Electronic Supplementary Material (ESI) for New Journal of Chemistry.

J-aggregation induced emission enhancement of thienyl substituted bis(difluoroboron)-1,2-bis((1H-pyrrol-2-yl)methylene) hydrazine (BOPHY) dye

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I. Materials and Instrumentations

II. Supporting Data

I. Materials and instrumentations

All reagents were obtained from commercial suppliers and used without further purification unless otherwise indicated. All reactions and manipulations of air-sensitive compounds were carried out under dry argon by using Schlenk techniques and/or vacuum line techniques. Solvents were dried prior to use by common methods in organometallic chemistry. Toluene was distilled over sodium. Chemicals were commercially obtained and used as received. ^{1}H and ^{13}C NMR spectra were recorded using Bruker DRX400 spectrometer instrument. Mass spectra were measured with a Bruker Daltonics AutoflexII TM MALDI–TOF spectrometer. Thin layer chromatography (TLC) was performed on plates coated with thick silica gel GF254 (Qingdao Haiyang Chemical Co., Ltd). Column chromatography was performed using silica gel (100-200 mesh, Qingdao Haiyang Chemical Co., Ltd).

II. Supporting Data

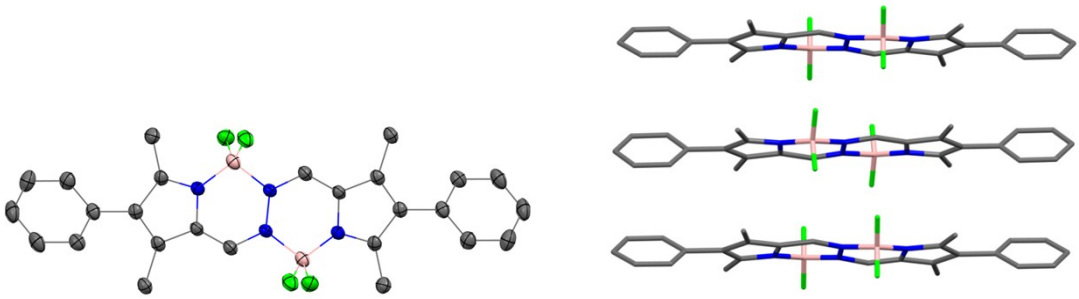


Figure S1. The conformation and *H*-aggregation of dye **1.**

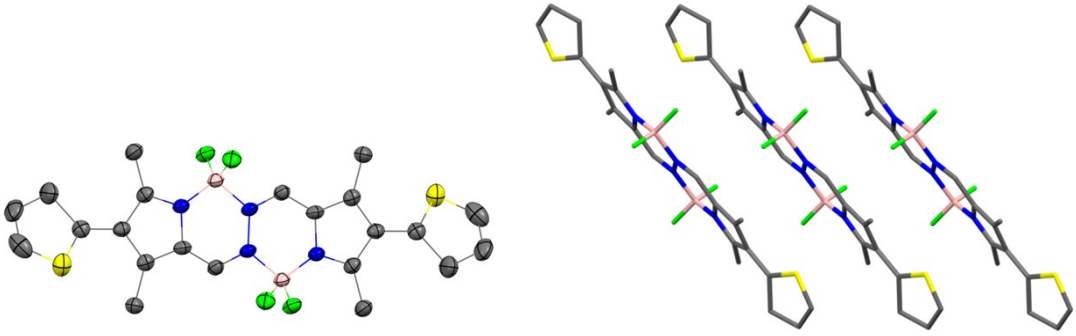


Figure S2. The conformation and *J*-aggregation of dye **2.**

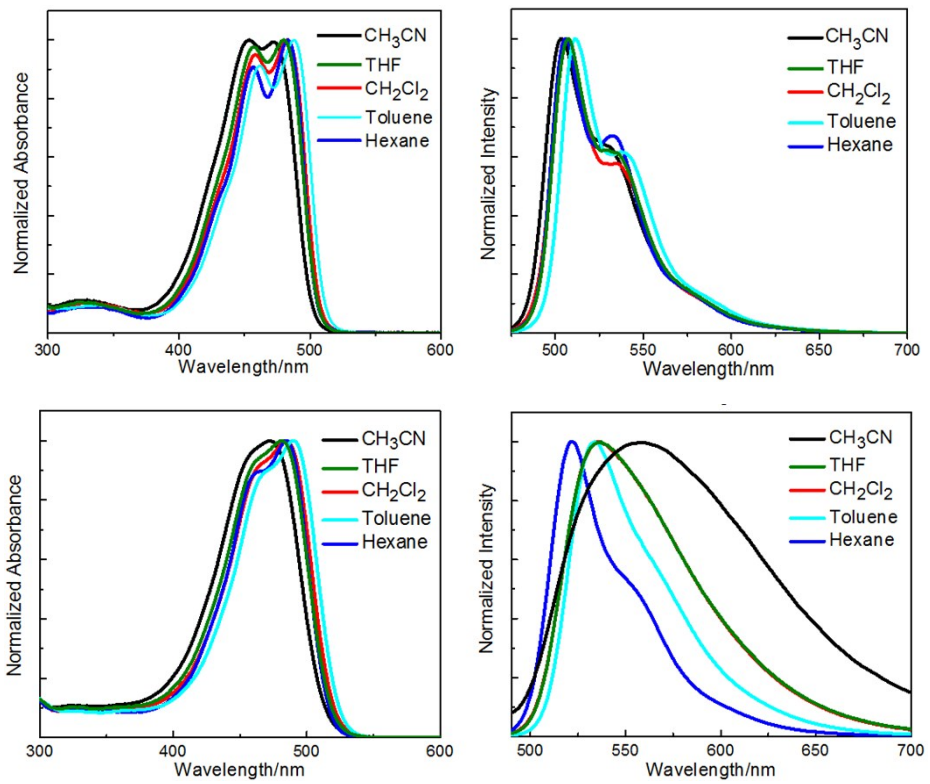


Figure S3. The absorption and emission spectra of **1** and **2** in hexane, toluene, DCM, THF, CH_3CN (top for **1**, bottom for **2**).

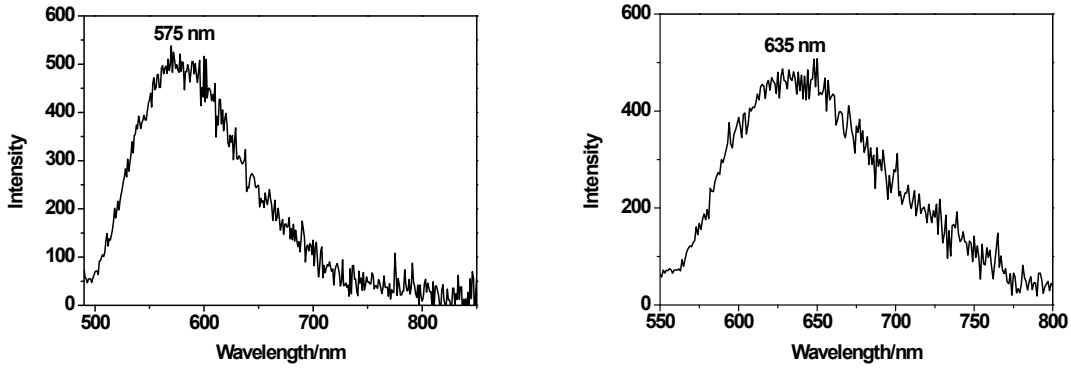


Figure S4. The solid-state emission spectra of **1** (left, excitation wavelength = 480 nm) and **2** (right, excitation wavelength = 450 nm) at room temperature.

