.890186000	1.671340000
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6	-5.983891000	1.709143000	1.583831000
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6	-5.360644000	3.675964000	3.497621000
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1	-8.617733000	3.797153000	1.100549000
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1	-7.636275000	3.254953000	-0.260995000
1	-9.060393000	1.448099000	1.755173000
1	4.493760000	-2.060411000	-1.901360000
1	-3.817134000	2.316662000	4.148604000
6	8.719452000	2.604470000	-1.510104000
6	8.464044000	-1.506862000	-0.926428000

1	7.773280000	-1.887314000	-1.671957000
1	9.097433000	1.605882000	-1.697137000
6	-4.941239000	1.512917000	2.503916000
1	-4.374524000	0.589383000	2.483327000
1	-3.959020000	2.102030000	-0.303152000
1	4.853778000	-5.484950000	0.680435000
6	5.875447000	-5.432579000	3.016535000
1	6.428393000	-6.074610000	2.319508000
1	6.282573000	-5.558361000	4.020423000
1	4.818431000	-5.727056000	3.016164000
1	6.252410000	-1.634303000	2.005308000
8	6.036027000	-4.057201000	2.700434000

7) BT-BZ-3g

6	7.865095000	5.019129000	-1.255784000
6	7.043852000	3.942260000	-0.931024000
6	7.508245000	2.621355000	-1.055569000
6	9.632348000	3.493238000	-1.855920000
6	9.165454000	4.801041000	-1.715491000
6	6.598730000	1.512157000	-0.713152000
6	8.153877000	-0.503591000	-0.107143000
6	6.879589000	0.204674000	-0.341928000
6	9.045712000	-0.030162000	0.870537000
1	8.781161000	0.852824000	1.443620000
6	10.256909000	-0.679916000	1.102051000
6	10.595492000	-1.817333000	0.366596000
6	9.718155000	-2.297588000	-0.606988000

1	7.488510000	6.032599000	-1.148813000
1	6.030555000	4.104797000	-0.580699000
1	10.636756000	3.310483000	-2.227436000
1	9.805971000	5.641167000	-1.967861000
1	10.933626000	-0.300772000	1.862031000
1	11.537027000	-2.325969000	0.550697000
1	9.977348000	-3.178473000	-1.186951000
6	4.666969000	0.564372000	-0.431488000
7	5.236966000	1.707120000	-0.754244000
7	5.627447000	-0.405137000	-0.174031000
6	0.375698000	0.221756000	-0.215269000
6	1.189963000	-0.540793000	0.638690000
6	2.577680000	-0.458376000	0.582387000
6	3.208642000	0.391197000	-0.341035000
6	2.398964000	1.170158000	-1.186369000
6	1.014233000	1.084409000	-1.124525000
6	-1.102045000	0.123679000	-0.153597000
6	-1.738312000	-1.103194000	0.101531000
6	-3.124999000	-1.197186000	0.152864000
6	-3.932942000	-0.063743000	-0.023985000
6	-3.301923000	1.161367000	-0.289355000
6	-1.915697000	1.251778000	-0.355994000
1	0.728962000	-1.180745000	1.384601000
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1	-1.139411000	-2.000224000	0.227835000
1	-3.601552000	-2.158114000	0.314115000
1	-1.455625000	2.216764000	-0.545589000
6	5.874504000	-2.334985000	1.305681000
6	5.661804000	-3.696627000	1.569818000
6	4.976174000	-4.500563000	0.644367000
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6	4.734921000	-2.588895000	-0.817642000
6	5.408691000	-1.786777000	0.110357000
1	3.987642000	-4.554708000	-1.263301000
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6	-9.861294000	-1.753228000	-1.827183000
6	-9.563004000	-0.956150000	-0.694695000
6	-10.618953000	-0.603164000	0.163431000
6	-11.936158000	-0.960314000	-0.121356000
6	-8.718944000	-2.263723000	-2.674973000
6	-8.143520000	-0.596318000	-0.429297000
6	-7.145041000	-1.471627000	-0.919665000
6	-7.550171000	-2.657794000	-1.763103000
6	-5.417986000	-0.211122000	-0.033734000
6	-6.323756000	0.701387000	0.553922000
6	-7.704254000	0.549750000	0.262683000
1	-9.047815000	-3.114437000	-3.280091000
1	-13.250446000	-1.973202000	-1.500816000
1	-11.397578000	-2.704031000	-2.981838000

1	-10.411545000	-0.071904000	1.083894000
1	-12.729919000	-0.673821000	0.562237000
1	-7.861432000	-3.490517000	-1.115815000
7	-5.842459000	-1.272051000	-0.744352000
1	-6.678961000	-2.990799000	-2.331598000
1	-8.382420000	-1.485349000	-3.375223000
6	-7.890235000	3.033364000	0.596658000
6	-6.690433000	2.975986000	1.505703000
6	-8.627907000	1.687465000	0.659463000
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6	-5.291582000	3.871985000	3.273130000
6	-4.561822000	2.682434000	3.294597000
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1	-9.499982000	1.702104000	0.001753000
1	-7.583899000	3.225816000	-0.441536000
1	-9.003076000	1.543129000	1.682897000
1	4.384312000	-2.148300000	-1.744501000
1	-3.747544000	2.553188000	4.001375000
6	8.812666000	2.412647000	-1.534283000
6	8.509017000	-1.645453000	-0.845213000
1	7.837515000	-2.016699000	-1.613205000
1	9.183408000	1.403158000	-1.670696000
6	-4.879740000	1.650488000	2.414573000

1	-4.314851000	0.726296000	2.450474000
1	-3.901275000	2.051689000	-0.446655000
1	4.814075000	-5.550338000	0.862105000
1	6.399264000	-1.714503000	2.022014000
6	6.140924000	-4.266583000	2.796444000
7	6.525290000	-4.733255000	3.790000000

SI4. Chemosensing Application

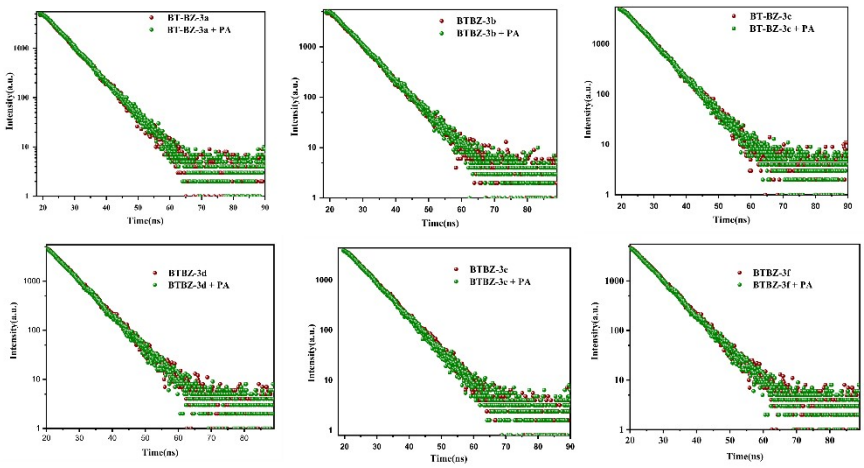

Fig S6. Lifetime of all the luminophores in the absence and presence of PA

Table S2: Lifetime of the respective compounds in the nanosecond range

Compounds	Lifetime without PA	Lifetime with PA
BTBZ-3a	4.56	4.43
BTBZ-3b	4.29	3.99
BTBZ-3c	4.16	3.98
BTBZ-3d	5.03	4.92
BTBZ-3e	3.97	3.68
BTBZ-3f	4.70	4.27
BTBZ-3g	5.06	4.99

