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Supporting Information

for

Solvatochromism, Acidochromism and Aggregation-Induced Emission of Propeller-shaped Spiroborates

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1. Materials and measurements

All the solvents were of analytical grade. Column flash chromatography was carried out on silica gel (200–400 mesh). Thin-layer chromatography (TLC) was performed on silica gel GF254. ^{1}H and ^{13}CNMR spectra were recorded on*a Varian Mercury-plus 400MHz spectrometer* and referenced to the residual proton signals of the solvent. HRMS spectra were recorded on an *Agilent 100 ABI-API4000 spectrometer.* X-ray data were collected on *Bruker Smart APEX II CCD diffractometer.*

Synthesis of Sborepy1–6

Compound 1

THF (20 mL) and NaH (2.2 g, 93.0 mmol) were mixed and then 2-benzylpyridine (5.2 g, 31.0 mmol) was added at room temperature. After stirring for 20 minutes, ethyl benzoate (4.7 g, 31.0 mmol) was added to the reaction system, and the mixture was heated at reflux for 10 hours. After cooling to room temperature, the reaction solution was added to the ice-water mixture, and then 2M HCl solution was added to adjust the pH to 7. The yellow precipitate was filtered, washed with water and dried to give a yellow product. Yield: 95%, ^{1}H NMR (400MHz, $CDCl_3$) δ/ppm = 8.55 (d, J = 4.1 Hz, 1H,), 8.03 (d, J = 7.4 Hz, 2H), 7.62 (t, J = 7.3Hz, 1H), 7.50 (t, J = 7.3 Hz, 1H), 7.37 (dt, J = 19.6, 7.8 Hz, 5H), 7.28 (s, 2H), 7.16 (dd, J = 12.3, 6.6 Hz, 2H), 6.29 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ/ppm = 197.5, 159.3, 149.3, 137.6, 136.7, 133.1, 129.2, 129.1, 128.9, 128.6, 127.5, 123.9, 122.0, 118.6, 62.1. HRMS (ESI): calcd: $[M+H]^+$ = 274.1232, found: $[M+H]^+$ = 274.1217.

Compound 2

The starting material for the synthesis of compound **2** is 2-benzylpyridine and ethyl *p*-anisate, and the synthesis method is the same as that of compound **1**. Yield: 90%, ^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm = 8.55 (d, J = 4.1 Hz, 1H), 8.02 (d, J = 8.7 Hz, 2H), 7.61 (td, J = 7.7, 1.6 Hz, 1H), 7.41–7.30 (m, 4H), 7.27 (dd, J=7.9, 2.6 Hz, 2H), 7.14 (dd, J=6.8, 5.2 Hz, 1H), 6.87 (d, J=8.8 Hz, 2H), 6.26 (s, 1H), 3.81 (s,

3H).^{13}C NMR (100 MHz, $CDCl_3$) δ/ppm = 195.9, 163.5, 159.5, 149.2, 137.9, 136.6, 131.4, 129.6, 129.1, 128.9, 127.4, 123.9, 121.9, 113.8, 61.8, 55.4. HRMS (ESI): calcd: $[M+H]^+$ = 304.1338, found: $[M+H]^+$ = 304.1386.

Compound 3

The synthetic material for compound **3** is 2-benzylpyridineand ethyl 4-dimethylaminobenzoate, and the synthesis method is the same as that of compound 1. Yield: 71%, 1H NMR (400 MHz, $CDCl_3$) δ/ppm = 8.57–8.53 (m, 1H), 8.02–7.92 (m, 2H), 7.63–7.55 (m, 1H), 7.41–7.37 (m, 1H), 7.30 (dd, *J*=7.3, 4.1 Hz, 3H), 7.21 (dd, *J*=9.3, 4.5 Hz, 1H), 7.16–7.08 (m, 2H), 6.59 (d, *J*= 9.1 Hz, 2H), 6.27 (s, 1H), 3.00 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ/ppm = 195.2, 159.9, 153.3, 149.1, 138.7, 136.5, 131.2, 129.1, 128.8, 126.4, 124.0, 123.1, 121.3, 110.7, 61.3, 39.9. HRMS (ESI): calcd: $[M+H]^+$ = 317.1576, found: $[M+H]^+$ = 317.1608.

Sborepy1

Compound **1** (1.0 g, 3.7 mmol) and catechol (0.5 g, 4.1 mmol) were dissolved with 1,2-dichloroethane (20 mL). Then, boric acid (0.2 g, 3.7 mmol) was added and the reaction solution was heated under for 6 hours. After completion of the reaction, the reaction solution was cooled and the solvent was evaporated. The crude product was purified by column chromatography on silica gel (petroleum ether: dichloromethane 1:3, v/v) to obtain **Sborepy1** (yield: 51%).^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm = 8.25 (d, *J*=5.7 Hz, 1H), 7.79 (dd, *J*=11.5, 4.3Hz, 1H), 7.38 (td, *J*=12.7, 6.4Hz, 5H), 7.27-7.16 (m, 4H), 7.12 (t, *J*=8.4 Hz, 3H), 6.89 (dt, *J*=7.7, 3.8Hz, 2H), 6.85-6.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ/ppm =160.3, 152.3, 150.7, 141.2, 140.6, 135.7, 135.1, 132.3, 129.6, 129.4, 129.3, 128.0, 127.4, 121.7, 120.6, 119.7, 109.7, 108.9. Elemental analysis (%) calcd for $C_{25}H_{18}BNO_3 \cdot 0.5H_2O$: C, 75.02; H, 4.78; N, 3.50. Found: C, 75.12; H, 4.45; N, 3.43. HRMS (ESI): calcd: $[M+H]^+$ = 392.1458, found: $[M+H]^+$ = 392.1465.

The synthesis method of **Sborepy2-6** is the same as for **Sborepy1**. For **Sborepy4-6**, the catechol is replaced by salicylic acid.

Sborepy2

Yield: 58%. ^{1}H NMR (400 MHz, $CDCl_3$) δ/ppm = 8.20 (d, *J*=6.0 Hz, 1H), 7.78–7.70 (m, 1H), 7.47–7.35 (m, 3H), 7.29 (dd, *J*=7.7, 5.4 Hz, 4H), 7.19 (t, *J*=6.7 Hz, 1H),

7.06 (d, *J*=8.6 Hz, 1H), 6.88 (dt, *J*=7.4, 3.8 Hz, 2H), 6.84–6.76 (m, 2H), 6.62 (d, *J*=9.1 Hz, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ/ppm = 160.4, 159.9, 159.9, 152.4, 150.8, 140.9, 140.4, 135.5, 132.3, 131.4, 129.5, 128.0, 121.5, 120.1, 119.6, 112.8, 109.7, 107.9, 55.2. Elemental analysis (%) calcd for $C_{26}H_{20}BNO_4$: C, 74.13; H, 4.79; N, 3.33. Found: C, 73.70; H, 4.74; N, 3.23. HRMS (ESI): calcd: $[M+H]^+$ = 422.1564, found: $[M+H]^+$ = 422.1579.

Sborepy3

Yield: 55%. ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm = 8.14 (d, *J*=5.9 Hz, 1H), 7.66 (dd, *J*=11.6, 4.3 Hz, 1H), 7.50–7.35 (m, 3H), 7.34–7.27 (m, 2H), 7.24 (s, 2H), 7.09 (t, *J* = 6.7 Hz, 1H), 6.98 (d, *J*=8.7 Hz, 1H), 6.88 (dt, *J*=7.6, 3.8 Hz, 2H), 6.84–6.75 (m, 2H), 6.38 (d, *J*=9.2 Hz, 2H), 2.90 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ*/ppm = 160.5, 152.7, 151.0, 150.8, 140.5, 140.1, 136.3, 132.5, 131.3, 129.6, 127.8, 122.5, 121.2, 119.5, 119.2, 110.4, 109.6, 106.7, 39.9. Elemental analysis (%) calcd for $C_{27}H_{23}BN_2O_3 \cdot H_2O$: C, 71.70; H, 5.57; N, 6.19. Found: C, 71.12; H, 5.66; N, 5.66. HRMS (ESI): calcd: $[M+H]^+$ = 435.1880, found: $[M+H]^+$ = 435.1887.

Sborepy4

Yield: 62%. ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm =8.39 (d, *J*=5.7 Hz, 1H), 8.07 (dd, *J*=8.1, 1.7Hz, 1H), 7.88-7.78 (m, 1H), 7.58-7.48 (m, 1H), 7.39 (q, *J*=5.5 Hz, 3H), 7.34-7.27 (m, 3H), 7.25 (s, 2H), 7.19 (t, *J*=7.4, 1H), 7.12 (dd, *J*=15.7, 8.0Hz, 3H), 7.04 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ*/ppm = 160.3, 152.3, 150.7, 141.2, 140.6, 135.7, 135.1, 132.3, 129.6, 129.4, 129.3, 128.0, 127.4, 121.7, 120.9, 120.6, 119.7, 115.2, 109.8, 108.9. Elemental analysis (%) calcd for $C_{26}H_{18}BNO_4 \cdot 0.5H_2O$: C, 72.92; H, 4.47, N, 3.27. Found: C, 73.24; H, 4.38; N, 3.23. HRMS (ESI): calcd: $[M+H]^+$ = 420.1407, found: $[M+H]^+$ = 420.1418.

Sborepy5

Yield: 53%. ^{1}H NMR (400 MHz, $CDCl_3$) *δ*/ppm = 8.34 (d, *J*=5.9 Hz, 1H), 8.07 (dd, *J*=8.0, 1.7 Hz, 1H), 7.78 (ddd, *J*=8.8, 7.3, 1.6 Hz, 1H), 7.56-7.48 (m, 1H), 7.47-7.35 (m, 3H), 7.28 (d, *J*=1.7 Hz, 2H), 7.23 (dd, *J*=11.0, 4.0 Hz, 3H), 7.13–6.96 (m, 3H), 6.61 (d, *J*=9.0 Hz, 2H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ*/ppm = 163.4, 160.4, 160.0, 158.6, 152.8, 141.2, 140.1, 135.4, 135.3, 132.3, 131.2, 130.3, 129.5,

128.1, 127.8, 121.9, 120.4, 120.2, 118.2, 115.0, 112.9, 108.1, 55.2. Elemental analysis (%) calcd for $C_{27}H_{20}BNO_5$: C, 72.18; H, 4.49, N, 3.12. Found: C, 71.96; H, 4.53, N, 3.06. HRMS (ESI): calcd: $[M+H]^+$ = 450.1513, found: $[M+H]^+$ = 450.1522.