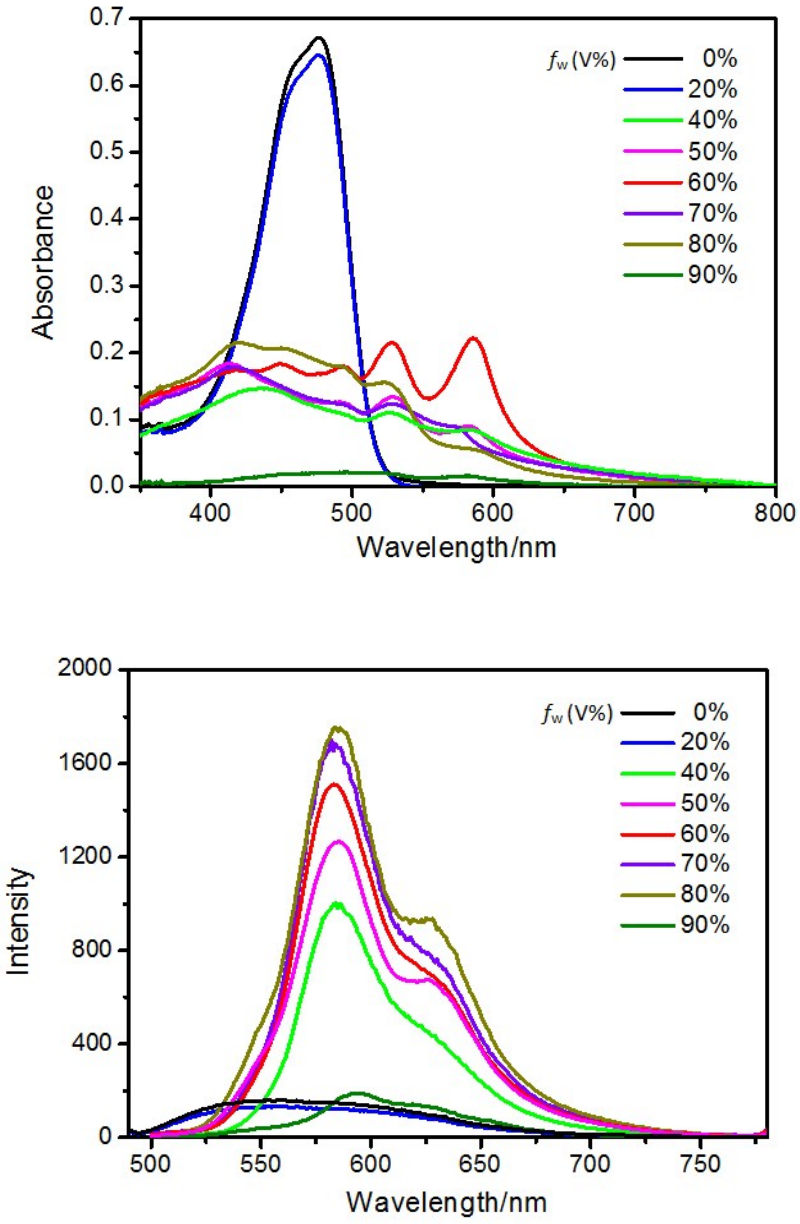
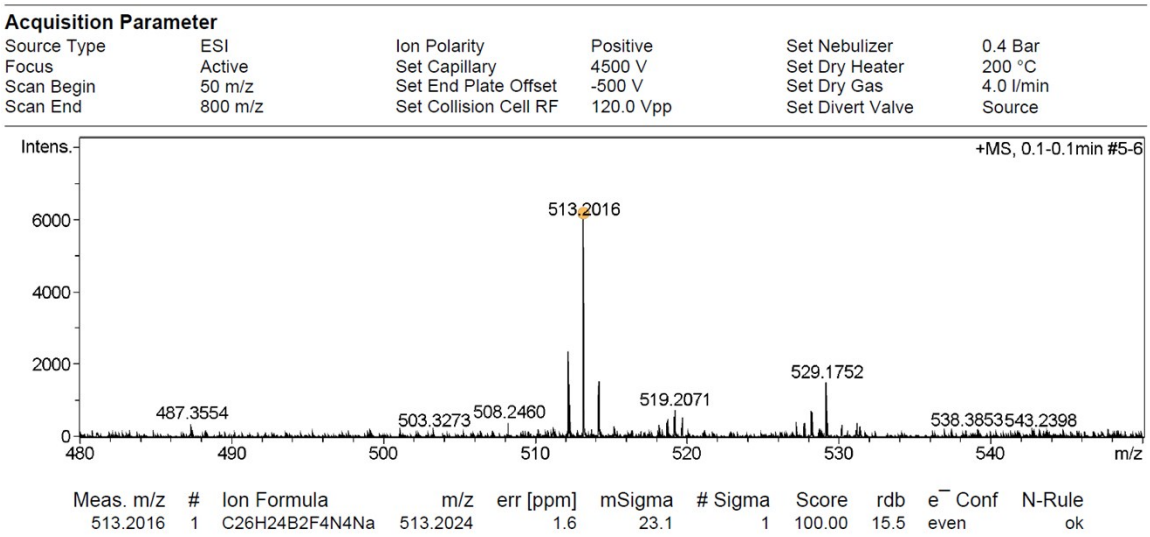


Figure S5. Absorption (up) and emission (bottom, excitation wavelength = 475nm) spectra changes of **2** (10^{-5} M) in CH_3OH-H_2O mixed solutions.