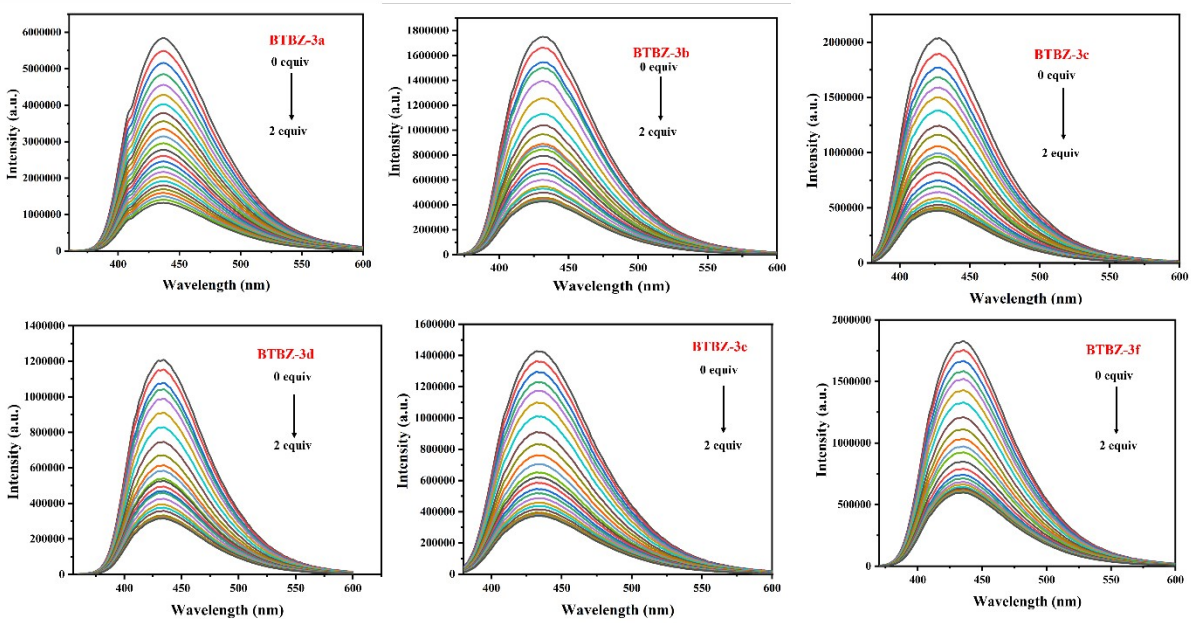

Figure S7. Change in the fluorescence of Fluorophores upon the addition of PA

Figure S8. Change in the fluorescence of Fluorophores upon the addition of other NACs