Sborepy6

Yield: 56%. ^{1}HNMR (400 MHz, $CDCl_3$) δ/ppm = 8.28 (d, *J*=5.8 Hz, 1H), 8.07 (dd, *J*=8.2, 1.7 Hz, 1H), 7.76–7.65 (m, 1H), 7.56–7.36 (m, 4H), 7.34–7.27 (m, 2H), 7.16 (dd, *J*=11.8, 4.7 Hz, 3H), 7.07–6.94 (m, 3H), 6.36 (d, *J*=9.1 Hz, 2H), 2.89 (s, 6H); ^{13}C NMR(100 MHz, $CDCl_3$) δ/ppm = 163.6, 160.6, 158.7, 153.1, 150.8, 140.7, 139.8, 136.0, 135.3, 132.5, 131.2, 130.3, 129.6, 129.0, 127.9, 122.3, 121.6, 120.2, 119.1, 118.2, 115.2, 110.4, 39.9. Elemental analysis (%) calcd for $C_{28}H_{23}BN_2O_4 \cdot H_2O$: C, 70.02; H, 5.25, N, 5.83. Found: C, 70.3; H, 4.99, N, 5.84. HRMS (ESI): calcd: $[M+H]^+$ = 463.1829, found: $[M+H]^+$ = 463.1840.

Solvatochromism[1]

The influence of the solvent on emission characteristics can be assessed by the relationship between the solvent polarity parameter (Δf) and the Stokes shift ($\Delta\upsilon$) of the absorption and emission maxima (Lippert-Mataga equations, equations 1 and 2).

$$\Delta\upsilon \equiv \Delta\upsilon_{ab} - \Delta\upsilon_{em} = \frac{2\Delta f}{hca^3}(\mu_e - \mu_g)^2 + const \qquad (1)$$

$$\Delta f = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \qquad (2)$$

Where, $\Delta\upsilon$ is the Stokes shift, h is the Planck constant, c is the speed of light, a is the Onsager cavity radius, μ_e and μ_g are the dipolar moments in the excited (e) and ground (g) states, and ε and n are the dielectric constant and refractive index of the solvent, respectively.

Fluorescence pH titration

The fluorescence titration experiments of **Sborepy6** were carried out by adding the diluted HCl aqueous solution to 3 mL of **Sborepy6** solution (50 μM, 1 : 99, THF–water v/v) in a cuvette. The spectra and pH values were recorded after the solution was completely mixed. All pH measurements were determined using a PHS-25 meter.

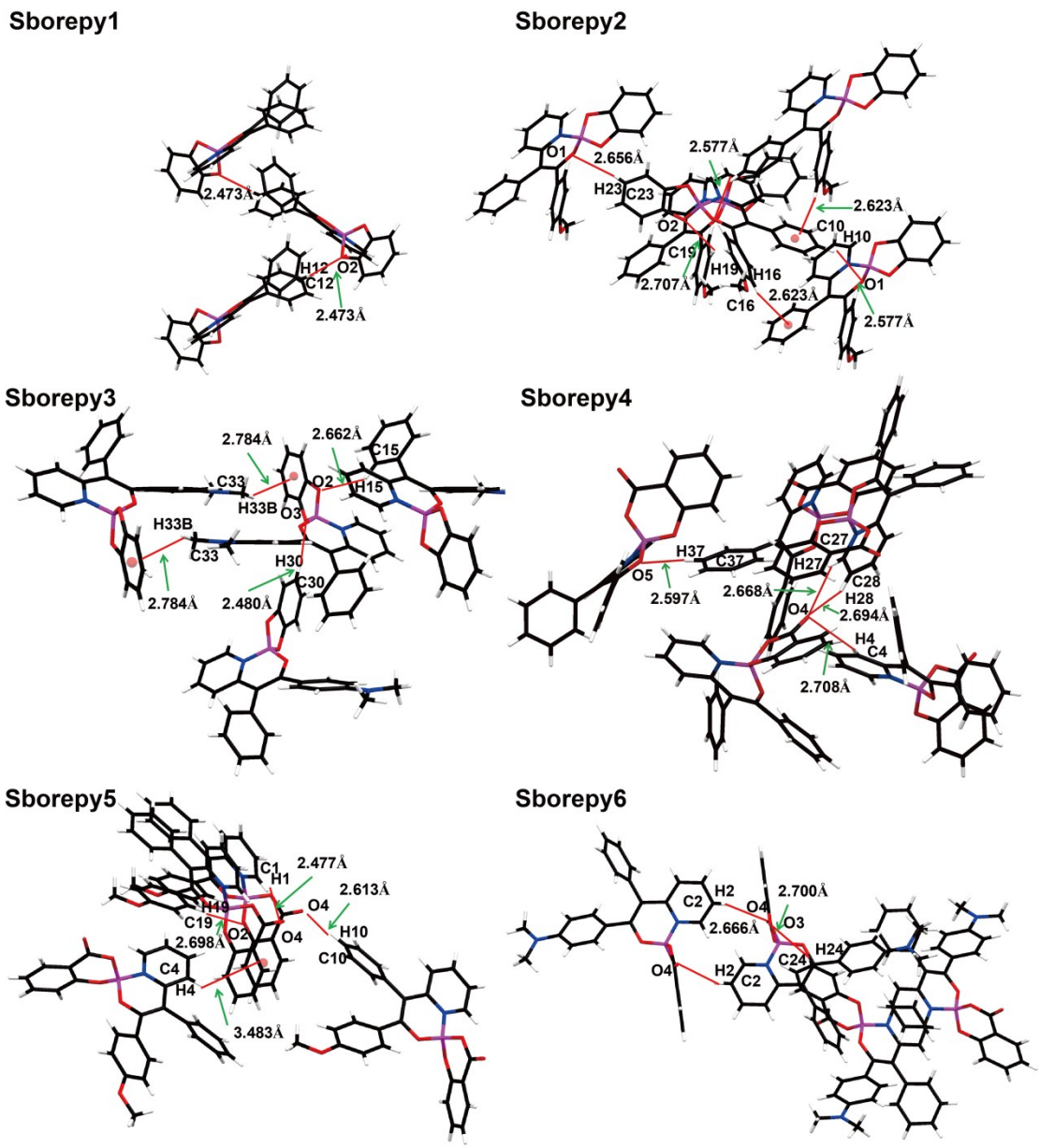


Figure S1. Crystal packing structures of **Sborepy1-6**.

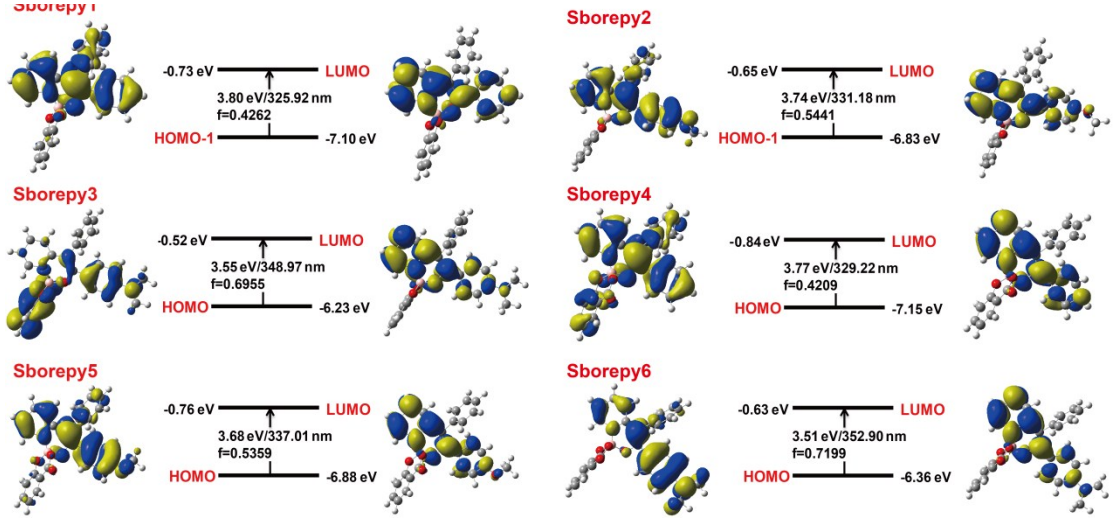


Figure S2. Molecular orbital energy diagram and isodensity surface plots of the HOMOs and LUMOs of **Sborepy1-6,** calculated by using CAM-B3LYP/6-31G(d) basis set with the G03 program package.

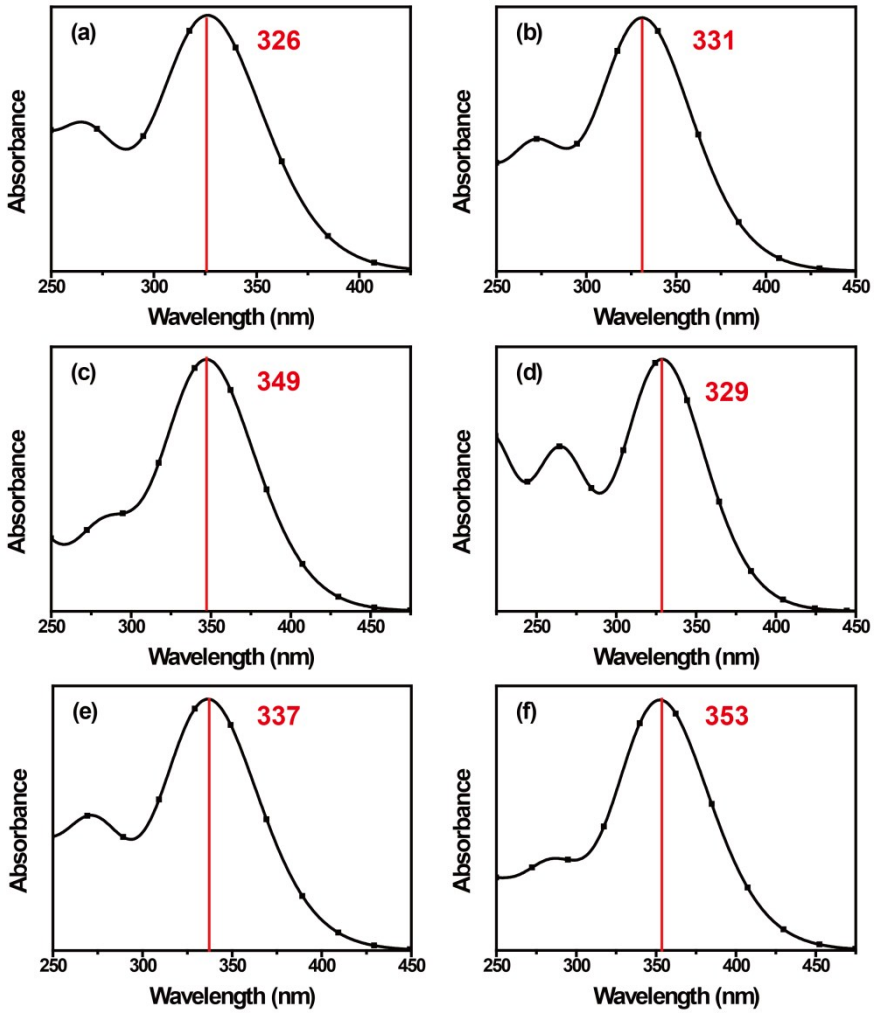


Figure S3. Calculated absorption spectra of **Sborepy1**(a), **Sborepy2**(b), **Sborepy3**(c), **Sborepy4**(d), **Sborepy5**(e) and **Sborepy6**(f).

