Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Data For

Modulation of ICT and PET processes in Boranil derivatives: ratiometric fluorescent probe for imaging of cysteine

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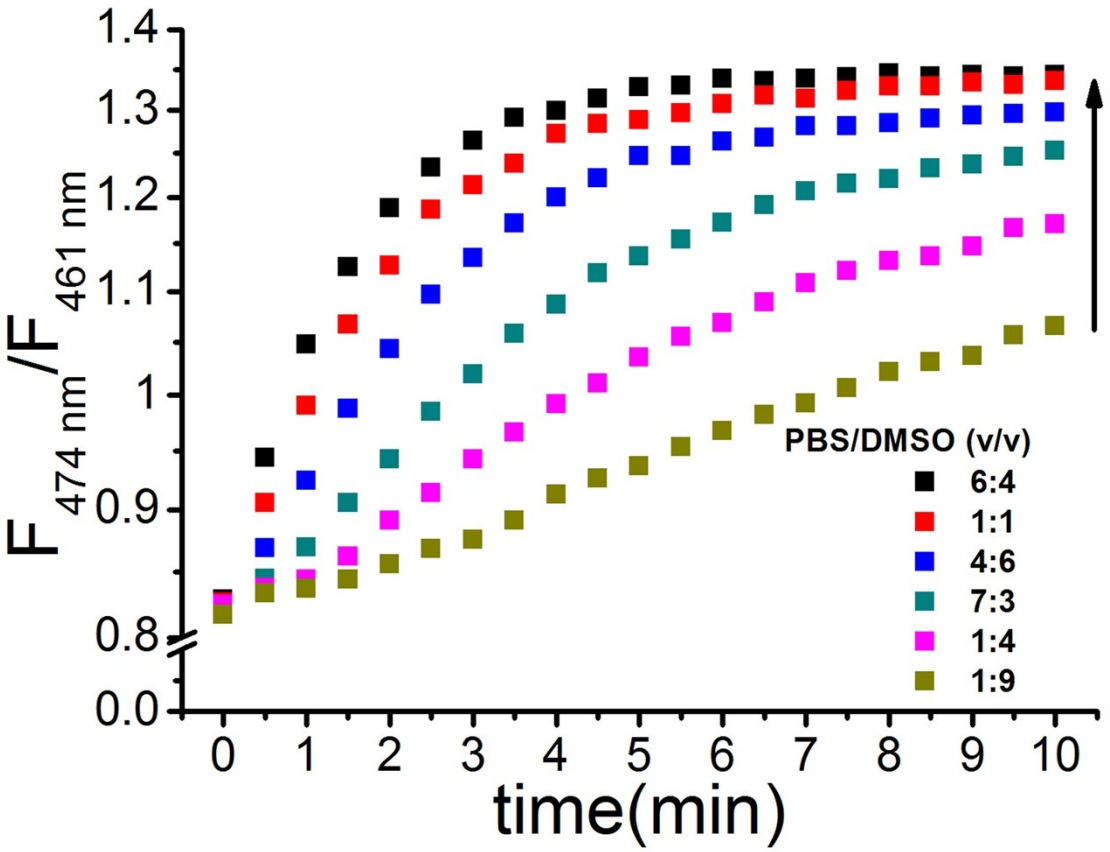


Fig. S1 Plot of fluorescence intensity ratio of $F_{474\ nm}/F_{461\ nm}$ versus the reaction time in the presence of Cys in PBS buffer solution (10 mM, pH 7.4, 25 °C) with different ratios of DMSO and PBS buffer solution.