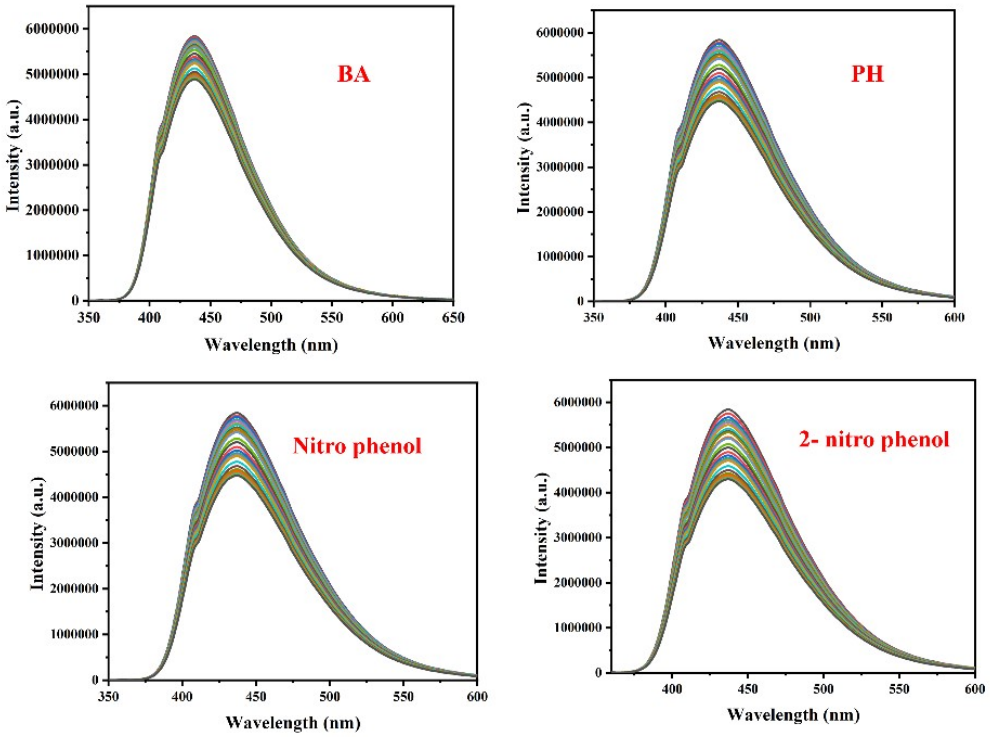

Figure S8a BTBZ-3a

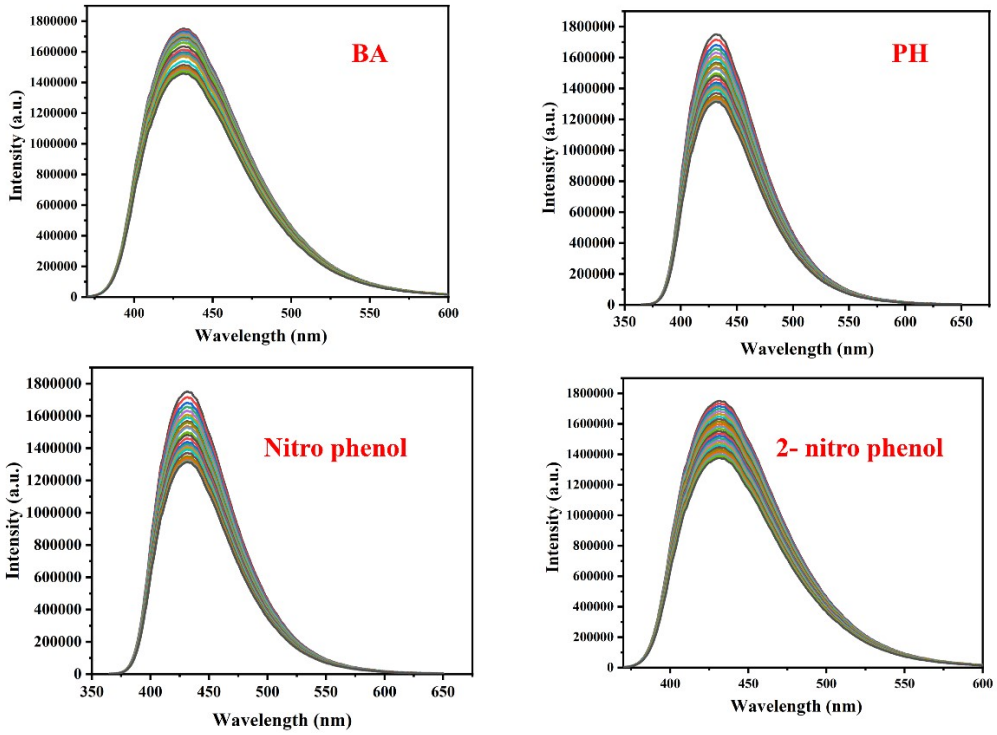

Figure S8b BTBZ-3b

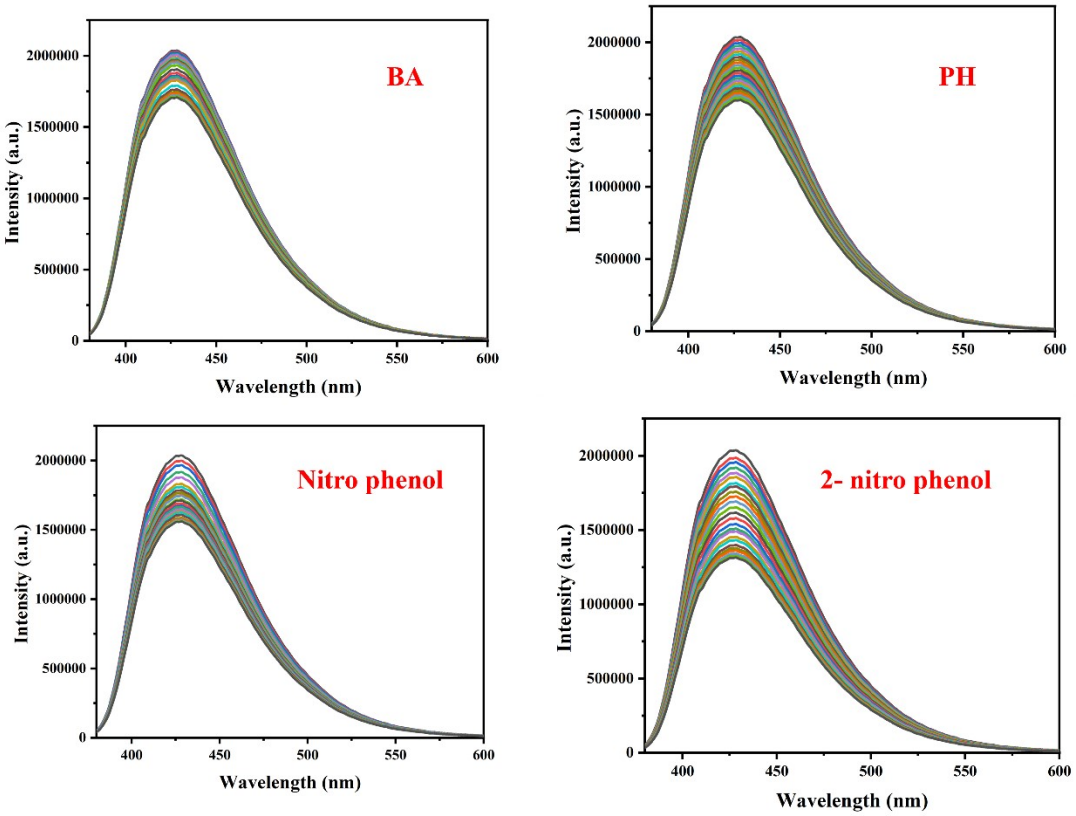

Figure S8c BTBZ-3c

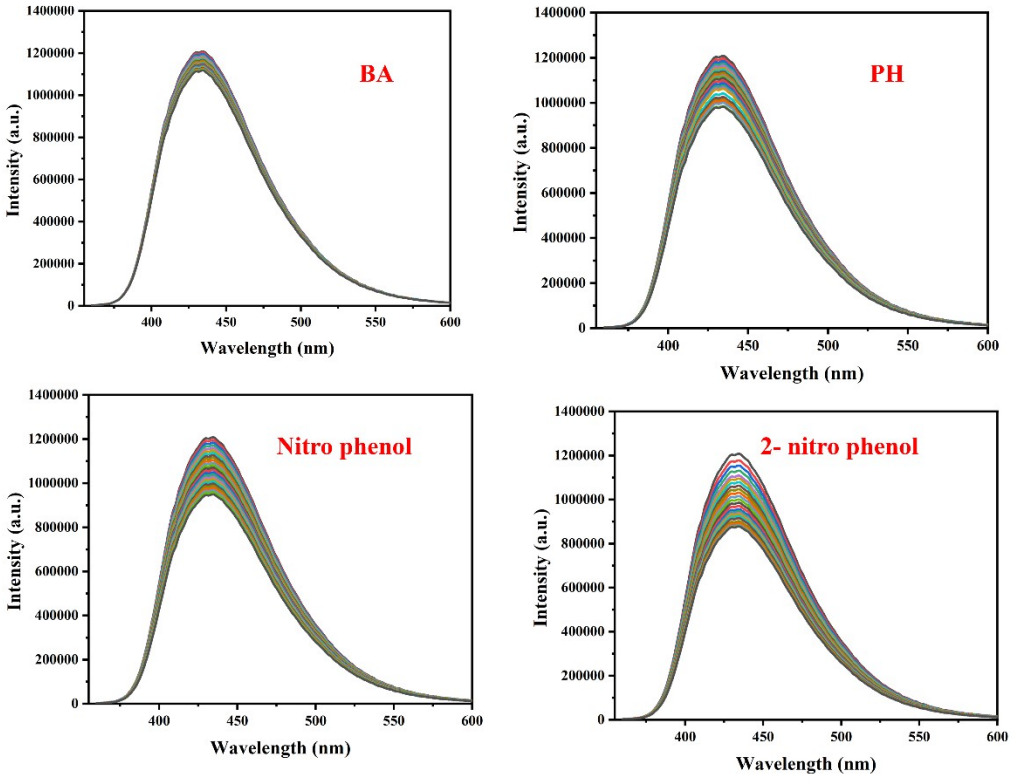

Figure S8d BTBZ-3d

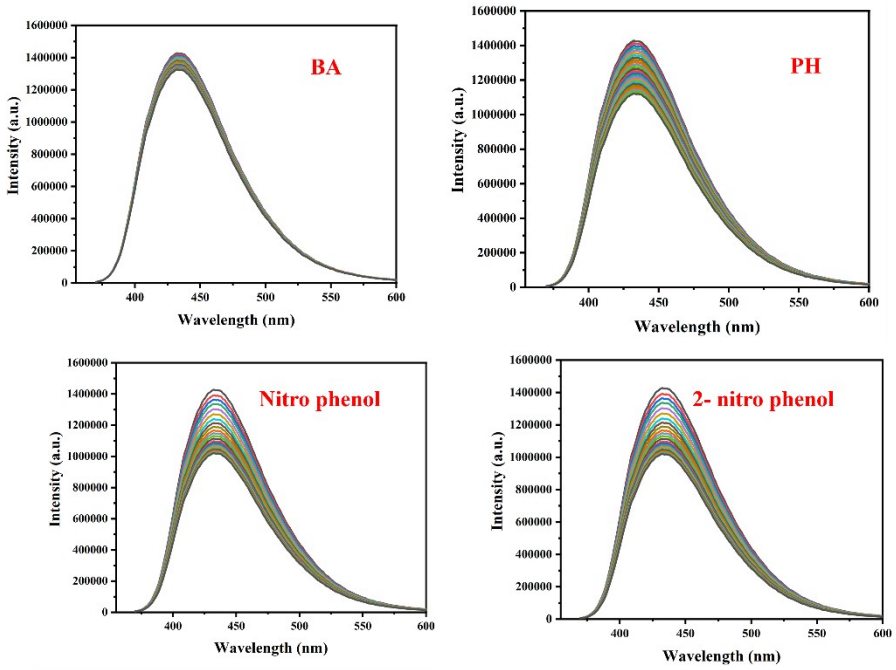

Figure S8e BTBZ-3e

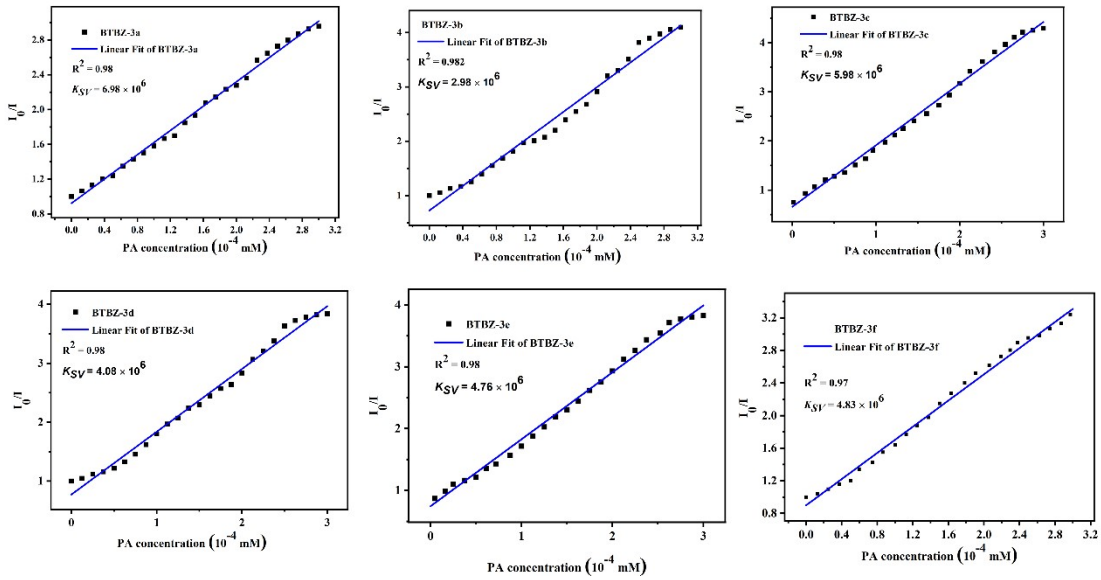