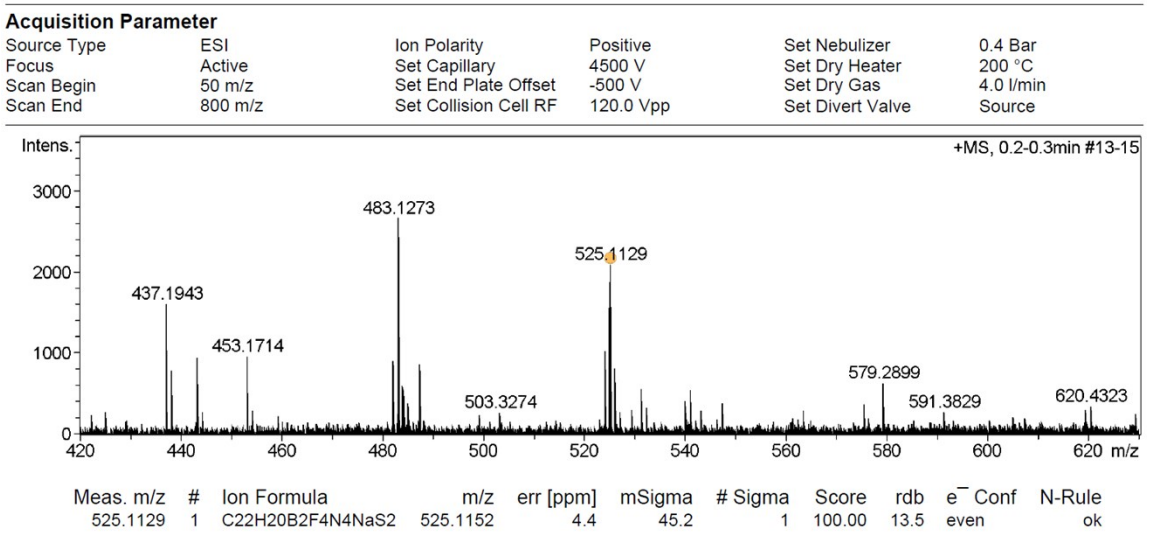


Figure S6. The HR-MS spectrum of **1** (up) and **2** (bottom).

