Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

An efficient colorimetric and fluorescent probe for detection fluoride based on benzothiadiazole derivative

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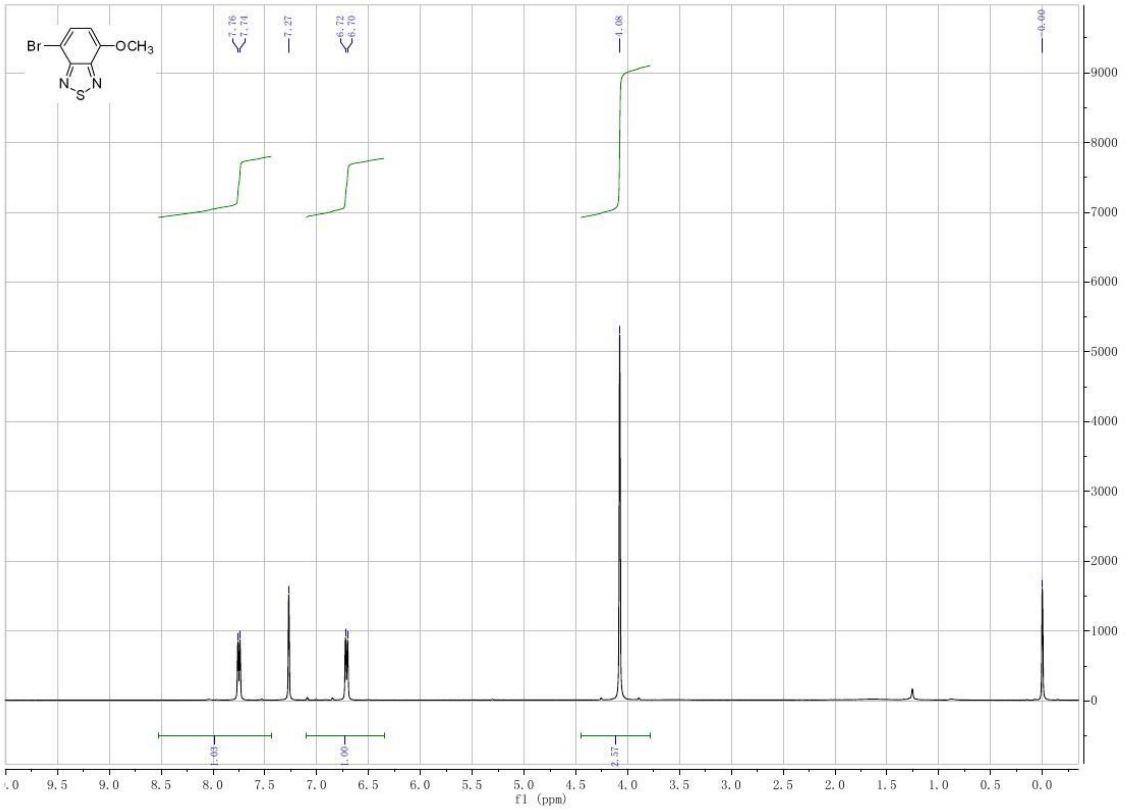
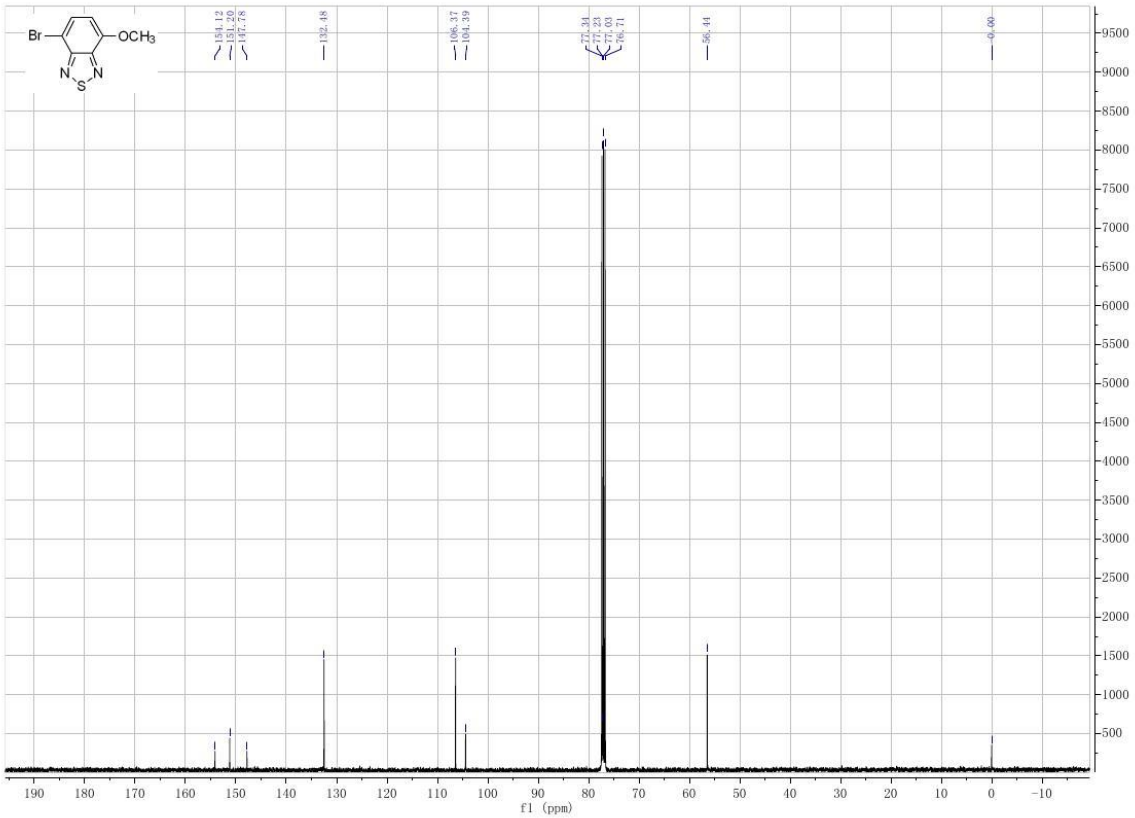
Contents

