Supporting Information

Triarylamine-BODIPYs exhibiting record hole mobility: synthesis, photophysical, electrochemical, spectroelectrochemical, and charge carrier mobility studies

Amiy Krishna, [a] Tarun, [b] Upendra Kumar Pandey, *[b] and Rajneesh Misra *[a]

[a] Department of Chemistry, Indian Institute of Technology Indore

Indore 453552, India. E-mail: rajneeshmisra@iiti.ac.in

[b] Organic & flexible electronics laboratory, Department of Electrical Engineering, School of Engineering, Shiv Nadar Institution of Eminence, Gautam Buddha Nagar, Uttar Pradesh 201314, India. E-mail: upendra.pandey@snu.edu.in

Synthesis of intermediate BTI_2

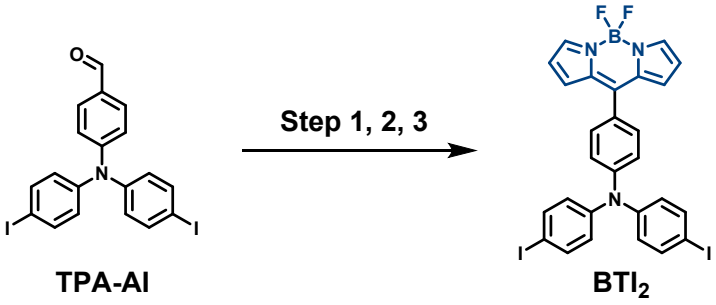

Fig. S1 Synthetic route of intermediate **BTI_2**.

(Note: Step1: pyrrole, TFA, r.t. Step2: DDQ, DCM, r.t. Step3: Et_3N, $BF_3 \cdot OEt_2$, DCM, r.t.).

Procedure: Pyrrole (2.5 mL, 36 mmol) and 4-N,N-bis(4-iodophenyl)-amino-benzaldehyde (0.756 g, 1.44 mmol) were added to a dry 25 mL round-bottomed flask and degassed with a stream of N_2 for 5 min. TFA (11.5 μL, 0.15 mmol) was added, and the solution was stirred for 20 minutes under N_2 at room temperature. The excess pyrrole was removed on a rotary evaporator under vacuum, and the crude compound was passed through flash silica gel column chromatography with a mixture of ethyl acetate and petroleum ether as eluent (1:6 by volume). The resultant compound was dissolved in freshly distilled dichloromethane and oxidized with DDQ (1.2 equivalent) for 30 min at room temperature. The reaction mixture was then treated with Et_3N (40 equivalent) followed by BF_3⍰OEt_2 (50 equivalent), and stirred for 1 h at room temperature. The solvent was removed on a rotary evaporator, and the resultant crude compound was purified by silica gel column chromatography with hexane/ethyl acetate (3:1) and afforded pure compound **BTI_2** in 28% yield; ^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC): δ 7.92 (s, 2H), 7.64 (d, J = 8.7 Hz, 4H), 7.47 (d, J = 8.5 Hz, 2H), 7.13 (d, J = 8.6 Hz, 2H), 7.02 (d, J = 3.9 Hz, 2H), 6.94 (d, J = 8.7 Hz, 4H), 6.56 (d, J = 2.4 Hz, 2H) ppm; ^{11}B NMR (160 MHz, $CDCl_3$,25 ºC) δ 0.46, 0.28, 0.10 ppm; ^{19}F NMR (470 MHz, $CDCl_3$,25 ºC) δ -145.04, -145.10, -145.16, -145.23 ppm; MALDI-TOF-MS: m/z calculated for chemical formula $C_{27}H_{18}BF_2I_2N_3$ $[M]^+$ 686.96; observed 686.9.

Solvatochromic studies

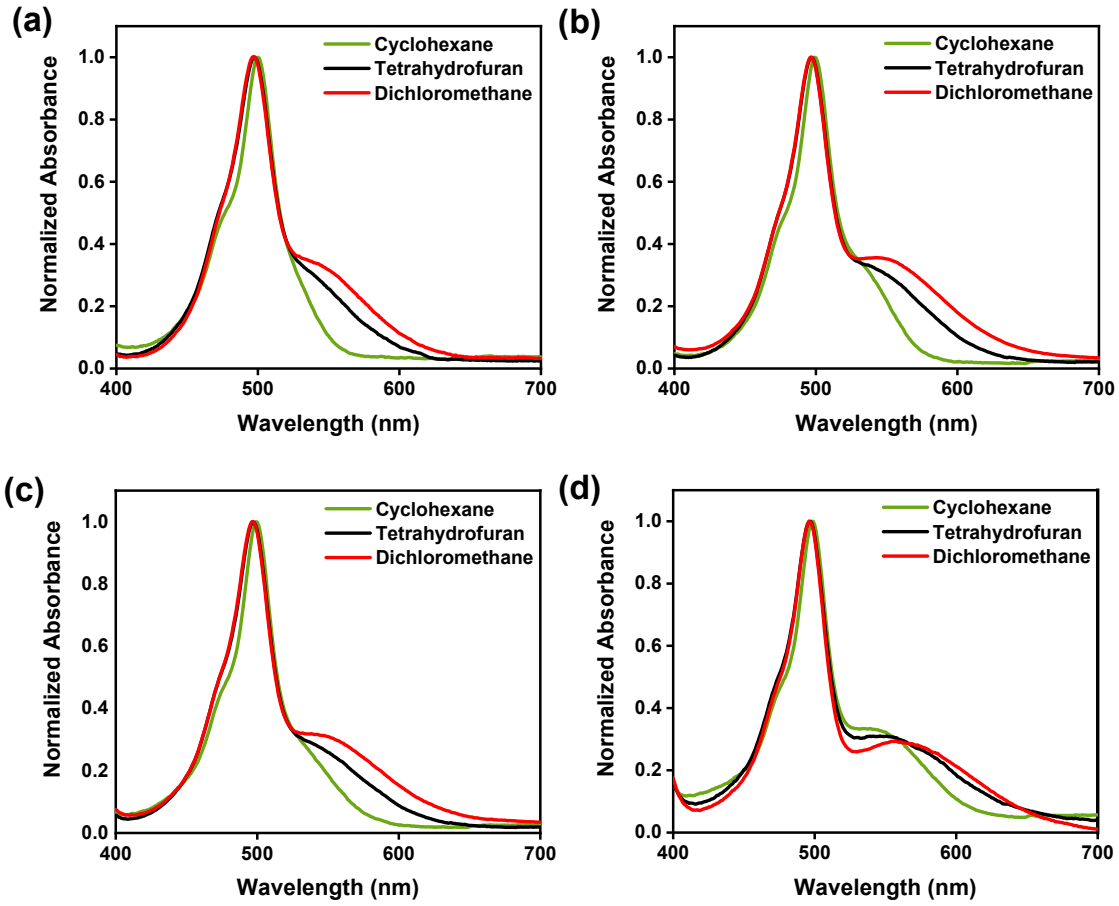

Fig. S2 Normalized electronic absorption spectra of the compounds **BTA1**–**BTA4** in solvents of different polarity.

Normalized absorption spectra in DCM and thin film

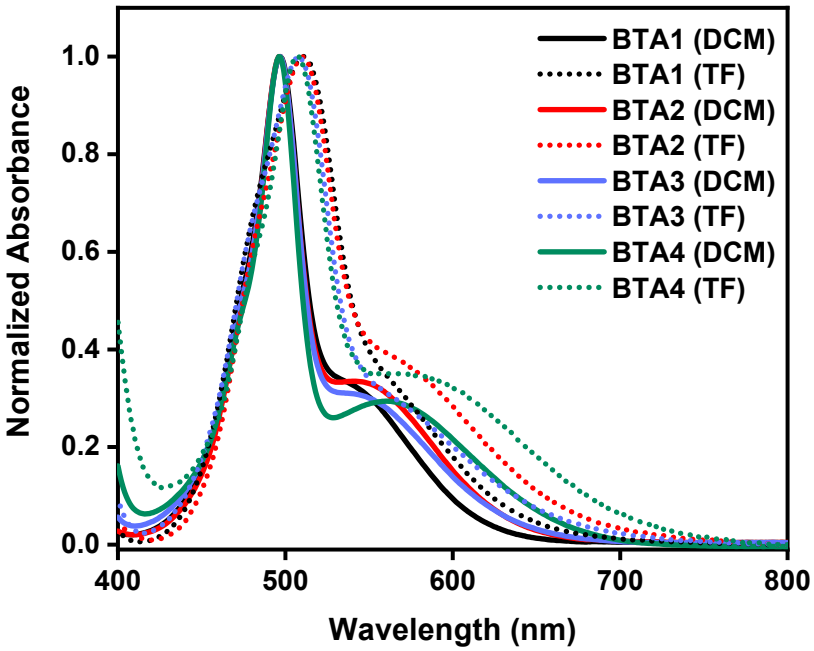

Fig. S3 Normalized electronic absorption spectra of the compounds **BTA1**–**BTA4** recorded in DCM and thin film.

Differential pulse voltammograms

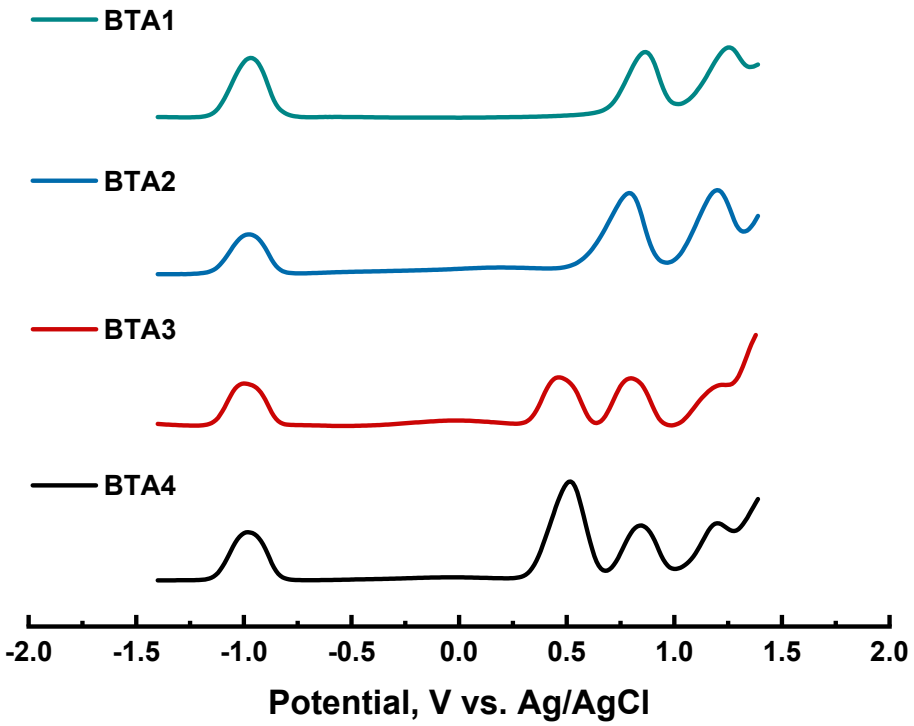

Fig. S4 DPVs of the compounds **BTA1**–**BTA4** in dichloromethane containing 0.1 M $TBAClO_4$ as the supporting electrolyte, recorded at a scan rate of 50 mV/s vs. Ag/AgCl.

Spectroelectrochemical studies

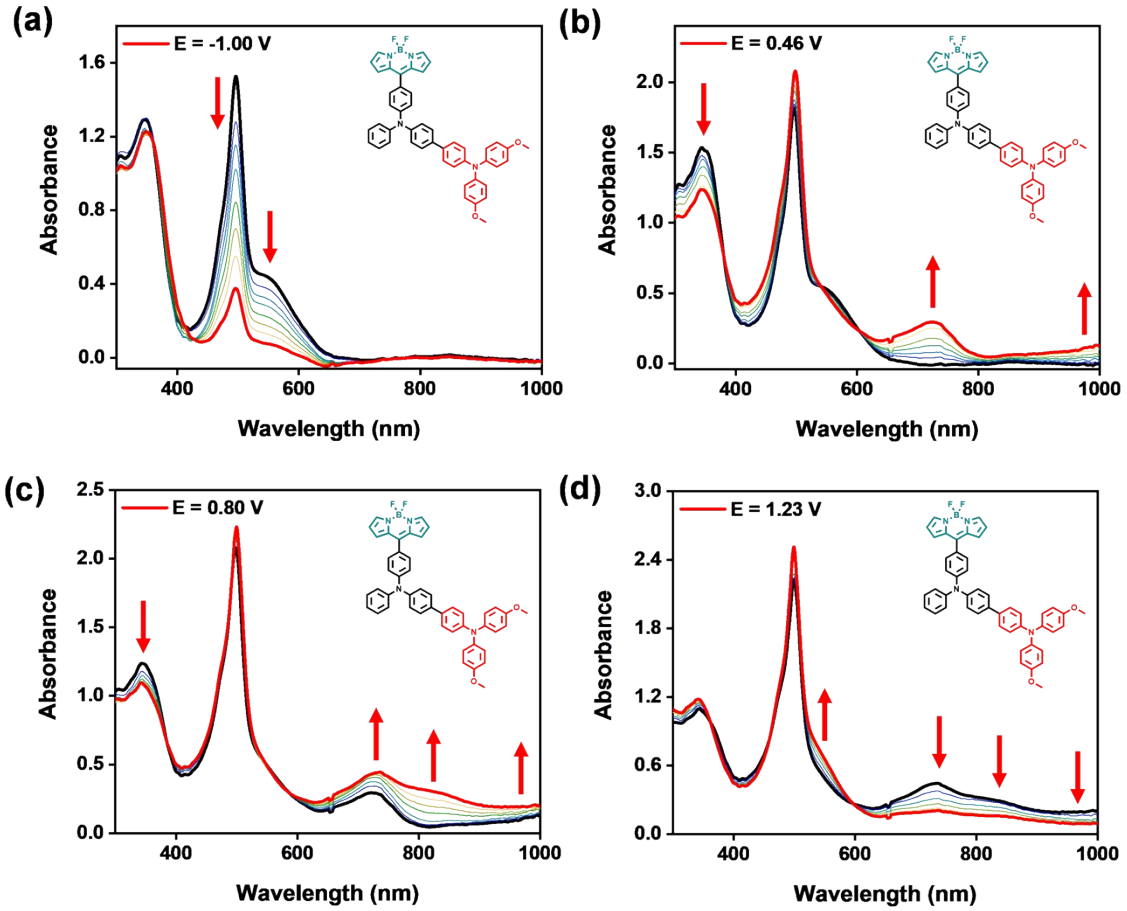

Fig. S5 Spectral changes observed for the compound **BTA3** at the indicated redox potentials.