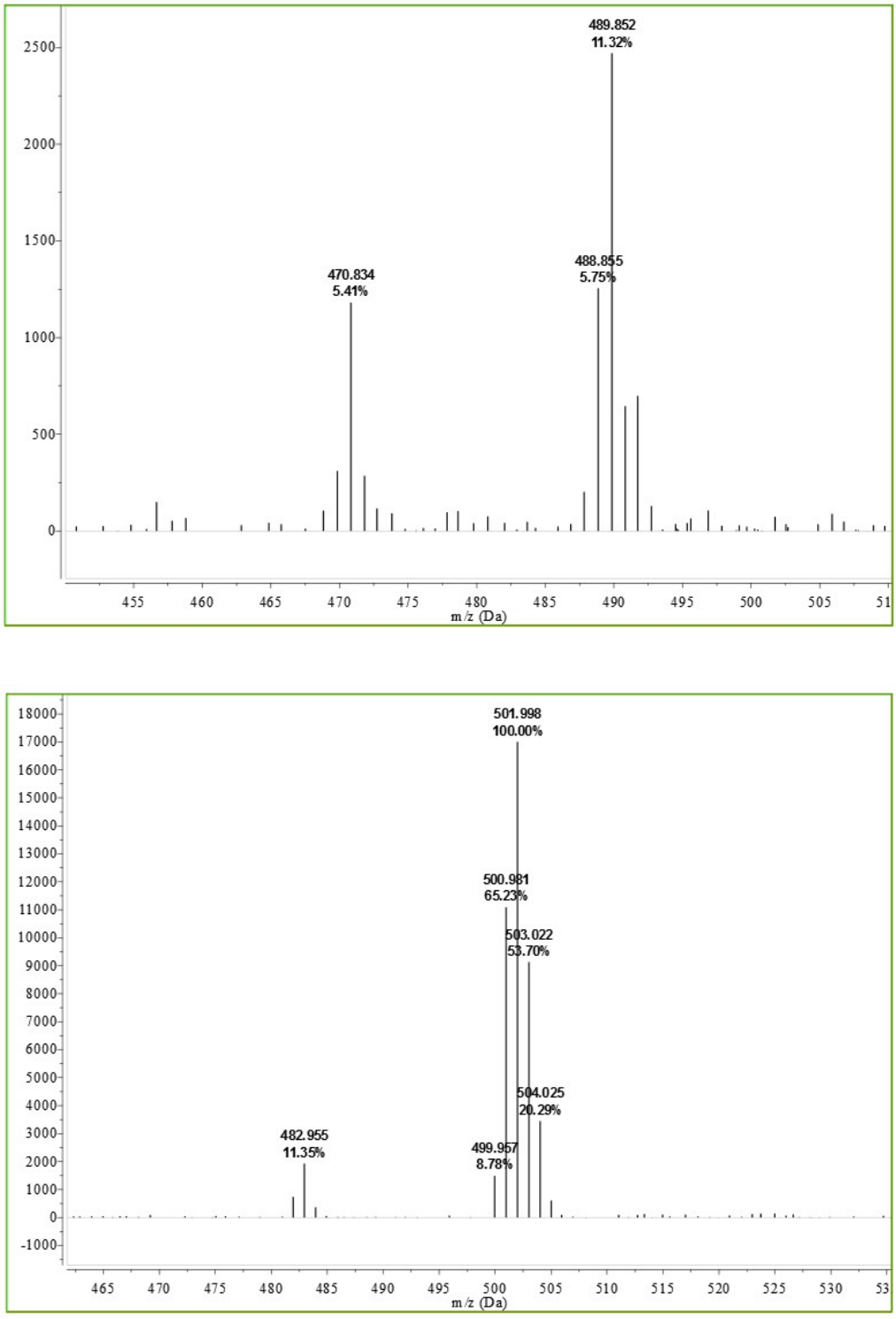
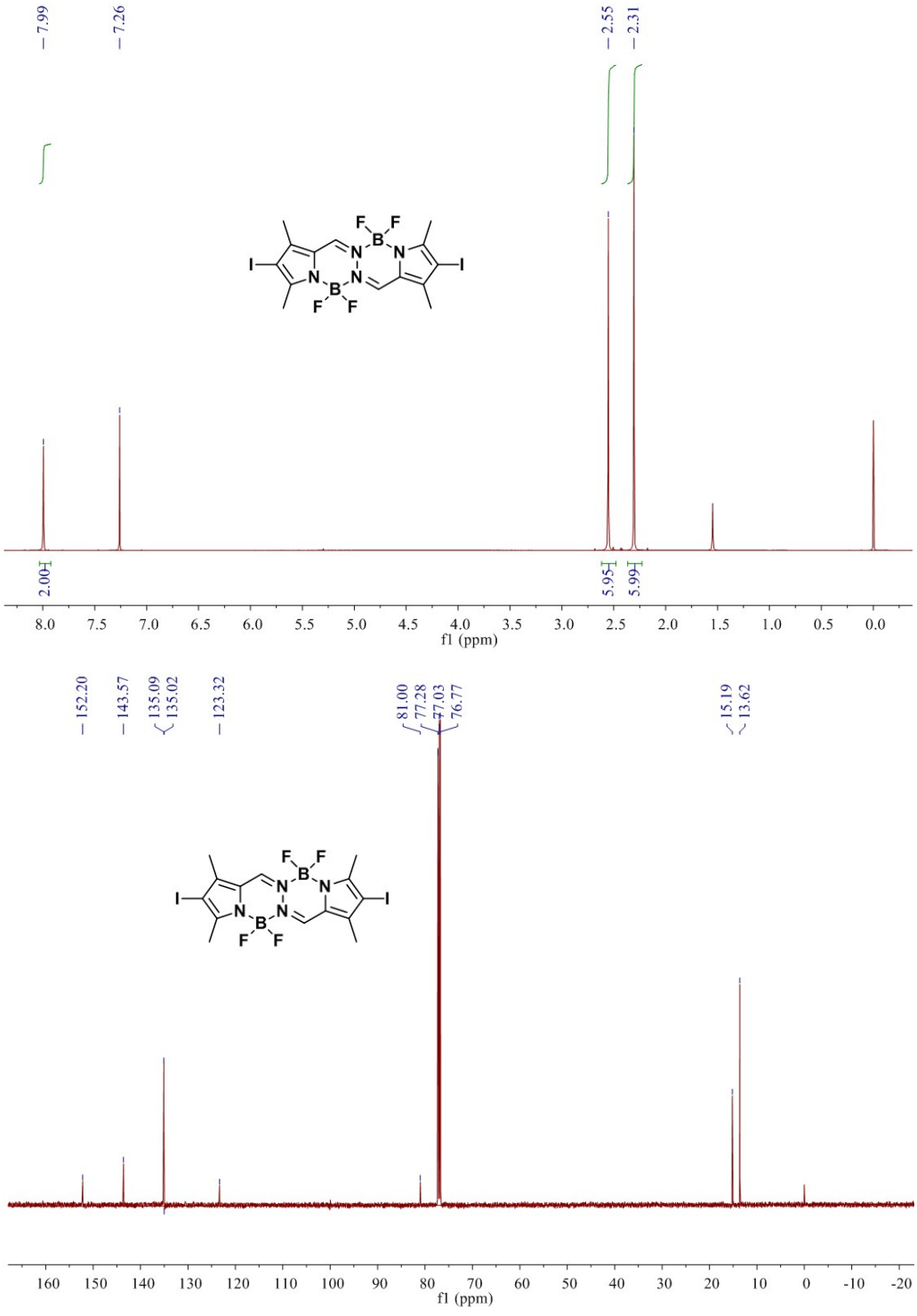
