Aggregation Caused Quenching to Aggregation Induced Emission Transformation: A Precise Tuning Based on BN-Doped Polycyclic Aromatic Hydrocarbons Toward Subcellular Organelle Specific Imaging

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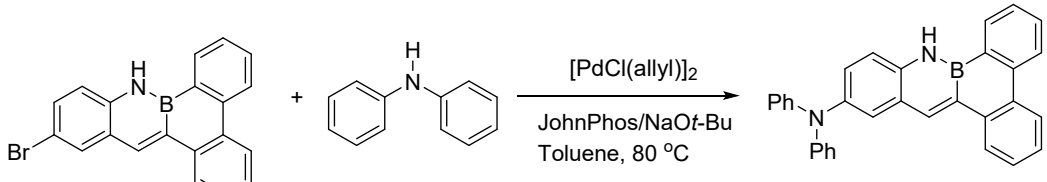
Contents

General Information. All operations involving air- and moisture-sensitive compounds were carried out under an atmosphere of dry argon by using a modified Schlenk line. All solvents were freshly distilled from Na or CaH_2. The ^{1}H, ^{13}C, ^{11}B spectra were recorded on a 400 MHz NMR spectrometer. Chemical shifts are referenced against external $BF_3{\cdot}Et_2O$ (^{11}B) and tetramethylsilane (TMS). High-resolution mass spectra (HRMS) were obtained on a Varian QFT-ESI spectrometer. The UV-vis spectra were recorded on a RAYLEIGH UV-2100 spectrometer. Fluorescence spectra and quantum yield were performed on Edinburgh Instruments FS5 fluorescence spectrophotometer. A suitable crystal was selected and on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. the crystal was kept at 150.00(10) K during data collection during data collection using graphite-monochromated CuKα radiation (λ = 1.54184Å). CCDC numbers: 2099086 (for compound DPA-BN-BFT) , 2099085 (for compound DMA-DPA-BN-BFT). The structures were solved by use of SHELXTL program[S1]. Refinements were performed on F^2 anisotropically for all the non-hydrogen atoms by the full-matrix least-squaresmethod. The commercially available catalysts and reagents were purchased from bidepharm.

Procedures for the Synthesis of BN-BFT and Br-BN-BFT.

The BN-BFT and Br-BN-BFT were synthesized according to the related synthetic routes. [S2]

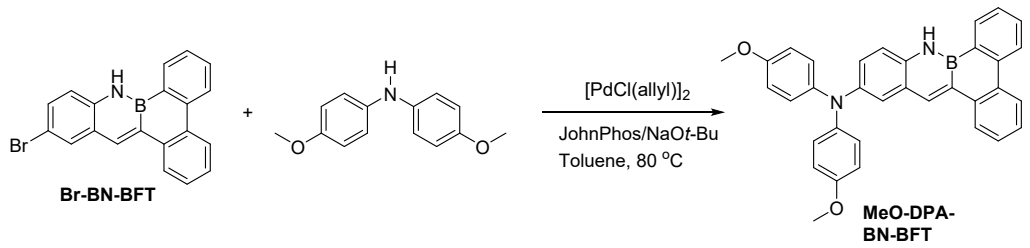
General Procedure for the Synthesis of DPA-BN-BFT



Br-BN-BFT **DPA-BN-BFT**

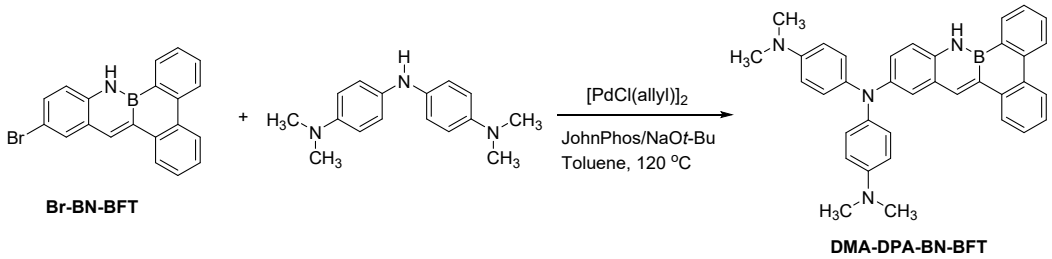
To an oven-dried schlenk tube with a stir bar was added Br-BN-BFT (0.5 mmol, 1 equiv) and diphenylamine (0.6 mmol, 1.2 equiv), $[PdCl(allyl)]_2$ dimer (0.005 mmol, 1 mol %), JohnPhos (0.01 mmol, 2 mol%), and NaOt-Bu (0.7 mmol, 1.4 equiv). The tube was sealed with schlenk system, evacuated under vacuum, and purged with Ar three times. Toluene (5 mL) was added, the resulting mixture was heated to 80°C and stirred 18 h. The reaction mixture was cooled to rt, and filtered over Celite. The solvent was removed in vacuo, and the product was purified by flash column chromatography on silica gel with hexanes and dichloromethane as the eluent.

General Procedure for the Synthesis of Compound MeO-DPA-BN-BFT



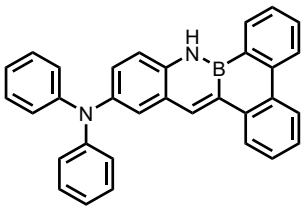
To an oven-dried schlenk tube with a stir bar was added Br-BN-BFT (0.5 mmol, 1 equiv) and methoxy substituted diphenylamine (0.6 mmol, 1.2 equiv), $[PdCl(allyl)]_2$ dimer (0.01 mmol, 2 mol %), JohnPhos (0.02 mmol, 4 mol%), and NaOt-Bu (0.7 mmol, 1.4 equiv). The tube was sealed with schlenk system, evacuated under vacuum, and purged with Ar three times. Toluene (8 mL) was added, the resulting mixture was heated to 120°C and stirred 18 h. The reaction mixture was cooled to rt, and filtered over Celite. The solvent was removed in vacuo, and the product was purified by flash column chromatography on silica gel with hexanes and dichloromethane as the eluent.

General Procedure for the Synthesis of Compound DMA-DPA-BN-BFT



To an oven-dried schlenk tube with a stir bar was added Br-BN-BFT (0.5 mmol, 1 equiv) and bindschedler (0.6 mmol, 1.2 equiv), $[PdCl(allyl)]_2$ dimer (0.005 mmol, 1 mol %), JohnPhos (0.01 mmol, 2 mol%), and NaOt-Bu (0.7 mmol, 1.4 equiv). The tube was sealed with schlenk system, evacuated under vacuum, and purged with Ar three times. Toluene (8 mL) was added, the resulting mixture was heated to 120°C and stirred 24 h. The reaction mixture was cooled to rt, and filtered over Celite. The solvent was removed in vacuo, and the product was purified by flash column chromatography on silica gel with hexanes and dichloromethane as the eluent.

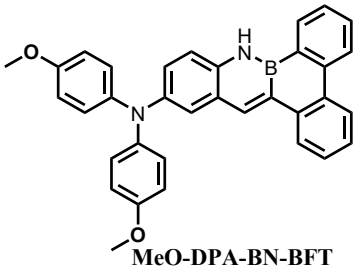
Characterization Data for the New Compounds



N, N-diphenyl-10H-benzo[e]dibenzo[3,4:5,6]borinino[1,2-b][1,2]azaborinin-13-amine

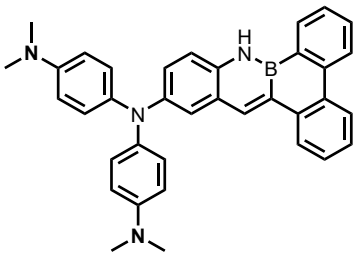
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (1H, s), 8.50 (1H, s, *NH*), 8.28-8.38 (3H, m), 8.09 (1H, d, *J* = 8 Hz), 7.57-7.61 (2H, m), 7.37-7.45(3H, m) 7.22-7.31 (6H, m), 7.11-7.13 (4H, m,), 6.97-7.01 (2H, m,). ^{13}C NMR (101 MHz, $CDCl_3$): δ 148.25, 141.40, 141.23, 136.33, 133.88, 133.45, 130.60, 129.84, 129.38, 127.42, 127.26, 127.17, 126.42, 126.19, 125.77, 125.00, 124.19, 123.53, 123.10, 122.42, 119.30. HRMS: calcd. for $[M]^+$: 357.0324, found: 357.0276. The carbons attaching to

boron were not observed.



MeO-DPA-BN-BFT

N,N-bis(4-methoxyphenyl)-10H-benzo[e]dibenzo[3,4:5,6]borinino[1,2-b][1,2]azaborinin-13-amine .^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (1H, s), 8.63 (1H, s, *NH*), 8.38-8.47 (3H, m), 8.20 (1H, d, *J*=8Hz), 7.65 (1H, t, *J*=8Hz), 7.29-7.51(6H, m), 7.22-7.31 (6H, m), 6.83-7.06 (8H, m,), 6.97-7.01 (2H, m,). ^{13}C NMR (101 MHz, $CDCl_3$): δ 155.42, 141.21, 136.49, 135.36, 134.06, 133.46, 130.55, 129.84, 127.20, 127.19, 126.34, 126.23, 125.59, 125.51, 125.05, 124.24, 123.09, 122.49, 118.95, 114.77(overlap), 55.64(-OMe). HRMS: calcd. for [M+H]+: 507.2244, found: 507.2241. The carbons attaching to boron were not observed.