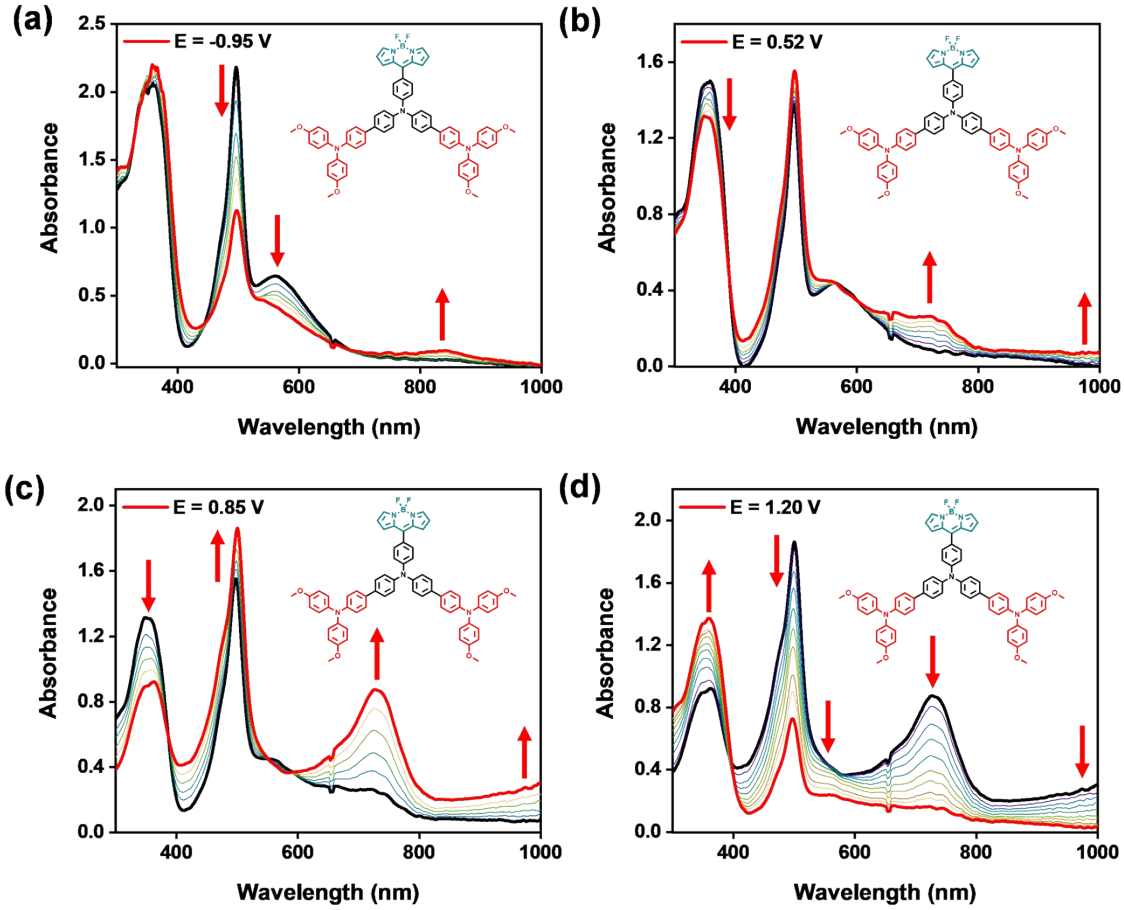

Fig. S6 Spectral changes observed for the compound **BTA4** at the indicated redox potentials.

Charge mobility studies and the corresponding data

ITO substrates (15 Ω/cm) were first patterned using 35M HCl solution. Subsequently, patterned ITO substrates were sequentially cleaned for 20 min each with 3% soap solution (Hellamanex III, Sigma Aldrich), then deionized water, acetone, and isopropyl alcohol in an ultrasonicator. Cleaned substrates were then dried under the gentle flow of ultra-pure nitrogen gas. The ITO substrates were then exposed to UV Ozone cleaner (BioBee, Bangalore, India) for 20 minutes at 70 °C.

Hole-only devices were fabricated in ITO/2PACz (~5-10 nm)/ **BTA1**–**BTA4**(~100 nm)/ MoO_3 (~ 10 nm)/Ag (~ 100 nm) architecture. For hole-only devices, 100 µl of 2PACz (1mg/ml in ethanol) was first spin-coated at 1500 rpm for 45 seconds on ITO substrates. The spin-coated substrates were then annealed at 80°C for 10 minutes under ambient conditions. Subsequently, **BTA1**–**BTA4** series compounds in chloroform (10 mg/ml) were spin-coated onto 2PACz coated substrate at 3000 rpm for 30 seconds to obtain ~100 nm thick films duly verified using dektek profilometer (Bruker). The samples were then placed in thermal evaporator (Hind High Vacuum, India) to deposit 7 nm of MoO_3 and 100 nm of Ag sequentially at 6×10^{-6} mbar base pressure to complete the hole-only devices.

For fabricating electron-only devices ITO/ZnO (~30-35 nm)/ **BTA1**–**BTA4**(~100 nm)/ LiF (~ 1 nm)/Al (~ 100 nm), the ZnO sol-gel solution was first prepared by vigorously stirring 200 mg of zinc acetate dihydrate in 52 mg of ethanolamine and 2 ml of 2-methoxyethanol overnight at room temperature. Subsequently, the ZnO sol-gel solution was spin-coated onto cleaned UV ozone-treated ITO substrates at 4000 rpm for 60 seconds. The spin-coated substrates were then annealed at 180°C for 1 hour. The active layer solution (same as hole only device) was spin-coated at 1500 rpm for 30 seconds to obtain 100 nm thick films. The devices were then completed by evaporating 1nm of LiF layer and subsequently 100 nm of aluminium under 6×10^{-6} mbar base pressure. The samples for both hole-only and electron-only devices

have an active area of 6.0 mm^2, calculated using the overlap area of both electrodes. All the devices were fabricated inside a glove box (GS Germany, O_2 < 100 PPM, H_2 <0.2 PPM). The mobility data of **BTA1**–**BTA4** materials for the best five devices are given in Table S1.

Table S1 Best five Hole and Electron mobility devices data of **BTA1**–**BTA4** materials under dark conditions.

Material	**BTA1 mobilities ($cm^2 V^{-1} s^{-1}$)**	
	Hole (× 10^{-3})	**Electron (× 10^{-3})**
	5.20	1.30
	4.00	1.60
	6.80	1.70
	5.30	1.40
	6.60	2.00
Average	5.58	1.60
STD	1.14	0.27

Material	**BTA2 mobilities ($cm^2 V^{-1} s^{-1}$)**	
	Hole (× 10^{-2})	**Electron (× 10^{-3})**
	1.60	4.60
	2.70	1.30
	2.10	2.30
	1.50	4.10
	1.00	2.20
Average	1.78	2.90
STD	0.64	1.39

Material	**BTA3 mobilities ($cm^2 V^{-1} s^{-1}$)**	
	Hole (× 10^{-2})	**Electron (× 10^{-3})**
	1.90	1.65
	1.10	1.70
	2.20	2.00
	1.10	2.40
	1.60	1.20
Average	1.58	1.79
STD	0.49	0.44

Material	**BTA4 mobilities ($cm^2 V^{-1} s^{-1}$)**	
	Hole (× 10^{-2})	**Electron (× 10^{-4})**

	0.81	6.40
	0.81	4.10
	1.20	6.00
	1.30	4.10
	1.32	5.40
Average	1.09	5.20
STD	0.26	1.07

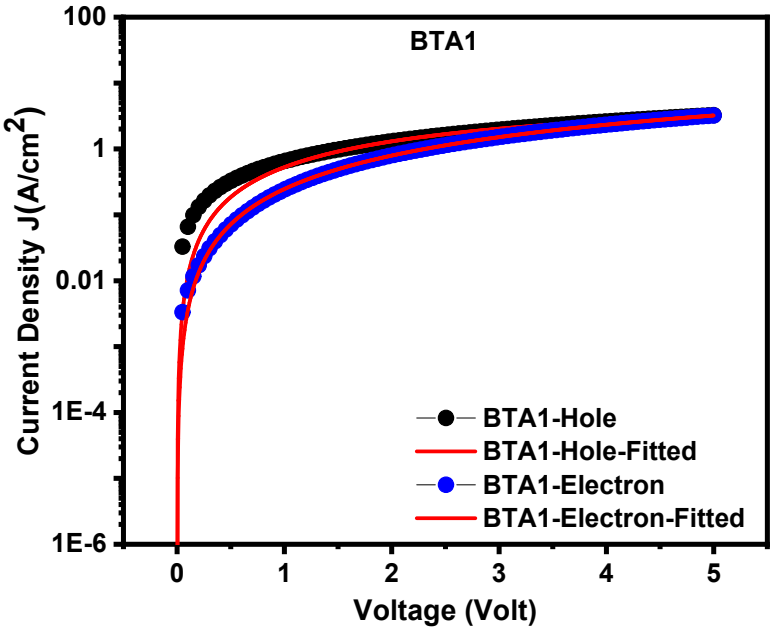

Fig. S7 Semi-logarithmic *J-V* characteristics of **BTA1** single carrier devices (either hole-only or electron-only) measured under dark conditions. The data were fitted using the modified Mott-Gurney law to extract charge carrier mobilities.

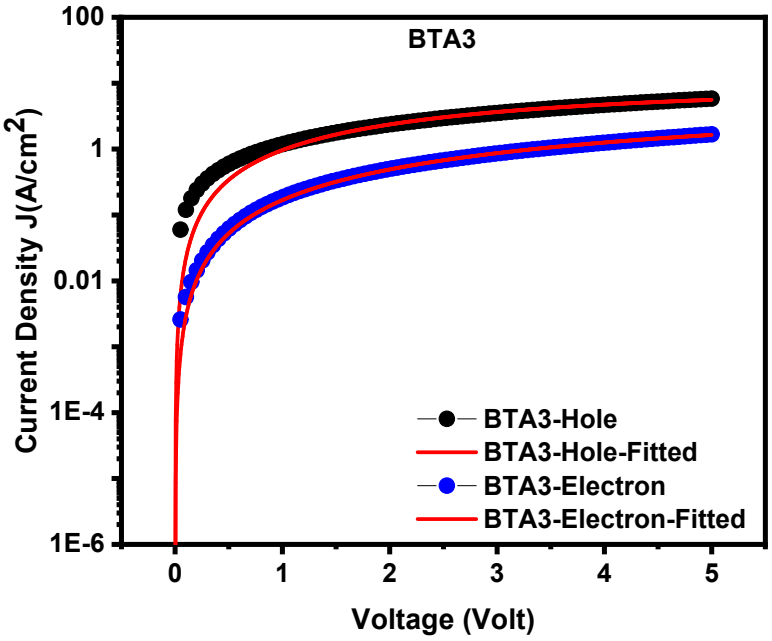

Fig. S8 Semi-logarithmic *J-V* characteristics of **BTA3** single carrier devices (either hole-only or electron-only) measured under dark conditions. The data were fitted using the modified Mott-Gurney law to extract charge carrier mobilities.

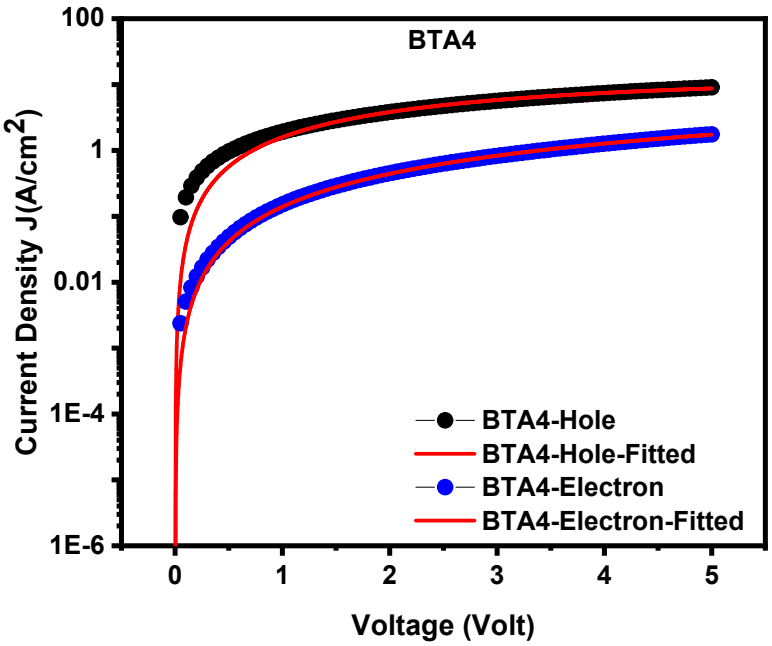

Fig. S9 Semi-logarithmic *J-V* characteristics of **BTA4** single carrier devices (either hole-only or electron-only) measured under dark conditions. The data were fitted using the modified Mott-Gurney law to extract charge carrier mobilities.

Table S2 Charge carrier mobilities of selected BODIPY-based conjugated small molecules evaluated using the SCLC method.

Entry	Compounds	Charge carrier mobility ($cm^2 V^{-1} s^{-1}$)		Ratio μ_e/μ_h	References
		Hole (μ_h)	Electron (μ_e)		
1	**BTA1**	**5.58×10^{-3}**	**1.60×10^{-3}**	**0.29**	**This work**
2	**BTA2**	**1.78×10^{-2}**	**2.90×10^{-3}**	**0.16**	**This work**
3	**BTA3**	**1.58×10^{-2}**	**1.75×10^{-3}**	**0.11**	**This work**
4	**BTA4**	**1.09×10^{-2}**	**5.20×10^{-4}**	**0.05**	**This work**
5	TM-01	7.61×10^{-5}	–	–	20
6	TM-02	4.32×10^{-4}	–	–	20
7	TM-03	7.74×10^{-5}	–	–	20
8	TM-04	1.69×10^{-4}	–	–	20
9	DIMER	1.16×10^{-3}	0.90×10^{-3}	0.78	21
10	Br-T-BO	4.71×10^{-4}	2.90×10^{-4}	0.62	21
11	H-T-BO	4.27×10^{-5}	1.00×10^{-5}	0.23	21
12	Py-BDP-1	6.54×10^{-5}	–	–	22
13	Py-BDP-2	6.04×10^{-5}	–	–	22
14	Py-BDP-3	6.41×10^{-5}	–	–	22
15	Py-BDP-4	5.76×10^{-5}	–	–	22
16	Py-BDP-5	4.86×10^{-5}	–	–	22
17	aza-BODIPY 1	4.60×10^{-4}			19
18	aza-BODIPY 2	3.20×10^{-4}	–	–	19
19	aza-BODIPY 3	1.20×10^{-4}	–	–	19
20	PTZ-PTZ-BDP	2.02×10^{-5}	–	–	23
21	CF3-BDP-Cz	2.45×10^{-4}	1.56×10^{-4}	0.64	24
22	CF3-BDP-TPA	2.18×10^{-4}	0.99×10^{-4}	0.45	24
23	D-A1-D	7.01×10^{-5}	–	–	25
24	D-A2-D	3.63×10^{-4}	–	–	25

Hole and electron mobilities (μ_h and μ_e) measured by the SCLC technique are listed for BODIPY-based CSMs from this work and the literature. Electron mobility is not reported for all compounds; where not available/applicable, a dash (–) is used.

Low-angle XRD patterns of spin-coated thin films of BTA1–BTA4

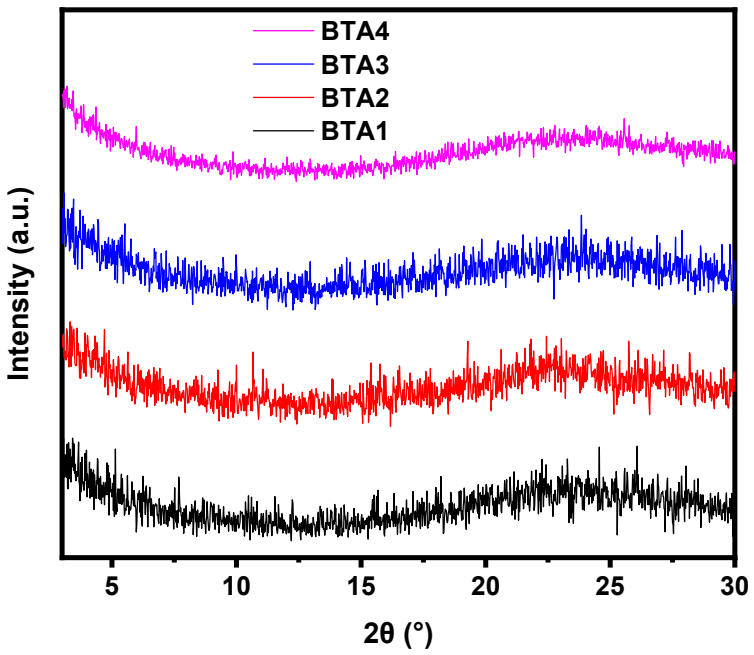

Fig. S10 Low-angle XRD patterns of spin-coated thin films of **BTA1**–**BTA4** measured on glass substrates.