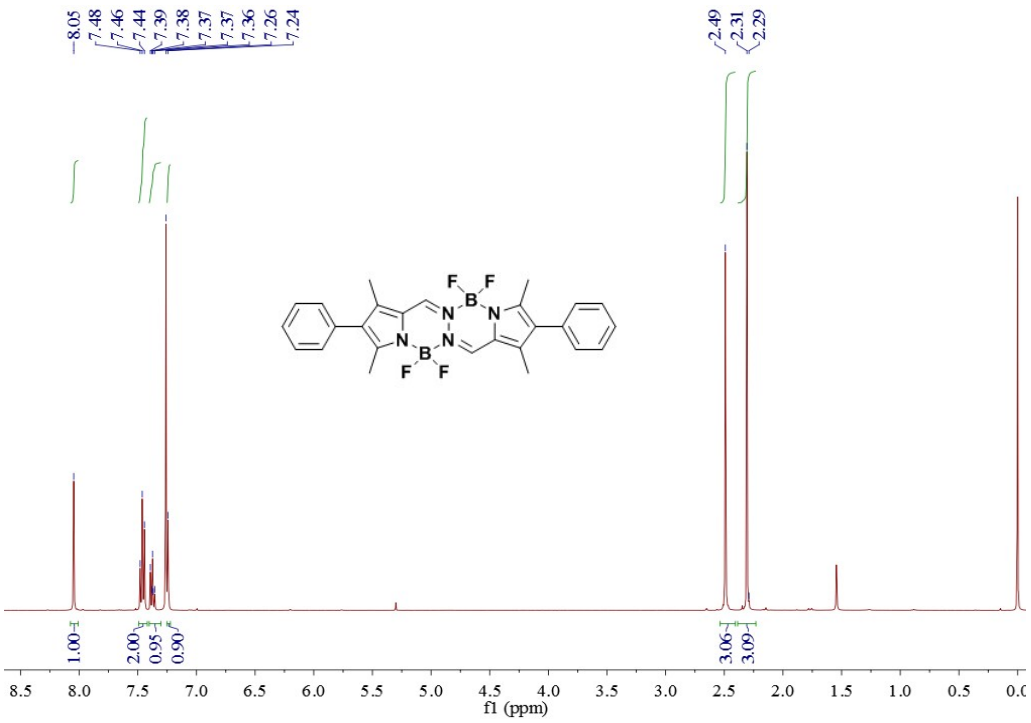