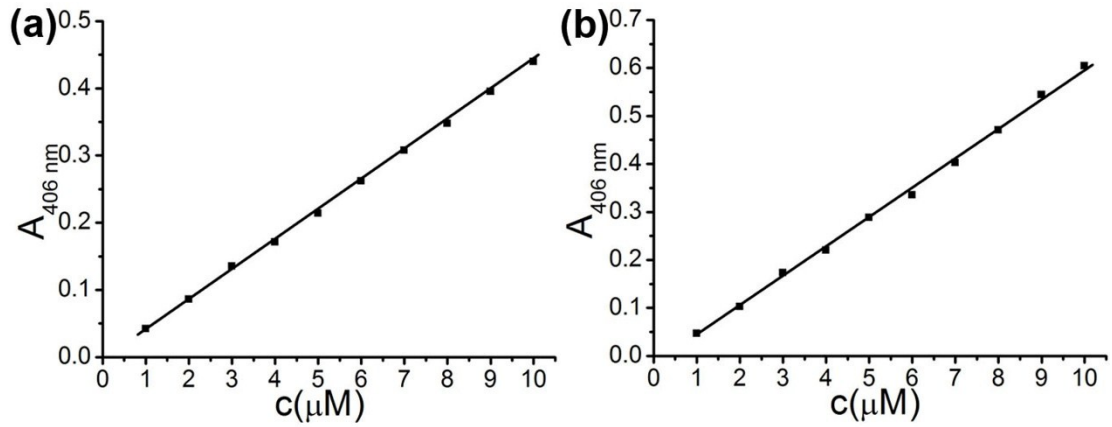


Fig. S2 (a) Plot of absorbance at 406 nm against **1** concentration in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C). (b) Plot of absorbance at 406 nm against **2** concentration in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C)

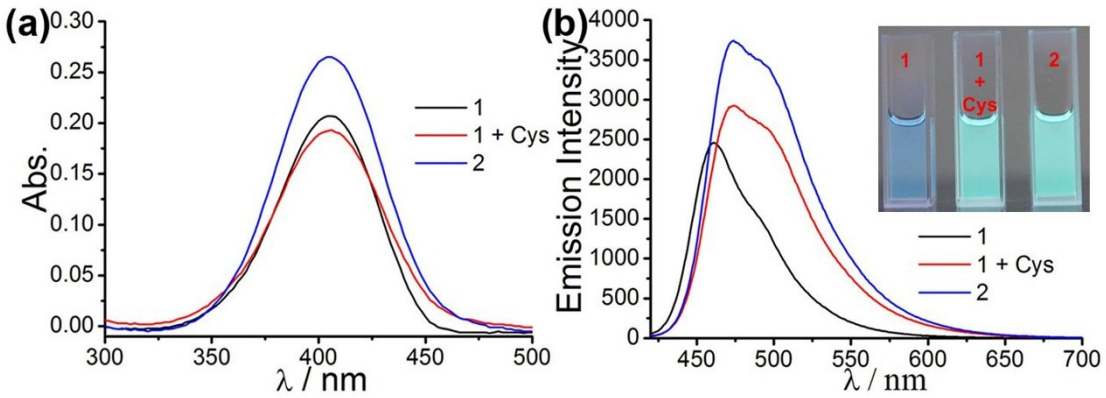


Fig. S3 (a) Absorption spectra of **2** (5 μM) (blue line), **1** (5 μM) (black line) before and after reaction with Cys (20 μM) (red line) in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C). (b) Fluorescence spectra of **2** (5 μM) (blue line), **1** (5 μM) (black line) before and after reaction with Cys (20 μM) (red line) in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C, λ_{ex} = 405 nm). The fluorescence color changes of **1** before and after the reaction and **2** in PBS buffer solution under illumination with a 365 nm UV lamp are shown in the inset.

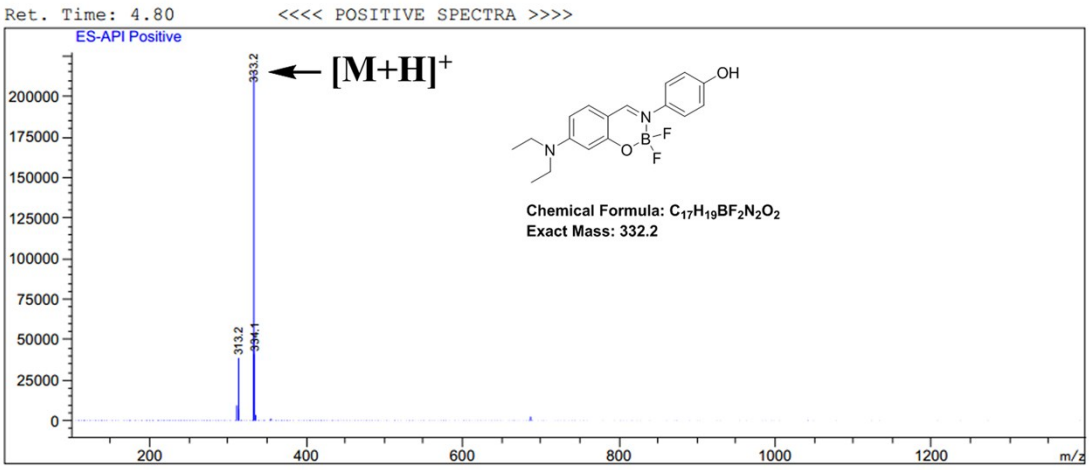


Fig. S4 ESI-MS spectrum of **1** after addition of Cys in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C).