Dielectric Constant

The relative dielectric constants (ε_r) of the **BTA1**–**BTA4** series materials were extracted from capacitance measurements using C-V measurements. The increasing dielectric constant from **BTA1** to **BTA4** reflects the enhanced donor-acceptor (D-A) interactions in the latter compounds, typically correlating with higher conductivity.[1]

Table S3 Dielectric constant of **BTA1**–**BTA4** materials.

Material	BTA 1	BTA 2	BTA 3	BTA 4
Dielectric (ε_r)	3.27	3.5	3.8	4.1

Molecular electrostatic potential surface plots

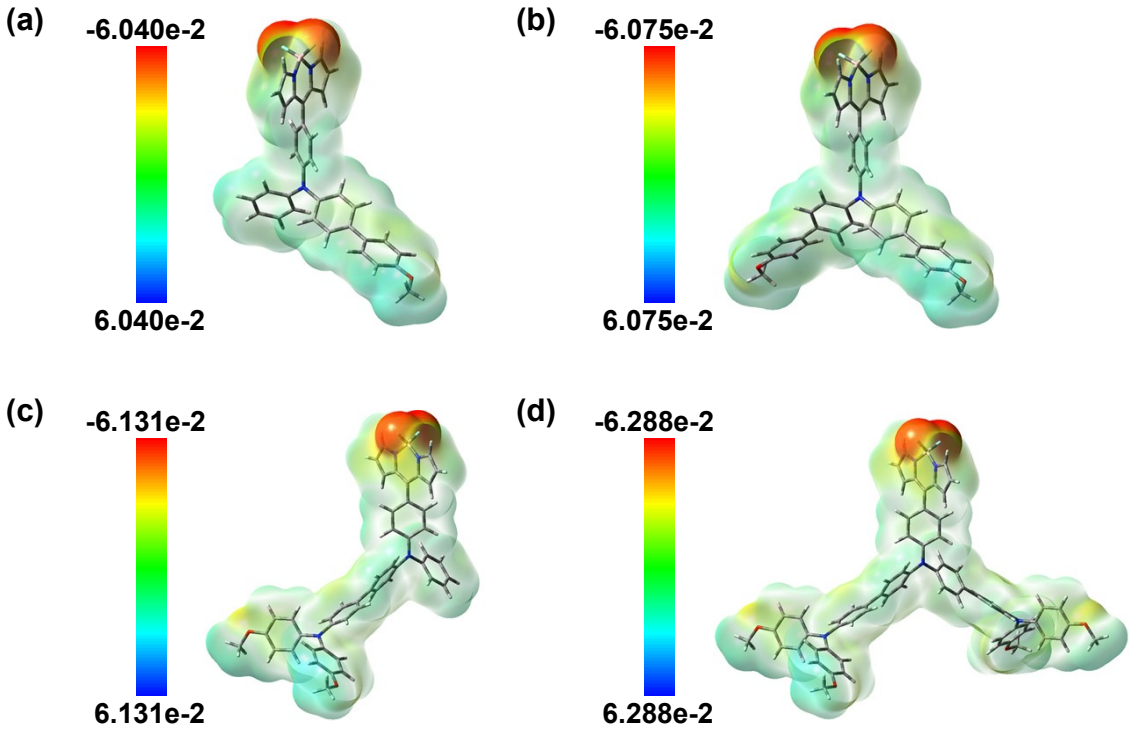

Fig. S11 Molecular electrostatic potential surface plots of the compounds (a) **BTA1**, (b) **BTA2**, (c) **BTA3**, and (d) **BTA4**.

DFT Calculation data

Calculation method: B3LYP/6-31G (d,p)

BTA1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.332914	1.363213	-0.032388
2	6	0	-1.446294	1.974893	0.575451
3	6	0	-0.510886	0.098670	-0.626097
4	6	0	-2.683803	1.346028	0.585105
5	1	0	-1.335344	2.948317	1.039147
6	6	0	-1.753296	-0.520690	-0.616936
7	1	0	0.332370	-0.396181	-1.094005
8	1	0	-3.529083	1.844491	1.047756
9	1	0	-1.859690	-1.501527	-1.067898
10	6	0	2.126793	1.235153	0.003008
11	6	0	2.274809	0.181545	0.916974
12	6	0	3.195625	1.537632	-0.852499
13	6	0	3.453950	-0.554952	0.958663
14	1	0	1.457627	-0.065055	1.586935
15	6	0	4.379370	0.810315	-0.786444
16	1	0	3.099388	2.356001	-1.558289
17	1	0	3.531046	-1.384131	1.655198
18	1	0	5.202559	1.085887	-1.438522
19	6	0	1.015638	3.421594	-0.110135
20	6	0	0.246083	4.143880	-1.034604
21	6	0	1.892369	4.111693	0.739609
22	6	0	0.344899	5.532605	-1.094716

23	1	0	-0.424813	3.612596	-1.701614
24	6	0	1.998077	5.498973	0.659702
25	1	0	2.487275	3.555420	1.456305
26	1	0	-0.257109	6.078761	-1.815048
27	1	0	2.681550	6.020212	1.323575
28	7	0	0.923630	1.999171	-0.044644
29	6	0	-2.869969	0.086193	-0.013330
30	6	0	-4.191864	-0.571534	-0.004809
31	6	0	-4.908289	-0.698507	1.202895
32	6	0	-4.738735	-1.088192	-1.197197
33	7	0	-6.169612	-1.288807	1.234264
34	6	0	-4.537135	-0.397992	2.540832
35	7	0	-5.976067	-1.729408	-1.201890
36	6	0	-4.253725	-1.073005	-2.532325
37	6	0	-6.569286	-1.348597	2.513611
38	5	0	-6.979715	-1.808098	-0.000541
39	6	0	-5.585899	-0.799577	3.358787
40	1	0	-3.597015	0.036605	2.846145
41	1	0	-3.327061	-0.624283	-2.857229
42	6	0	-5.195748	-1.723233	-3.319882
43	1	0	-7.524740	-1.785685	2.768870
44	9	0	-8.061672	-0.980229	-0.245128
45	9	0	-7.378589	-3.114443	0.211289
46	1	0	-5.644445	-0.728893	4.435424
47	1	0	-5.152000	-1.901527	-4.384713
48	6	0	-6.244209	-2.105683	-2.461570
49	1	0	-7.169690	-2.613408	-2.695865
50	6	0	1.222937	6.217608	-0.252478
51	6	0	4.537911	-0.257409	0.114216
52	6	0	5.797871	-1.036211	0.173668

53	6	0	6.537567	-1.316956	-0.983147
54	6	0	6.299582	-1.523102	1.396597
55	6	0	7.726592	-2.046681	-0.939576
56	1	0	6.167961	-0.982462	-1.947950
57	6	0	7.478506	-2.250846	1.457684
58	1	0	5.768595	-1.303886	2.318061
59	6	0	8.204293	-2.519587	0.287771
60	1	0	8.259125	-2.247733	-1.861420
61	1	0	7.866836	-2.614915	2.403125
62	8	0	9.349761	-3.242138	0.452223
63	6	0	10.129138	-3.536203	-0.696837
64	1	0	10.988083	-4.106163	-0.340190
65	1	0	9.570229	-4.142121	-1.421346
66	1	0	10.482635	-2.622347	-1.191202
67	1	0	1.303127	7.298763	-0.307510

Electronic Energy: -1775.503573 Hartree

BTA2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.662820	-0.028401	-0.008625
2	6	0	-1.408050	1.005453	0.591124
3	6	0	-1.365631	-1.092346	-0.607232
4	6	0	-2.795660	0.971527	0.591848
5	1	0	-0.891676	1.837143	1.056175
6	6	0	-2.753530	-1.115362	-0.607119
7	1	0	-0.815832	-1.903213	-1.070822

8	1	0	-3.345924	1.786985	1.049275
9	1	0	-3.269251	-1.955425	-1.059973
10	6	0	1.499316	-1.208033	0.032687
11	6	0	1.167382	-2.233384	0.930281
12	6	0	2.603421	-1.386378	-0.812913
13	6	0	1.909966	-3.408930	0.963321
14	1	0	0.317248	-2.109909	1.593081
15	6	0	3.353732	-2.556124	-0.755509
16	1	0	2.878917	-0.597137	-1.504561
17	1	0	1.613155	-4.198917	1.646317
18	1	0	4.222011	-2.655781	-1.399589
19	6	0	1.444239	1.244027	-0.047977
20	6	0	1.078715	2.246570	-0.957968
21	6	0	2.524397	1.479284	0.814225
22	6	0	1.765592	3.455669	-0.987587
23	1	0	0.245823	2.078614	-1.632845
24	6	0	3.219595	2.682821	0.760761
25	1	0	2.824634	0.708207	1.516047
26	1	0	1.443370	4.226739	-1.680560
27	1	0	4.071257	2.827894	1.418248
28	7	0	0.744761	0.001315	-0.009160
29	6	0	-3.503592	-0.086192	-0.008556
30	6	0	-4.979484	-0.111889	-0.003391
31	6	0	-5.682698	0.087820	1.202510
32	6	0	-5.694128	-0.352282	-1.194962
33	7	0	-7.075255	0.097774	1.231632
34	6	0	-5.220858	0.203326	2.540955
35	7	0	-7.086915	-0.402323	-1.200066
36	6	0	-5.248606	-0.558030	-2.527947
37	6	0	-7.464220	0.219800	2.509872

38	5	0	-8.027449	-0.024982	-0.004492
39	6	0	-6.341874	0.294547	3.356749
40	1	0	-4.185956	0.191160	2.848624
41	1	0	-4.218989	-0.551157	-2.852649
42	6	0	-6.377830	-0.750605	-3.314413
43	1	0	-8.515334	0.236832	2.762666
44	9	0	-8.638179	1.190512	-0.260624
45	9	0	-8.958372	-1.023325	0.213127
46	1	0	-6.366049	0.386289	4.433122
47	1	0	-6.413771	-0.940688	-4.377502
48	6	0	-7.489547	-0.639942	-2.457808
49	1	0	-8.543130	-0.705505	-2.692010
50	6	0	2.854996	3.703917	-0.134151
51	6	0	3.590136	4.990518	-0.178480
52	6	0	4.100353	5.580124	0.986163
53	6	0	3.802103	5.670091	-1.394003
54	6	0	4.793713	6.791080	0.957326
55	1	0	3.932285	5.100297	1.945740
56	6	0	4.487583	6.874730	-1.440487
57	1	0	3.445002	5.232180	-2.321263
58	6	0	4.990960	7.447113	-0.262943
59	1	0	5.160700	7.213898	1.884892
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62	6	0	3.817331	-4.850870	0.175146
63	6	0	4.374212	-5.408139	-0.984050
64	6	0	4.040059	-5.528337	1.389941
65	6	0	5.122391	-6.585927	-0.950566
66	1	0	4.200646	-4.929953	-1.943482
67	6	0	4.779638	-6.700316	1.440957

68	1	0	3.647414	-5.113799	2.313563
69	6	0	5.328792	-7.240785	0.268791
70	1	0	5.524453	-6.984686	-1.874240
71	1	0	4.957110	-7.213319	2.380399
72	8	0	6.039774	-8.394866	0.423284
73	8	0	5.650647	8.631725	-0.413414
74	6	0	6.187866	9.253320	0.743803
75	1	0	6.669337	10.168871	0.397642
76	1	0	5.403359	9.510145	1.467055
77	1	0	6.934448	8.616978	1.235857
78	6	0	6.623514	-8.983620	-0.728579
79	1	0	7.139382	-9.879365	-0.380154
80	1	0	5.863447	-9.269708	-1.466762
81	1	0	7.349235	-8.311278	-1.203704

Electronic Energy: -2121.092608 Hartree

BTA3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.896326	1.553998	-0.669179
2	6	0	-5.122519	2.090018	-0.228723
3	6	0	-3.763938	0.152180	-0.715493
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5	1	0	-5.252257	3.165163	-0.184501
6	6	0	-4.815648	-0.673020	-0.342089
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8	1	0	-7.105511	1.696567	0.469018

9	1	0	-4.680375	-1.748968	-0.371539
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11	6	0	-1.045583	1.433801	0.345103
12	6	0	-0.549755	2.129286	-1.910401
13	6	0	0.276189	1.031822	0.506057
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15	6	0	0.775176	1.746549	-1.731551
16	1	0	-0.868619	2.559832	-2.853996
17	1	0	0.577393	0.583045	1.447548
18	1	0	1.480025	1.901046	-2.542559
19	6	0	-3.084635	3.673633	-1.627880
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21	6	0	-2.373571	4.798469	-1.184931
22	6	0	-4.259290	5.072317	-3.221476
23	1	0	-4.568866	2.949176	-3.012425
24	6	0	-2.600683	6.044309	-1.766514
25	1	0	-1.644969	4.687652	-0.388827
26	1	0	-4.991044	5.170452	-4.018038
27	1	0	-2.042701	6.906724	-1.413702
28	7	0	-2.833385	2.394175	-1.048482
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45	9	0	-9.536673	-3.933014	2.048881
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54	6	0	3.280612	0.871146	0.896634
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68	6	0	8.467229	-1.364598	-1.251338

69	6	0	8.423018	2.216883	2.105698
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71	6	0	9.145272	0.060955	2.930333
72	1	0	8.247270	-1.643970	1.976808
73	6	0	7.088501	-3.766079	-1.516396
74	1	0	5.591151	-2.873362	-0.266560
75	6	0	9.027478	-2.403080	-1.998032
76	1	0	9.003710	-0.426467	-1.153175
77	6	0	9.206746	1.457624	2.987477
78	1	0	8.487829	3.298818	2.155161
79	1	0	9.735928	-0.552624	3.599994
80	6	0	8.335386	-3.610707	-2.140384
81	1	0	6.567340	-4.711201	-1.627588
82	1	0	9.990839	-2.252049	-2.470079
83	8	0	9.989172	2.170520	3.851742
84	8	0	8.782083	-4.687476	-2.853431
85	1	0	-3.725748	7.163370	-3.229246
86	6	0	10.797270	1.452153	4.769622
87	1	0	11.331904	2.203057	5.353101
88	1	0	10.192304	0.834227	5.445782
89	1	0	11.524638	0.810961	4.254954
90	6	0	10.035846	-4.581933	-3.508043
91	1	0	10.197178	-5.538362	-4.007386
92	1	0	10.036308	-3.779789	-4.257421
93	1	0	10.852143	-4.405234	-2.795606

Electronic Energy: -2407.489791 Hartree

BTA4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005146	3.319302	-0.012898
2	6	0	1.055038	4.039202	0.590981
3	6	0	-1.038860	4.049248	-0.615157
4	6	0	1.055201	5.427014	0.592408
5	1	0	1.872142	3.502492	1.058739
6	6	0	-1.026986	5.437029	-0.615102
7	1	0	-1.861708	3.520247	-1.081641
8	1	0	1.882648	5.956512	1.052782
9	1	0	-1.852384	5.973336	-1.071040
10	6	0	-1.230478	1.189215	0.007598
11	6	0	-2.254989	1.537023	0.899990
12	6	0	-1.430022	0.101244	-0.853797
13	6	0	-3.450420	0.826522	0.912132
14	1	0	-2.114817	2.375151	1.574772
15	6	0	-2.620452	-0.617036	-0.818183
16	1	0	-0.641486	-0.186337	-1.541425
17	1	0	-4.238555	1.136159	1.591454
18	1	0	-2.737139	-1.472946	-1.475702
19	6	0	1.222927	1.179405	-0.031774
20	6	0	2.249797	1.515781	-0.925762
21	6	0	1.414546	0.094179	0.834795
22	6	0	3.440300	0.796983	-0.934262
23	1	0	2.115533	2.351817	-1.604347
24	6	0	2.600075	-0.632380	0.803018
25	1	0	0.623914	-0.184613	1.523645
26	1	0	4.230752	1.097909	-1.614813
27	1	0	2.710931	-1.485781	1.464803