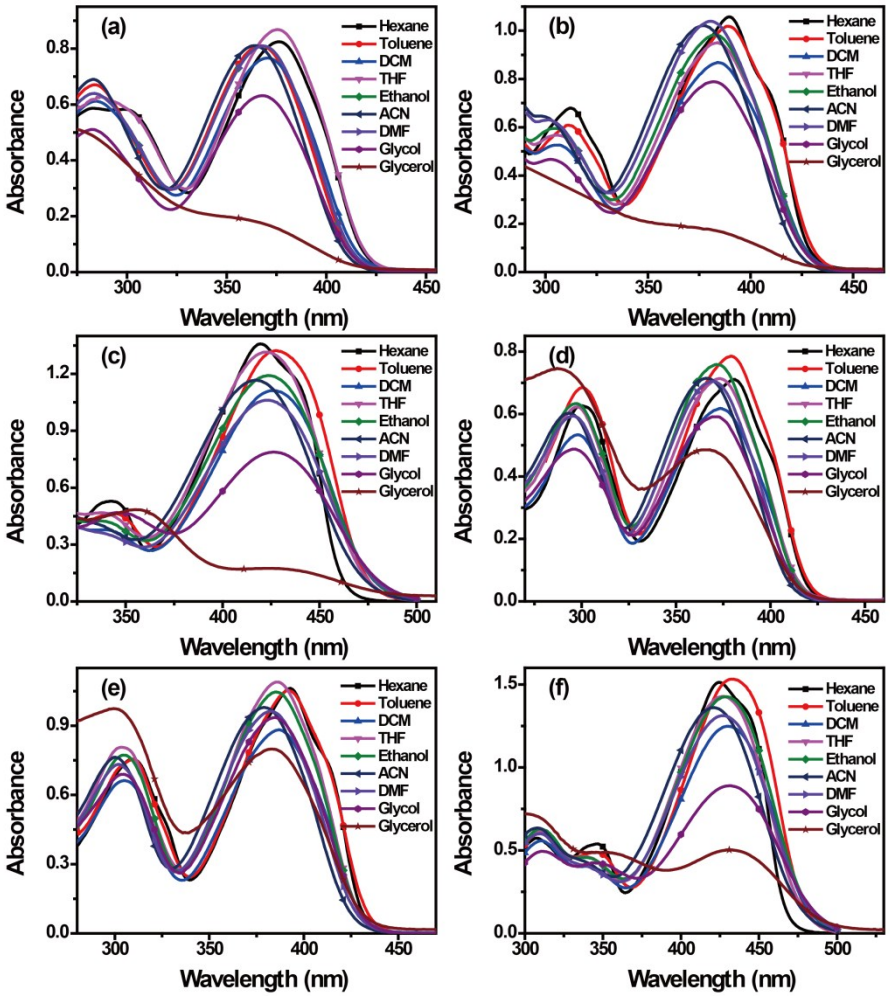


Figure S4. Absorption spectra of **Sborepy1**(a), **Sborepy2**(b), **Sborepy3**(c), **Sborepy4**(d), **Sborepy5**(e) and **Sborepy6**(f) in various solvents such as hexane, toluene, dichloromethane (DCM), tetrahydrofuran (THF), ethanol, acetonitrile (ACN), dimethylformamide (DMF), ethylene glycol (glycol) and glycerol, respectively.

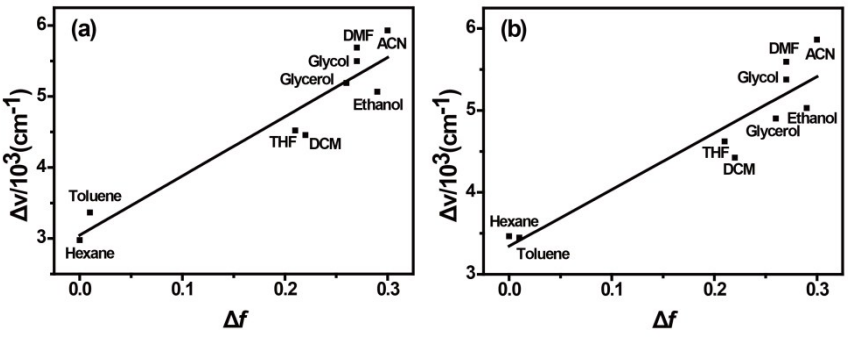


Figure S5. Plots of Stokes shift (Δν) of **Sborepy3** (a) and **Sborepy6** (b) versus solvent

orientation polariz ability (Δf) in different solvents. [2]

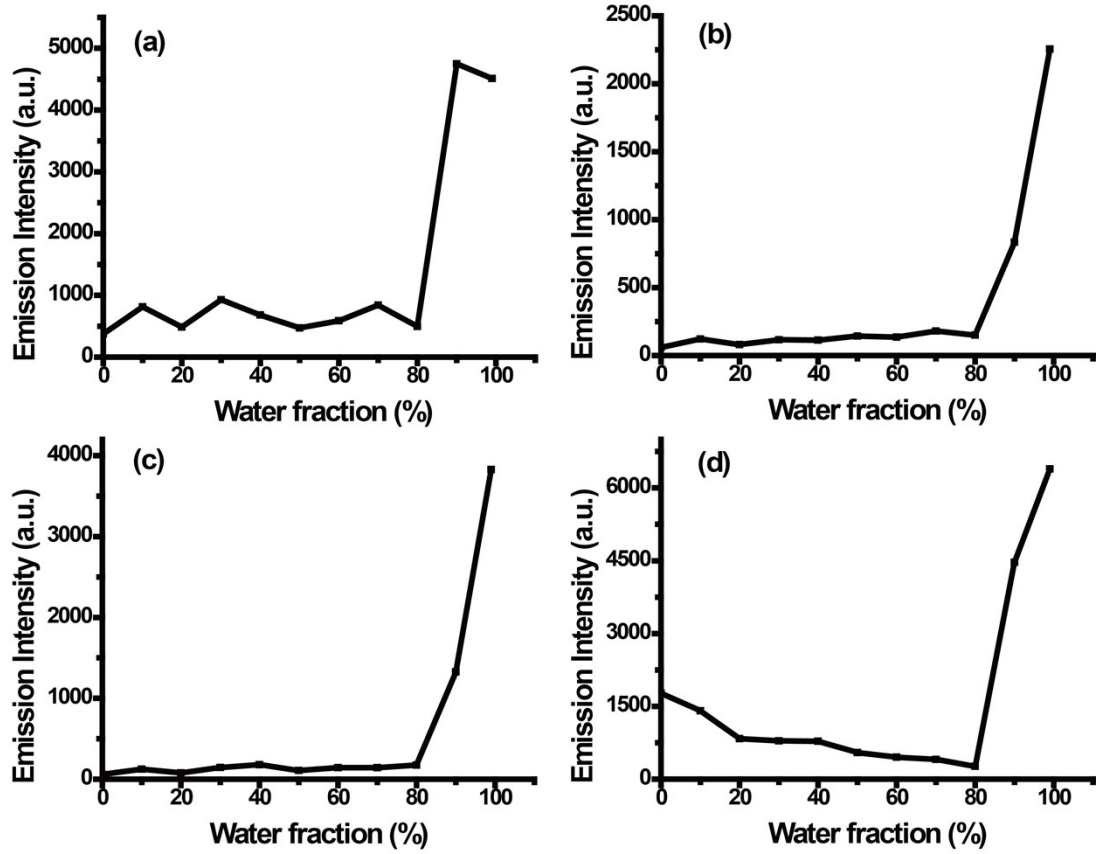


Figure S6. Changes in the F_{max} of **Sborepy3**(a), **Sborepy4**(b), **Sborepy5**(c) and **Sborepy6**(d) in THF/water mixtures (50 μM) with varied volumetric fractions of water (f_w).

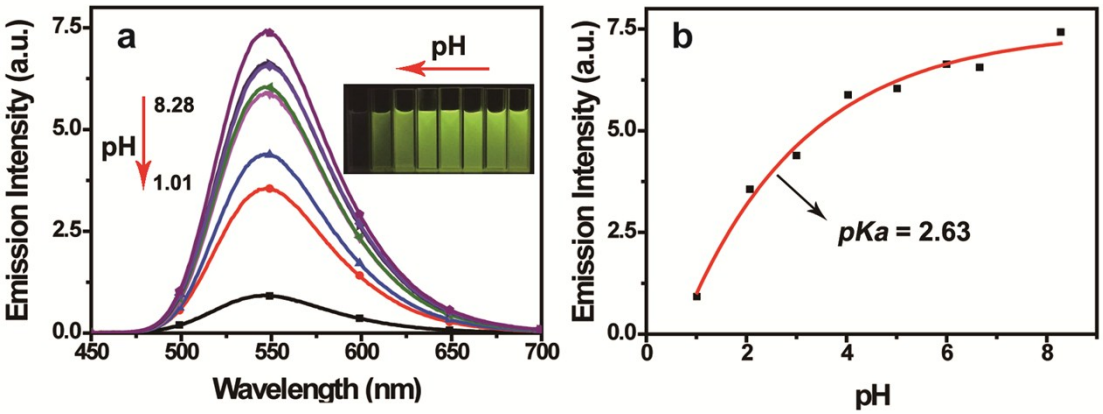


Figure S7. (a) Emission spectra (λ_{ex} = 424 nm) of **Sborepy6** (50 μM) in aqueous solutions (THF–water = 1 : 99, v/v) at different pH, (b) emission intensity at 549 nm versus pH in acidic conditions according to the fluorescent pH titration

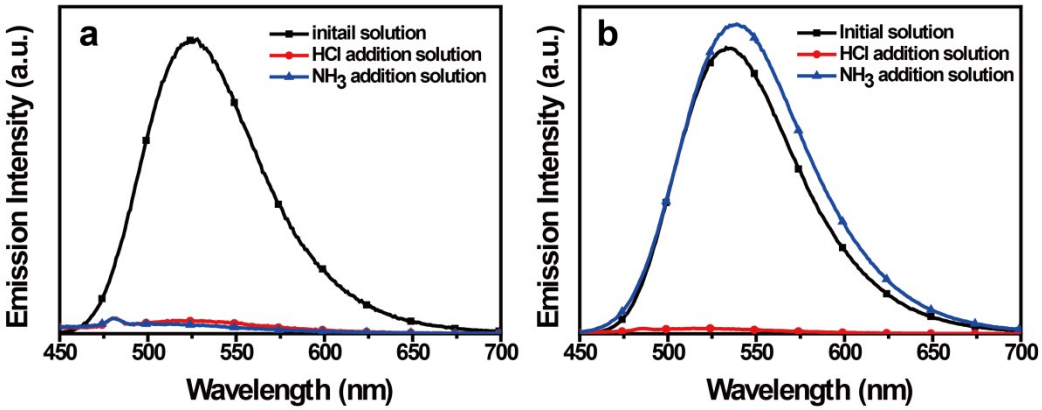


Figure S8. Emission spectra of initial, HCl (aq) and NH_3 (aq) of **Sborepy3** (a) and **Sborepy6** (b) in THF.