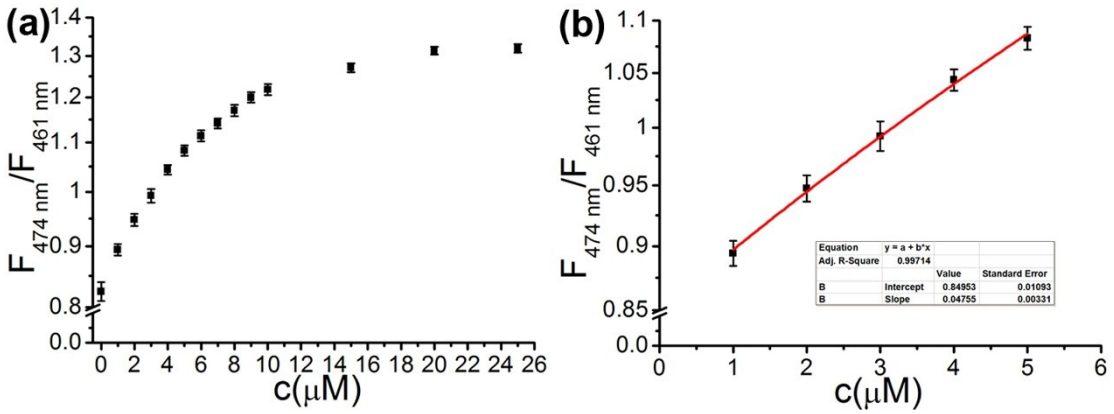


Fig. S5 (a) The ratios of fluorescence intensities ($F_{474\ nm}/F_{461\ nm}$) of **1** (5 μM) with varied concentrations of Cys in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C, λ_{ex} = 405 nm). (b) The ratios of fluorescence intensities ($F_{474\ nm}/F_{461\ nm}$) of **1** as a function of the concentrations of Cys in the range of 1 - 5 μM upon excitation at 405 nm and the calculation of the detection limit of probe **1** for Cys.

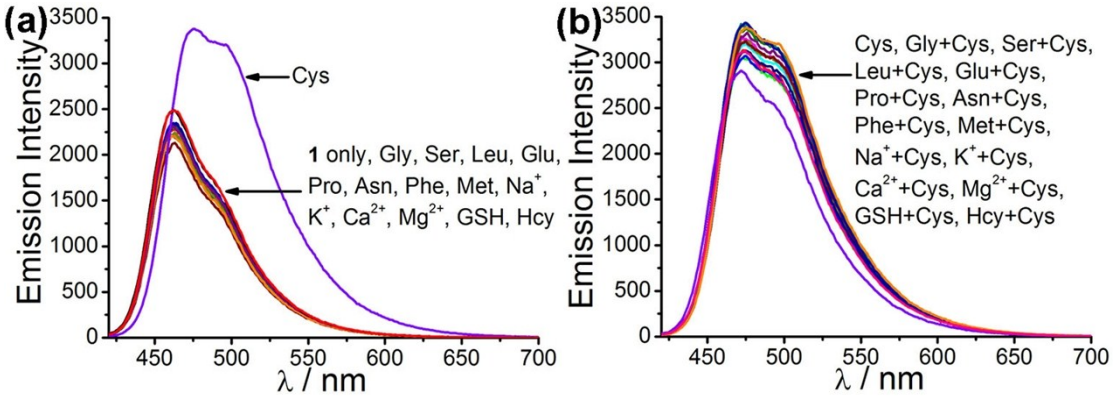


Fig. S6 Fluorescence spectra of **1** (5 μM) after addition of various analytes: **1** (none), Gly (100 μM), Ser (100 μM), Leu (100 μM), Glu (100 μM), Pro (100 μM), Asn (100 μM), Phe (100 μM), Met (100 μM), NaCl (1 mM), KCl (1 mM), $CaCl_2$ (1 mM), $MgCl_2$ (1 mM), Cys (20 μM), GSH (20 μM), Hcy (20 μM). (a): free probe and probe treated with the marked analytes. (b): probe treated with Cys in the presence of the marked analytes. Data were acquired in PBS buffer solution (10 mM, H_2O/DMSO, 1:1, v/v, pH 7.4, 25 °C, λ_{ex} = 405 nm).