28	7	0	-0.000989	1.912535	-0.013655
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30	6	0	0.028839	7.637201	-0.007319
31	6	0	0.247643	8.336426	1.197942
32	6	0	-0.194806	8.357544	-1.199110
33	7	0	0.292894	9.728277	1.226091
34	6	0	0.354777	7.872728	2.536292
35	7	0	-0.211072	9.751123	-1.204740
36	6	0	-0.408904	7.916755	-2.532186
37	6	0	0.428169	10.114853	2.503903
38	5	0	0.183364	10.683530	-0.008679
39	6	0	0.476844	8.991649	3.351189
40	1	0	0.317135	6.838691	2.844754
41	1	0	-0.425580	6.887175	-2.856562
42	6	0	-0.572941	9.050107	-3.319441
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46	1	0	0.572392	9.014005	4.427279
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49	1	0	-0.476425	11.213761	-2.697810
50	6	0	3.646370	-0.297161	-0.074815
51	6	0	4.913613	-1.064011	-0.094799
52	6	0	5.462731	-1.605881	1.080239
53	6	0	5.622556	-1.279778	-1.289197
54	6	0	6.649506	-2.328553	1.068154
55	1	0	4.958775	-1.447395	2.029129
56	6	0	6.817708	-1.988228	-1.313234
57	1	0	5.225428	-0.895996	-2.224351

58	6	0	7.355336	-2.531526	-0.131953
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63	6	0	9.449304	-3.221322	0.968832
64	6	0	8.016663	-4.912746	-1.888024
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66	6	0	9.807319	-1.999648	1.565727
67	6	0	9.997076	-4.400488	1.483875
68	6	0	8.377699	-5.666458	-2.995456
69	1	0	7.016011	-5.000244	-1.477681
70	6	0	10.598347	-4.710878	-2.929866
71	1	0	10.938030	-3.261493	-1.378918
72	6	0	10.672921	-1.966703	2.649462
73	1	0	9.397306	-1.074690	1.173685
74	6	0	10.887128	-4.373885	2.559528
75	1	0	9.730810	-5.351095	1.033366
76	6	0	9.673812	-5.576395	-3.524612
77	1	0	7.673979	-6.348575	-3.461024
78	1	0	11.605816	-4.616839	-3.317270
79	6	0	11.225168	-3.153364	3.154254
80	1	0	10.950979	-1.026624	3.114406
81	1	0	11.294938	-5.307390	2.928477
82	6	0	-3.664187	-0.270591	0.058379
83	6	0	-4.936106	-1.029507	0.083402
84	6	0	-5.488248	-1.576877	-1.087677
85	6	0	-5.646494	-1.232576	1.279177
86	6	0	-6.678968	-2.292923	-1.070475
87	1	0	-4.983368	-1.428276	-2.037673

88	6	0	-6.845649	-1.934007	1.308236
89	1	0	-5.247297	-0.844490	2.211659
90	6	0	-7.386169	-2.483141	0.130960
91	1	0	-7.073032	-2.703429	-1.993429
92	1	0	-7.367921	-2.067081	2.249062
93	7	0	-8.600110	-3.202349	0.153552
94	6	0	-8.974246	-3.959629	1.302200
95	6	0	-9.482628	-3.171774	-0.966000
96	6	0	-8.064847	-4.842864	1.910380
97	6	0	-10.261717	-3.855343	1.838022
98	6	0	-9.833729	-1.953877	-1.574576
99	6	0	-10.036165	-4.352801	-1.470488
100	6	0	-8.432395	-5.582277	3.025281
101	1	0	-7.064156	-4.941232	1.502607
102	6	0	-10.646730	-4.613190	2.945924
103	1	0	-10.974682	-3.178335	1.379024
104	6	0	-10.698112	-1.926537	-2.659454
105	1	0	-9.419239	-1.027442	-1.190813
106	6	0	-10.925059	-4.331614	-2.547203
107	1	0	-9.775288	-5.300534	-1.010867
108	6	0	-9.728675	-5.478126	3.551448
109	1	0	-7.733795	-6.263887	3.499221
110	1	0	-11.654169	-4.508587	3.330667
111	6	0	-11.256055	-3.114965	-3.153724
112	1	0	-10.970794	-0.989405	-3.133446
113	1	0	-11.337447	-5.266380	-2.907771
114	8	0	-12.103897	-2.977106	-4.216738
115	8	0	-9.992198	-6.257146	4.643142
116	8	0	12.074895	-3.009968	4.215047
117	8	0	9.930632	-6.368916	-4.608176

118	6	0	12.657951	-4.179037	4.766835
119	1	0	13.291971	-3.841573	5.587995
120	1	0	11.896884	-4.866395	5.158438
121	1	0	13.274622	-4.711381	4.030943
122	6	0	11.224502	-6.311110	-5.185758
123	1	0	11.213050	-7.010456	-6.022989
124	1	0	11.457653	-5.305681	-5.559521
125	1	0	12.001595	-6.615805	-4.472683
126	6	0	-11.286270	-6.184039	5.218571
127	1	0	-11.280385	-6.873719	6.063836
128	1	0	-11.513053	-5.172792	5.580384
129	1	0	-12.064627	-6.491737	4.508169
130	6	0	-12.692973	-4.148226	-4.757733
131	1	0	-13.324206	-3.815238	-5.582855
132	1	0	-11.935384	-4.843655	-5.141734
133	1	0	-13.313401	-4.669837	-4.017330

Electronic Energy: -3385.065059 Hartree

Copies of ^{1}H-NMR, ^{13}C-NMR, ^{11}B-NMR, ^{19}F-NMR and HRMS/MALDI spectra

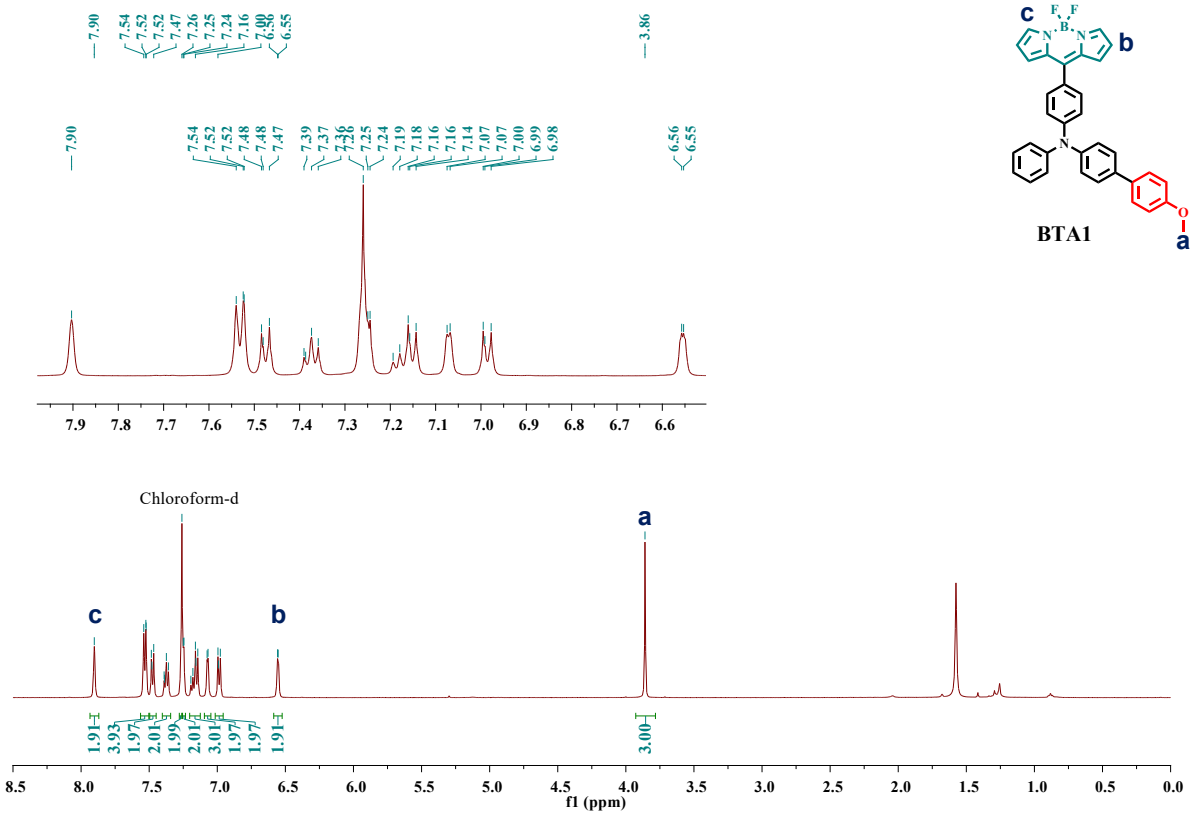

Fig. S12 ^{1}H NMR ($CDCl_3$) spectra of **BTA1**.

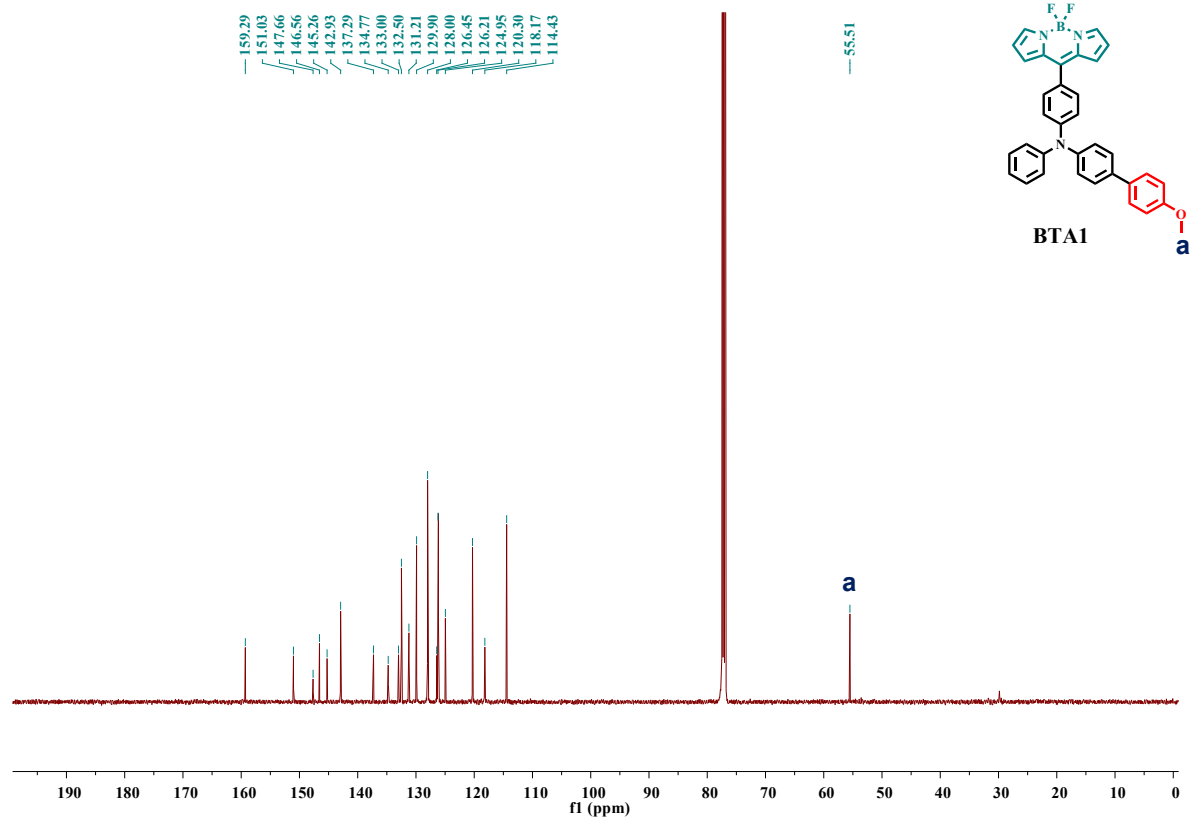

Fig. S13 ^{13}C{^{1}H} NMR ($CDCl_3$) spectra of **BTA1**.

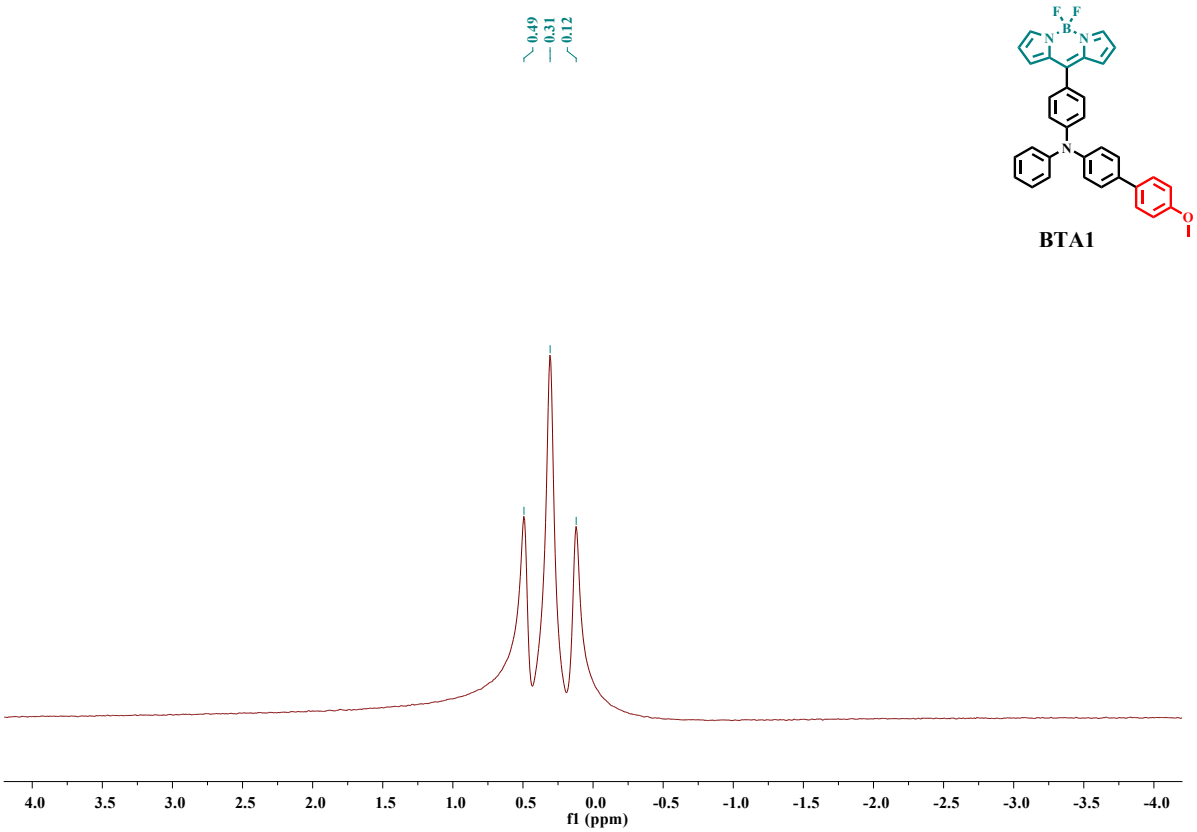

Fig. S14 ^{11}B NMR ($CDCl_3$) spectra of **BTA1**.