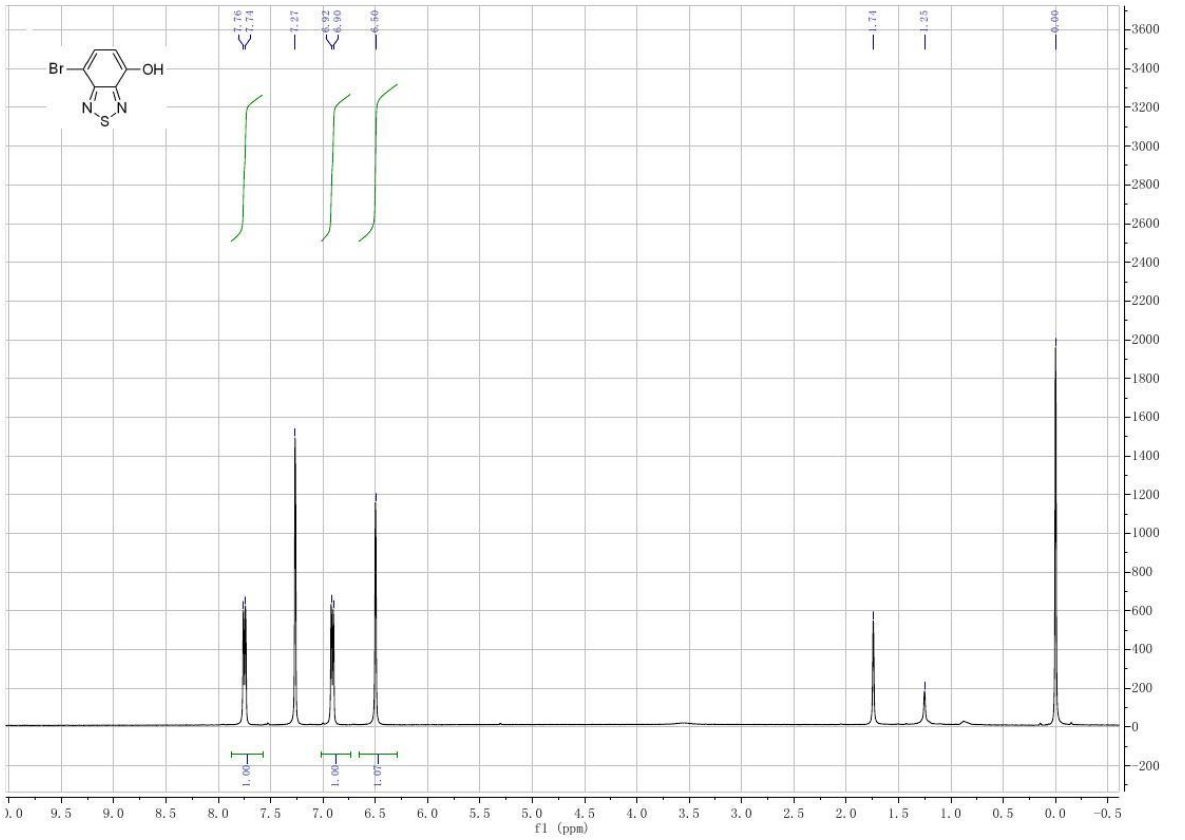
^{1}H NMR and ^{13}C NMR spectra of compound 1 to 3