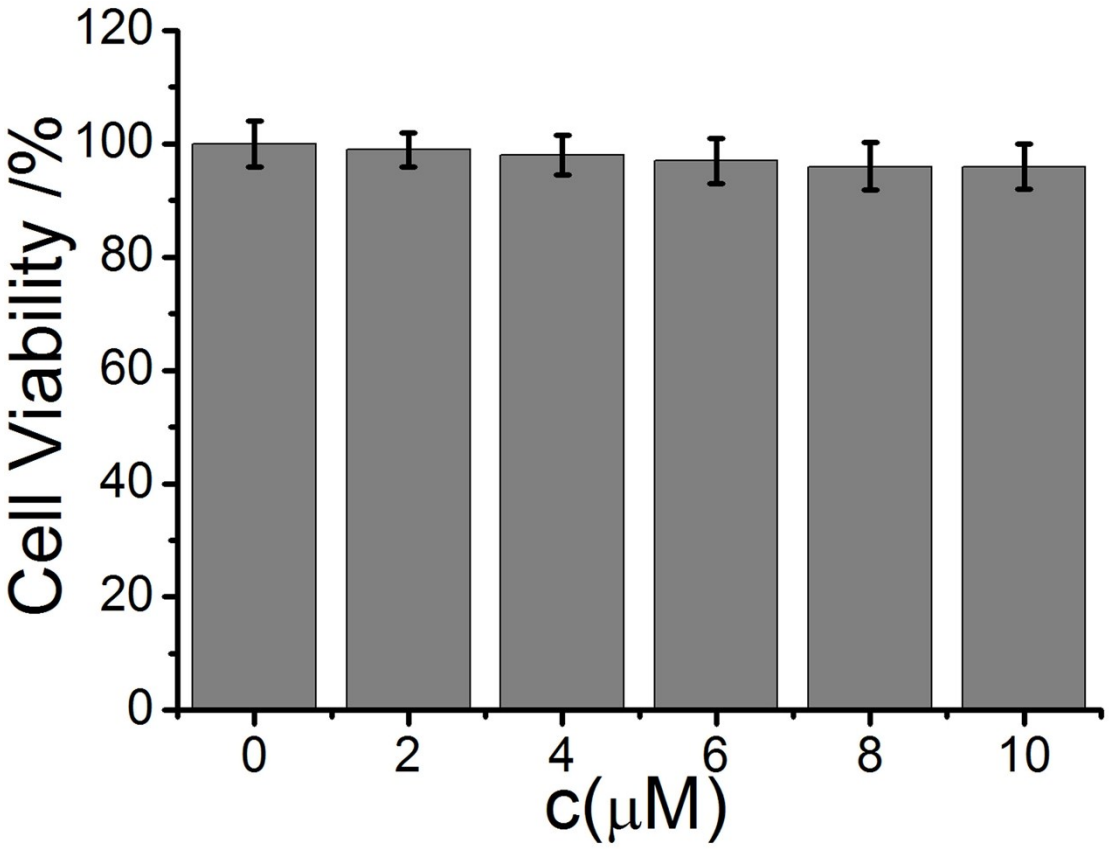
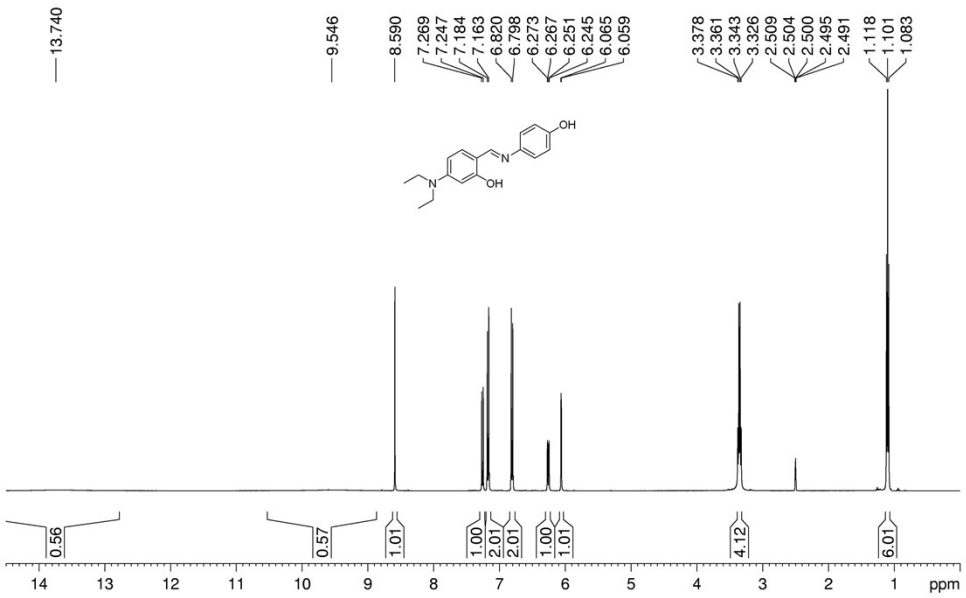