Figure S7. The MALDI-TOF spectrum of **1** (up) and **2** (bottom).

^{1}H and ^{13}C NMR of **1, 2** and **4**

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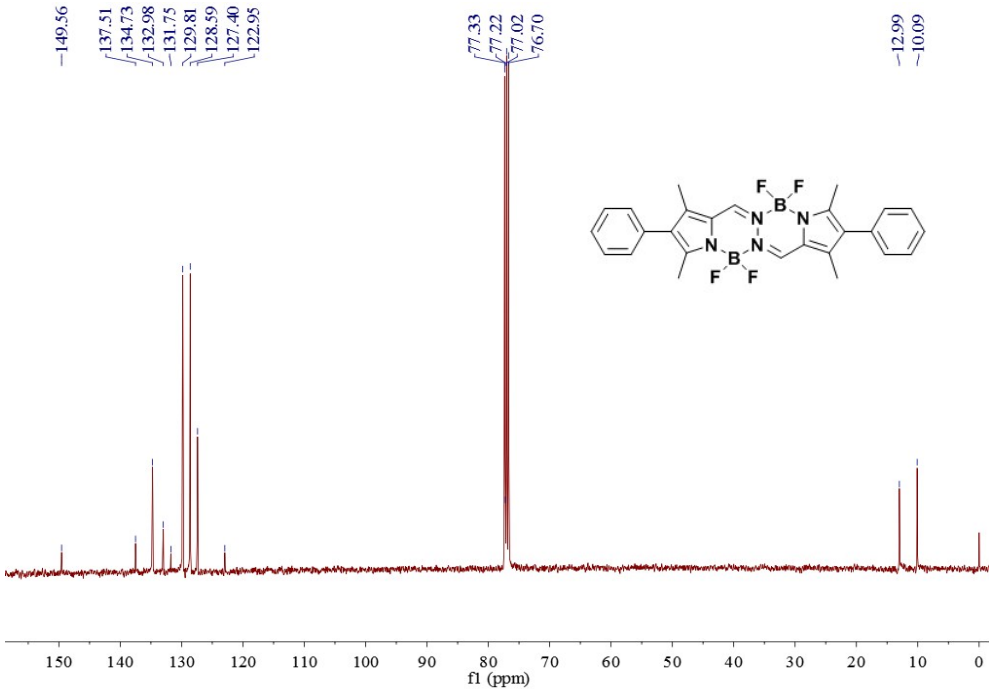
7.46
7.44
7.39
7.38
7.37
7.37
7.36
7.26
7.24
2.49
2.31
2.29
F
F
B
N
N
N
B
F
F
1.00
2.00
0.95
0.90
3.06
3.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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131.75
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127.40
122.95
77.33
77.22
77.02
76.70
12.99
10.09
F
F
B
N
N
N
B
F
F
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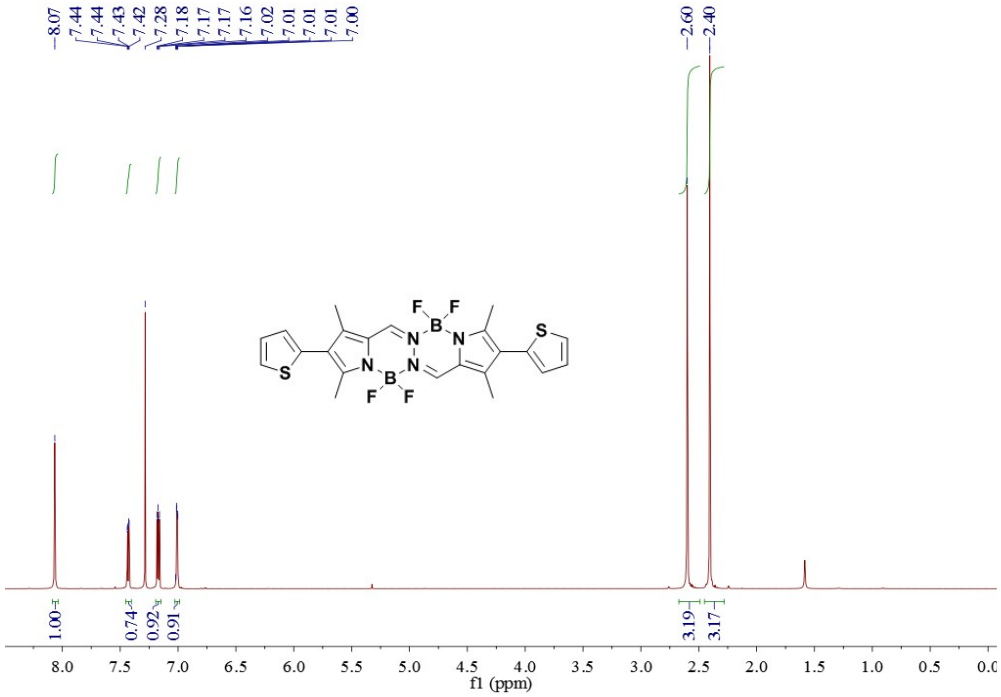