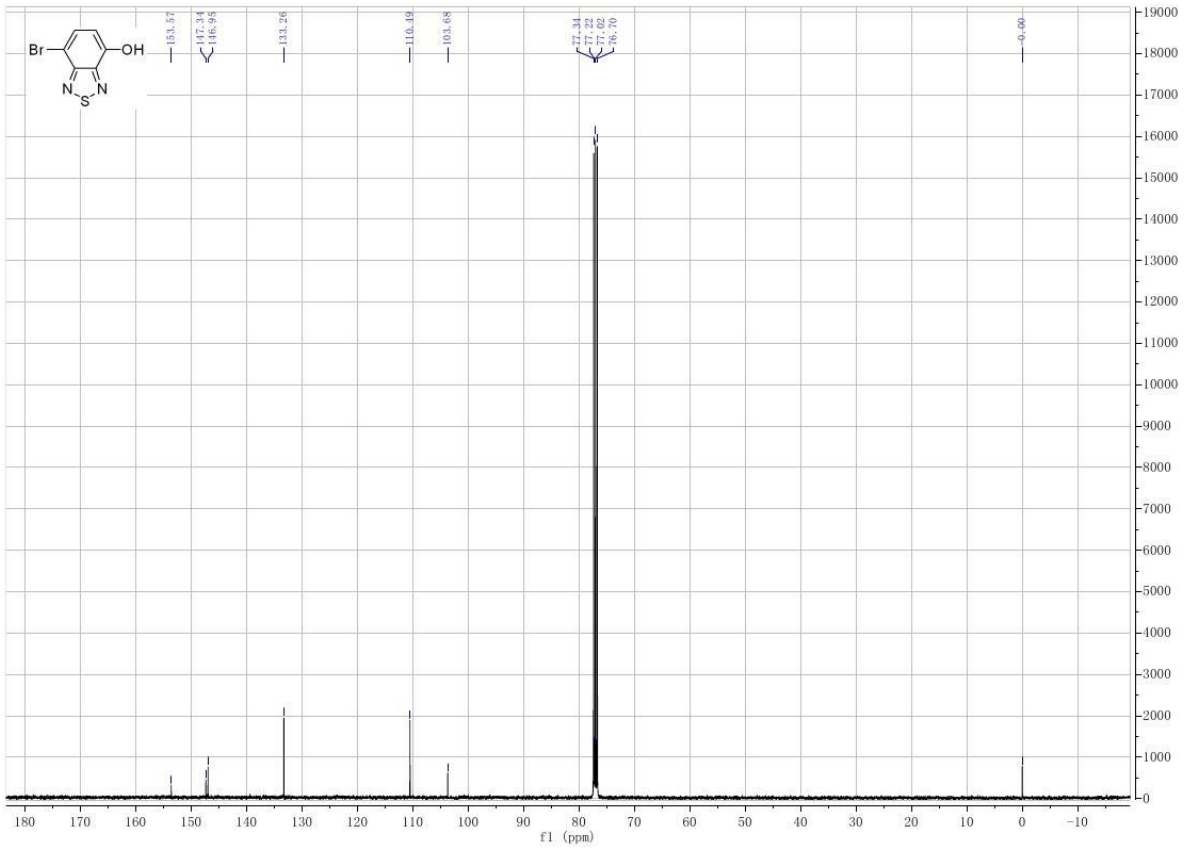
Compound 1



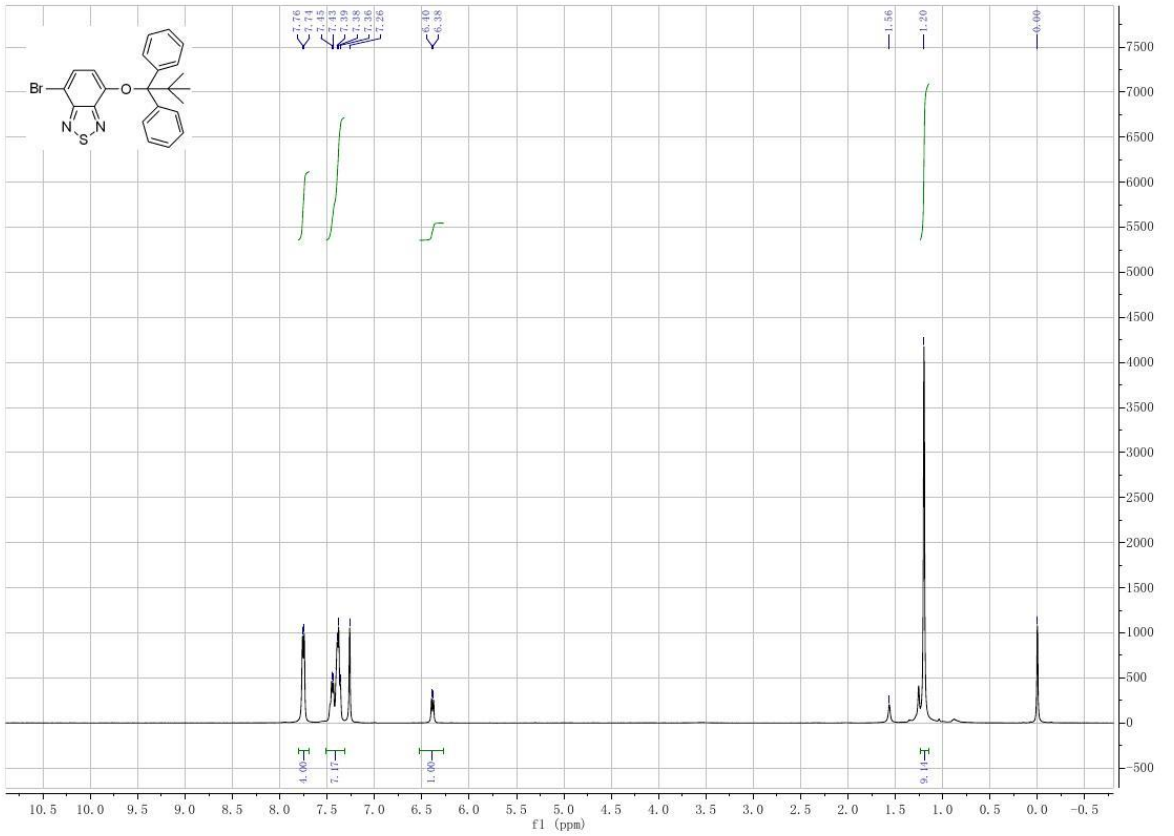


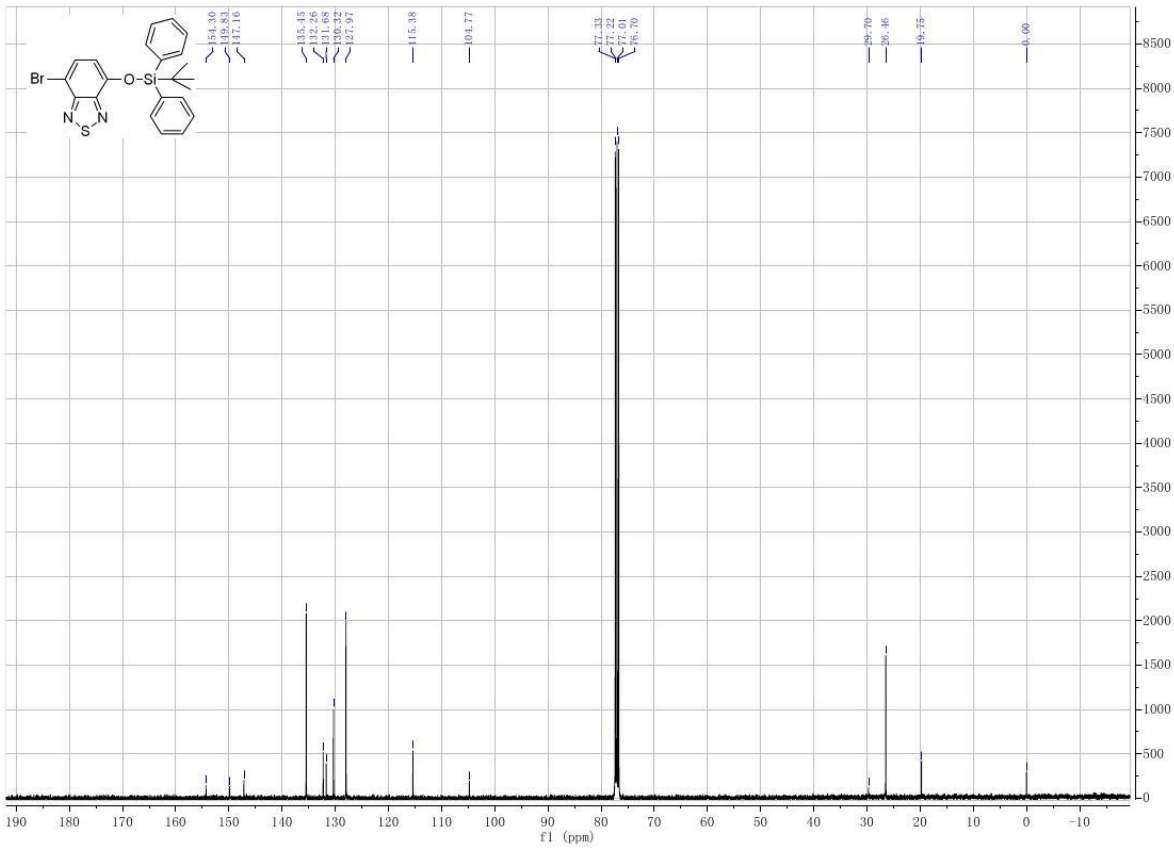
Compound 2


Br
OH
N
S
N
7.76
7.74
7.27
6.92
6.90
6.50
1.74
1.25
0.00
1.00
1.02
1.07
f1 (ppm)


Br
OH
N
S
N
153.57
147.34
146.95
133.26
110.49
103.68
77.34
77.22
77.02
76.70
0.00
f1 (ppm)

Compound 3


Br
O
N
S
N
7.76
7.74
7.45
7.43
7.39
7.38
7.36
7.26
6.40
6.38
1.56
1.20
0.00
4.00
7.17
1.00
9.14
f1 (ppm)


Br
O
Si
N
S
N
154.30
149.83
147.16
135.45
132.26
131.68
130.32
127.97