DMA-DPA-BN-BFT

N1-(10H-benzo[e]dibenzo[3,4:5,6]borinino[1,2-b][1,2]azaborinin-13-yl)-N1-(4-(dimethylamino)phenyl)-N4,N4-dimethylbenzene-1,4-diamine.^{1}H NMR (400 MHz, THF-d_8): δ 10.22 (1H, s), 8.88 (1H, s, *NH*), 8.41-8.50 (4H, m), 7.54-7.58 (1H, m), 7.49-7.51 (1H, m), 7.35-7.49(4H, m), 7.21 (1H, b), 6.97 (4H, m,), 6.66-6.68(4H, m), 2.52 (12H, m). ^{13}C NMR (Solid-state nuclear magnetic): δ 146.33, 145.26, 141.44, 140.02, 137.51, 135.59, 133.72, 132.22, 129.10, 128.14, 126.72, 124.51, 123.80, 119.40, 117.66, 112.38, 111.27, 39.40 (-$N(CH_3)_2$). HRMS: calcd. for [M]+: 532.2798, found: 532.2798. The carbons attaching to boron were not observed.

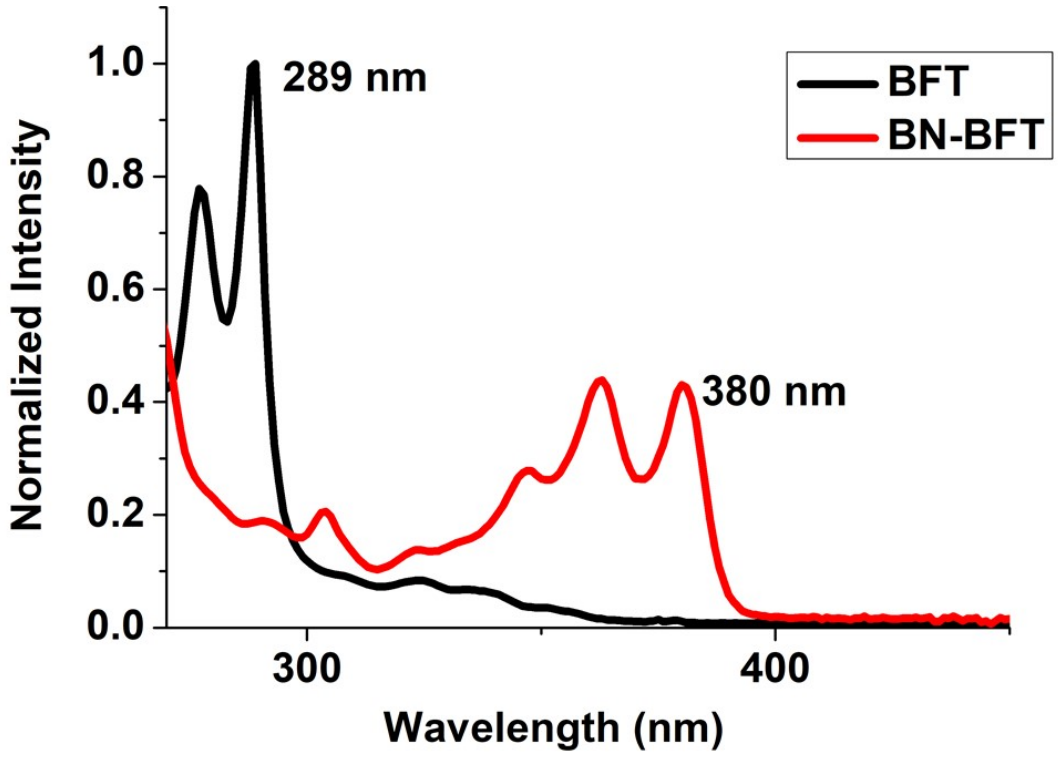


Figure S1. The UV−vis spectra of BN-BFT and BFT in CH_2Cl_2 (Concentration = 10^{-5} M)

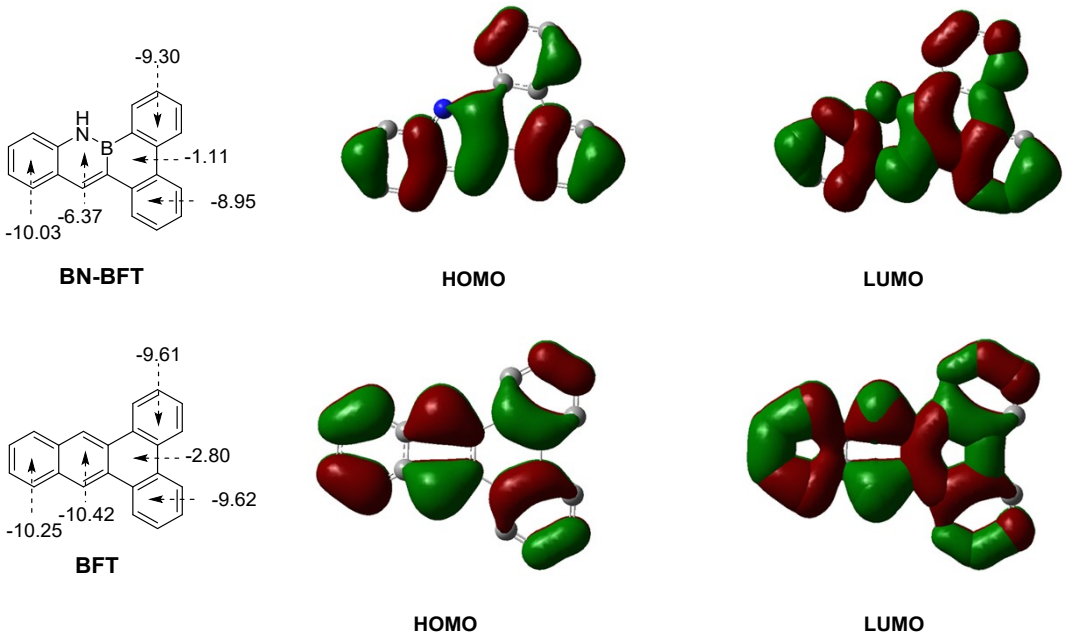
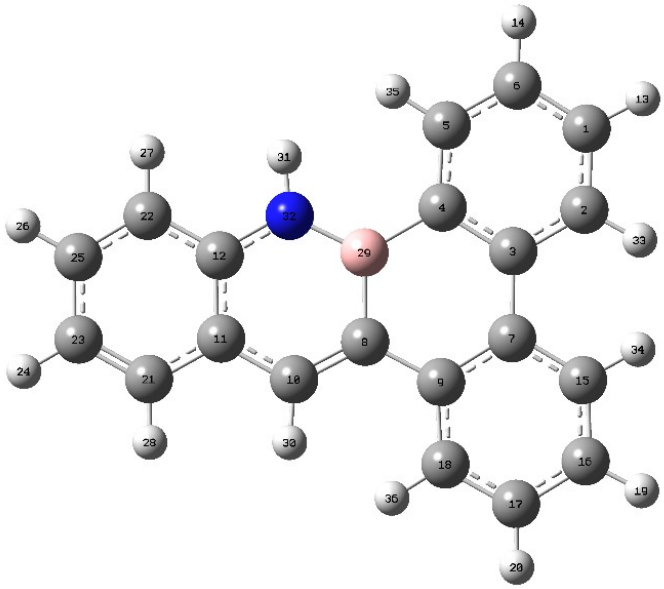


Figure S2. Calculated NICS (1) $_{zz}$ values (in ppm, calculated at the GLAO-B3LYP16-311+G (d. p) level), and the electronic distribution of HOMO and LUMO BN-BFT (up) and its hydrocarbon analogue BFT (down).