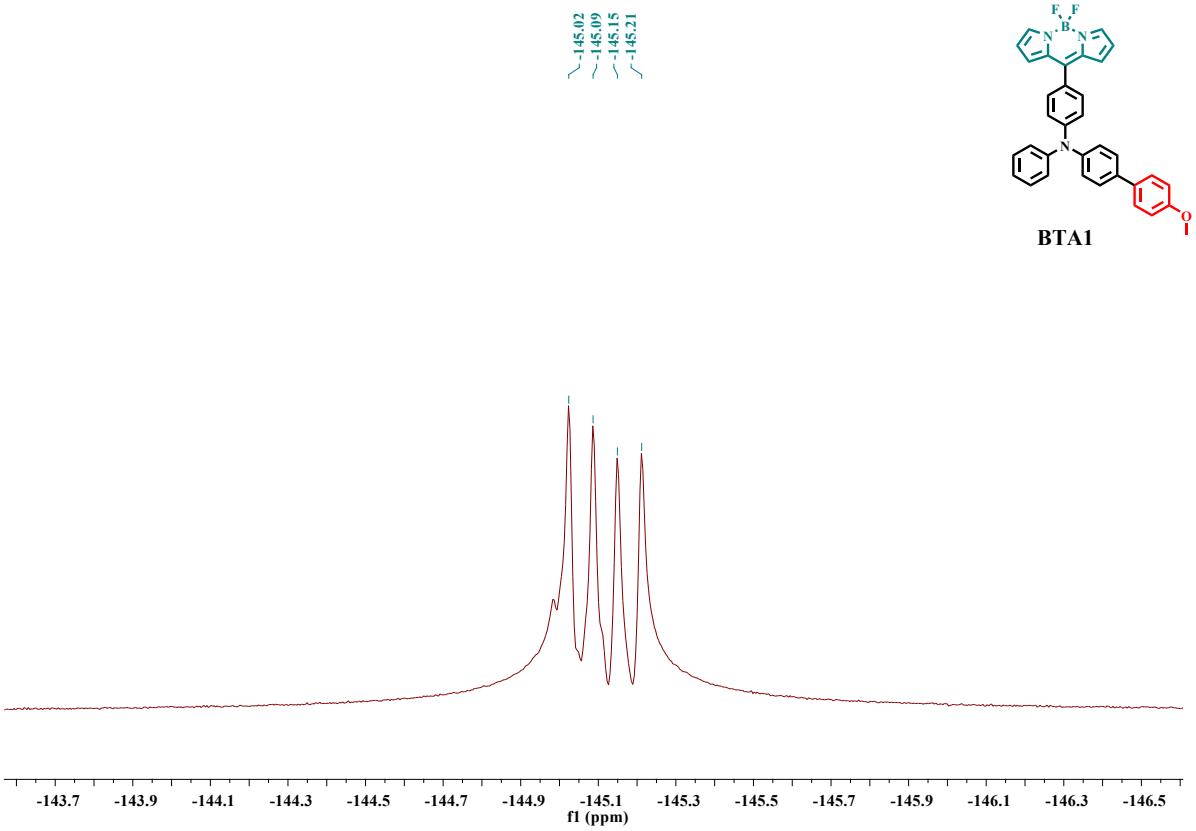

Fig. S15 ^{19}F NMR ($CDCl_3$) spectra of **BTA1**.

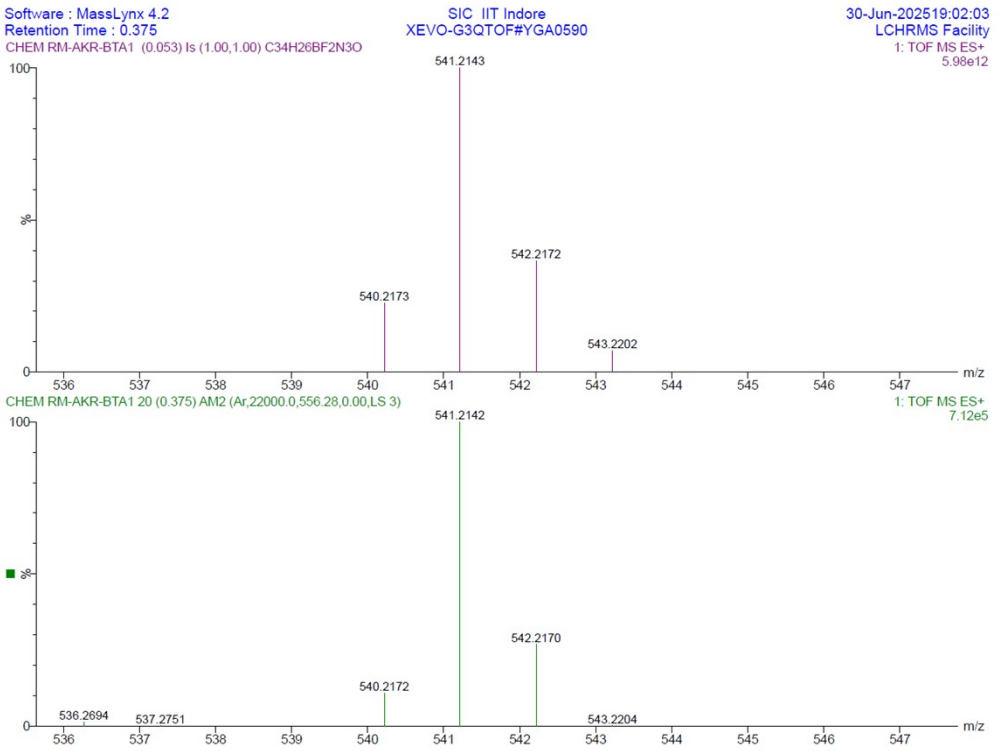

Fig. S16 HRMS of **BTA1**.

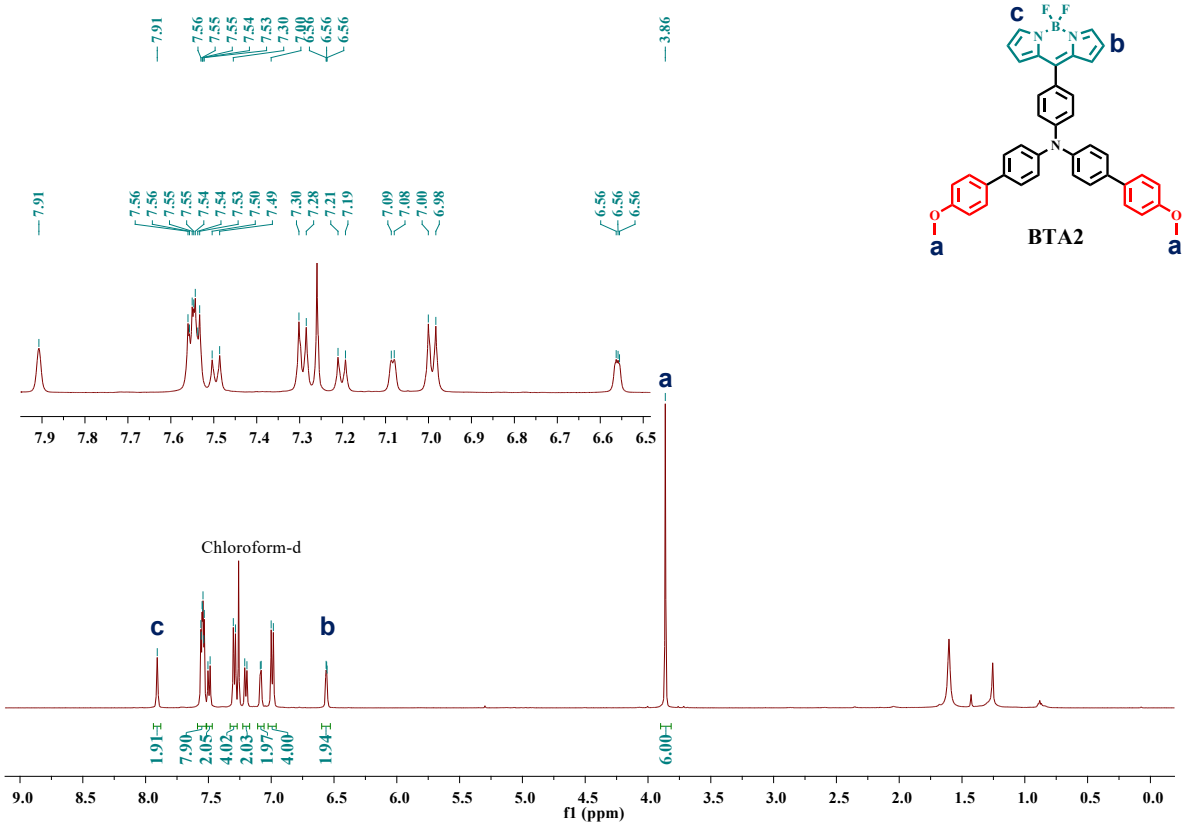

Fig. S17 ^{1}H NMR ($CDCl_3$) spectra of **BTA2**.

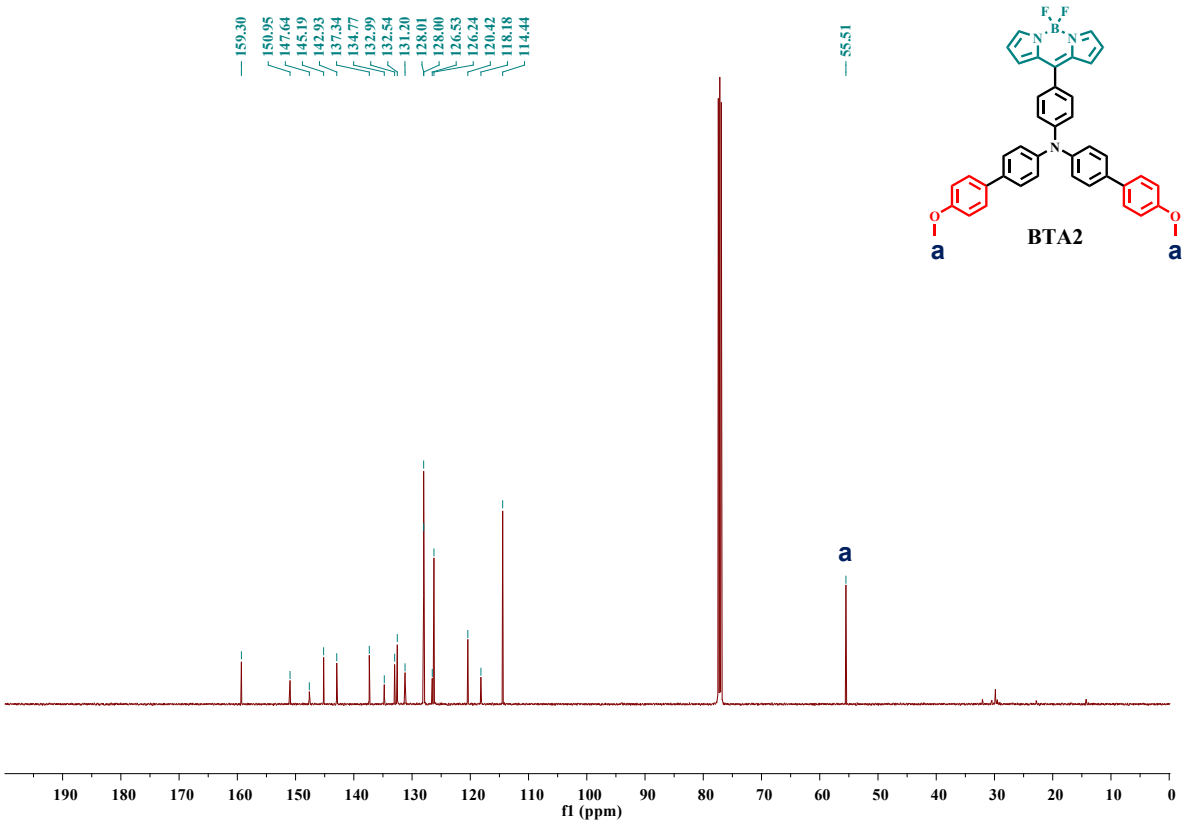

Fig. S18 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **BTA2**.

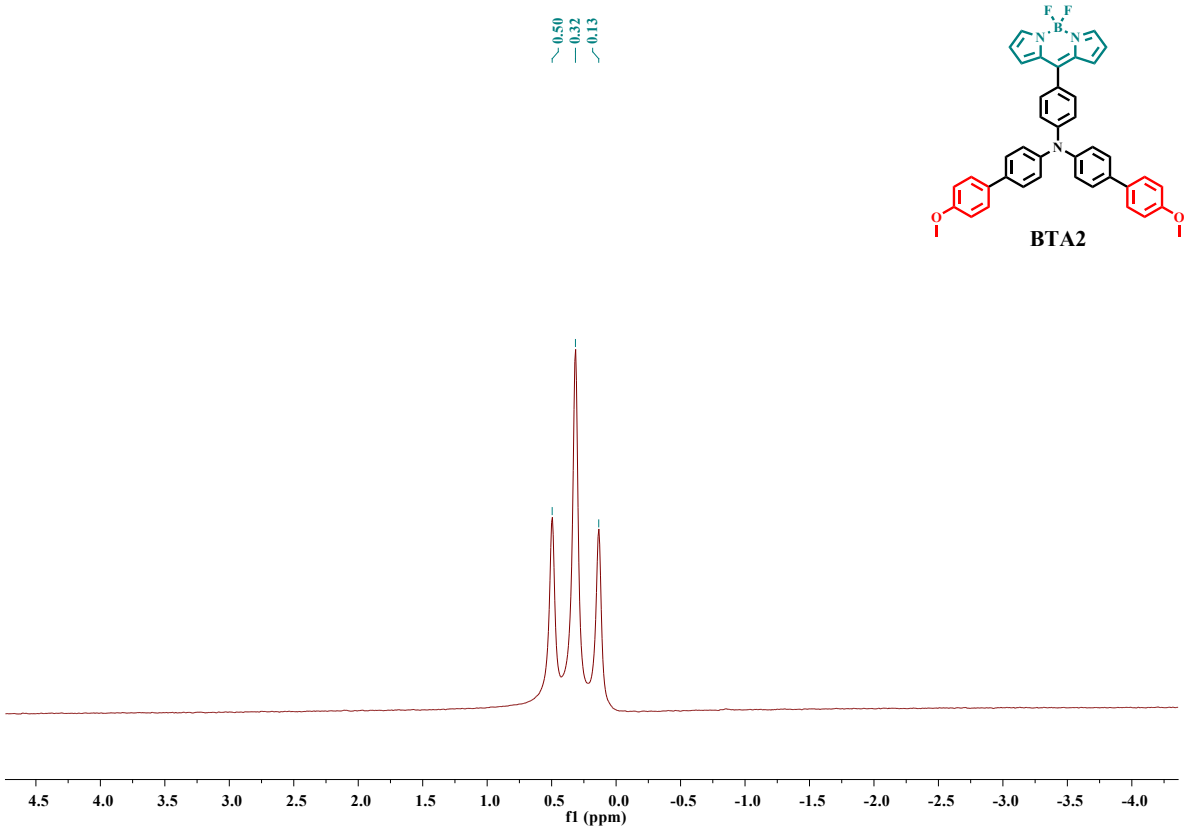

Fig. S19 ^{11}B NMR ($CDCl_3$) spectra of **BTA2**.