Figure S9. Stern–Volmer plots for fluorophores using PA as a quencher

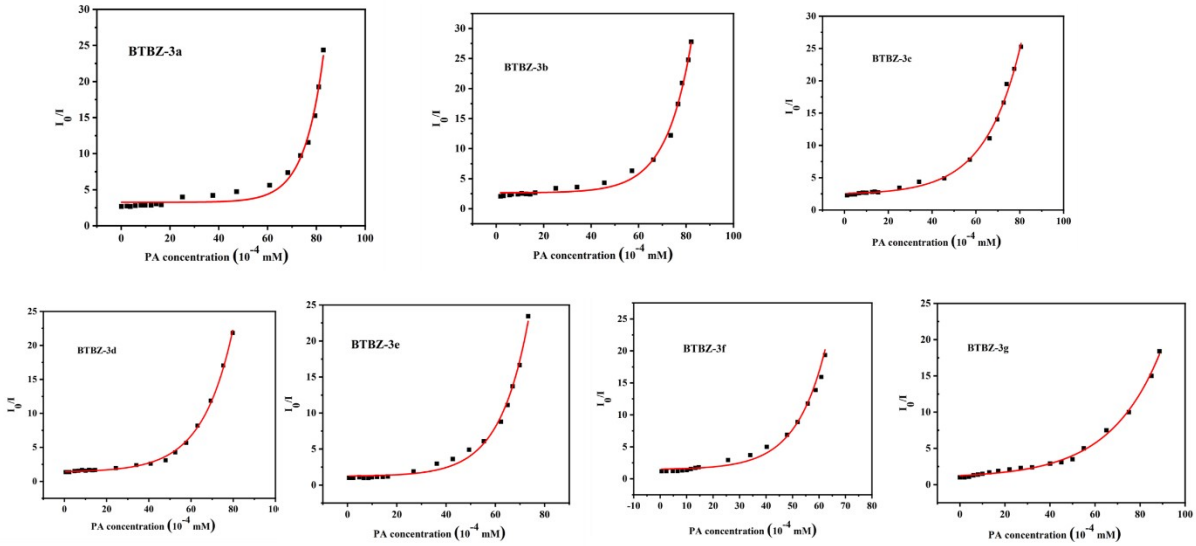

Figure S10. Stern–Volmer plots for fluorophores using PA as a quencher at higher concentrations of PA (curve fitting)

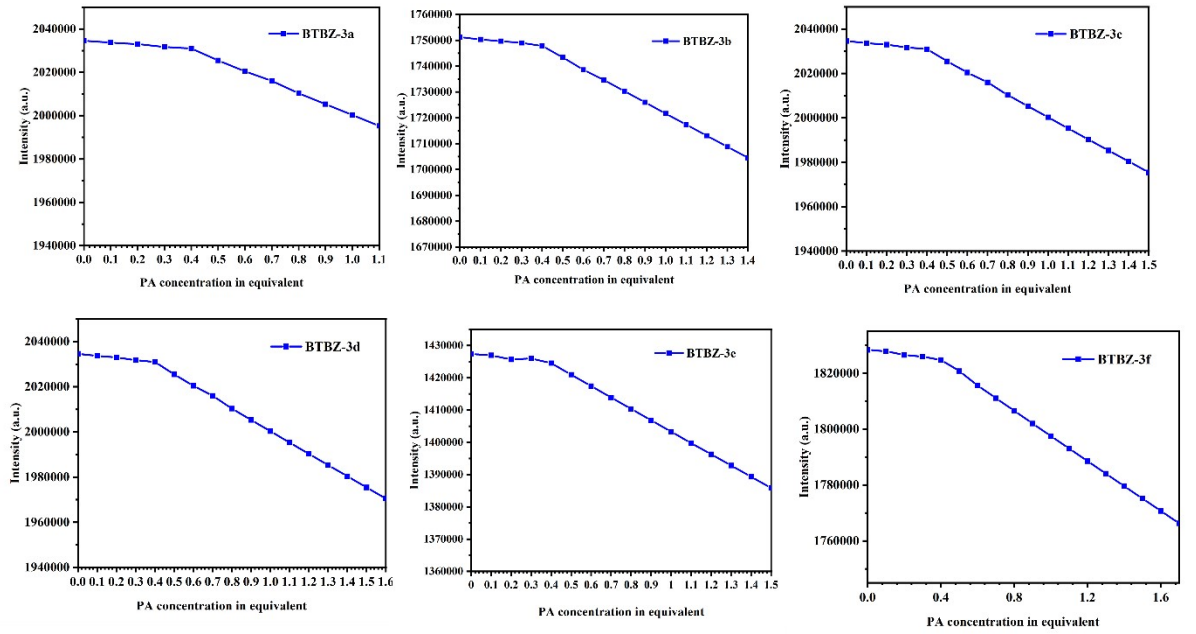

Figure S11. Fluorescence intensity of fluorophores as a function of PA concentration.