Table S1. The summary data of dual descriptor evaluation.



atoms	Atom No.	q_N	q_{N-1}	q_{N+1}	Δf
C	1	-0.22462	-0.09891	-0.15649	-0.19384
C	2	-0.22101	-0.12711	-0.10441	-0.2105
C	5	-0.19265	-0.09885	-0.10737	-0.17908
C	6	-0.24199	-0.12591	-0.14352	-0.21455
C	10	-0.12905	-0.07468	-0.28368	0.10026
C	15	-0.21522	-0.0772	-0.09762	-0.25562
C	16	-0.23747	-0.15362	-0.17757	-0.14375
C	17	-0.23524	-0.09755	-0.1313	-0.24163
C	18	-0.21503	-0.12135	-0.12918	-0.17953
C	21	-0.20014	-0.10866	-0.2011	-0.09052
C	22	-0.27086	-0.11146	-0.16377	-0.26649
C	23	-0.26292	-0.11459	-0.11578	-0.29547
C	25	-0.21794	-0.13349	-0.20356	-0.09883

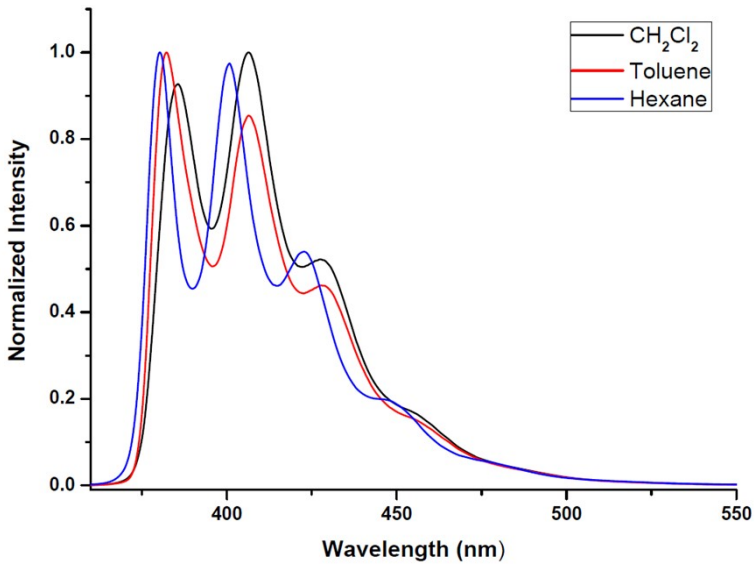


Figure S3. Normalized fluorescence emission spectra of BN-BFT in CH_2Cl_2, *n*-hexane and toluene, respectively. All experiments upon excitation at the absorption maximum wavelength. [S2]

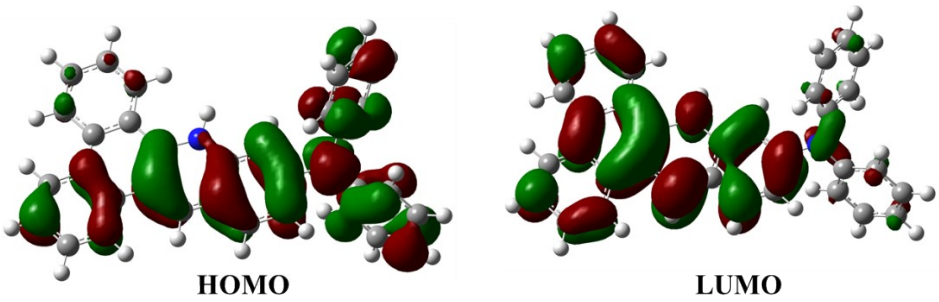


Figure S4. Calculated frontier orbitals of DPA-BN-BFT.

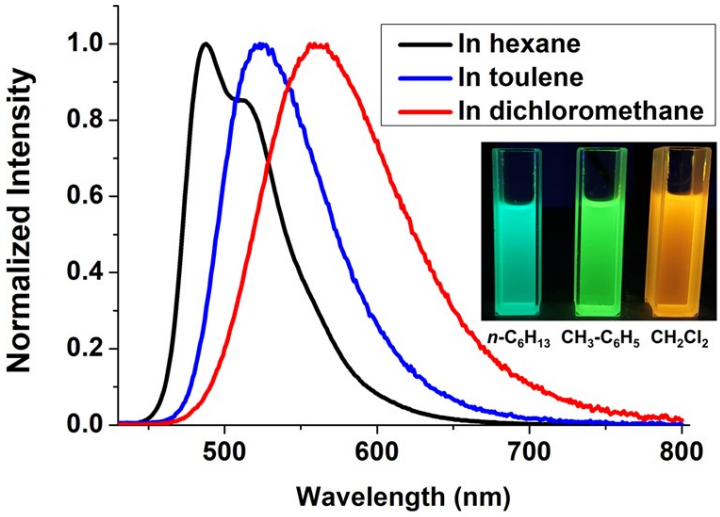


Figure S5. Normalized solvent-dependent fluorescence spectra of MeO-DPA-BN-BFT in n-hexane (black), toluene (red), dichloromethane (blue) solutions at 10^{-6} M (Inset: Fluorescent photographs of MeO-DPA-BN-BFT in different solvents).

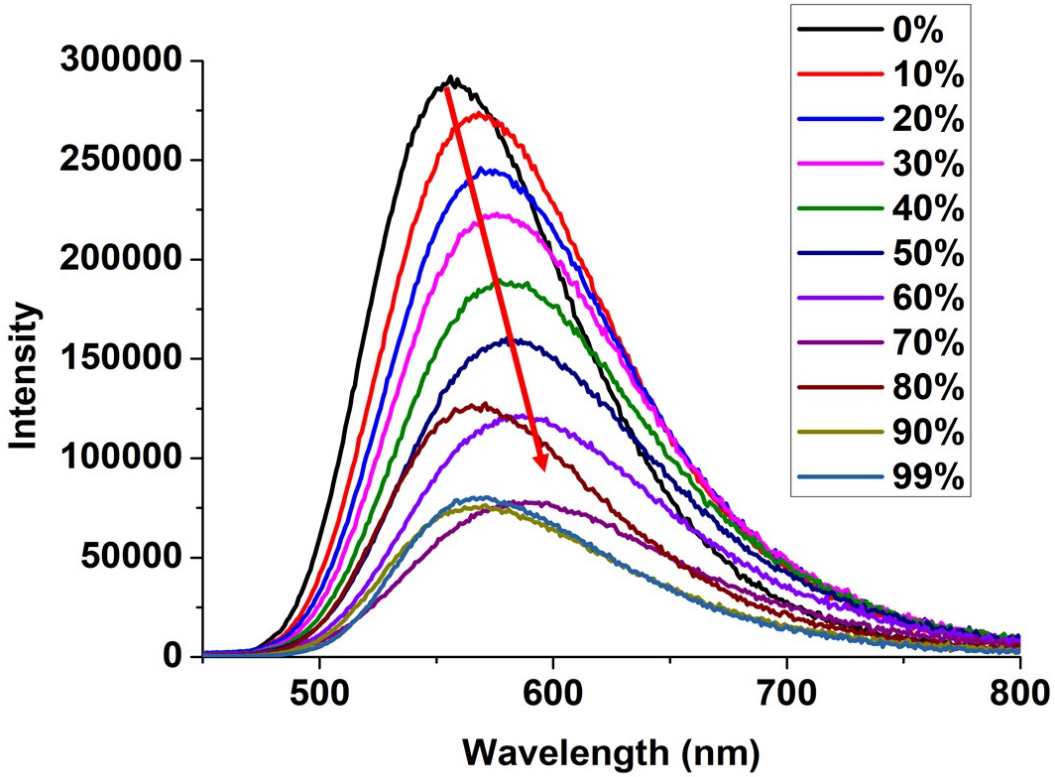


Figure S6. PL spectra of MeO-DPA-BN-BFT in THF/water mixtures with different water fractions (fw). excitation wavelength: 420 nm.

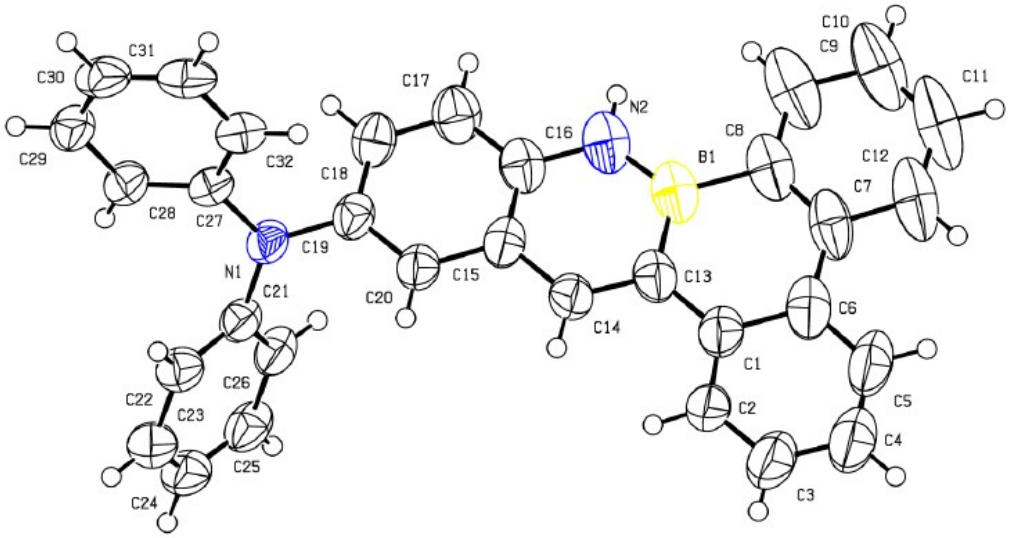


Figure S7. Molecular structure of DPA-BN-BFT

Table S2 Crystal data and structure refinement for DPA-BN-BFT

Identification code	DPA-BN-BFT
Empirical formula	$C_{32}H_{23}BN_2$

Formula weight	446.33
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.1281(4)
b/Å	14.6359(10)
c/Å	22.9977(13)
α/°	90
β/°	93.688(5)
γ/°	90
Volume/Å^3	2730.2(3)
Z	4
ρ_{calc}g/cm^3	1.086
μ/mm^{-1}	0.480
F(000)	936.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.164 to 133.192
Index ranges	$-9 \leq h \leq 9$, $-16 \leq k \leq 17$, $-19 \leq l \leq 27$
Reflections collected	10196
Independent reflections	4826 [R_{int} = 0.0251, R_{sigma} = 0.0253]
Data/restraints/parameters	4826/7/317
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0933, wR_2 = 0.2568
Final R indexes [all data]	R_1 = 0.1053, wR_2 = 0.2696
Largest diff. peak/hole / e Å^{-3}	0.67/-0.25