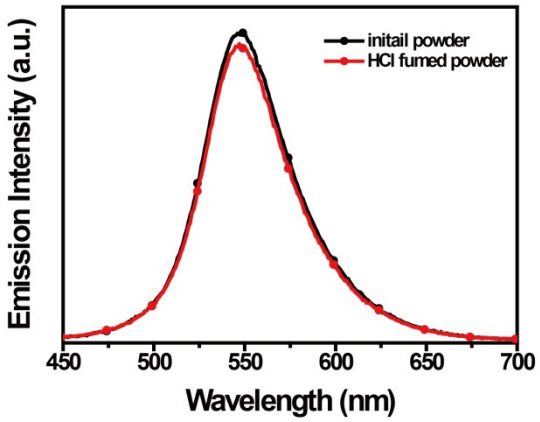


Figure S9. Emission spectra of initial and HCl (g) fumed powders of **Sborepy3**.

Table S1. Related wave functions, oscillator strengths, and calculated electronic excitation energies of **Sborepy1-6**.

Compound	State	λ [nm]	*f*	E_g (eV)	Orbital (coefficient)
Sborepy1	S_1	343.08	0.0299	3.61	H-L (69.4%)
	S_2	325.92	0.4262	3.80	H_{-1}-L (68.7%)
	S_5	255.71	0.0254	4.85	H_{-2}-L (67.9%)
Sborepy2	S_1	341.48	0.0444	3.63	H-L (68.2%)
	S_2	331.38	0.5441	3.74	H_{-1}-L (66.1%)
	S_4	274.17	0.2482	4.52	H_{-1}-L_{+1}(56.6%)
Sborepy3	S_1	348.97	0.6955	3.55	H_{-1}-L (45.9%)
	S_2	334.41	0.0578	3.71	H-L (57.2%)
	S_3	286.37	0.2462	4.33	H_{-1}-L_{+1}(42.0%)
Sborepy4	S_1	329.22	0.4209	3.77	H-L (66.1%)
	S_3	268.71	0.2224	4.61	H-L_{+1} (63.0%)

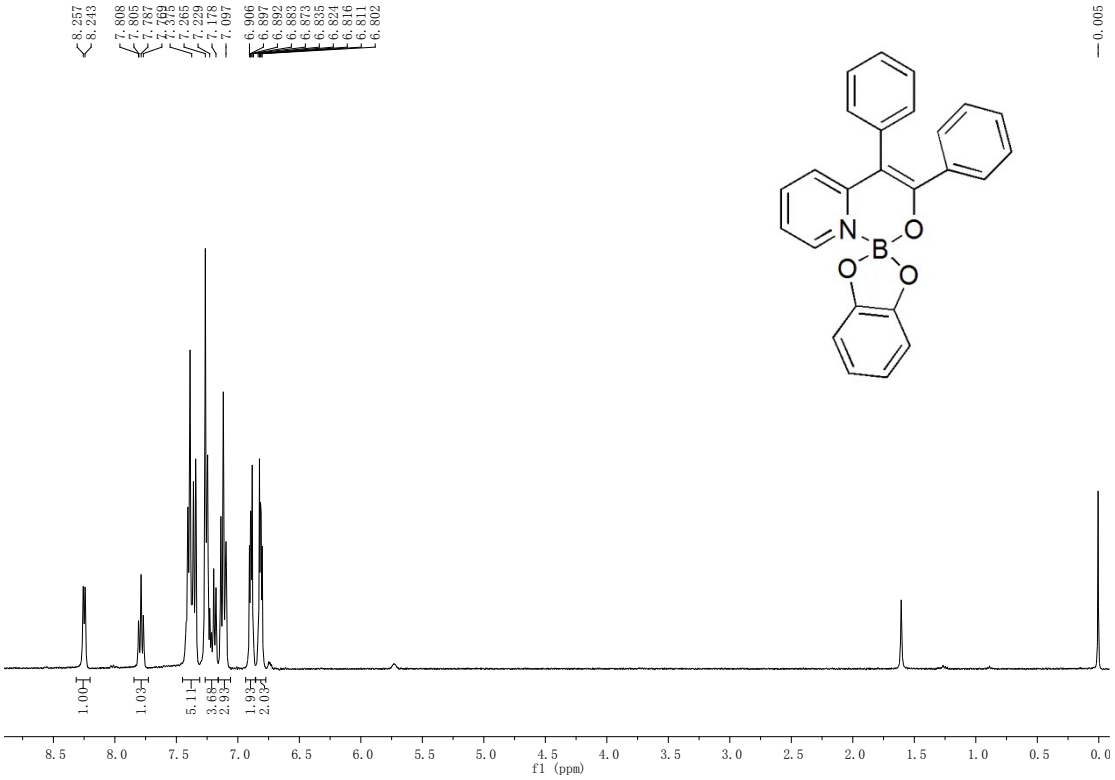
Sborepy5	S_1	337.01	0.5359	3.68	H-L (67.3%)
	S_2	275.21	0.2456	4.51	$H\text{-}L_{+1}$ (63.8%)
Sborepy6	S_1	352.90	0.7199	3.51	H-L (64.1%)
	S_2	288.18	0.2251	4.30	$H\text{-}L_{+1}$ (54.3%)

References

[1] C. Reichardt, *Chem. Rev.*, 1994, **94**, 2319.

[2]Y. P. Zhang, D. D. Li, Y Li, J. H. Yu, *Chem. Sci*., 2014, **5**, 2710.

NMR spectra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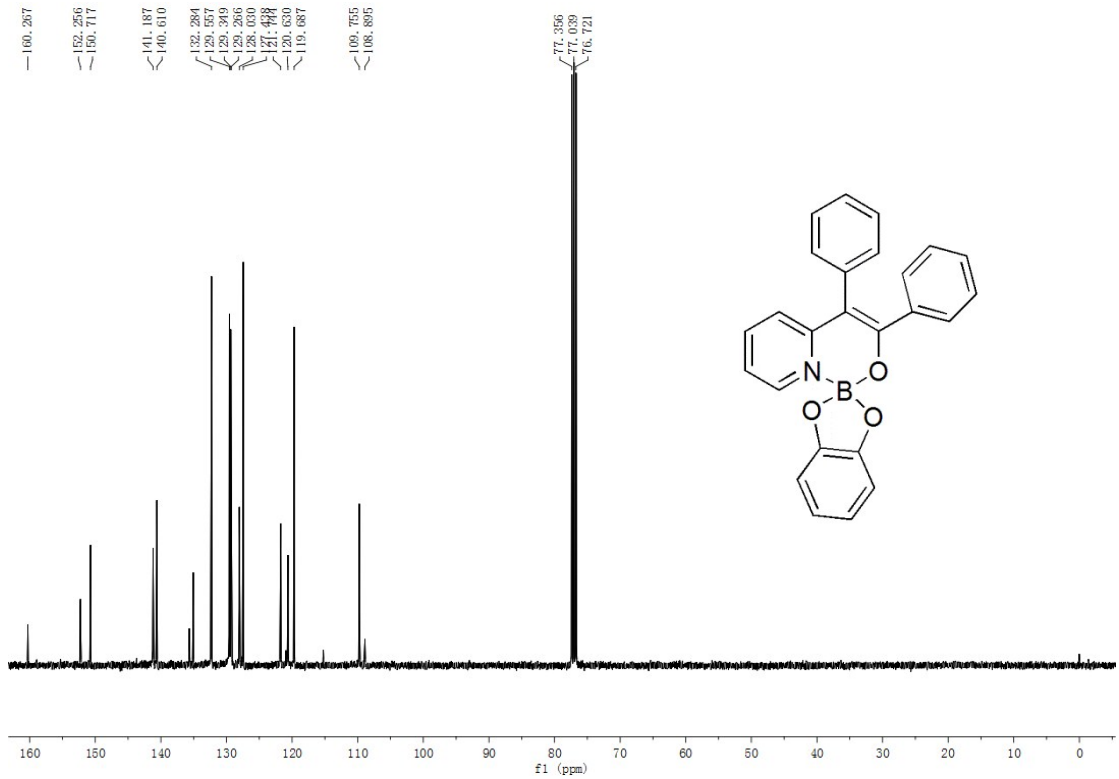
8.243
7.808
7.805
7.787
7.395
7.265
7.229
7.178
7.097
6.906
6.897
6.892
6.883
6.873
6.835
6.824
6.816
6.811
6.802
0.005
1.00
1.03
5.11
3.66
2.93
1.93
2.03
f1 (ppm)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152.256
150.717
141.187
140.610
132.284
129.557
129.349
129.266
128.030
120.630
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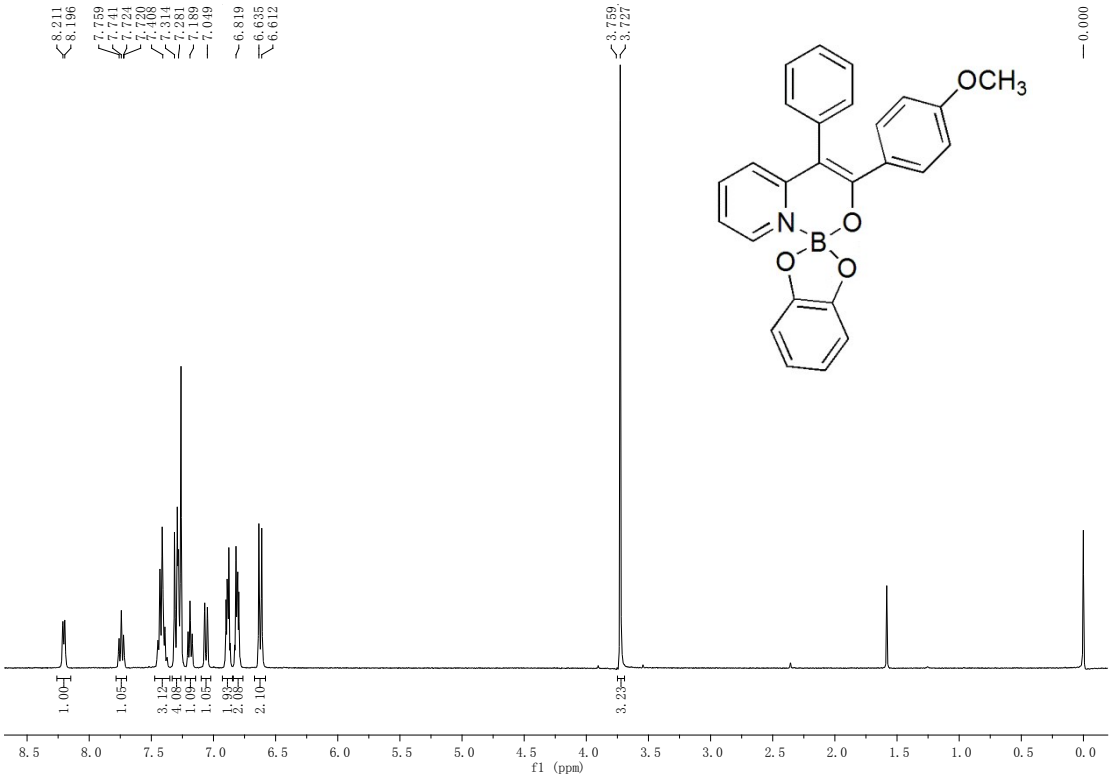
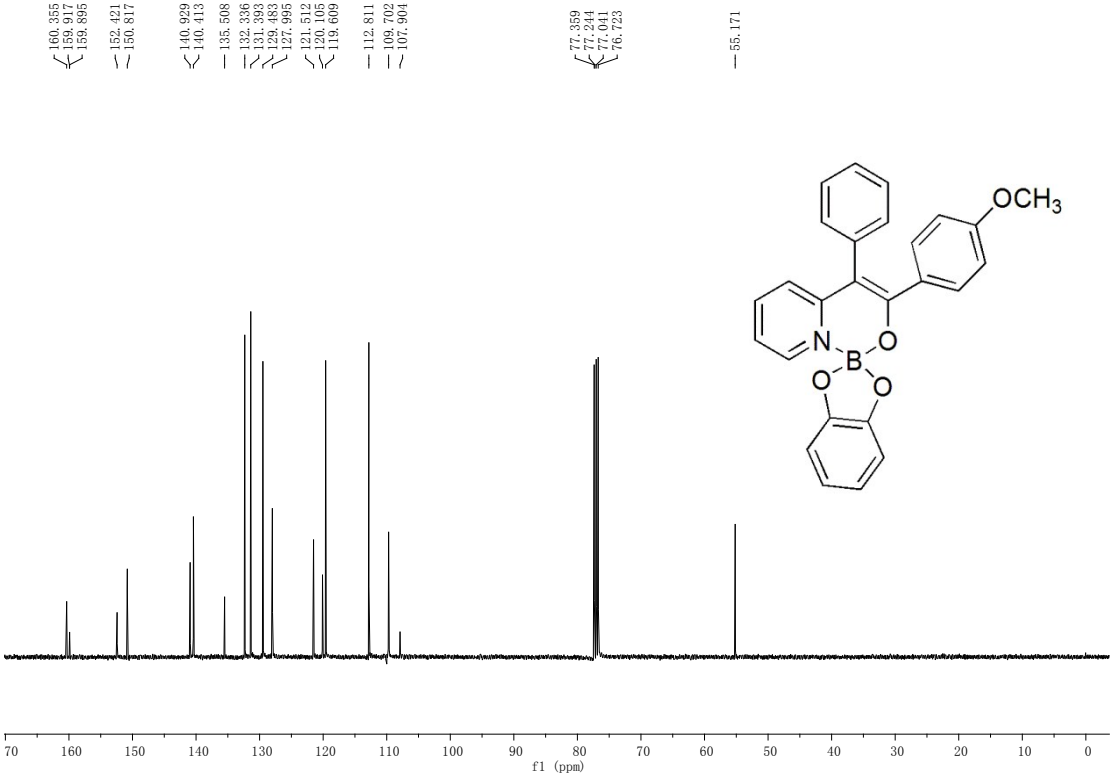
77.356
77.039
76.721
f1 (ppm)