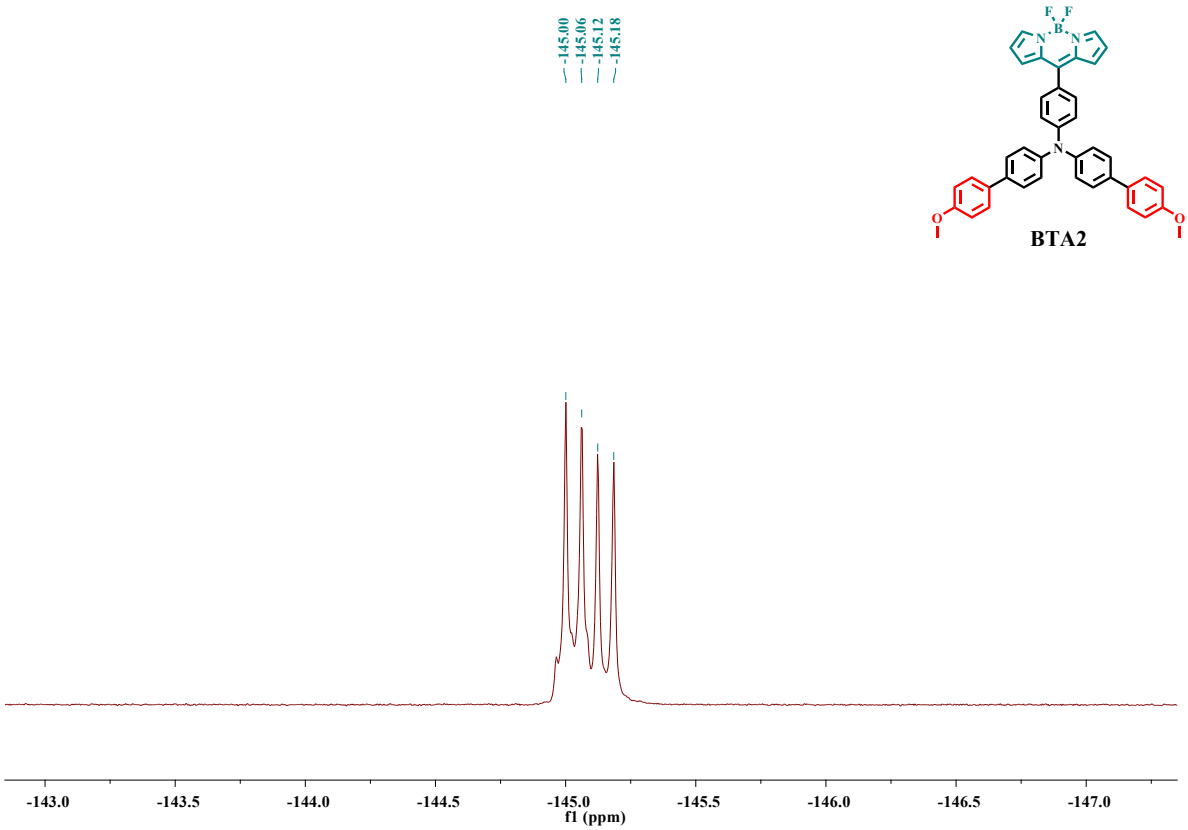

Fig. S20 ^{19}F NMR ($CDCl_3$) spectra of **BTA2**.

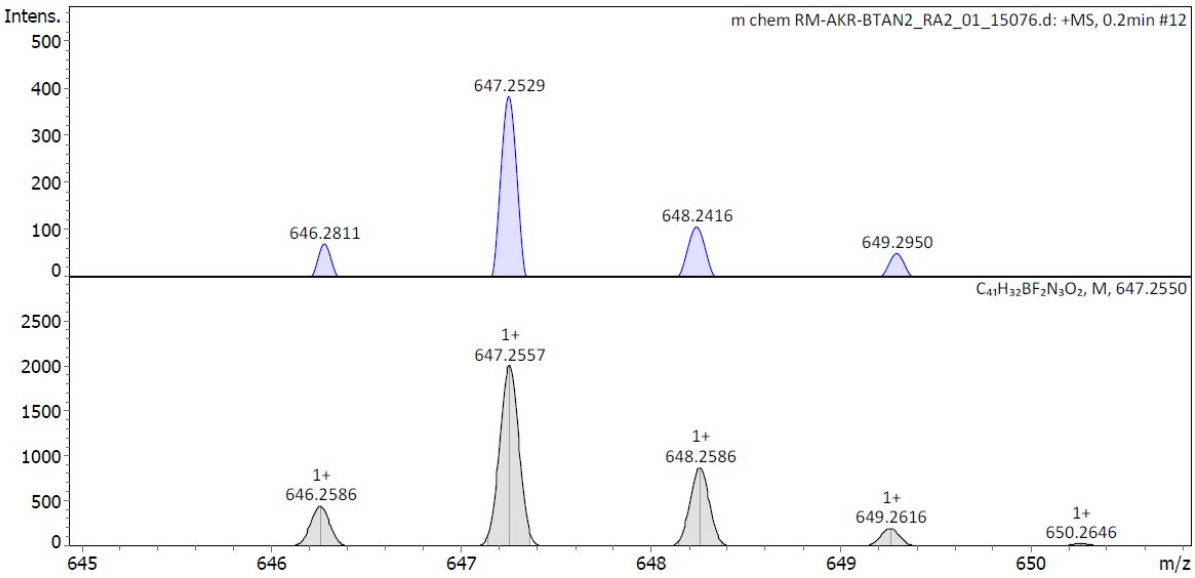

Fig. S21 HRMS of **BTA2**.

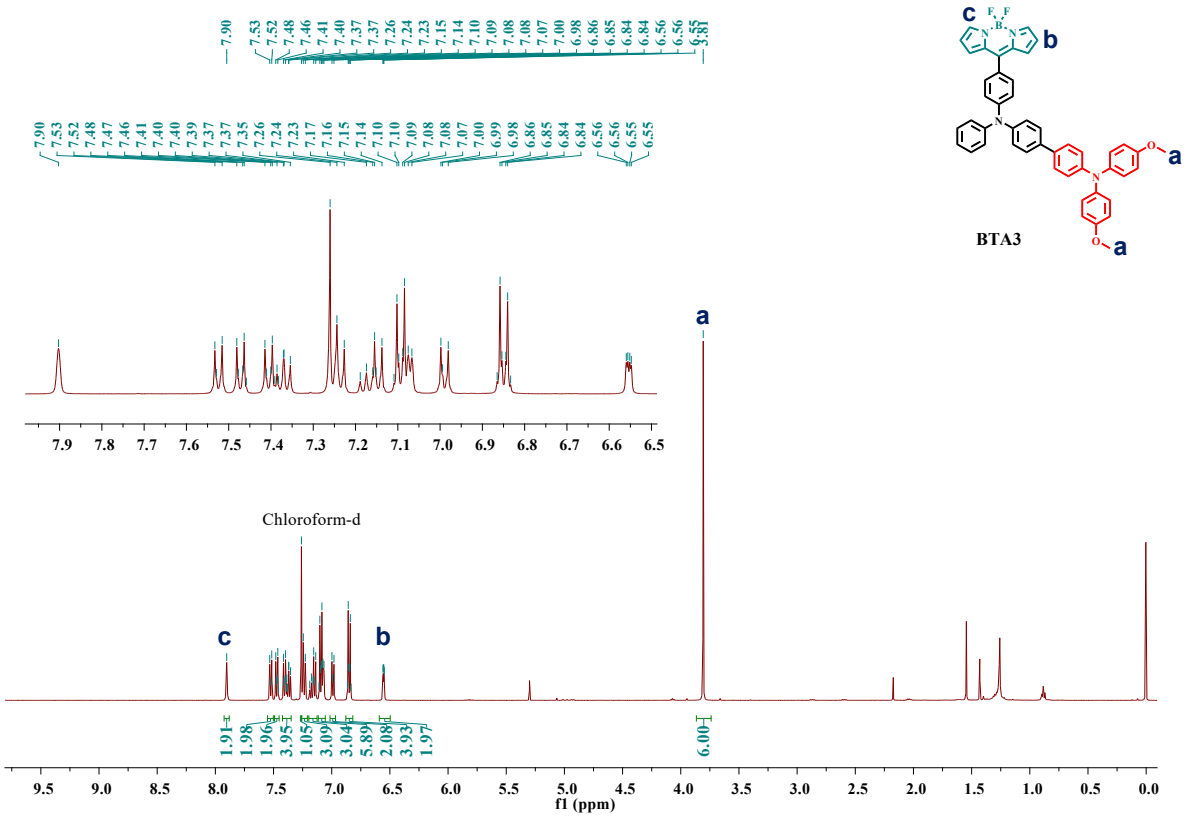

Fig. S22 ^{1}H NMR ($CDCl_3$) spectra of **BTA3**.

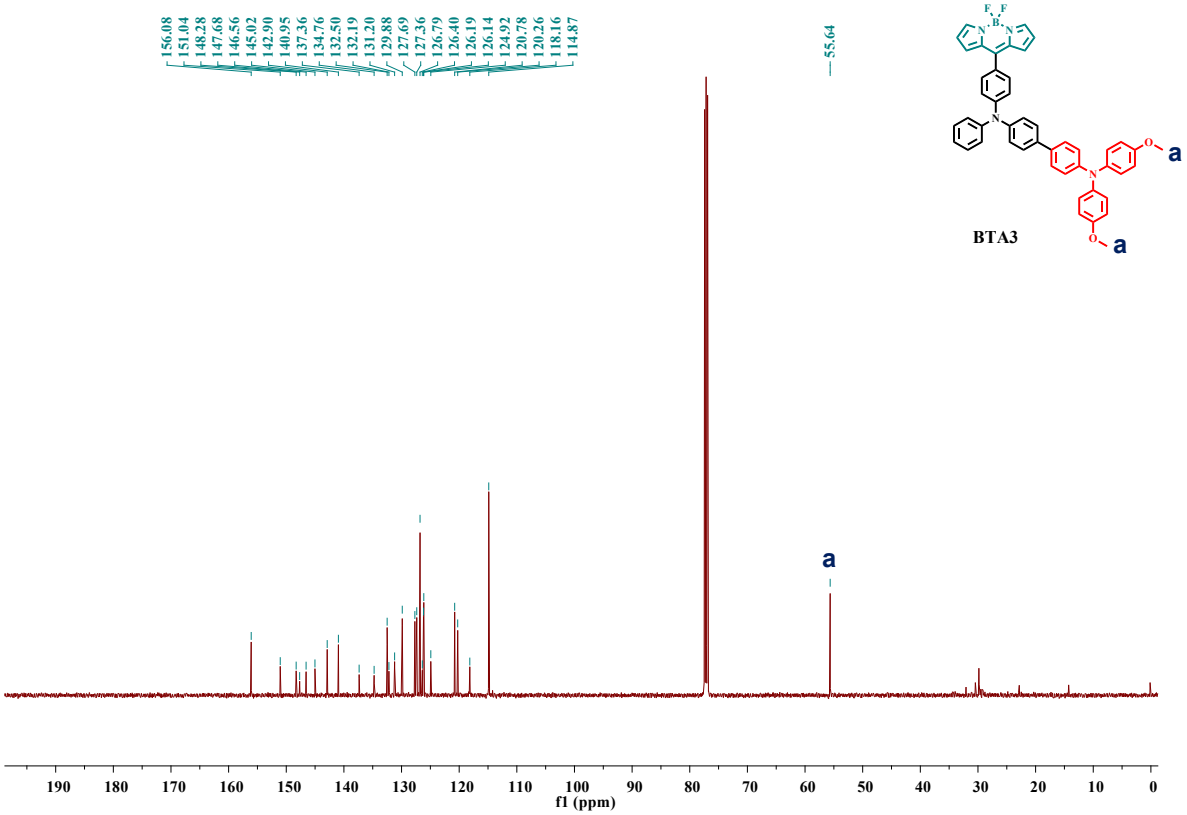

Fig. S23 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **BTA3**.

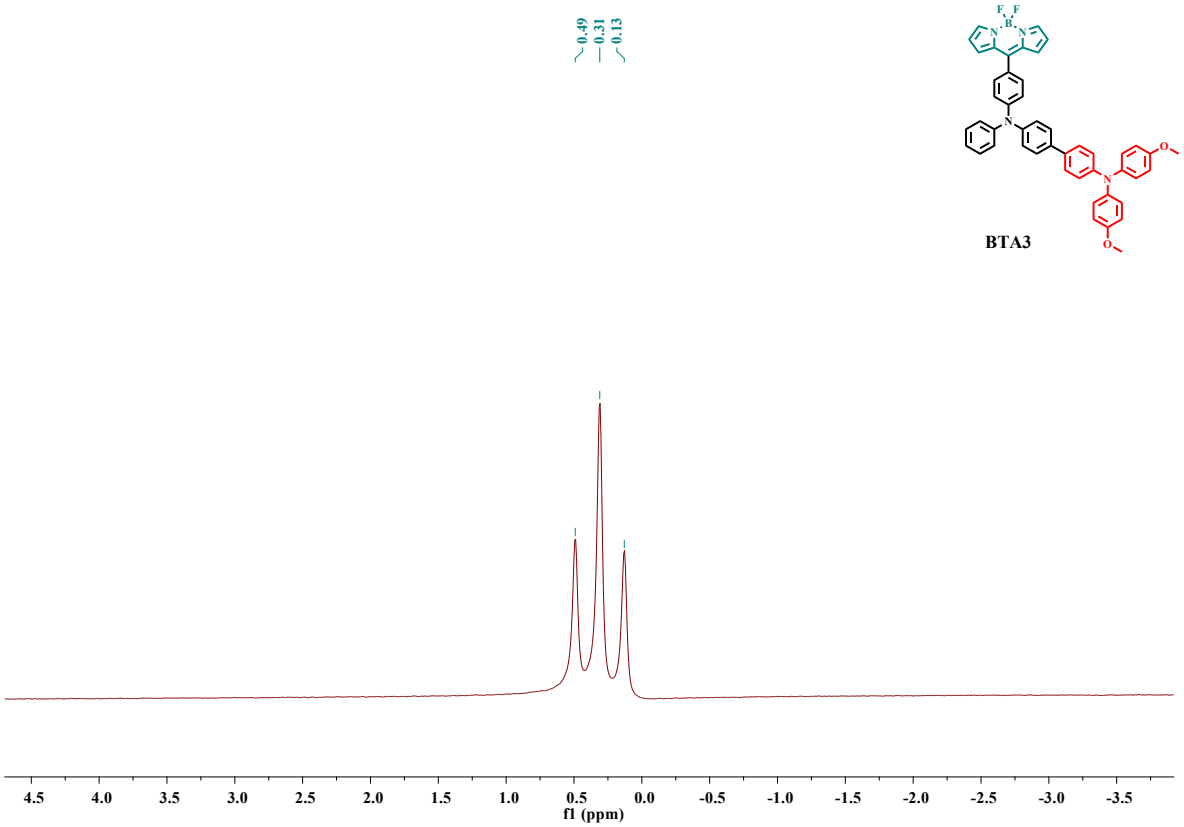

Fig. S24 ^{11}B NMR ($CDCl_3$) spectra of **BTA3**.

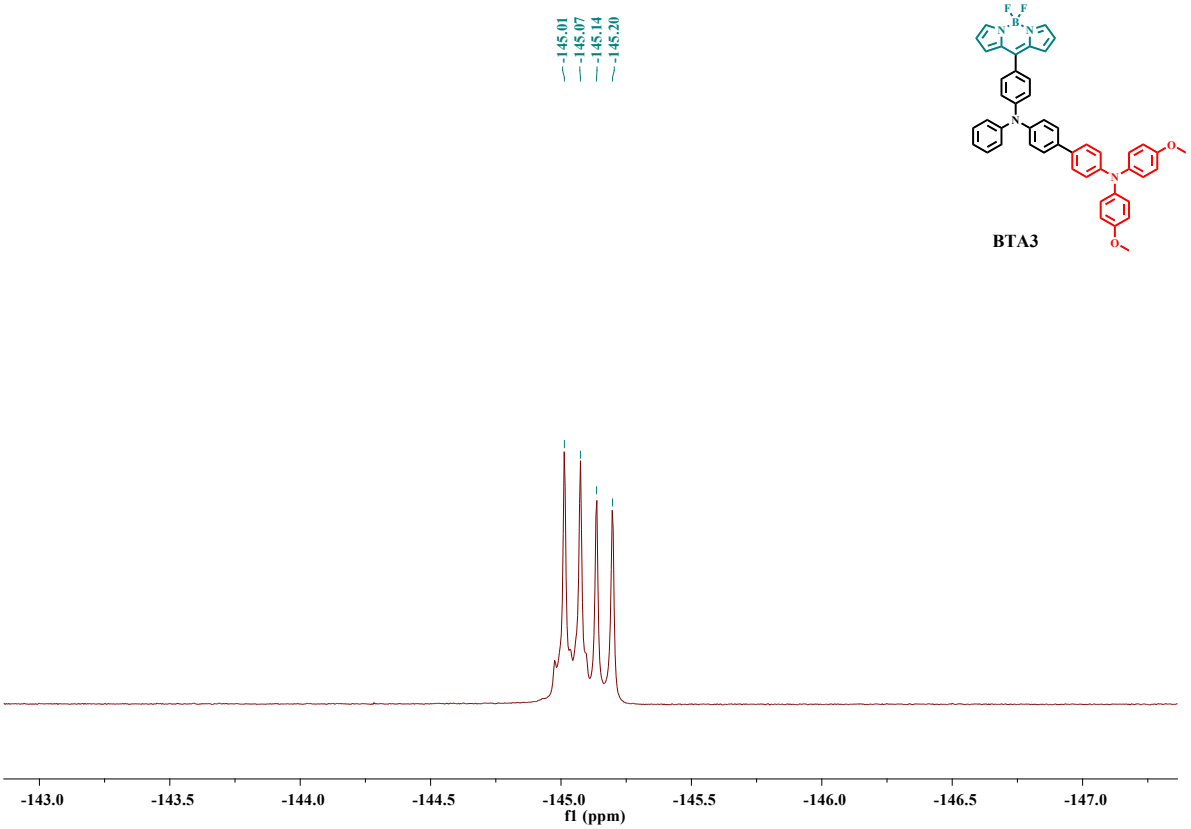

Fig. S25 ^{19}F NMR ($CDCl_3$) spectra of **BTA3**.