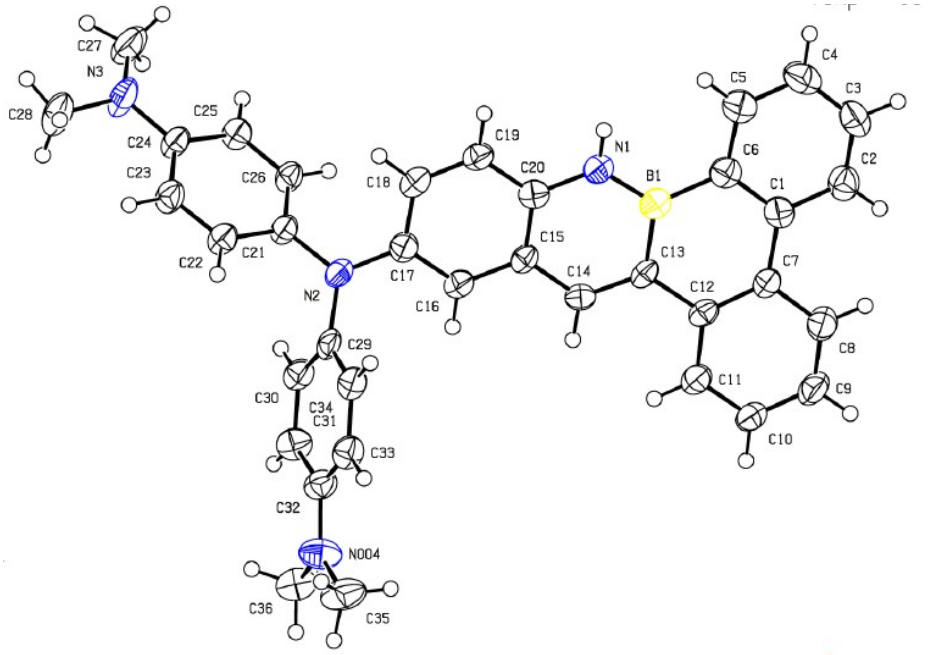


Figure S8. Molecular structure of DMA-DPA-BN-BFT

Table S3 Crystal data and structure refinement for DMA-DPA-BN-BFT

Identification code	DMA-DPA-BN-BFT
Empirical formula	$C_{36}H_{33}BN_4$
Formula weight	532.47
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.3480(15)
b/Å	9.7155(7)
c/Å	20.1083(19)
α/°	90
β/°	95.494(9)
γ/°	90
Volume/Å^3	2790.2(4)
Z	4
ρ_{calc}g/cm^3	1.268
μ/mm^{-1}	0.572
F(000)	1128.0
Crystal size/mm^3	0.12 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	7.252 to 133.198
Index ranges	$-17 \leq h \leq 16$, $-11 \leq k \leq 11$, $-20 \leq l \leq 23$
Reflections collected	4941
Independent reflections	4941 [R_{int} = 0.0560, R_{sigma} = 0.0659]
Data/restraints/parameters	4941/0/375
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.1150, wR_2 = 0.3236
Final R indexes [all data]	R_1 = 0.1400, wR_2 = 0.3393
Largest diff. peak/hole / e $Å^{-3}$	0.44/-0.40

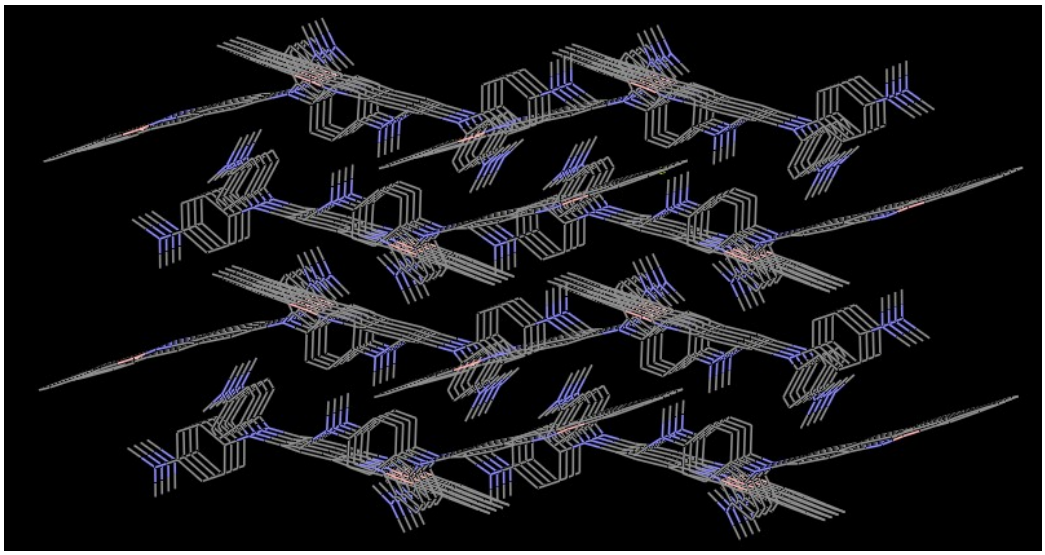


Figure S9. Molecular packing arrangement of DMA-DPA-BN-BFT

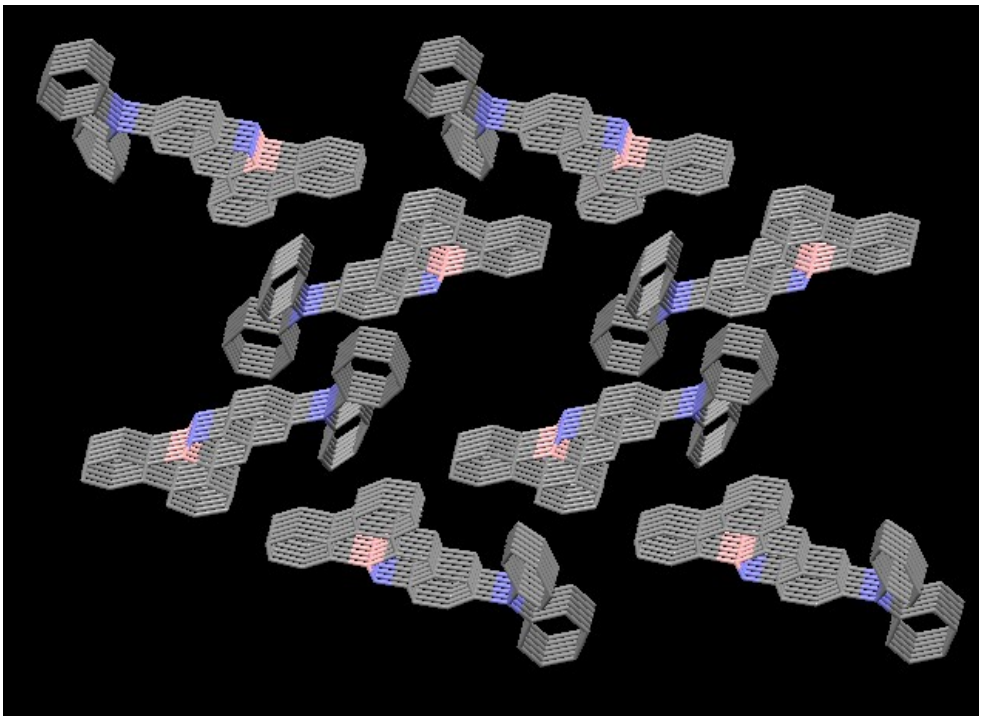


Figure S10. Molecular packing arrangement of DPA-BN-BFT

Table S4. Cartesian coordinates of BN-BFT for NICS and frontier orbitals calculations

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	-1.955330	-0.098743	-0.110357
2	6	0	0.142261	1.183985	0.202714
3	6	0	-0.509051	2.366432	0.602950
4	6	0	1.547056	1.214425	-0.017110
5	6	0	2.315401	-0.026984	-0.200735
6	6	0	1.694735	-1.253071	0.143608
7	6	0	3.654943	-0.031310	-0.636735
8	6	0	2.198991	2.461884	0.059746
9	6	0	1.529334	3.632720	0.377833
10	6	0	0.166523	3.575699	0.679292
11	1	0	-0.367166	4.466632	0.996188
12	1	0	2.070278	4.572151	0.434179
13	6	0	-2.686676	-1.263073	0.261104
14	6	0	-2.007016	-2.428602	0.772059
15	6	0	-0.653238	-2.512313	0.777064
16	1	0	-2.636467	-3.259405	1.090168
17	6	0	2.460049	-2.434729	0.097041
18	6	0	4.381232	-1.213893	-0.684668
19	1	0	5.412910	-1.196424	-1.024837
20	6	0	3.789957	-2.424344	-0.301471