8.211
8.196
7.759
7.741
7.724
7.720
7.468
7.314
7.281
7.189
7.049
6.819
6.635
6.612
3.759
3.727
0.000
OCH3
N
B
O
1.00
1.05
3.12
4.08
1.09
1.05
1.93
2.08
2.10
3.23
f1 (ppm)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140.929
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121.512
120.105
119.609
112.811
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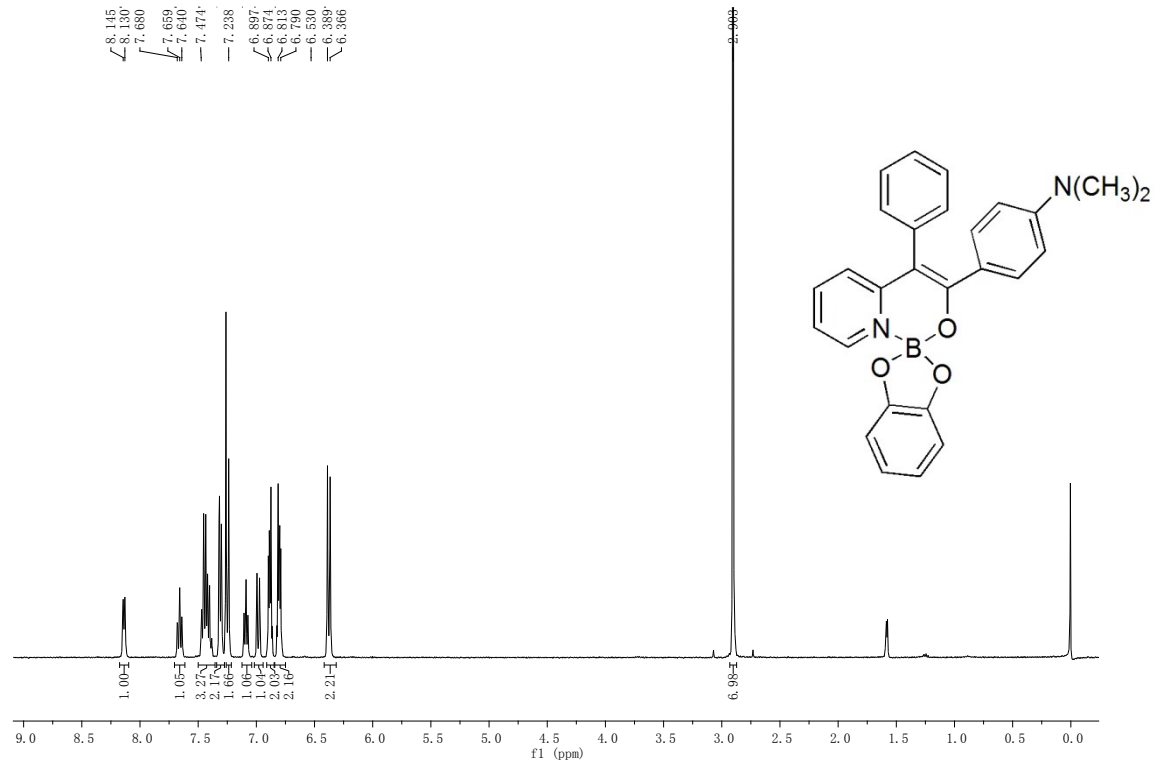
77.244
77.041
76.723
55.171
OCH3
N
B
O
f1 (ppm)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7.659
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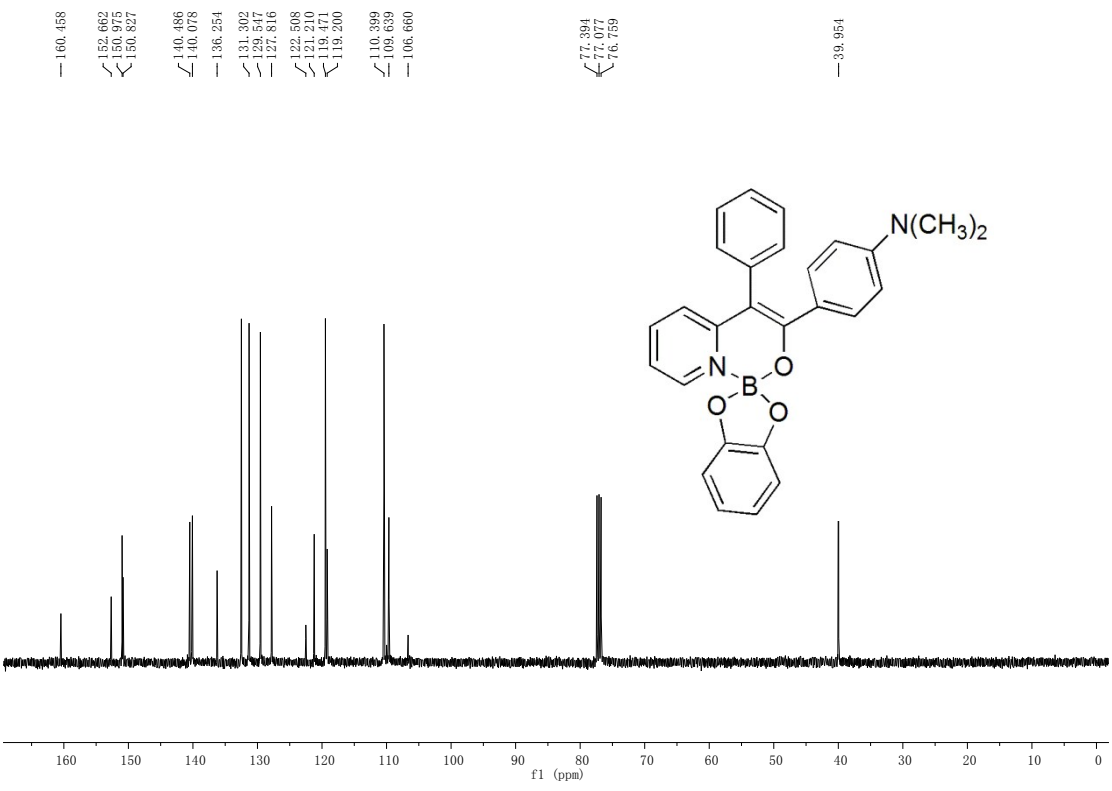