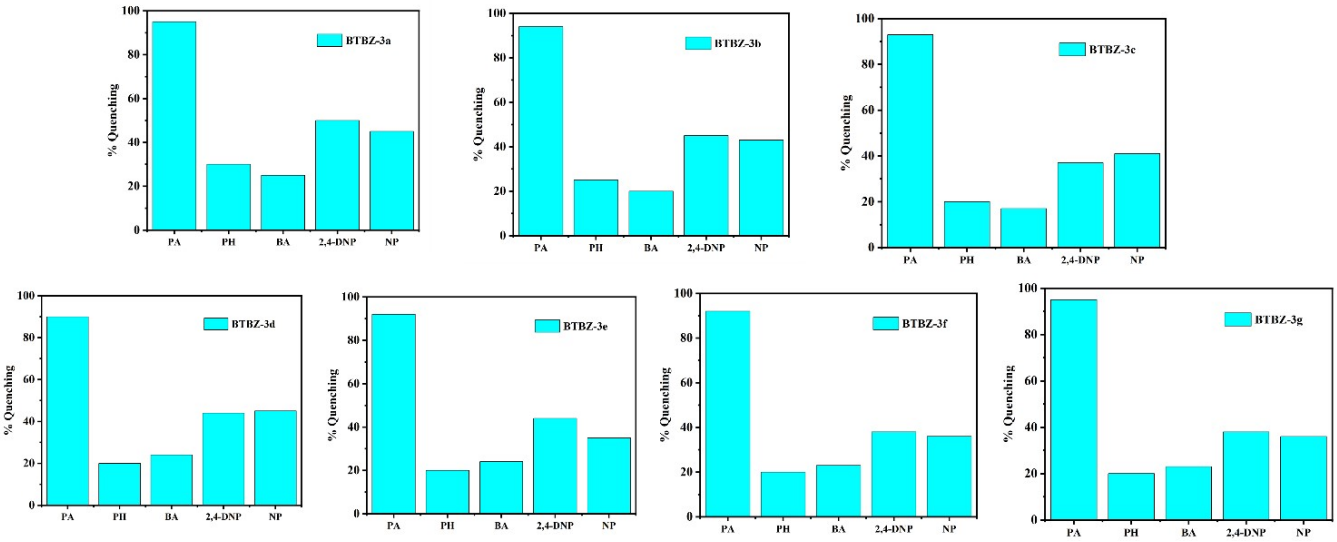

Figure S12. Fluorescence quenching efficiency of the different nitroaromatic quenchers towards the luminophores.

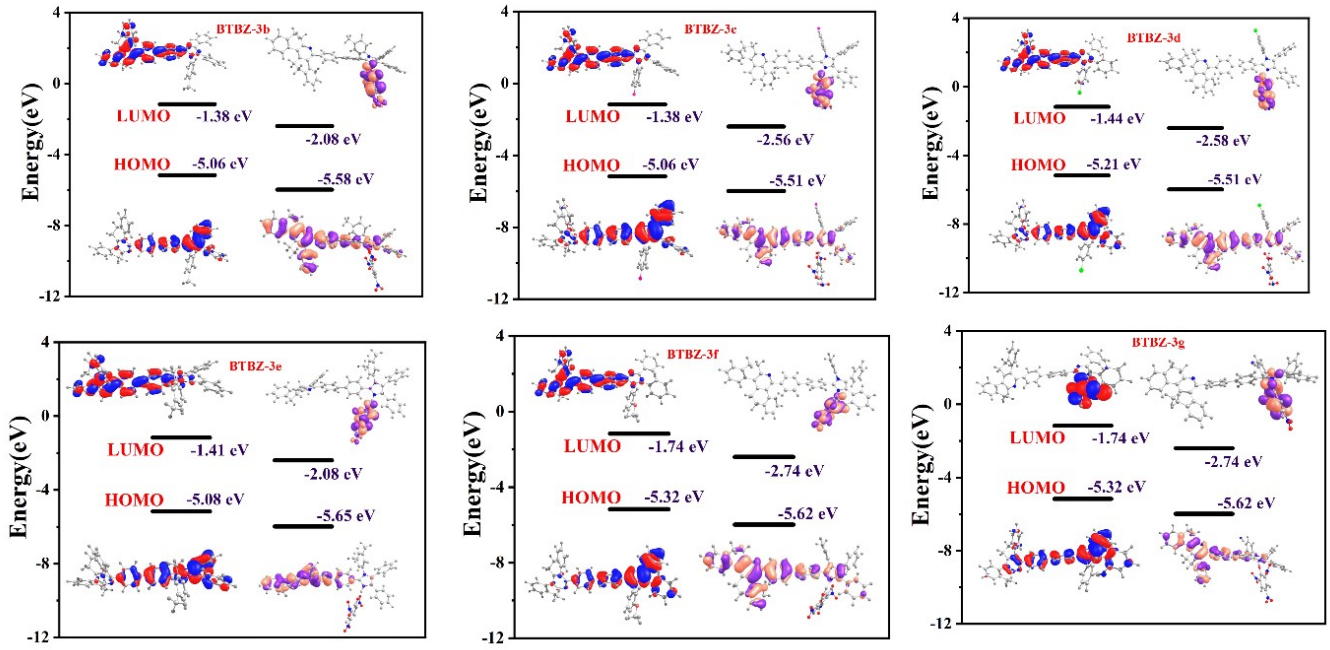

Figure S13. Frontier molecular orbitals of Fluorophores and Fluorophores + PA obtained from DFT calculations using Gaussian 09

SI1.5. Photophysical properties of fluorophores

Table S3. Key photophysical details of the fluorophores

Solvents	**Δ *f***	**BTBZ-3a**				**BTBZ-3b**			
		λ_{abs} (nm)	**λ_{em} (nm)**	**Stokes' shift^{-1} (cm)**	**FWHM (nm)**	**λ_{abs} (nm)**	**λ_{em} (nm)**	**Stokes' shift^{-1} (cm)**	**FWHM (nm)**
Hexane	0.0012	338	426	6650	55	345	408	4988	57
Benzene	0.002	331	427	6792	63	350	417	5460	68
Toluene	0.0131	339	426	6024	65	360	422	5457	65
Dioxane	0.022	330	428	6938	69	361	430	5678	69
$CHCl_3$	0.153	340	430	6736	70	360	432	6543	69
THF	0.210	336	436	6826	72	358	434	6457	78
Acetone	0.284	334	442	6678	72	359	443	7012	76
EtOAc	0.200	343	442	6520	73	365	445	7034	77
DMF	0.276	335	458	8016	78	360	457	7867	75
DMSO	0.263	335	464	8478	79	356	460	7893	81
ACN	0.305	334	469	8368	85	350	480	8034	88