21	1	0	4.362745	-3.346564	-0.333554
22	1	0	3.271958	2.500234	-0.088112
23	1	0	4.133408	0.888860	-0.954235
24	1	0	-1.553429	2.328448	0.882884
25	1	0	-0.195201	-3.442391	1.106256
26	1	0	1.991526	-3.379395	0.357933
27	7	0	-0.564217	-0.053004	0.139272
28	5	0	0.168563	-1.284654	0.381342
29	6	0	-2.636859	0.920084	-0.808167
30	6	0	-4.080083	-1.296340	0.043577
31	6	0	-4.743928	-0.256717	-0.582529
32	1	0	-5.815309	-0.306505	-0.748922
33	6	0	-4.002952	0.842728	-1.036974
34	1	0	-2.084242	1.764851	-1.197707
35	1	0	-4.492748	1.641247	-1.586388
36	1	0	-4.623650	-2.184472	0.355069

Table S5. Cartesian coordinates of BFT for NICS and frontier orbitals calculations

Center Number	Atomic Number	Atomic Type	Coordinates(Angstroms)		
			X	Y	Z
1	6	0	2.003134	-0.056984	-0.090143
2	6	0	-0.198290	1.243632	0.133682
3	6	0	0.409509	2.479879	0.464367
4	6	0	-1.614114	1.221376	-0.026689
5	6	0	-2.307541	-0.057550	-0.160484
6	6	0	-1.588890	-1.260105	0.078489
7	6	0	-3.684229	-0.137153	-0.465203
8	6	0	-2.324593	2.440748	0.026173
9	6	0	-1.690818	3.644821	0.274188
10	6	0	-0.312782	3.658351	0.525733
11	1	0	0.187652	4.584221	0.793348
12	1	0	-2.267773	4.563737	0.317213
13	6	0	2.704740	-1.263461	0.229976
14	6	0	1.960726	-2.414119	0.612947
15	6	0	0.597356	-2.406068	0.562938
16	1	0	2.496079	-3.318086	0.890330
17	6	0	-2.297107	-2.483743	0.045560
18	6	0	-4.351162	-1.348255	-0.499143
19	1	0	-5.409817	-1.378401	-0.738841
20	6	0	-3.651502	-2.532994	-0.230108
21	1	0	-4.163767	-3.490103	-0.256213
22	1	0	-3.402046	2.437834	-0.087370
23	1	0	-4.237632	0.766549	-0.691563

24	1	0	1.458250	2.500237	0.727536
25	1	0	0.063160	-3.317432	0.800615
26	1	0	-1.772255	-3.417159	0.207110
27	6	0	2.767430	0.996879	-0.663672
28	6	0	4.115427	-1.318472	0.108379
29	6	0	4.828947	-0.248928	-0.385681
30	1	0	5.908685	-0.306069	-0.485661
31	6	0	4.137544	0.904784	-0.807632
32	1	0	2.262287	1.873445	-1.047237
33	1	0	4.682891	1.723969	-1.267096
34	1	0	4.622214	-2.238993	0.386241
35	6	0	0.561889	-0.007466	0.086309
36	6	0	-0.136996	-1.219133	0.255280

Table S6. Cartesian coordinates of DPA-BN-BFT for ESPs and frontier orbitals calculations

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-5.938324	-3.150080	0.823343
2	6	0	-6.966064	-2.246122	0.534318
3	6	0	-6.650940	-0.948374	0.154507
4	6	0	-5.319369	-0.489522	0.043638
5	6	0	-4.270482	-1.417403	0.339601
6	6	0	-4.620312	-2.730668	0.724183
7	6	0	-5.046055	0.917160	-0.369055
8	6	0	-6.103979	1.807379	-0.662364
9	6	0	-5.868800	3.122148	-1.048128
10	1	0	-6.711379	3.773720	-1.264707
11	6	0	-4.559451	3.604161	-1.157943
12	6	0	-3.505682	2.744520	-0.874606
13	6	0	-3.712541	1.407235	-0.480623
14	1	0	-6.165245	-4.169659	1.122954
15	1	0	-8.006720	-2.550273	0.605137
16	1	0	-3.834504	-3.442983	0.953149
17	1	0	-4.371813	4.630949	-1.459775
18	1	0	-2.489768	3.124692	-0.963863
19	1	0	-7.136142	1.485522	-0.594494
20	1	0	-7.474558	-0.278408	-0.059547
21	6	0	-2.862882	-1.000885	0.243926
22	6	0	-1.790871	-1.830749	0.500839
23	6	0	-0.433146	-1.397626	0.402219

24	6	0	-0.125607	-0.055879	0.031445
25	1	0	0.437508	-3.290903	0.963453
26	1	0	-1.926365	-2.871348	0.793325
27	6	0	0.653944	-2.267734	0.666028
28	6	0	1.210782	0.365544	-0.075047
29	1	0	-0.885466	1.743563	-0.494996
30	6	0	2.261316	-0.512148	0.197123
31	6	0	1.963352	-1.849058	0.575821
32	1	0	1.421673	1.386698	-0.376582
33	1	0	2.772550	-2.533047	0.804591
34	7	0	3.602841	-0.083175	0.114657
35	6	0	3.953654	1.264565	0.427821
36	6	0	3.495529	1.860954	1.613511
37	6	0	4.773709	2.002950	-0.439067
38	6	0	3.845336	3.176300	1.917305
39	1	0	2.868682	1.290294	2.291577
40	6	0	5.132887	3.312944	-0.119675
41	1	0	5.126150	1.547284	-1.359146
42	6	0	4.668254	3.908317	1.056045
43	1	0	3.484460	3.624591	2.839030
44	1	0	5.768629	3.872492	-0.800469
45	1	0	4.944672	4.930144	1.299344
46	6	0	4.621416	-0.972714	-0.335790
47	6	0	5.859233	-1.019587	0.325789
48	6	0	4.407976	-1.802656	-1.448264
49	6	0	6.862587	-1.878443	-0.122067
50	1	0	6.028091	-0.383474	1.189004
51	6	0	5.410699	-2.672057	-1.878300
52	1	0	3.458789	-1.761503	-1.973180
53	6	0	6.643903	-2.712973	-1.222031
54	1	0	7.814768	-1.903650	0.400941
55	1	0	5.229881	-3.308385	-2.740394
56	1	0	7.425129	-3.385616	-1.563965
57	7	0	-1.169537	0.804408	-0.236117
58	5	0	-2.550518	0.436735	-0.165638

Table S7. Cartesian coordinates of DMA-DPA-BN-BFT for ESPs calculation

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	7.039422	-3.474223	-0.870921
2	6	0	8.085718	-2.613052	-0.522362
3	6	0	7.798173	-1.321134	-0.103129
4	6	0	6.477963	-0.826223	-0.010152
5	6	0	5.409392	-1.710882	-0.365286
6	6	0	5.732067	-3.019633	-0.789287
7	6	0	6.234602	0.572515	0.444349
8	6	0	7.310226	1.424327	0.785320
9	6	0	7.103172	2.731518	1.210334
10	1	0	7.958663	3.352762	1.462699
11	6	0	5.805018	3.245079	1.312683
12	6	0	4.734446	2.424109	0.982035
13	6	0	4.912368	1.094756	0.548084
14	1	0	7.244284	-4.488833	-1.202043
15	1	0	9.118489	-2.946125	-0.577204
16	1	0	4.931987	-3.699851	-1.062528
17	1	0	5.639150	4.266380	1.644586
18	1	0	3.727541	2.829367	1.064030
19	1	0	8.334679	1.077482	0.723033
20	1	0	8.634873	-0.684745	0.157996
21	6	0	4.013465	-1.257387	-0.285417
22	6	0	2.922369	-2.044714	-0.601270
23	6	0	1.577865	-1.579346	-0.511675
24	6	0	1.295105	-0.247070	-0.086006
25	1	0	0.662168	-3.418000	-1.175765
26	1	0	3.036403	-3.075280	-0.936670
27	6	0	0.469615	-2.402941	-0.836027
28	6	0	-0.028568	0.209106	0.012180
29	1	0	2.094462	1.504980	0.532856
30	6	0	-1.105963	-0.624544	-0.313765
31	6	0	-0.828181	-1.954551	-0.747949
32	1	0	-0.212338	1.222882	0.352359
33	1	0	-1.648360	-2.608227	-1.019730
34	7	0	-2.426124	-0.173762	-0.233424
35	6	0	-2.734051	1.225036	-0.233982