6.897
6.874
6.813
6.790
6.530
6.389
6.366
2.903
1.00
1.05
3.27
2.17
1.66
1.06
1.04
2.03
2.16
2.21
6.98
N(CH3)2
f1 (ppm)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131.302
129.547
127.816
122.508
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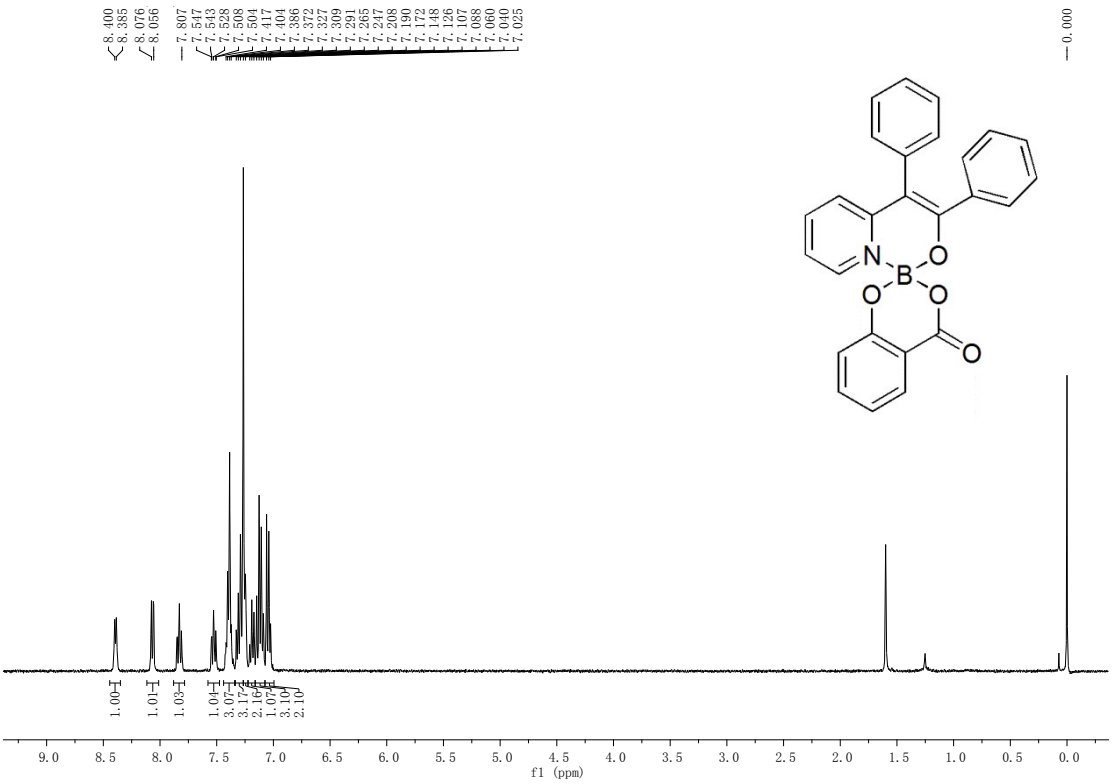
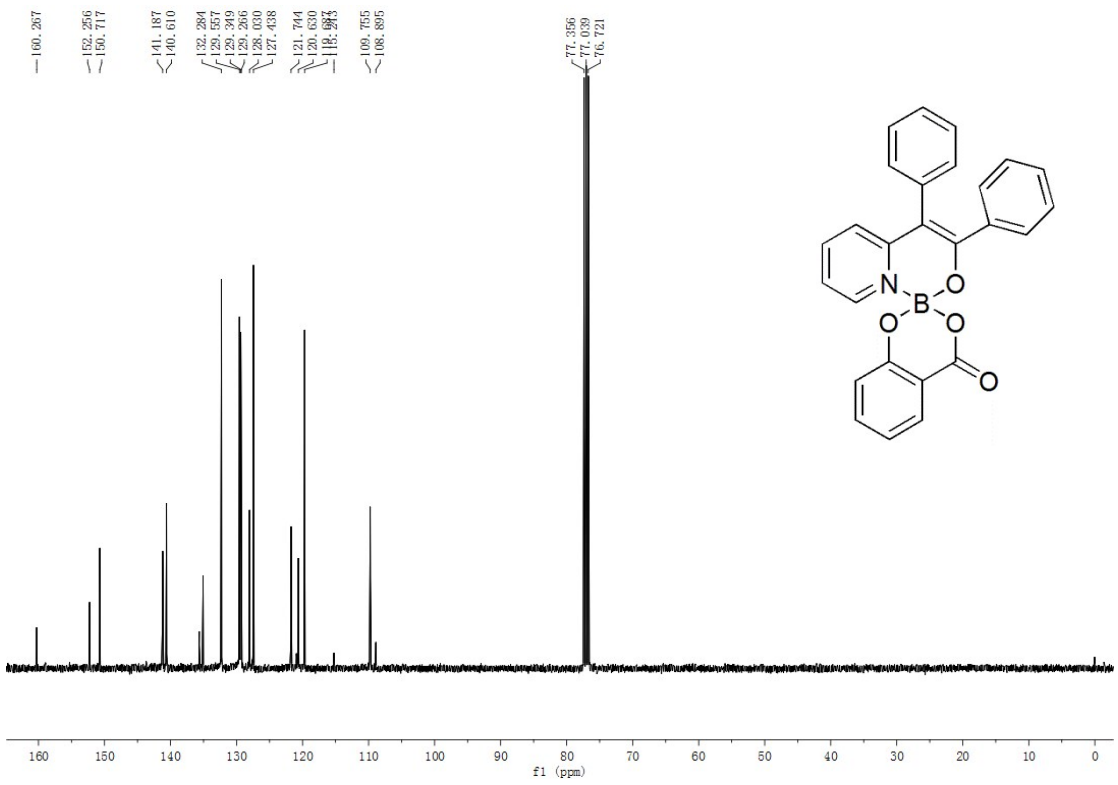
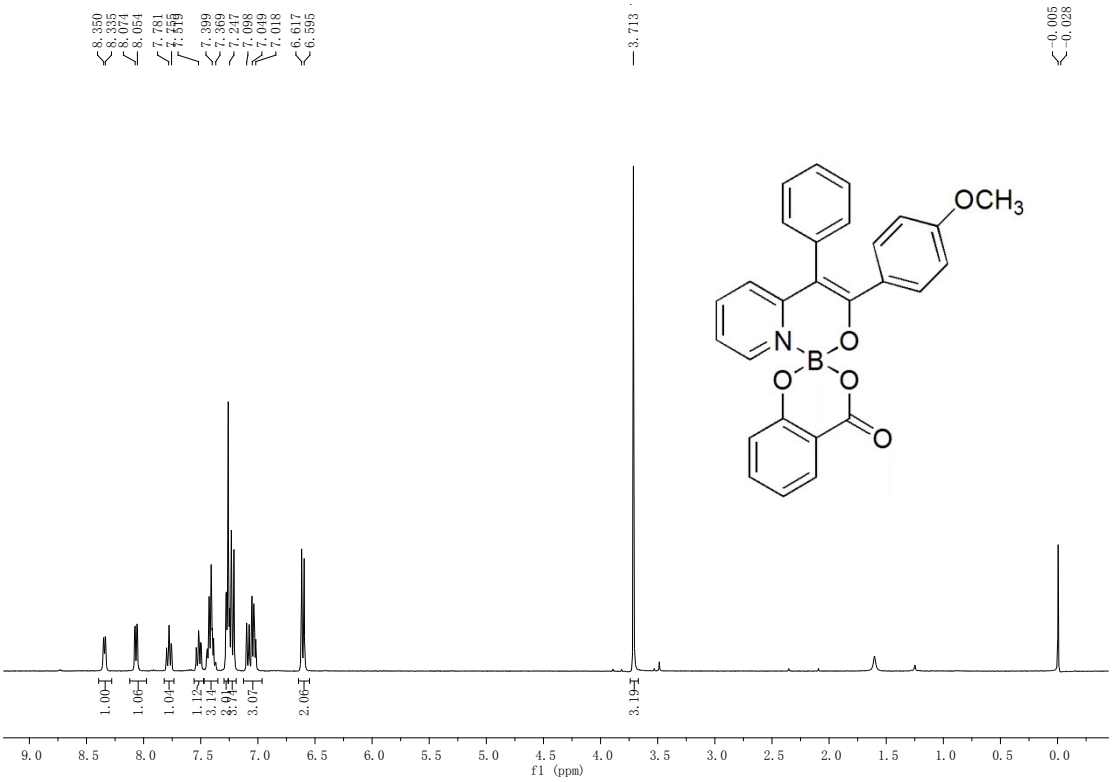
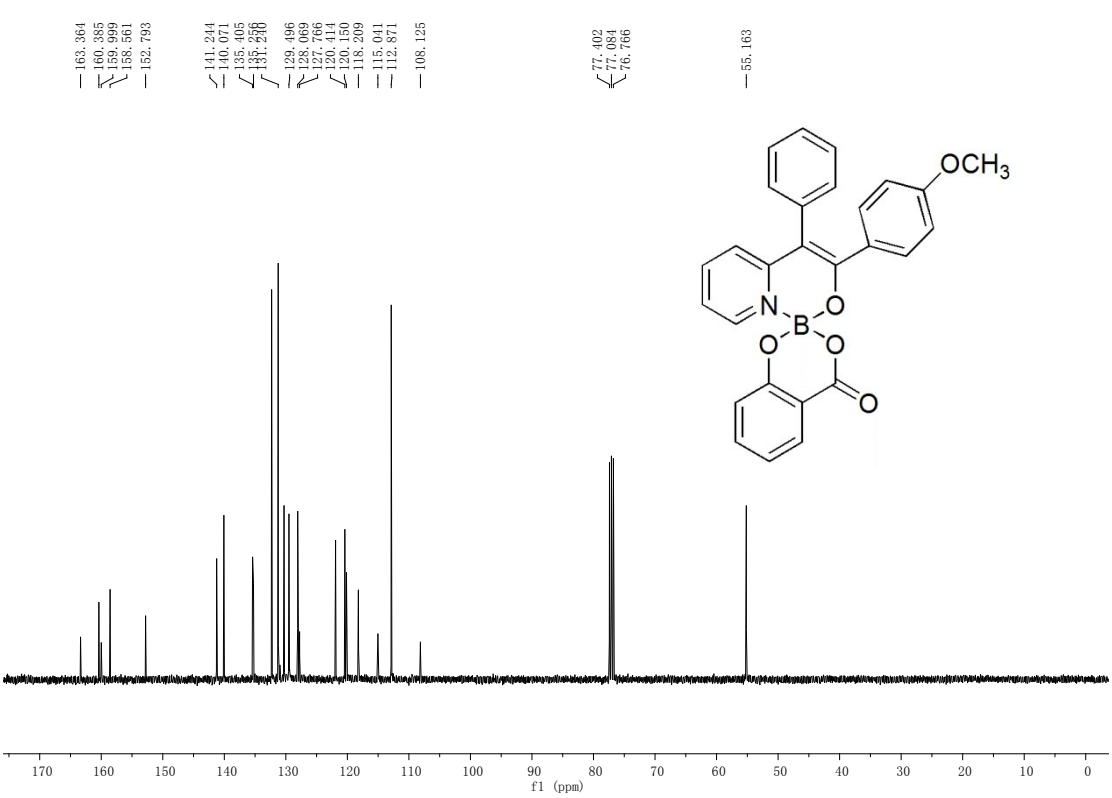
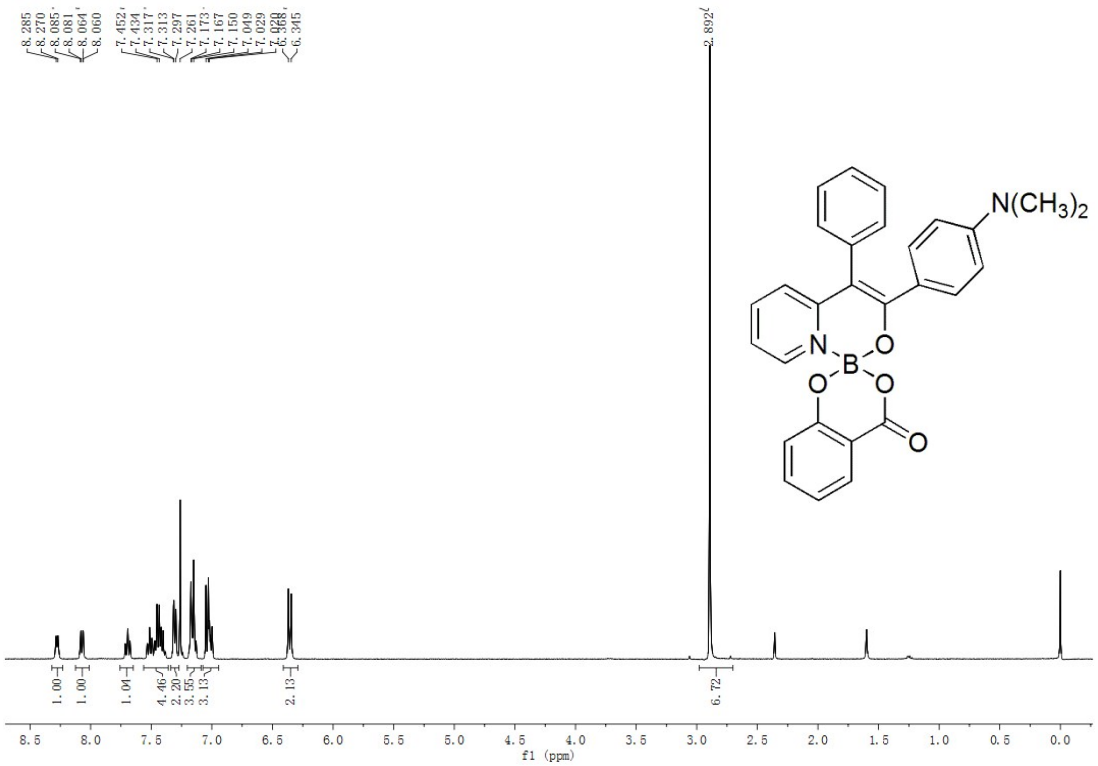
119.471
119.200
110.399
109.639
106.660
77.394
77.077
76.759
39.954
N(CH3)2
f1 (ppm)