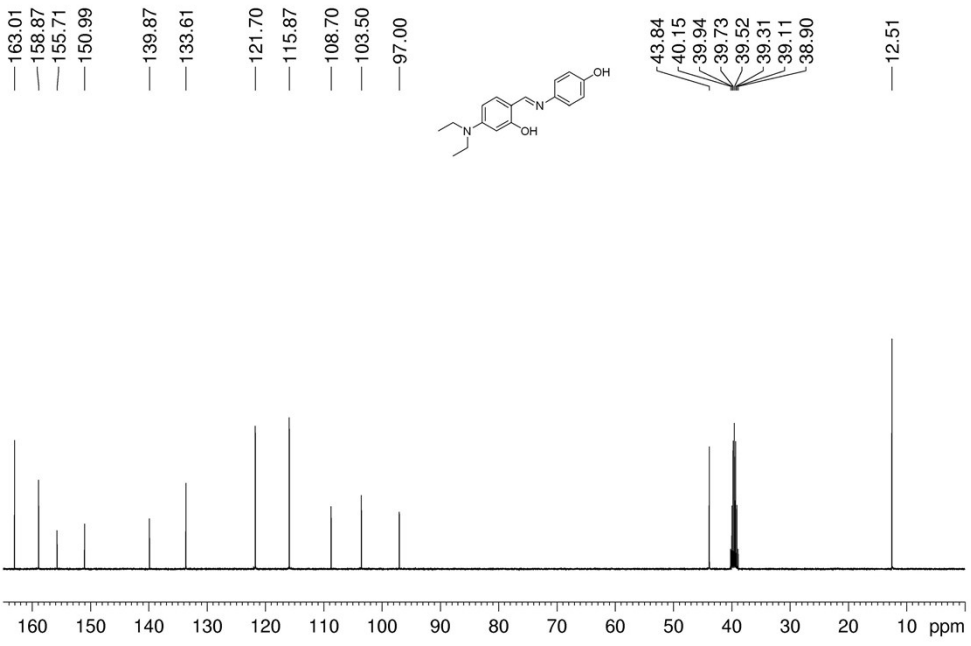
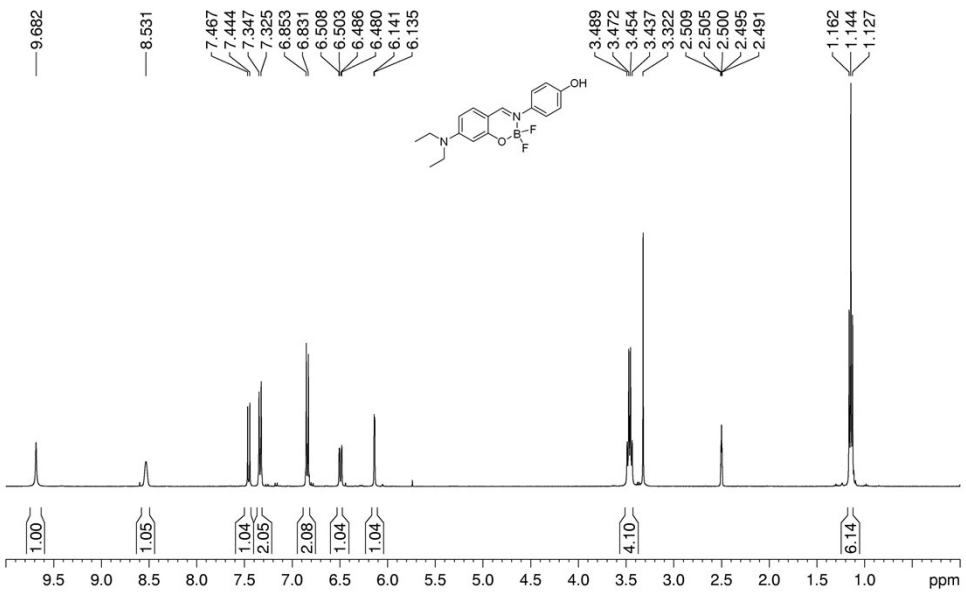