36	6	0	-2.338019	2.053395	-1.292826
37	6	0	-3.476718	1.798002	0.805604
38	6	0	-2.652367	3.408368	-1.306054
39	1	0	-1.776132	1.630475	-2.120894
40	6	0	-3.813073	3.148429	0.794874
41	1	0	-3.808096	1.174281	1.631026
42	6	0	-3.394922	4.001635	-0.255232
43	1	0	-2.327655	4.002274	-2.151857
44	1	0	-4.399562	3.538127	1.618104
45	6	0	-3.509573	-1.092416	-0.052319
46	6	0	-4.617100	-1.067814	-0.909292
47	6	0	-3.516432	-2.012418	1.004673
48	6	0	-5.692262	-1.931512	-0.725352
49	1	0	-4.641467	-0.353797	-1.727809
50	6	0	-4.577187	-2.893843	1.188125
51	1	0	-2.678924	-2.038582	1.696202
52	6	0	-5.697516	-2.886112	0.321431
53	1	0	-6.529069	-1.864700	-1.410012
54	1	0	-4.534837	-3.581438	2.024121
55	7	0	2.358278	0.570584	0.238183
56	5	0	3.730863	0.168172	0.176321
57	7	0	-6.746523	-3.779219	0.484594
58	7	0	-3.689626	5.357555	-0.250507
59	6	0	-7.969131	-3.589323	-0.282914
60	1	0	-8.669901	-4.389290	-0.038631
61	1	0	-8.458803	-2.624913	-0.074187
62	1	0	-7.769476	-3.641787	-1.359374
63	6	0	-6.821590	-4.572870	1.703026
64	1	0	-7.696504	-5.222796	1.650572
65	1	0	-5.938999	-5.214141	1.809475
66	1	0	-6.904217	-3.954303	2.610668
67	6	0	-4.640161	5.874508	0.723821
68	1	0	-4.736310	6.953009	0.588845
69	1	0	-5.640176	5.423017	0.625884
70	1	0	-4.288276	5.699229	1.746941
71	6	0	-3.455612	6.140870	-1.455458
72	1	0	-3.723923	7.180582	-1.261177
73	1	0	-2.396785	6.120396	-1.737952

74	1	0	-4.044610	5.786724	-2.316272

Reference

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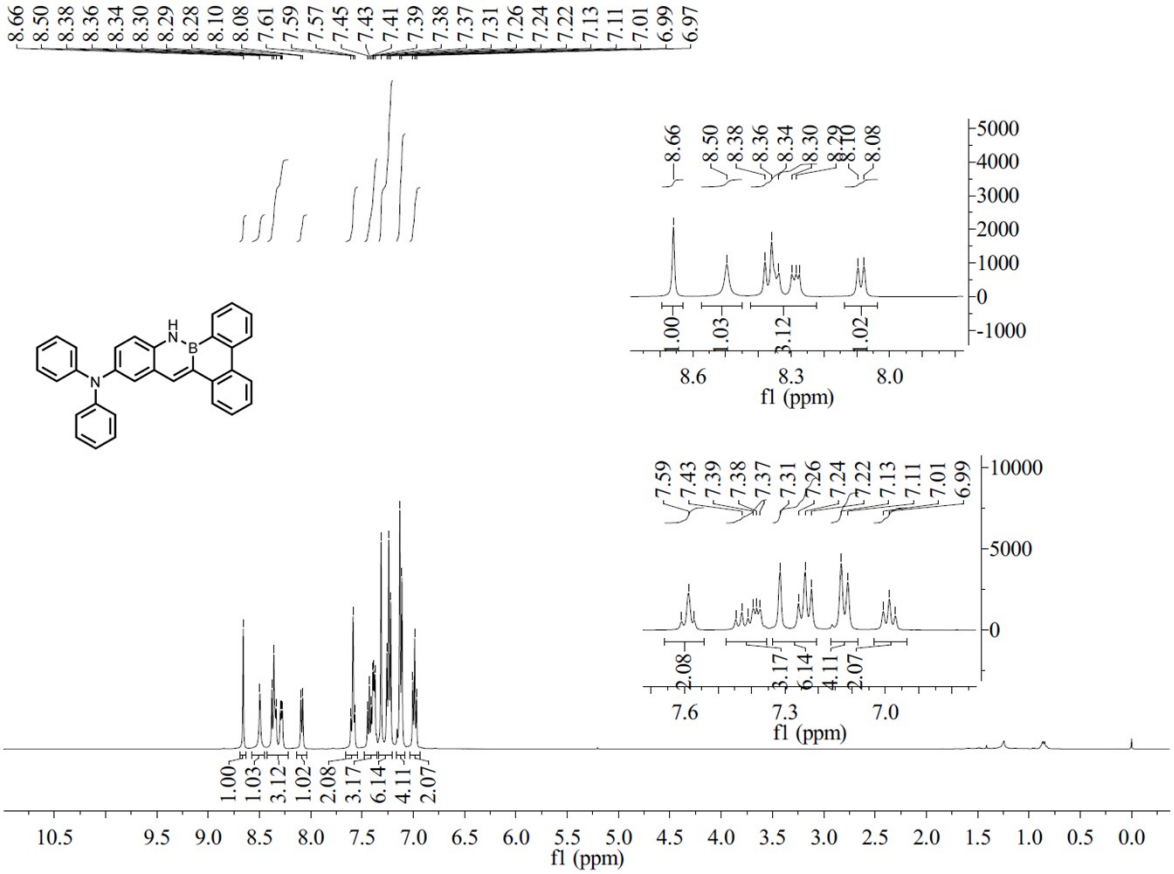
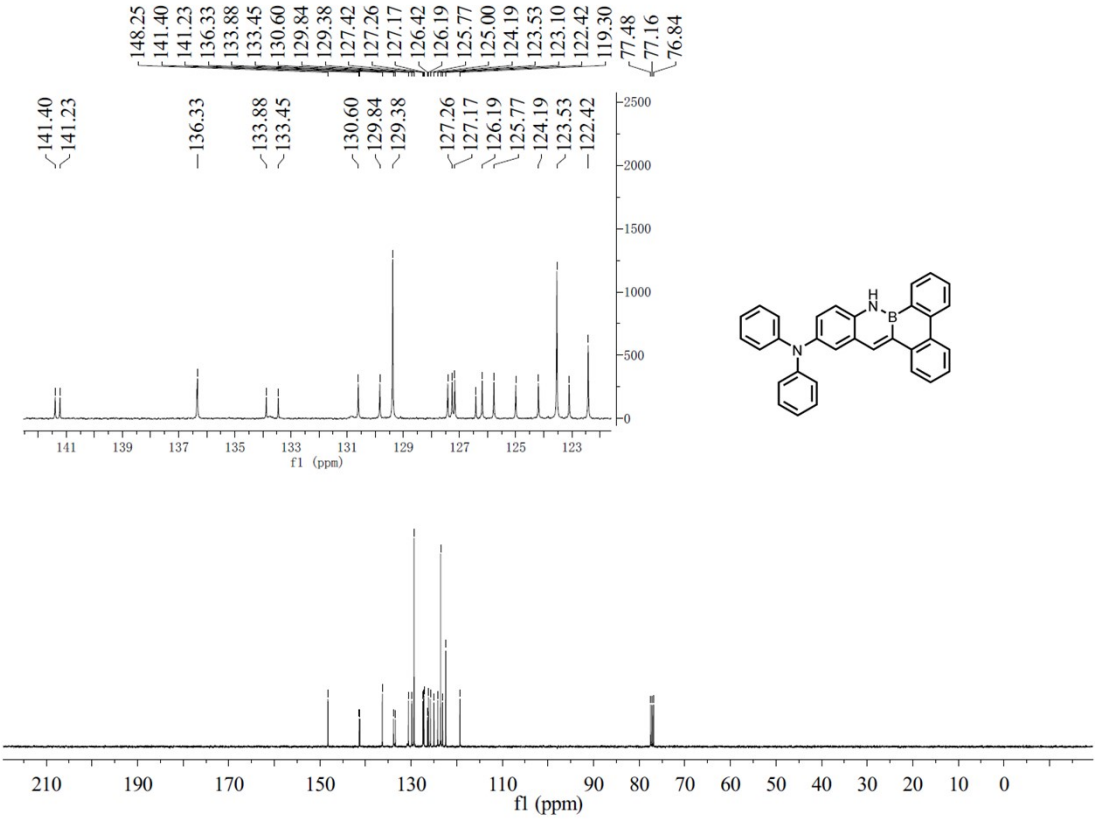
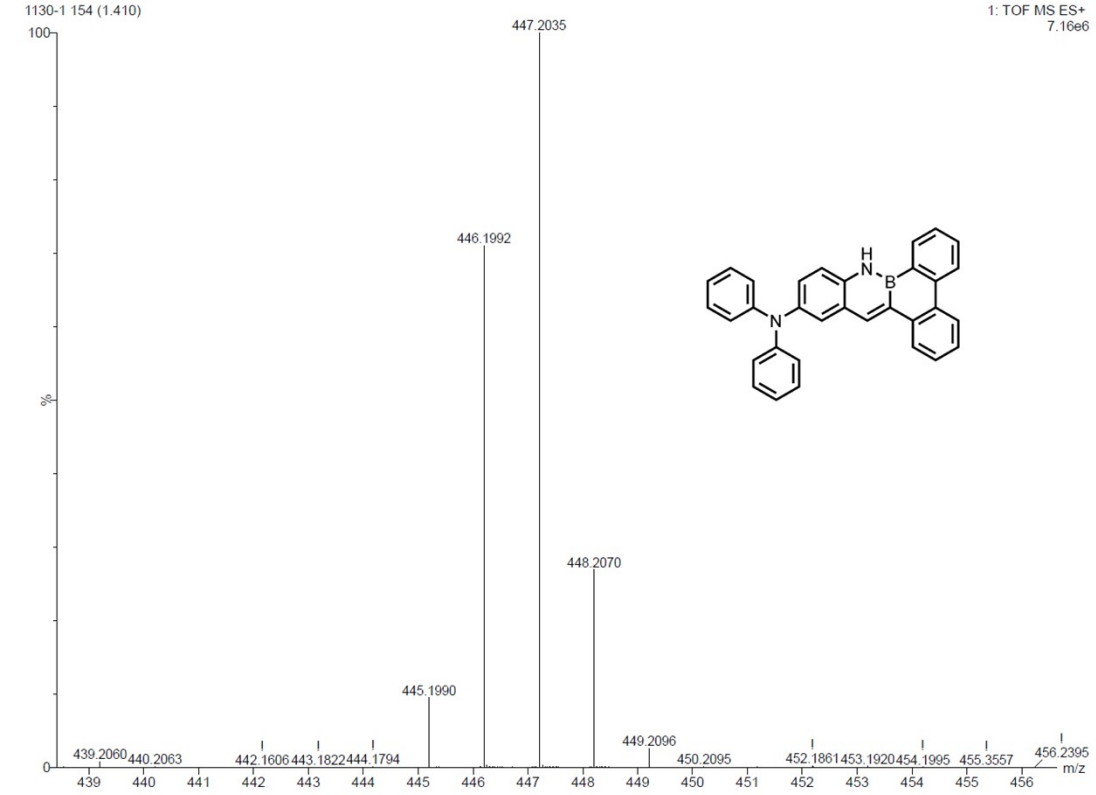
S2. H. N. Huang, Y. Zhou, Y. W. Wang, X. H. Cao, C. Han, G. C. Liu, Z. X. Xu, C. C. Zhan, H. H. Hu, Y. Peng, P. Yan, D. P. Cao, *J. Mater. Chem. A*, **2020**, **8**, 22023-22031.