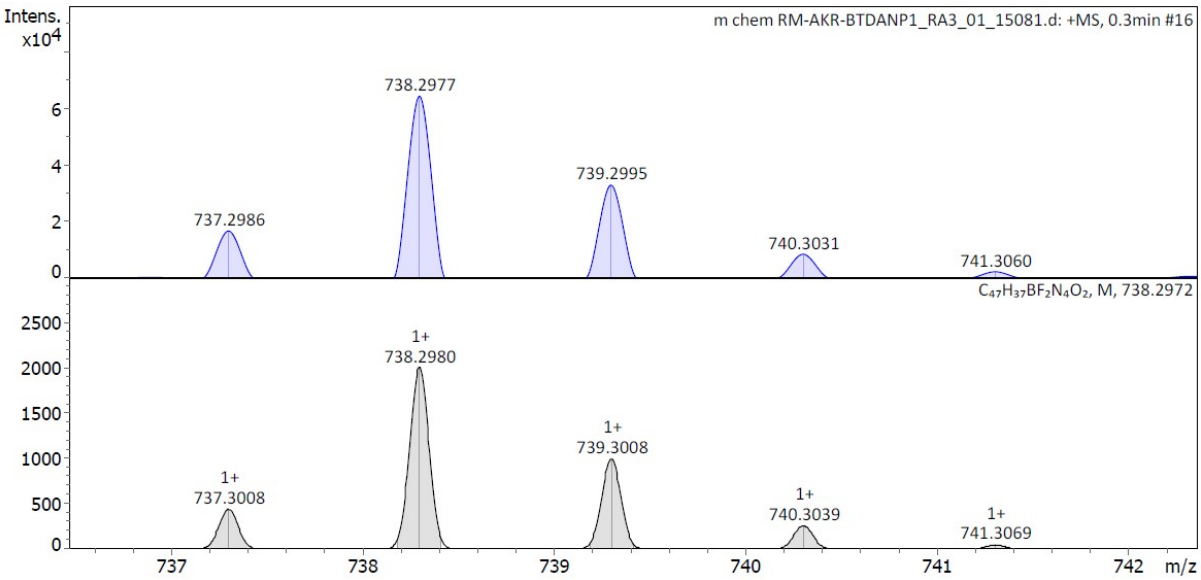

Fig. S26 HRMS of **BTA3**.

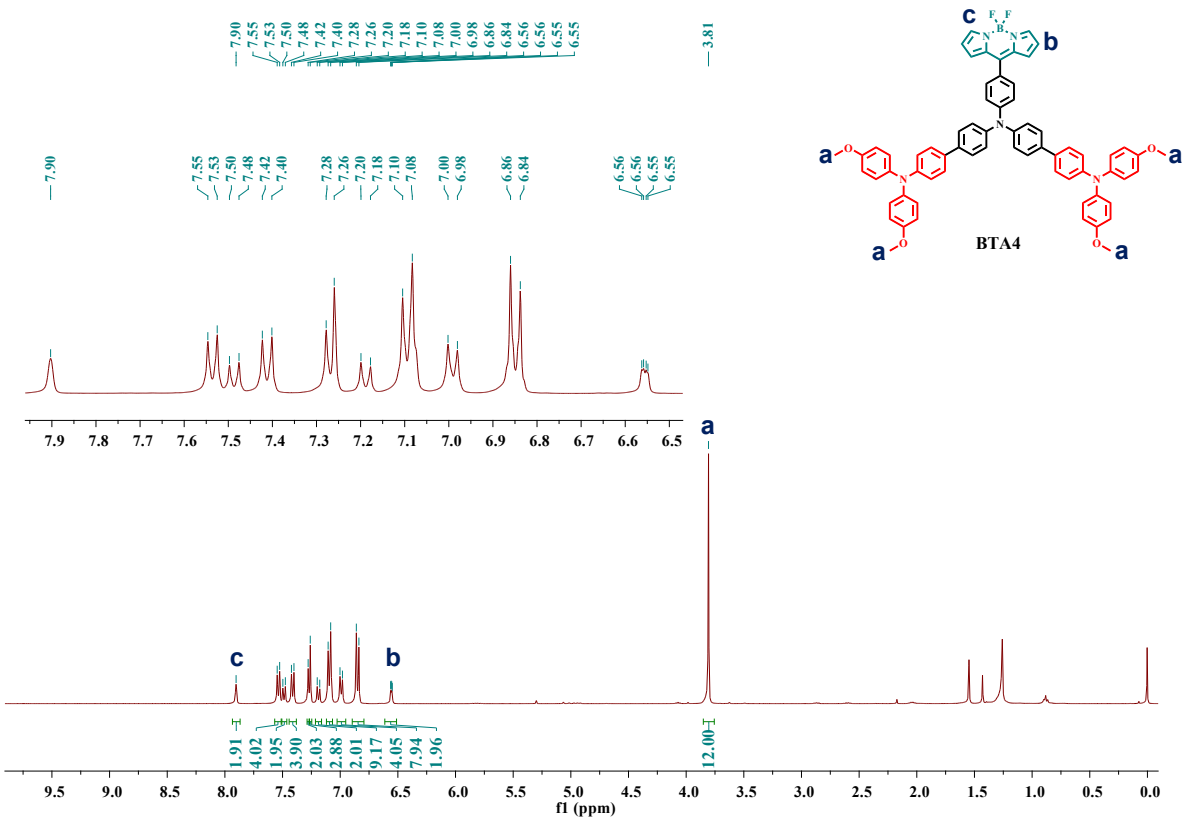

Fig. S27 ^{1}H NMR ($CDCl_3$) spectra of **BTA4**.

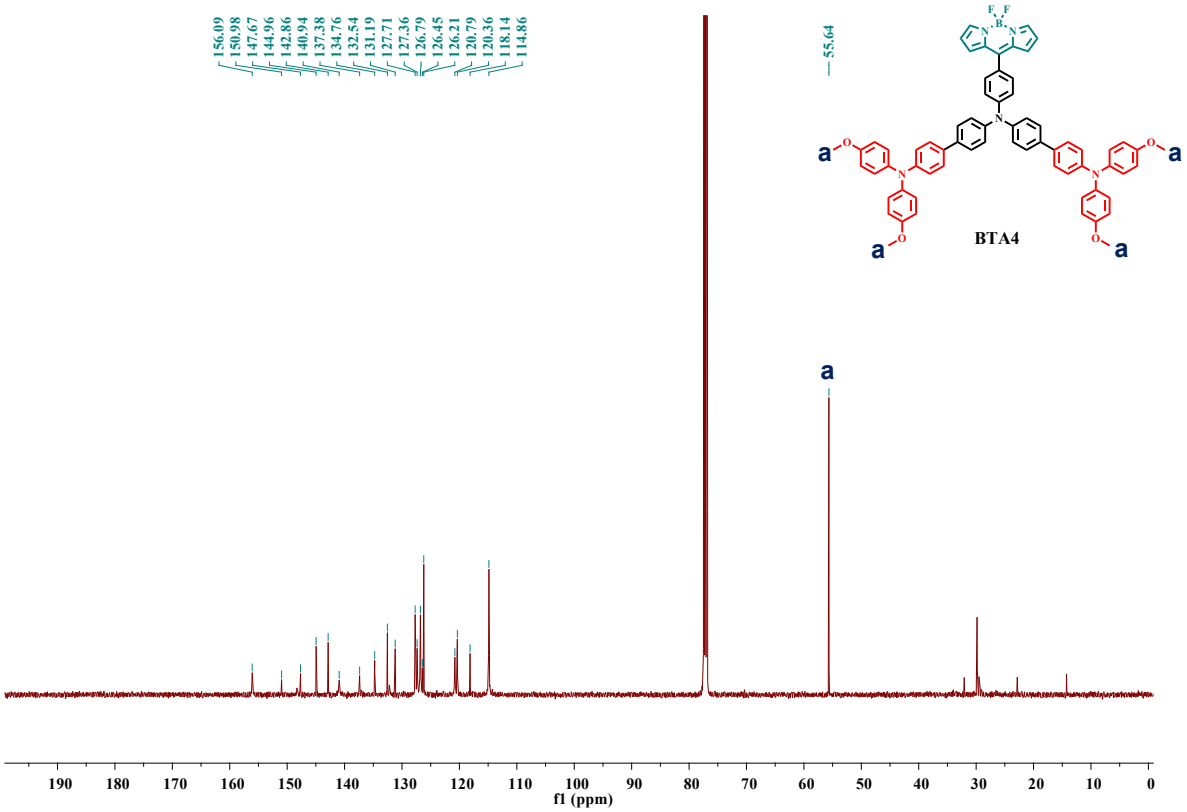

Fig. S28 $^{13}C\{^{1}H\}$ NMR ($CDCl_3$) spectra of **BTA4**.

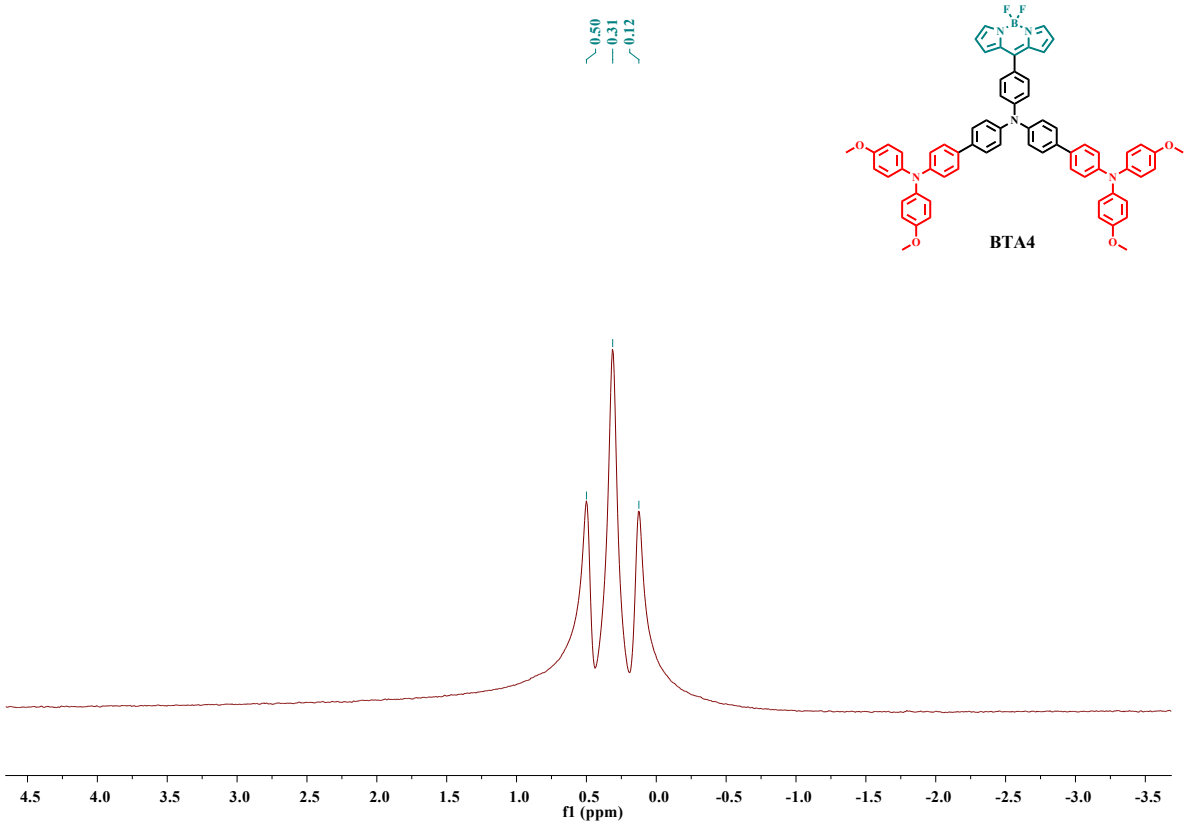

Fig. S29 ^{11}B NMR ($CDCl_3$) spectra of **BTA4**.

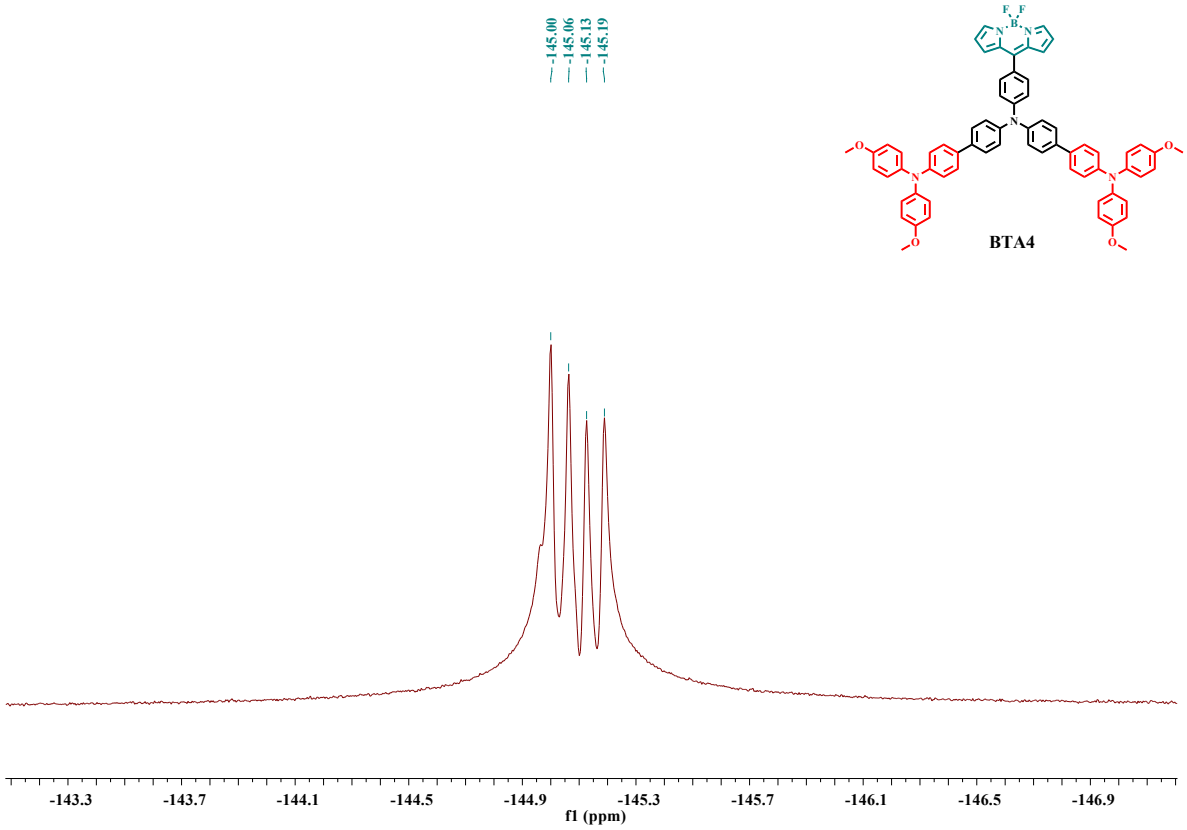

Fig. S30 ^{19}F NMR ($CDCl_3$) spectra of **BTA4**.