115.38
104.77
77.33
77.22
77.01
76.70
29.70
26.46
19.75
0.00
f1 (ppm)

Determination of the detection limit

$$\text{Detection limit} = 3\sigma/k$$

Where σ is the standard deviation of blank measurement, k is the slop between the absorbance versus F^- concentration.

The detection limit was calculated based on the absorption titration. The absorption spectrum of probe 3 was measured by 15 times and the standard deviation of blank measurement was calculated to give 4.87E-4.

To gain the slop, the absorbance at 519 nm was plotted as a concentration of F^- from 2.5 to 30 μ M. The slop is 860.12.

So the detection limit was calculated with equation:

$$\text{Detection limit} = 3\sigma/k$$
$$= 3*4.87E\text{-}4/860.12$$
$$= 1.7\ \mu M$$

Fluorescence intensity of probe 3 versus low concentration of F^-

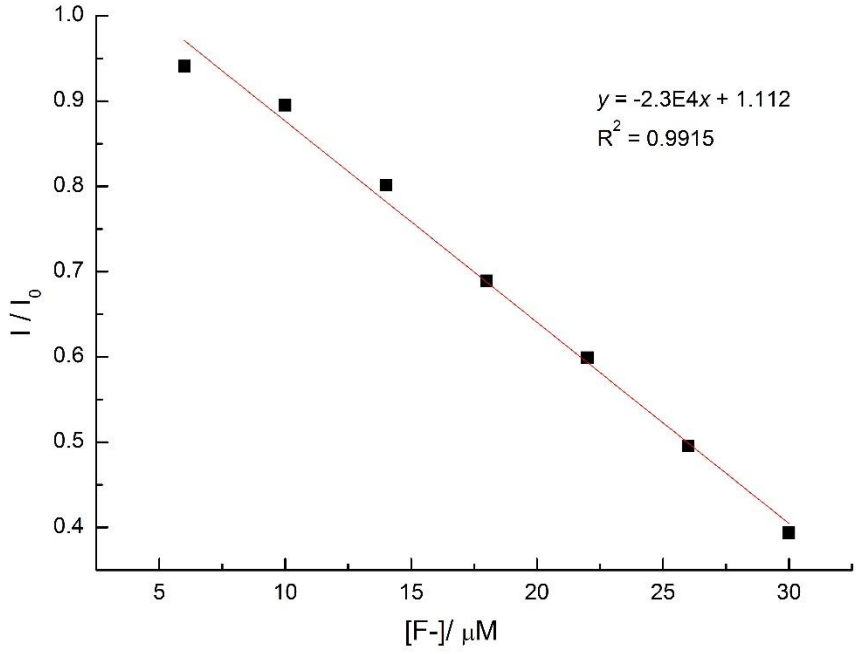


Fig. **S1** Relative fluorescence intensity of probe **3** at low concentrations of F^- from 5 to 30 μM in the mixture of acetonitrile and Tris-HCl buffer (v/v = 9:1, pH = 7.5)