Fig. S7 CCK-8 assay of Hela cells in the presence of various concentrations of **1** (0, 2, 4, 6, 8, 10 μM) for 24 h at 37 °C.

NMR Spectra


13.740
9.546
8.590
7.269
7.247
7.184
7.163
6.820
6.798
6.273
6.267
6.251
6.245
6.065
6.059
3.378
3.361
3.343
3.326
2.509
2.504
2.500
2.495
2.491
1.118
1.101
1.083
OH
N
OH
0.56
0.57
1.01
1.00
2.01
2.01
1.00
1.01
4.12
6.01
14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm


163.01
158.87
155.71
150.99
139.87
133.61
121.70
115.87
108.70
103.50
97.00
43.84
40.15
39.94
39.73
39.52
39.31
39.11
38.90
12.51
OH
N
OH
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


9.682
8.531
7.467
7.444
7.347
7.325
6.853
6.831
6.508
6.503
6.486
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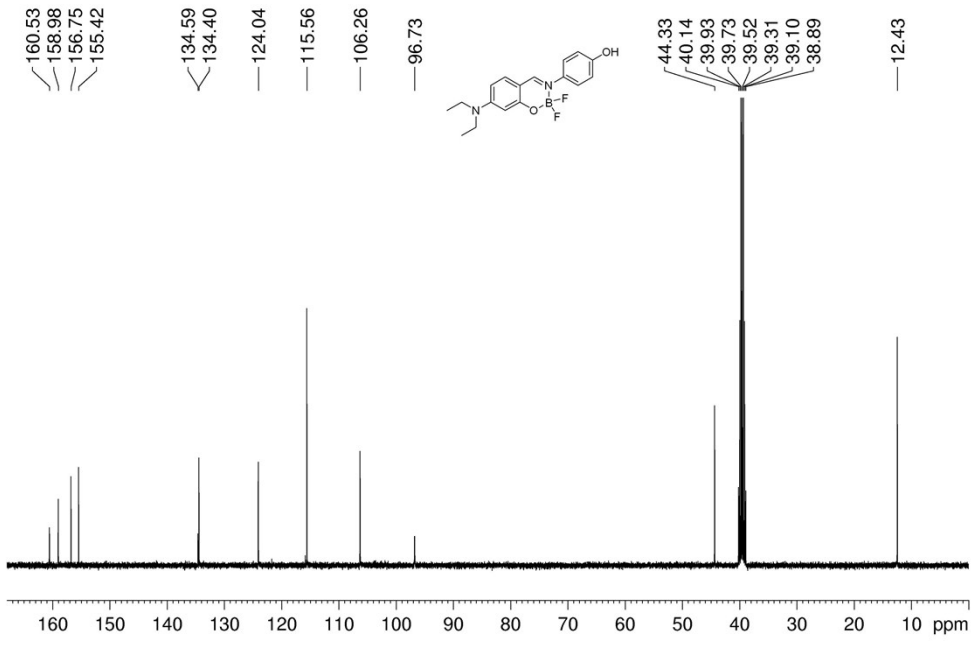
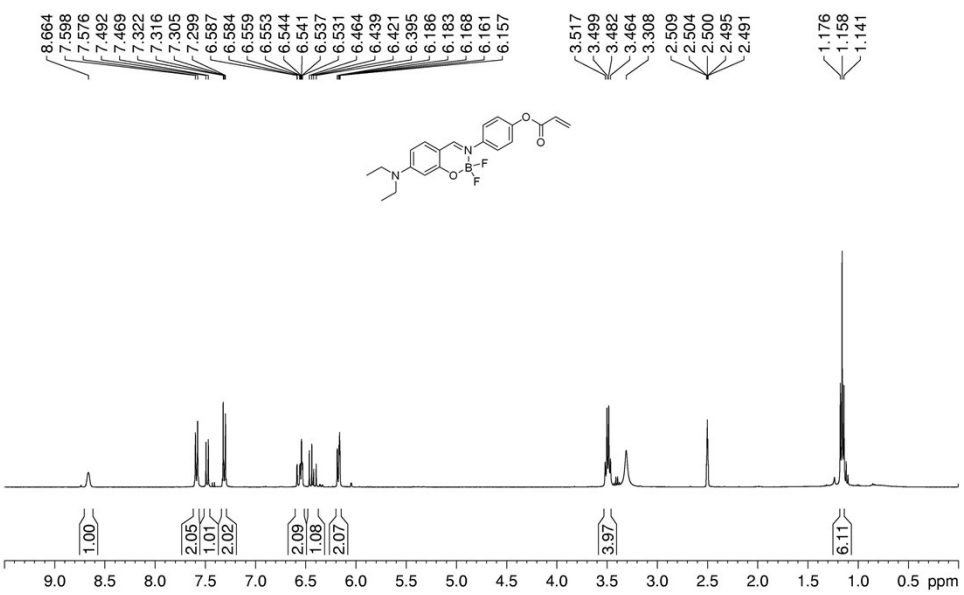
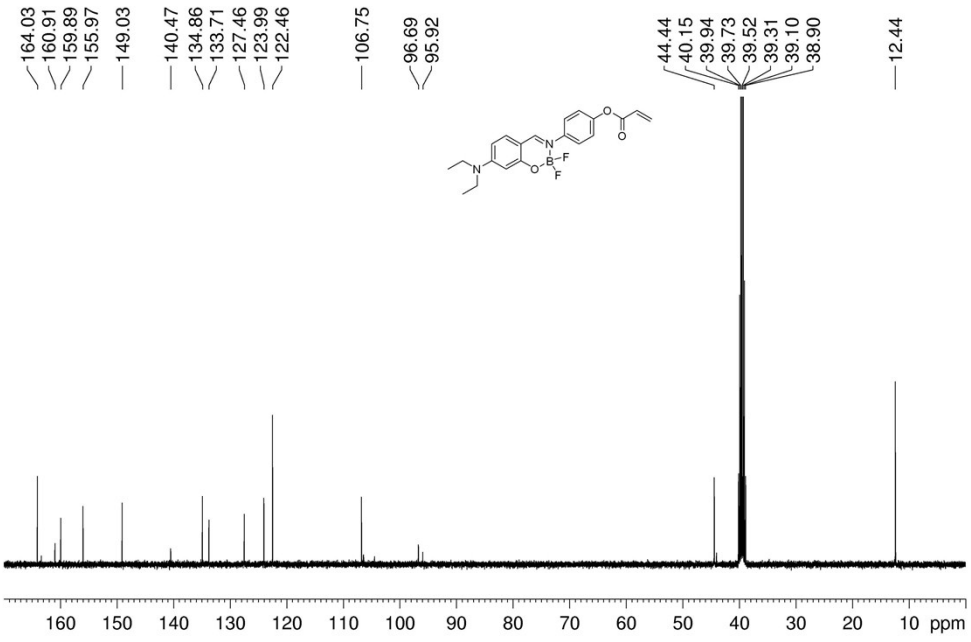
6.141
6.135
3.489
3.472
3.454
3.437
3.322
2.509
2.505
2.500
2.495
2.491
1.162
1.144
1.127
OH
N
B
F
F
O
1.00
1.05
1.04
2.05
2.08
1.04
1.04
4.10
6.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm


160.53
158.98
156.75
155.42
134.59
134.40
124.04
115.56
106.26
96.73
44.33
40.14
39.93
39.73
39.52
39.31
39.10
38.89
12.43
OH
N
B
F
F
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.664
7.598
7.576
7.492
7.469
7.322
7.316
7.305
7.299
6.587
6.584
6.559
6.553
6.544
6.541
6.537
6.531
6.464
6.439
6.421
6.395
6.186
6.183
6.168
6.161
6.157
3.517
3.499
3.482
3.464
3.308
2.509
2.504
2.500
2.495
2.491
1.176
1.158
1.141
1.00
2.05
1.01
2.02
2.09
1.08
2.07
3.97
6.11
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 ppm


164.03
160.91
159.89
155.97
149.03
140.47
134.86
133.71
127.46
123.99
122.46
106.75
96.69
95.92
44.44
40.15
39.94
39.73
39.52
39.31
39.10
38.90
12.44
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

ESI-MS Spectra