Solvents	**Δ *f***	**BTBZ-3c**				**BTBZ-3d**			
		λ_{abs} (nm)	**λ_{em} (nm)**	**Stokes' shift^{-1} (cm)**	**FWHM (nm)**	**λ_{abs} (nm)**	**λ_{em} (nm)**	**Stokes' shift^{-1} (cm)**	**FWHM (nm)**
Hexane	0.0012	339	408	5226	52	338	403	5191	61
Benzene	0.002	341	412	5430	66	340	409	5643	64
Toluene	0.0131	351	423	5446	68	335	417	6872	59
Dioxane	0.022	352	427	5345	70	344	425	7152	68
$CHCl_3$	0.153	337	433	5558	74	347	430	7098	62
THF	0.210	340	430	6579	76	345	435	7150	63
Acetone	0.284	354	434	6789	78	341	439	7865	65
EtOAc	0.200	334	436	7756	79	339	439	7982	68
DMF	0.276	348	457	7876	75	345	466	8797	71
DMSO	0.263	339	469	7965	80	347	471	8885	79
ACN	0.305	337	471	8094	91	332	461	8849	89

Solvents	Δ *f*	BTBZ-3e				BTBZ-3f				BTBZ-3g			
		λ_{abs} (nm)	λ_{em} (nm)	Stokes' shift^{-1} (cm)	FWHM (nm)	λ_{abs} (nm)	λ_{em} (nm)	Stokes' shift^{-1} (cm)	FWHM (nm)	λ_{abs} (nm)	λ_{em} (nm)	Stokes' shift^{-1} (cm)	FWHM (nm)
Hexane	0.0012	337	409	5825	61	341	420	5543	64	341	415	5563	67
Benzene	0.002	341	418	5789	65	334	423	5678	66	342	425	5587	69
Toluene	0.0131	335	427	5686	68	340	431	6784	67	331	431	6746	75
Dioxane	0.022	340	429	6678	64	345	434	6678	72	349	436	6871	78
$CHCl_3$	0.153	340	433	6698	69	354	433	6987	74	337	442	6945	79
THF	0.210	336	438	6870	68	356	439	7012	78	350	444	6896	76
Acetone	0.284	334	439	6987	75	350	445	7123	79	343	448	7856	82
EtOAc	0.200	343	440	7897	78	334	449	7345	80	351	449	7981	87
DMF	0.276	335	464	7980	79	340	466	7546	89	346	477	8407	84
DMSO	0.263	335	479	8948	82	351	469	8012	94	359	479	8469	86
CAN	0.305	334	483	8765	95	347	476	8564	98	360	495	8744	92

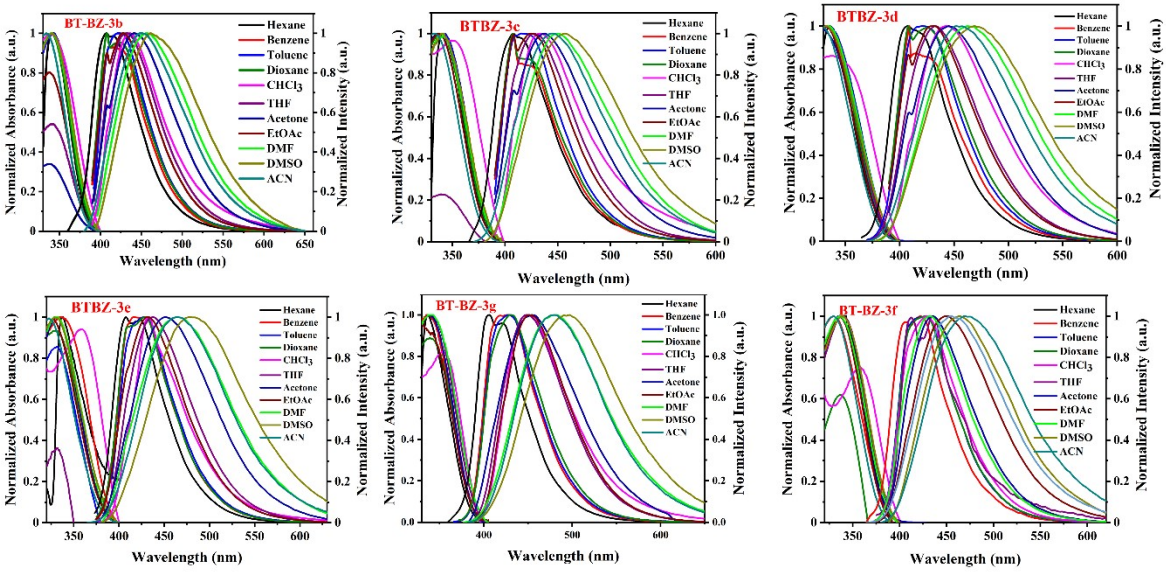

Figure S14. Absorption and emission spectra of fluorophores (BTBZ-3a-g) in different solvents

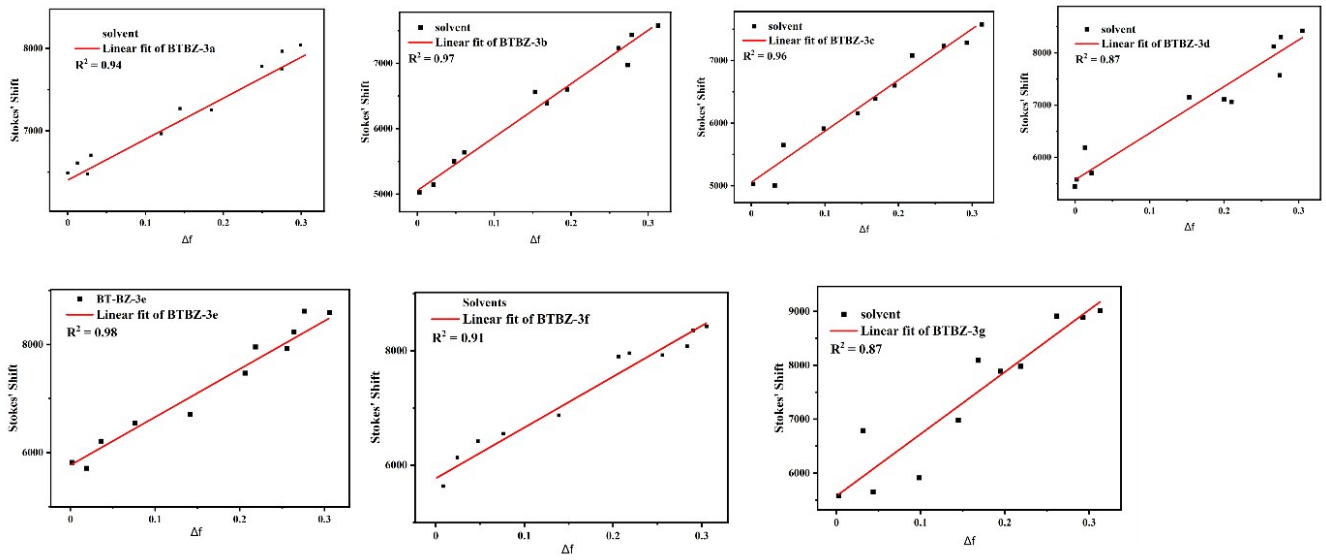

Fig S15. Plot of stokes'shift versus orientation polarizability(Δf) and linear fitting of the fluorophores (BTBZ-3a-g)