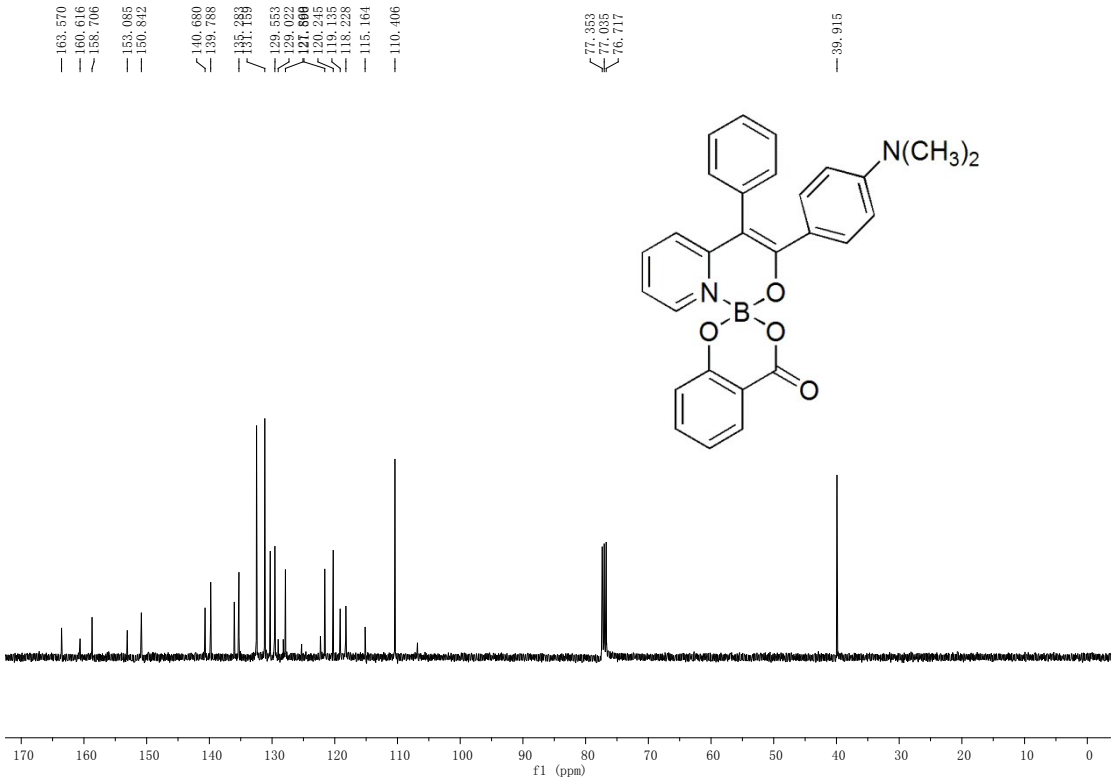

8.400
8.385
8.076
8.056
7.807
7.547
7.543
7.528
7.508
7.504
7.417
7.404
7.386
7.372
7.327
7.309
7.291
7.265
7.247
7.208
7.190
7.172
7.148
7.126
7.107
7.088
7.060
7.040
7.025
0.000
1.00
1.01
1.03
1.04
3.07
3.17
2.16
1.07
3.10
2.10
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
N
B
O
O
O
O


160.267
152.256
150.717
141.187
140.610
132.284
129.557
129.349
129.266
128.030
127.438
121.744
120.630
109.755
108.895
77.356
77.039
76.721
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
N
B
O
O
O
O


8.350
8.335
8.074
8.054
7.781
7.399
7.369
7.247
7.098
7.049
7.018
6.617
6.595
3.713
0.005
0.028
1.00
1.06
1.04
1.12
3.14
3.07
2.06
3.19
OCH3
N
B
O
O
O
O
f1 (ppm)


163.364
160.385
159.999
158.561
152.793
141.244
140.071
135.405
129.496
128.069
127.766
120.414
120.150
118.209
115.041
112.871
108.125
77.402
77.084
76.766
55.163
OCH3
N
B
O
O
O
O
f1 (ppm)


8.285
8.270
8.085
8.081
8.064
8.060
7.452
7.434
7.317
7.313
7.297
7.261
7.173
7.167
7.150
7.049
7.029
6.345
2.892
N(CH3)2
O
B
1.00
1.00
1.04
4.46
2.20
3.55
3.13
2.13
6.72
f1 (ppm)


163.570
160.616
158.706
153.085
150.842
140.680
139.788
135.283
131.199
129.553
129.022
120.245
119.135
118.228
115.164
110.406
77.353
77.035
76.717
39.915
N(CH3)2
O
B
f1 (ppm)

Z-matrix and total energy of Sborepy1-6

Sborepy1

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	0.52526	0.82999	-0.78726
O	2.04435	0.1142	0.95394
O	2.76344	0.08638	-1.26859
N	1.01066	-1.54735	-0.57143
C	-1.19611	-0.64877	-0.15404
C	-0.30166	-1.77705	-0.30436
C	-1.54221	1.85449	-0.48398
C	-3.53142	-1.54479	-0.48518
H	-3.2499	-1.85272	-1.48868
C	-0.73556	0.60865	-0.4617
C	-4.82215	-1.7793	-0.02606
H	-5.54155	-2.2771	-0.66923
C	-2.86569	1.90571	-0.92818
H	-3.36018	1.00505	-1.26845
C	5.09681	0.71829	-0.78231
H	5.41576	0.71085	-1.81898
C	-2.97245	-0.50063	1.60342
H	-2.24751	-0.00175	2.23883
C	-0.91511	3.0389	-0.08327
H	0.11896	3.00166	0.23876
C	-2.58826	-0.90012	0.32204
C	-0.72748	-3.11709	-0.20536
H	-1.76023	-3.31847	0.04208
C	-1.60661	4.24151	-0.09621
H	-1.1106	5.15064	0.22891
C	1.87094	-2.55679	-0.81218
H	2.88211	-2.24402	-1.03819
C	0.15404	-4.14791	-0.43223
H	-0.18815	-5.17526	-0.35661
C	4.22592	0.73784	1.91804
H	3.88111	0.74318	2.94632
C	-2.92661	4.28237	-0.53214
H	-3.4664	5.22429	-0.54927
C	3.79492	0.42665	-0.44279
C	3.36287	0.43635	0.88696
C	-5.19285	-1.36873	1.25022
H	-6.20156	-1.54786	1.60927
C	-3.54991	3.11356	-0.95455

H	-4.57477	3.14049	-1.31128
C	-4.26489	-0.72733	2.06242
H	-4.54597	-0.40383	3.05991
C	5.55411	1.03647	1.5825
H	6.2577	1.27974	2.3726
C	1.48472	-3.87095	-0.76427
H	2.20182	-4.6578	-0.96191
C	5.98101	1.0274	0.26147
H	7.01437	1.26409	0.02821
B	1.60356	-0.07735	-0.42332

Sborepy2

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	2.34565	-0.39223	1.03163
O	0.58187	-0.68783	-0.6064
N	1.83941	1.39484	-0.61098
O	2.90863	-0.781	-1.20216
O	-4.88225	-3.59756	0.12271
C	0.68059	2.06339	-0.37778
C	-0.51821	-0.04577	-0.24993
C	-1.68662	-0.9488	-0.14643
C	-3.8094	-2.78035	-0.01213
C	-0.52179	1.319	-0.07777
C	-1.75137	2.10194	0.24013
C	-2.76821	2.25857	-0.7045
H	-2.66533	1.78296	-1.67488
C	3.47201	-1.14754	0.96028
C	-3.90582	3.00005	-0.40822
H	-4.68937	3.10506	-1.15239
C	-1.69652	-2.10081	-0.93509
H	-0.85942	-2.28985	-1.59647
C	3.80971	-1.38646	-0.37553
C	-3.79897	-1.64768	0.80597
H	-4.62213	-1.50174	1.49652
C	-2.75655	-0.74476	0.73634
H	-2.76673	0.1152	1.39289
C	-1.89399	2.72383	1.48401
H	-1.10804	2.60978	2.22525
C	0.69441	3.46883	-0.4986
H	-0.22133	4.01427	-0.31727
C	-3.02886	3.46997	1.78114
H	-3.12541	3.94081	2.75473
C	2.96664	2.03815	-0.97492