Scanned NMR Spectra for the New Compounds



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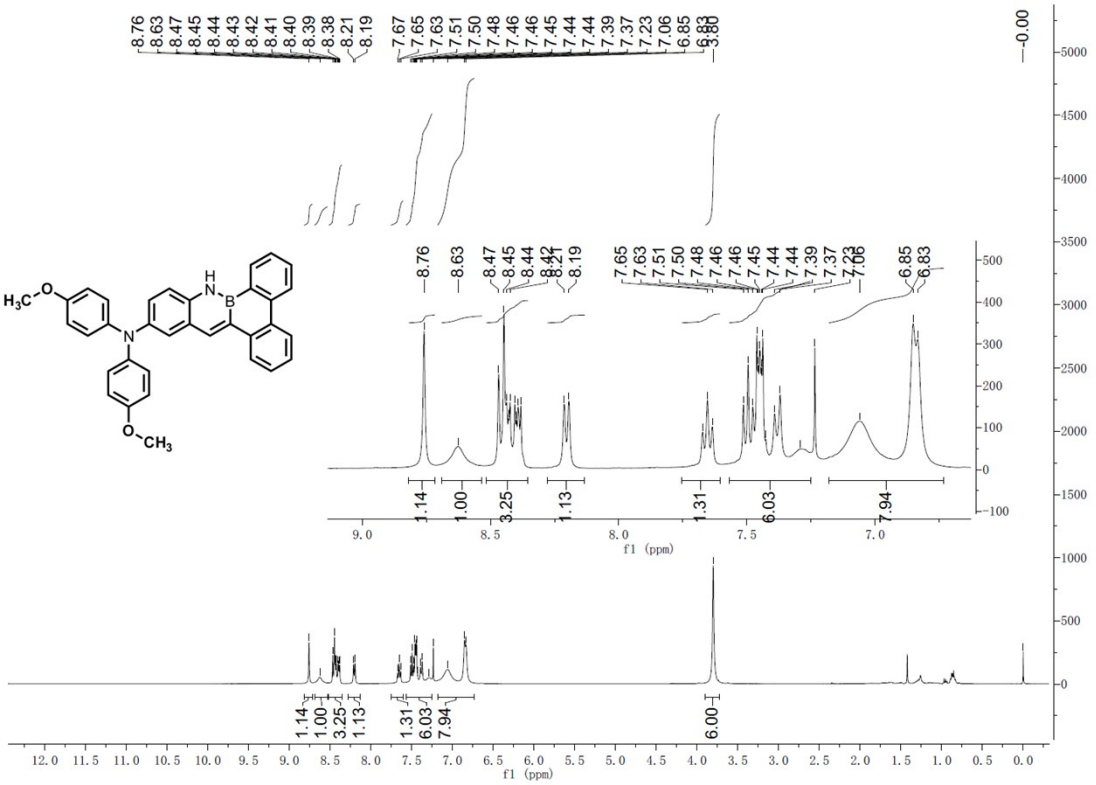
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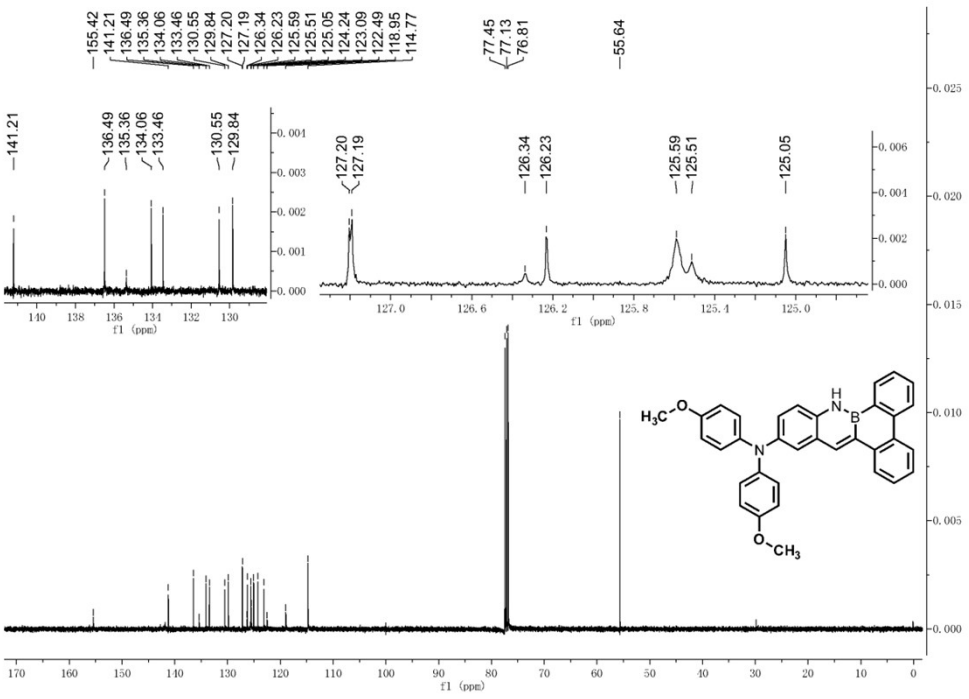
f1 (ppm)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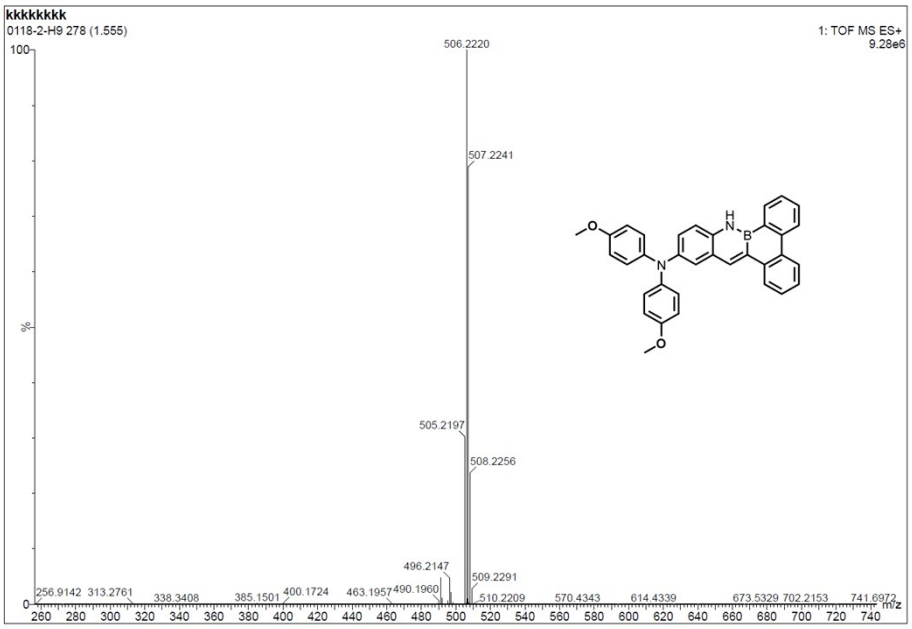
f1 (ppm)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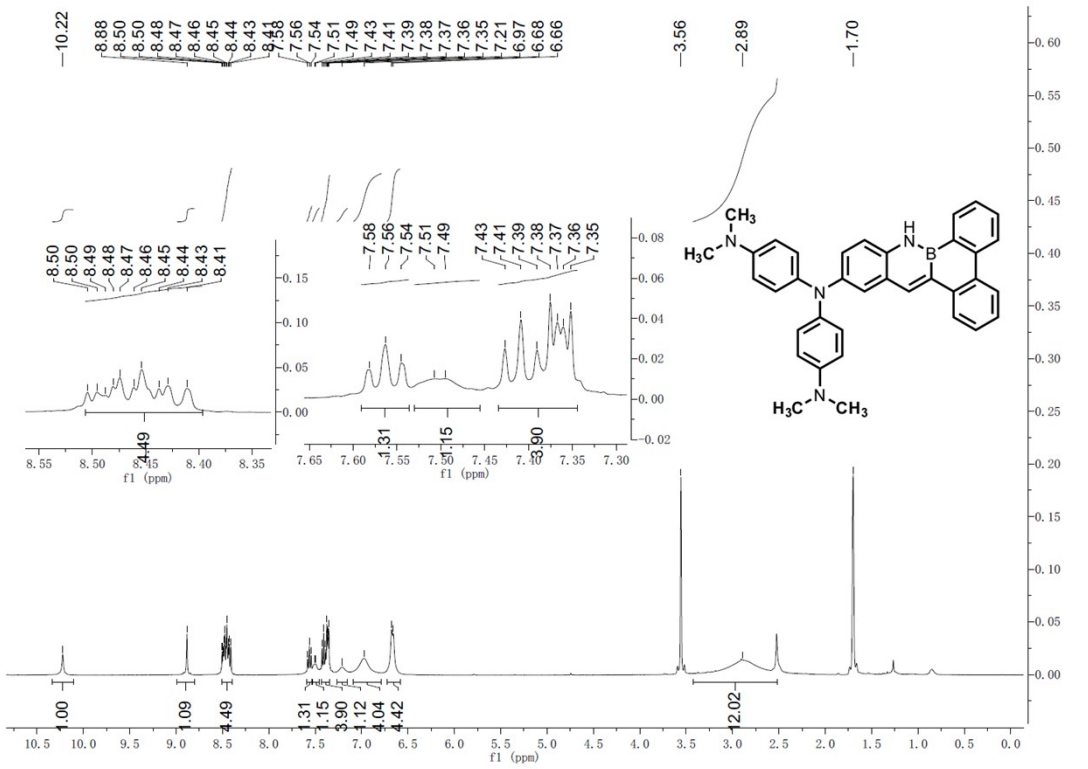