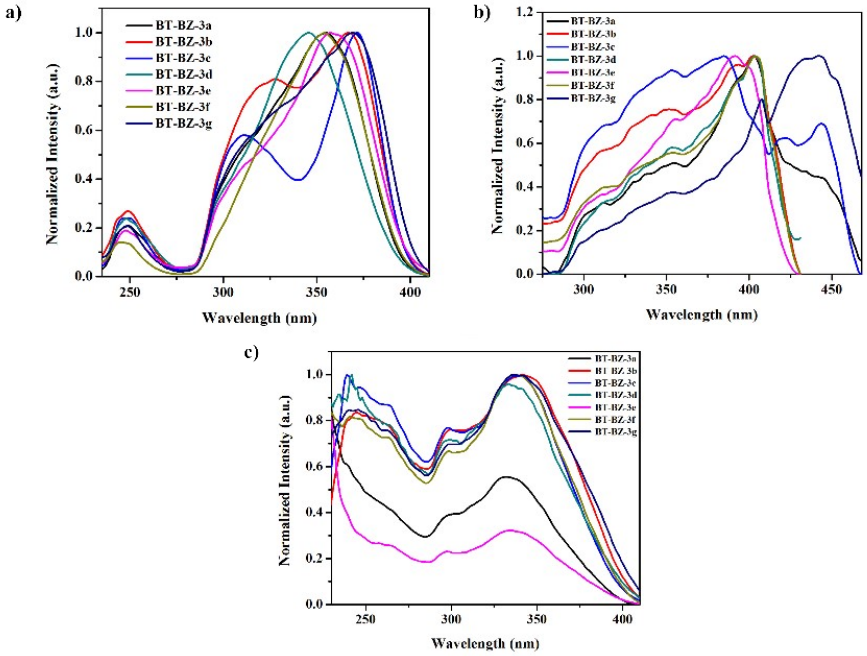

Fig S16. PL Excitation spectra of the fluorophores (BTBZ-3a-g) a) solution (THF) b) solid c) thin film

SI6. Vapoluminescence study of the fluorophores

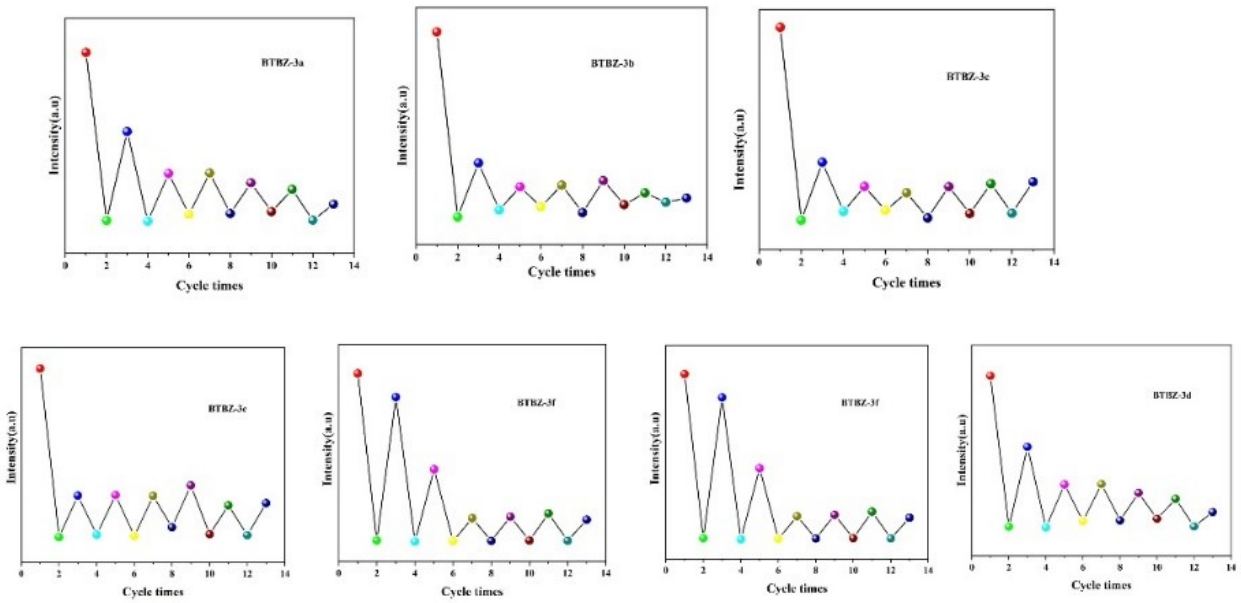

Fig S17. The reversible on-off-on fluorescence switching response upon sequential alternate addition of acid-base

SI7. Electroluminescence (EL) properties of the fabricated LEDs

Table S4. EL properties of the fabricated Blue LEDs

Fluorophores	**CIE (x,y)**	**LER**	**Color Purity**
BTBZ-3a	0.15,0.08	237	80
BTBZ-3b	0.15,0.09	232	78
BTBZ-3c	0.16,0.09	230	76
BTBZ-3d	0.14,0.11	230	78
BTBZ-3e	0.18,0.09	215	81
BTBZ-3f	0.16,0.11	221	85
BTBZ-3g	0.17,0.11	229	83

Table S5. EL properties of the fabricated White LEDs

Fluorophores	CIE (x,y)	CRI	CCT	LER	Ra
BTBZ-3a	0.37,0.32	82	4696	230	80
BTBZ-3b	0.32,0.28	79	4194	226	78
BTBZ-3c	0.31,0.27	80	5182	210	81
BTBZ-3d	0.32,0.26	81	5489	218	83
BTBZ-3e	0.37,0.32	83	5241	220	79
BTBZ-3f	0.33,0.29	84	5246	238	81
BTBZ-3g	0.37,0.32	86	5155	234	79