H	3.81789	1.39387	-1.15241
C	-2.74775	-3.00618	-0.88708
H	-2.72267	-3.88149	-1.52406
C	-4.03966	3.60724	0.83565
H	-4.92812	4.1865	1.06731
B	1.91725	-0.17157	-0.34443
C	3.01696	3.40087	-1.11096
H	3.93999	3.88601	-1.40265
C	1.84682	4.12639	-0.85788
H	1.84306	5.2078	-0.95194
C	4.91913	-2.12512	-0.72016
H	5.16605	-2.30431	-1.76109
C	4.23967	-1.64292	1.99183
H	3.96895	-1.45326	3.02478
C	5.37166	-2.39696	1.65111
H	5.99518	-2.80231	2.44197
C	5.70492	-2.63362	0.32442
H	6.58585	-3.2219	0.08729
C	-4.93319	-4.76891	-0.66427
H	-4.94546	-4.53343	-1.73506
H	-5.86238	-5.27213	-0.39617
H	-4.08737	-5.43306	-0.45131

Sborepy3

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	2.45992	-0.63619	0.96688
O	3.00544	-1.05143	-1.26715
C	-6.38102	-2.25196	-0.62318
H	-6.63017	-1.36019	-0.037
H	-7.18478	-2.97501	-0.48201
H	-6.36042	-1.96564	-1.68437
C	-5.06359	-4.26396	0.04771
H	-4.50173	-4.78942	-0.73719
H	-6.07438	-4.67184	0.07355
H	-4.59058	-4.48836	1.01035
N	-5.13337	-2.83692	-0.18273
C	-3.97306	-2.09765	-0.24262
C	-3.98832	-0.73578	-0.60337
H	-4.91831	-0.2511	-0.87093
C	-2.82458	0.00961	-0.6338
H	-2.89002	1.04884	-0.92814
C	-1.58417	-0.5575	-0.32368
C	-1.56481	-1.9198	0.00118

H	-0.61346	-2.39012	0.21979
C	-2.72088	-2.67292	0.05166
H	-2.64688	-3.71958	0.31695
C	-0.29872	0.16291	-0.37369
C	-0.0966	1.5065	-0.13398
C	1.21066	2.07177	-0.36729
N	2.25394	1.24292	-0.6406
B	2.09564	-0.3201	-0.41213
O	0.70559	-0.6322	-0.70172
C	-1.18288	2.40727	0.3515
C	-1.74988	3.38233	-0.47598
H	-1.40469	3.47272	-1.50244
C	-2.75603	4.21968	-0.00791
H	-3.18592	4.96774	-0.66733
C	-3.21647	4.0926	1.29838
H	-4.00466	4.74308	1.66487
C	-2.66134	3.12791	2.13142
H	-3.01411	3.02257	3.15285
C	-1.64993	2.29734	1.6629
H	-1.21563	1.54521	2.3139
C	1.46902	3.45994	-0.3405
H	0.66317	4.13413	-0.08711
C	2.71825	3.94447	-0.64331
H	2.89949	5.01461	-0.62299
C	3.75119	3.06096	-0.98155
H	4.74351	3.41004	-1.23807
C	3.47546	1.71978	-0.95613
H	4.21225	0.95894	-1.17911
C	3.46545	-1.5455	0.89419
C	3.79055	-1.80074	-0.44207
C	4.13141	-2.17292	1.92479
H	3.872	-1.96837	2.95787
C	5.14626	-3.07836	1.58325
H	5.68787	-3.58914	2.37345
C	5.46677	-3.33109	0.25643
H	6.25575	-4.03764	0.01831
C	4.78535	-2.68771	-0.78718
H	5.02323	-2.87764	-1.82831

Sborepy4

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

B	1.32254	-0.55976	-0.22224
N	0.50275	-1.89601	-0.42175

O	0.46116	0.53409	-0.66264
O	1.57868	-0.4558	1.20001
O	2.49472	-0.62331	-1.042
O	2.79288	0.31808	2.89371
C	1.18384	-3.04702	-0.59417
H	2.25097	-2.92445	-0.72515
C	0.56321	-4.26816	-0.59364
H	1.1404	-5.17358	-0.7327
C	-0.82029	-4.29592	-0.38384
H	-1.349	-5.24326	-0.34976
C	-1.51582	-3.12108	-0.22318
H	-2.58535	-3.12975	-0.06778
C	-0.84801	-1.88031	-0.26766
C	-1.53688	-0.61083	-0.17564
C	-2.98238	-0.60856	0.19756
C	-3.96749	-1.06669	-0.68334
H	-3.67728	-1.41602	-1.67077
C	-5.30834	-1.06337	-0.31715
H	-6.05956	-1.41839	-1.01619
C	-5.68641	-0.59762	0.93782
H	-6.73356	-0.59081	1.22405
C	-4.71658	-0.14079	1.82263
H	-5.00308	0.22353	2.80432
C	-3.37542	-0.15174	1.45683
H	-2.61782	0.20222	2.14888
C	-0.84	0.54458	-0.43295
C	-1.40974	1.91262	-0.50356
C	-2.66151	2.19416	-1.05619
H	-3.27431	1.39348	-1.44976
C	-3.12042	3.50287	-1.12108
H	-4.091	3.70867	-1.56141
C	-2.34162	4.54453	-0.6296
H	-2.70626	5.56613	-0.67654
C	-1.09098	4.27385	-0.08498
H	-0.47468	5.08184	0.29634
C	-0.62275	2.96903	-0.03337
H	0.3572	2.75368	0.376
C	2.69388	0.0896	1.71114
C	3.77652	0.35125	0.73243
C	4.96764	0.9437	1.15238
H	5.05035	1.2218	2.19756
C	6.00177	1.15643	0.25739
H	6.92595	1.61961	0.5864
C	5.84513	0.76513	-1.07382

H	6.65171	0.92703	-1.78293
C	4.67006	0.17295	-1.50806
H	4.53122	-0.13142	-2.53967
C	3.62802	-0.03255	-0.60429

Sborepy5

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	0.60725	0.36029	-0.59312
O	2.87992	-0.09969	-1.08048
N	1.38405	-1.95233	-0.53188
O	2.0326	-0.36738	1.17936
O	3.02385	0.61122	2.91183
C	-1.5807	1.10007	-0.32154
O	-3.99245	4.48494	-0.21558
C	-1.93807	3.44723	0.1645
H	-1.58483	4.40602	0.52734
C	-0.93603	-1.36141	-0.1586
C	2.95369	0.44766	1.71637
C	2.14613	-4.17929	-0.87971
H	2.96208	-4.85755	-1.0952
C	-0.63057	-0.03235	-0.34555
C	0.8431	-4.63632	-0.64769
H	0.6242	-5.69916	-0.67368
C	3.87399	1.08924	0.74677
C	-2.89805	1.01849	-0.77064
H	-3.28518	0.08364	-1.15413
C	-1.11225	2.34338	0.13209
H	-0.08491	2.42809	0.46532
C	-2.29837	-1.82229	0.24122
C	3.79958	0.77206	-0.6134
C	-3.13487	-2.50103	-0.65116
H	-2.7927	-2.68239	-1.66667
C	0.0965	-2.35349	-0.35482
B	1.77082	-0.4492	-0.24391
C	2.37154	-2.83095	-0.80072
H	3.347	-2.38376	-0.94029
C	-3.25951	3.34756	-0.28085
C	-3.73557	2.12715	-0.75759
H	-4.74953	2.02705	-1.12396
C	5.73962	2.55596	0.30617
H	6.49459	3.25116	0.6578
C	-0.1654	-3.73954	-0.38944
H	-1.17596	-4.08152	-0.21661

C	-2.76005	-1.58732	1.53781
H	-2.11675	-1.06525	2.23906
C	4.70038	1.34314	-1.51213
H	4.62221	1.08335	-2.56215
C	4.84832	1.98109	1.19547
H	4.8812	2.19784	2.25778
C	-4.39864	-2.92818	-0.26
H	-5.03511	-3.4502	-0.96818
C	5.65984	2.22907	-1.04902
H	6.35575	2.67445	-1.75402
C	-4.84861	-2.67942	1.03239
H	-5.83639	-3.00945	1.3389
C	-5.33441	4.44369	-0.65238
H	-5.40346	4.17717	-1.71368
H	-5.72957	5.44934	-0.50784
H	-5.92679	3.73378	-0.06315
C	-4.02634	-2.00672	1.92905
H	-4.36922	-1.81009	2.94019

Sborepy6

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	-0.70161	-0.26802	-0.57864
O	-3.01642	-0.19124	-1.07306
O	-2.23528	0.21088	1.18997
N	-1.85111	1.88219	-0.51929
C	0.53713	1.68552	-0.15744
C	0.45906	0.31991	-0.33856
C	1.57737	-0.63879	-0.31828
C	-0.64507	2.48974	-0.34903
C	2.29861	-2.92222	0.10042
H	2.03719	-3.92292	0.41909
C	3.62122	-2.61576	-0.27754
C	1.31095	-1.95847	0.06915
H	0.30094	-2.2257	0.35582
C	1.80351	2.3715	0.23466
C	-3.7628	-1.56736	0.73994
C	2.88621	-0.33897	-0.71119
H	3.13711	0.6558	-1.05488
C	-4.53212	-1.94745	-1.52146
H	-4.50783	-1.66504	-2.56829
C	-3.75313	-1.226	-0.61664
N	4.6155	-3.56578	-0.23806
C	-2.97402	3.95221	-0.86104
H	-3.89204	4.48623	-1.0714

C	2.51196	3.17511	-0.66481
H	2.14257	3.28741	-1.68071
C	3.8821	-1.29707	-0.70053
H	4.873	-1.01483	-1.03196
C	-0.61856	3.9018	-0.38286
H	0.32174	4.40693	-0.21392
C	3.47755	2.85999	1.91668
H	3.85012	2.7324	2.92844
C	-4.54867	-2.63325	1.17818
H	-4.53766	-2.86375	2.23807
C	3.68536	3.81369	-0.28024
H	4.2231	4.43051	-0.99408
C	2.30047	2.22861	1.53175
H	1.75618	1.6097	2.23802
C	-1.76226	4.61851	-0.63506
H	-1.72235	5.70298	-0.66085
C	-2.9722	2.5859	-0.78186
H	-3.8608	1.98311	-0.9161
B	-1.98149	0.33905	-0.23317
C	-5.30454	-3.00487	-1.06865
H	-5.90549	-3.56578	-1.77858
O	-3.02186	-0.95592	2.91142
C	4.2868	-4.93875	0.08081
H	3.84346	-5.0213	1.07978
H	5.19876	-5.53603	0.07264
H	3.58353	-5.37829	-0.63994
C	-2.98194	-0.77028	1.71742
C	4.17273	3.65535	1.01286
H	5.09065	4.15058	1.31424
C	-5.31671	-3.35705	0.28252
H	-5.92505	-4.18698	0.62629
C	5.93657	-3.24726	-0.73405
H	5.9331	-2.99078	-1.8028
H	6.58877	-4.10968	-0.59465
H	6.37561	-2.40601	-0.18549