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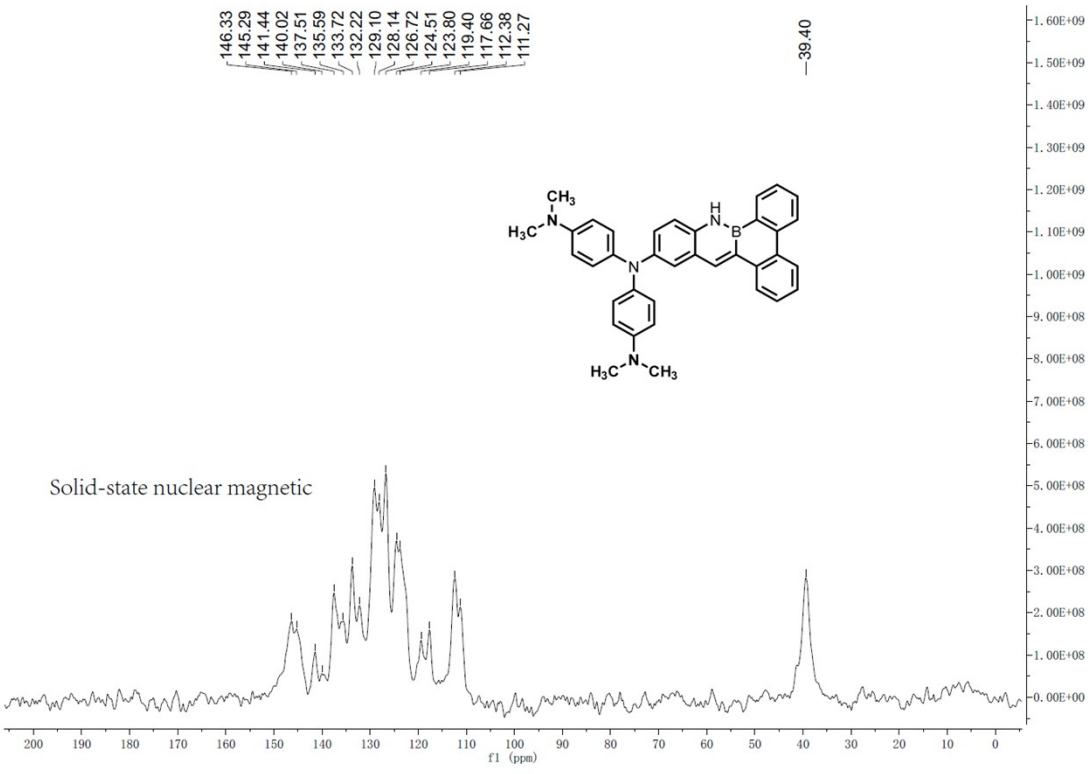
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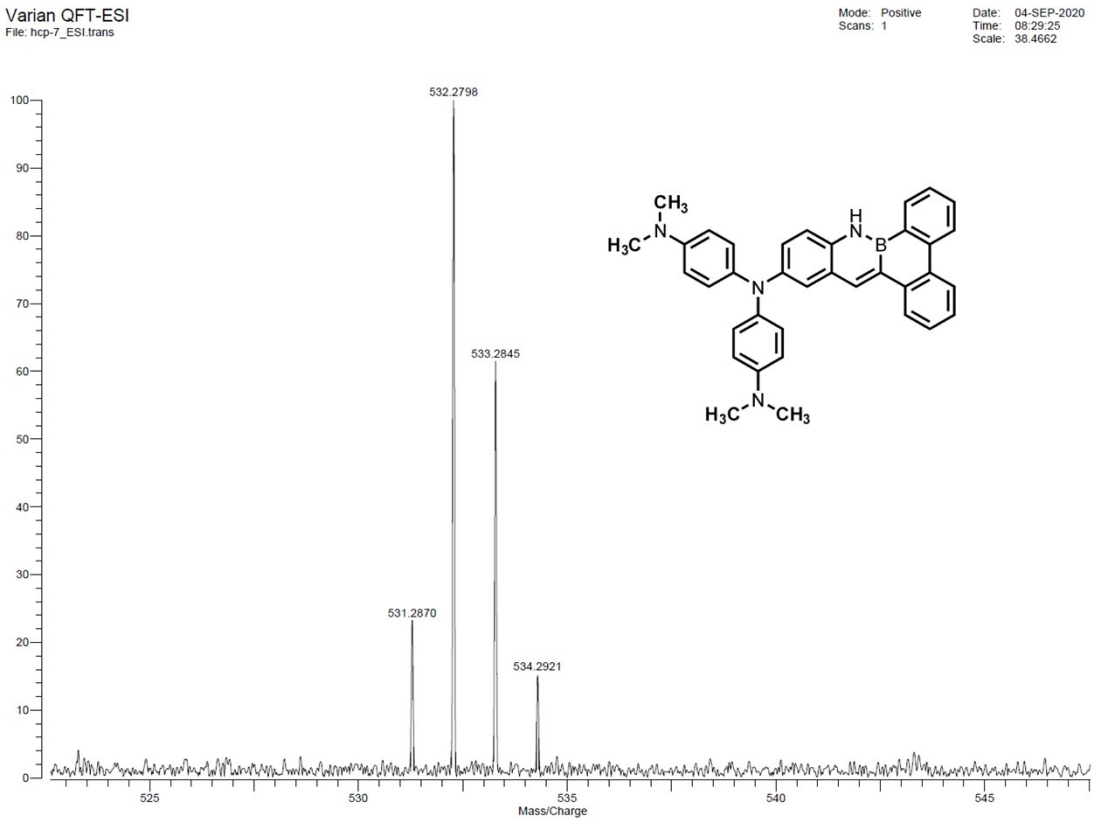
Solid-state nuclear magnetic
f1 (ppm)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Mass/Charge
CH3
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N
H
N
B
N
H3C
N
CH3