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.28
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7.17
7.17
7.16
7.02
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7.01
7.01
7.00
2.60
2.40
1.00
0.74
0.92
0.91
3.19
3.17
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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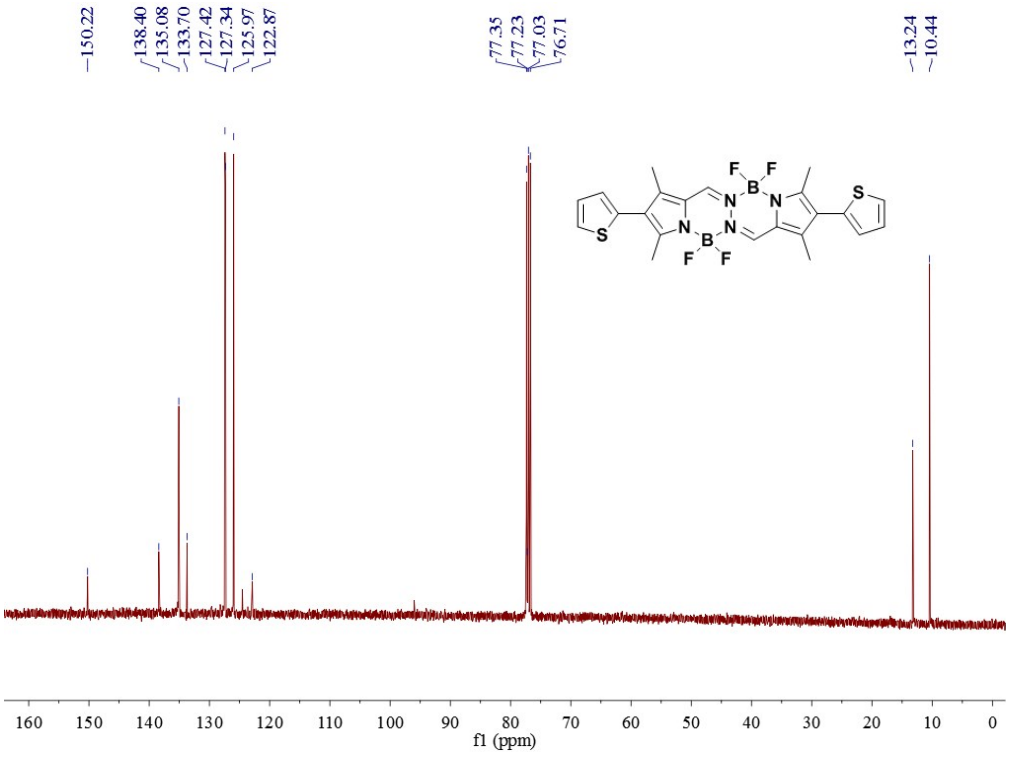
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.42
127.34
125.97
122.87
77.35
77.23
77.03
76.71
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10.44
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)