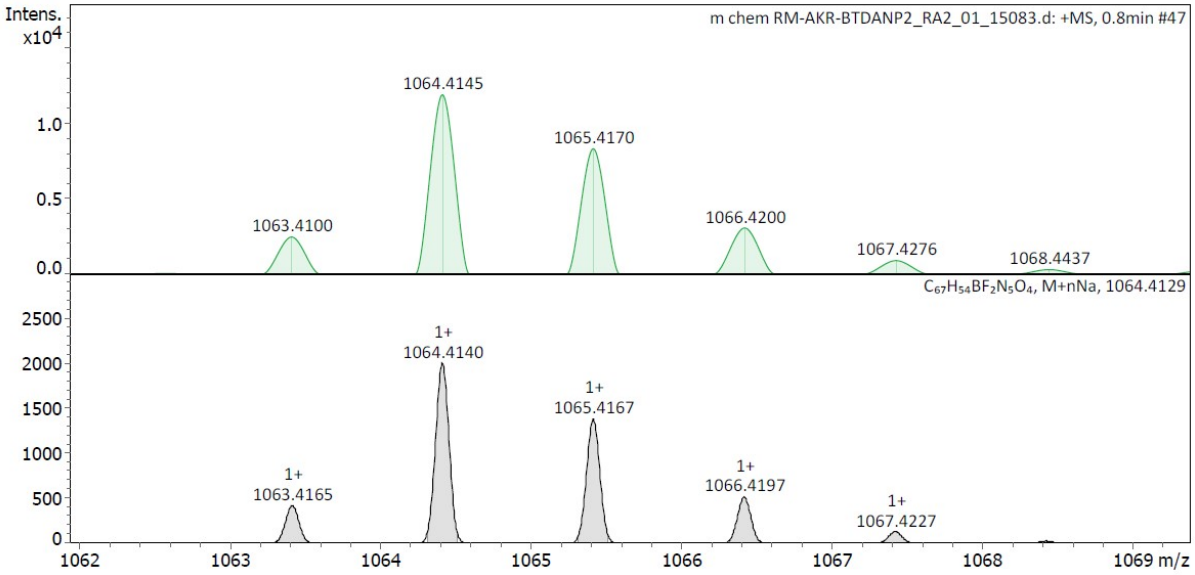

Fig. S31 HRMS of **BTA4**.

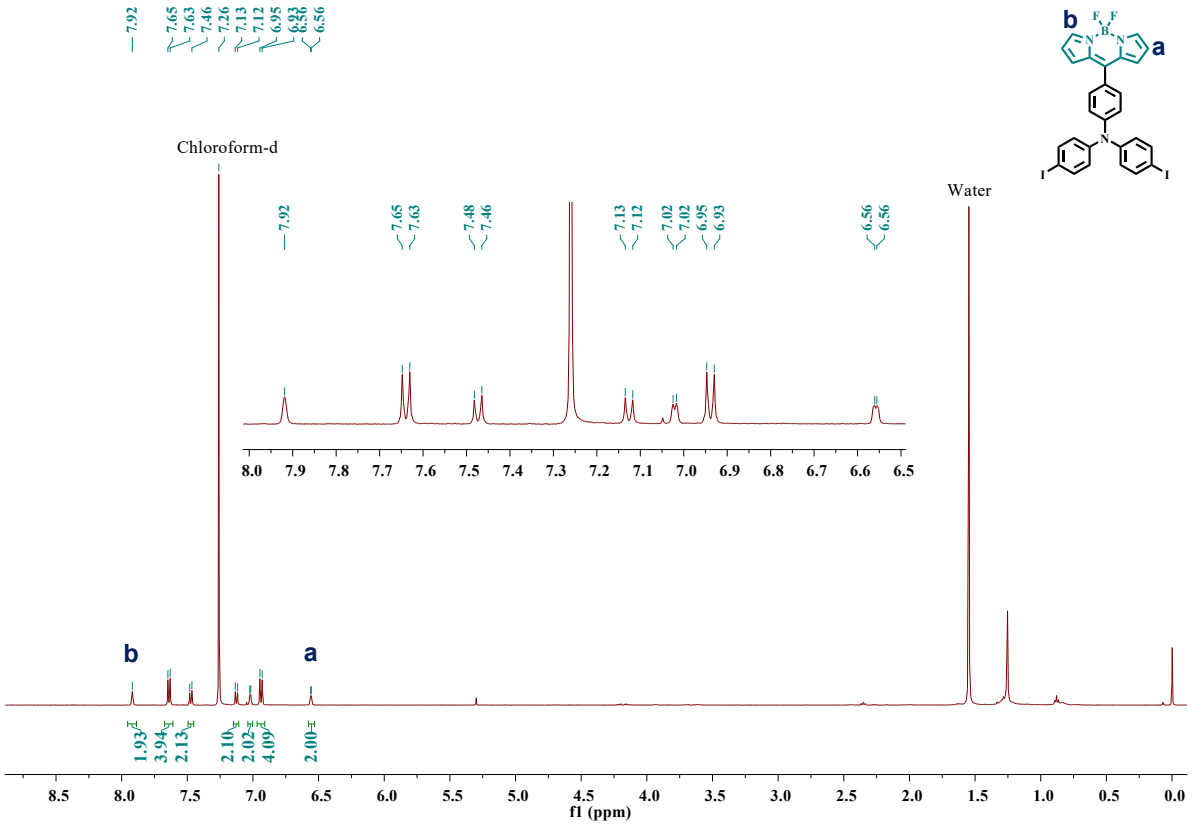

Fig. S32 ^{1}H NMR ($CDCl_3$) spectra of **BTI_2**.

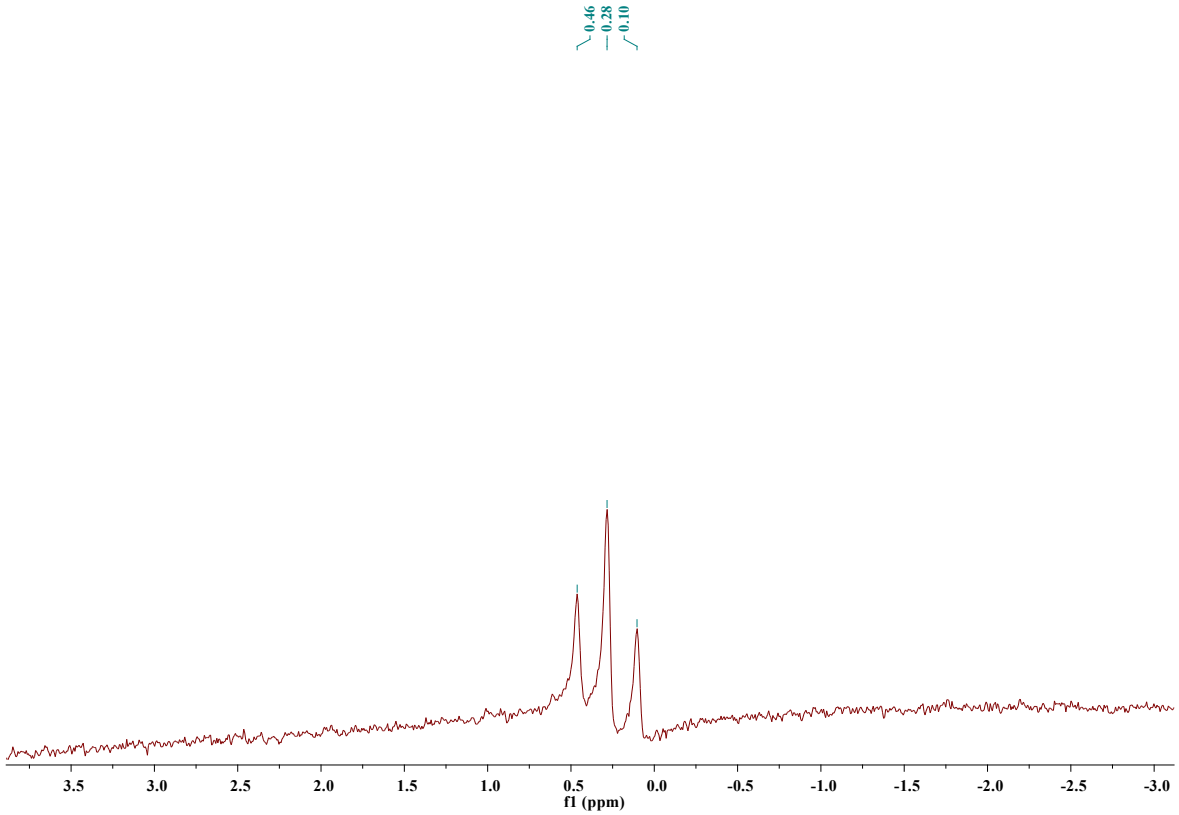

Fig. S33 ^{11}B NMR ($CDCl_3$) spectra of **BTI_2**.

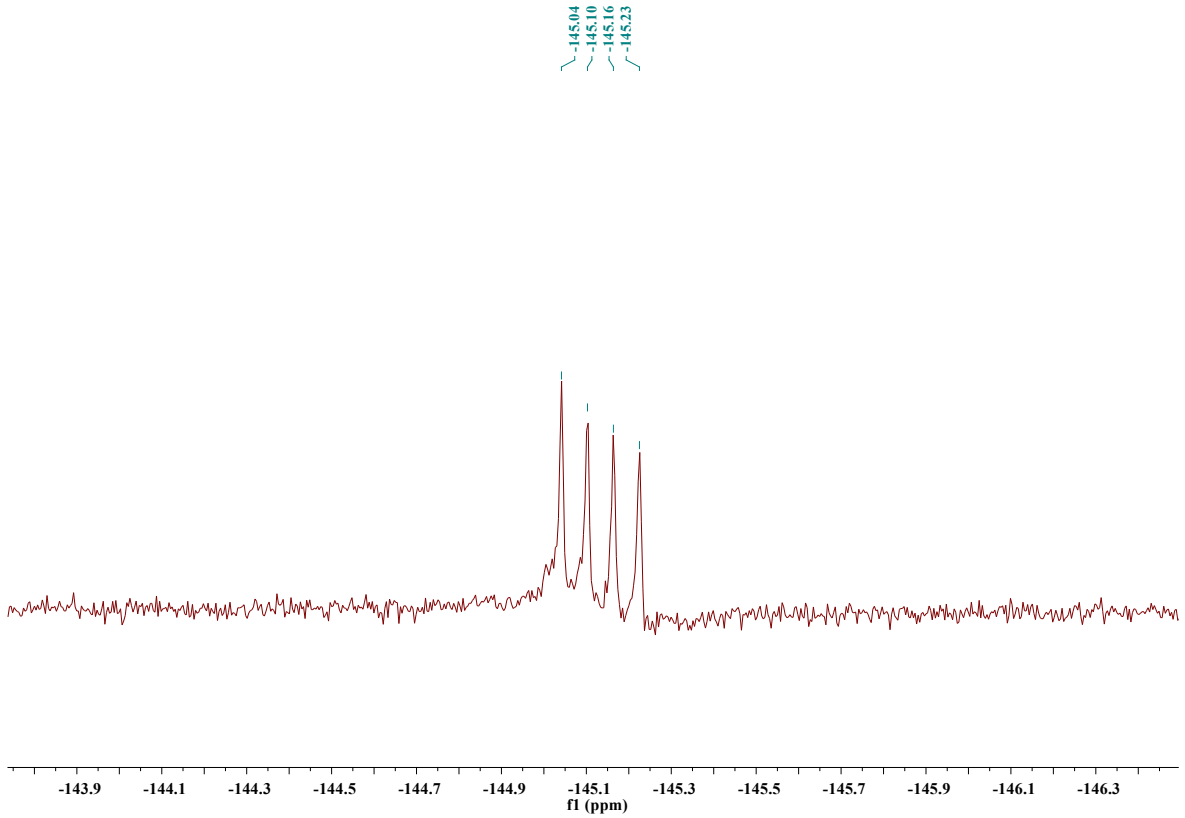

Fig. S34 ^{19}F NMR ($CDCl_3$) spectra of **BTI_2**.

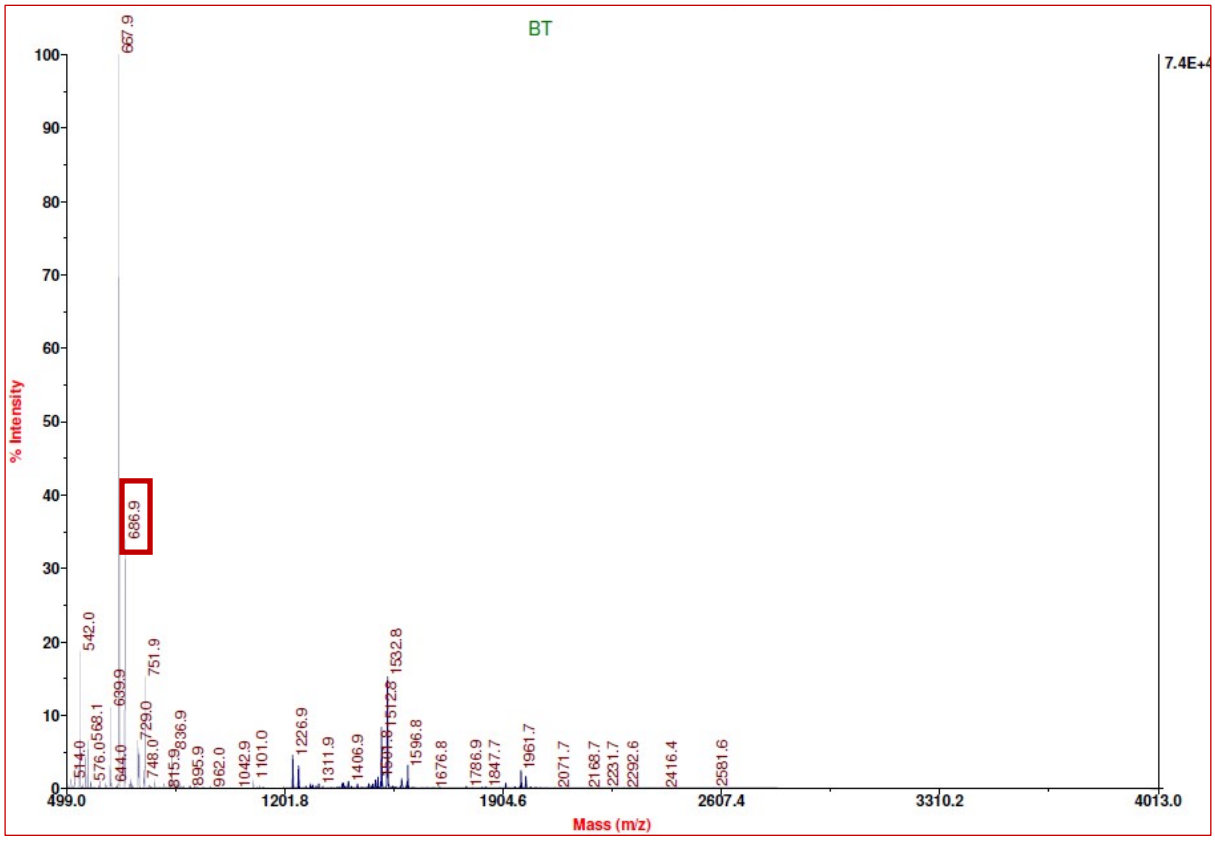

Fig. S35 MALDI-TOF-MS of **BTI_2**.

Reference

1 B. G. Kim, X. Ma, C. Chen, Y. Ie, E. W. Coir, H. Hashemi, Y. Aso, P. F. Green, J. Kieffer and J. Kim, *Adv. Funct. Mater.*, 2013, **23**, 439–445.