SI8. Photophysical properties of developed fingerprints

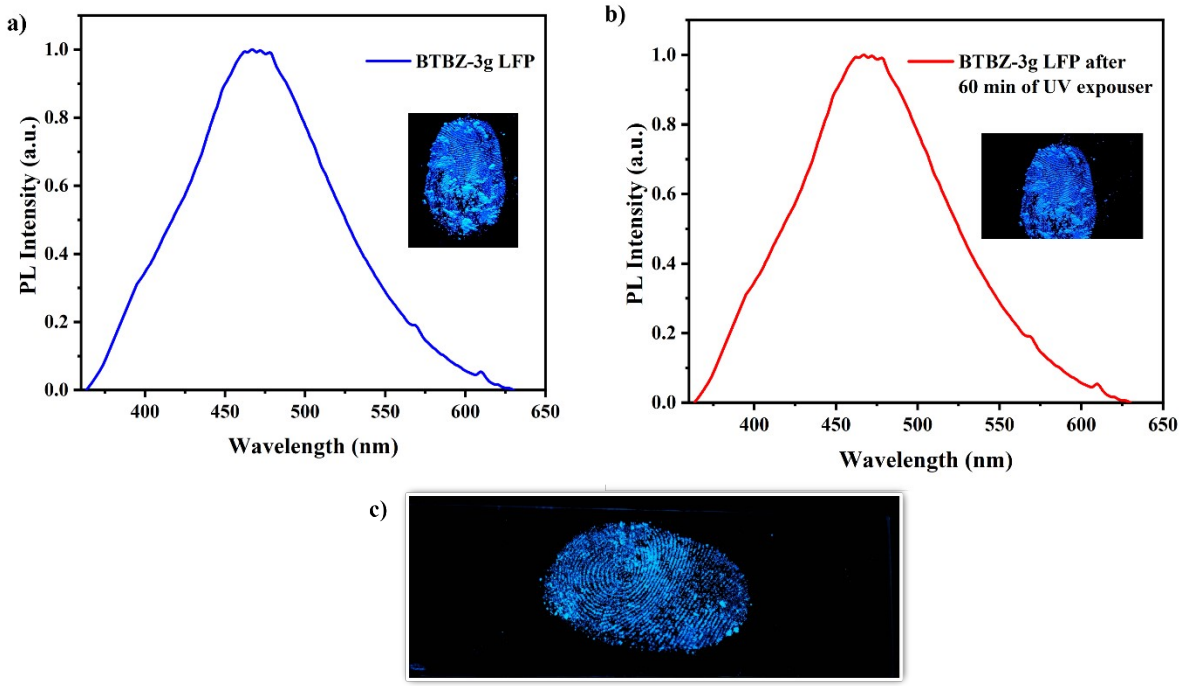

Fig S18. a) PL emission spectra of developed fingerprints (λexcit = 370) b) PL emission spectra of developed fingerprints after expouser to UV light for 60 min c) developed LFP after 30 days

SI9. Temperature dependent PL study of the fluorophores

S

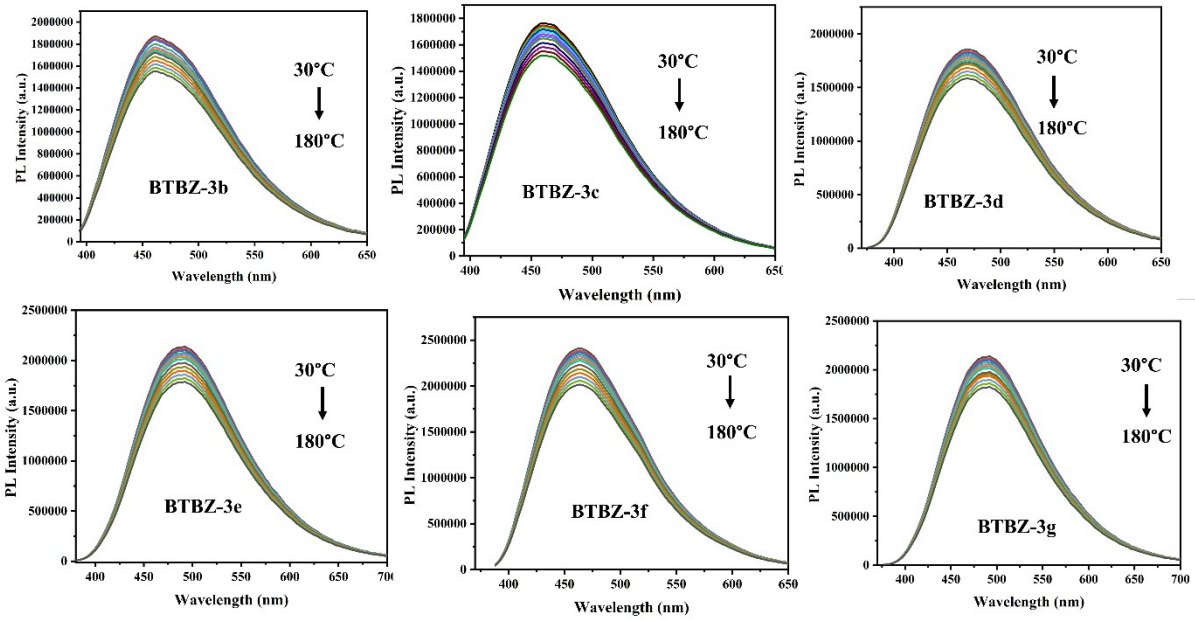

Fig S19. PL Spectra of the fluorophores BTBZ-3(b-g) in DMSO under different temperatures (30°C to180°C) at excitation 380 nm

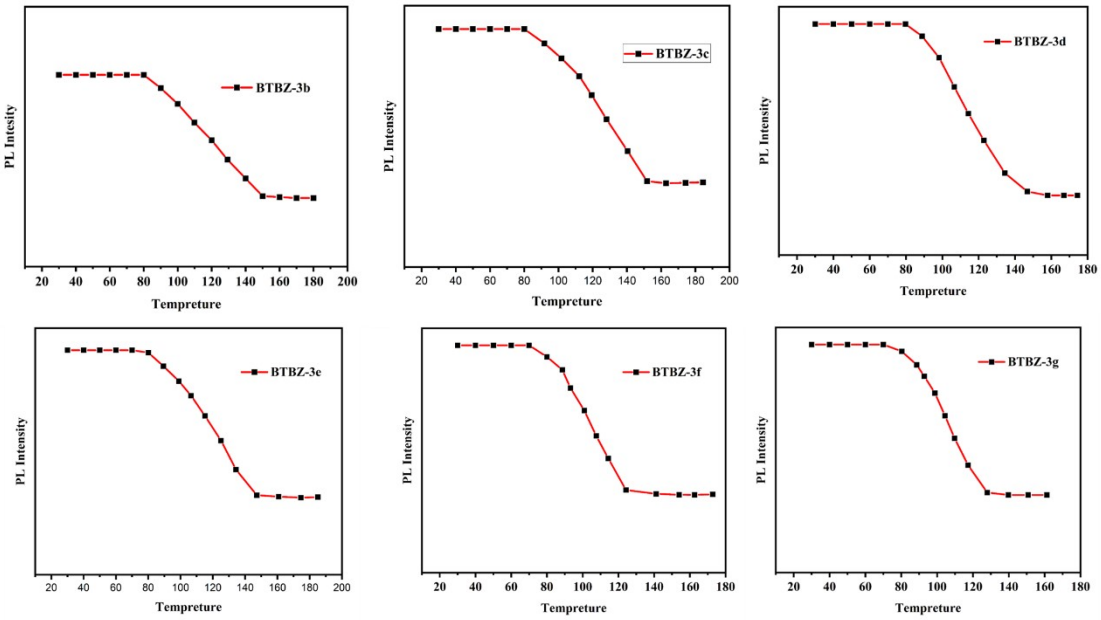

Fig S20. Plot of temperature vs PL intensity of the fluorophores BTBZ-3(b-g) in DMSO solvent at excitation 380 nm