Supporting Information

Investigation of thiolysis of 4-substituted SBD derivatives and rational design of a GSH-selective fluorescent probe

Chao Yang,[a] Xiaoqiang Tu,[b] Xiuru Ji,[c] Haishun Ye,[b] Shan Li,[b] Lu Sun,[c] Long Yi[b]* and Zhen Xi[a]*

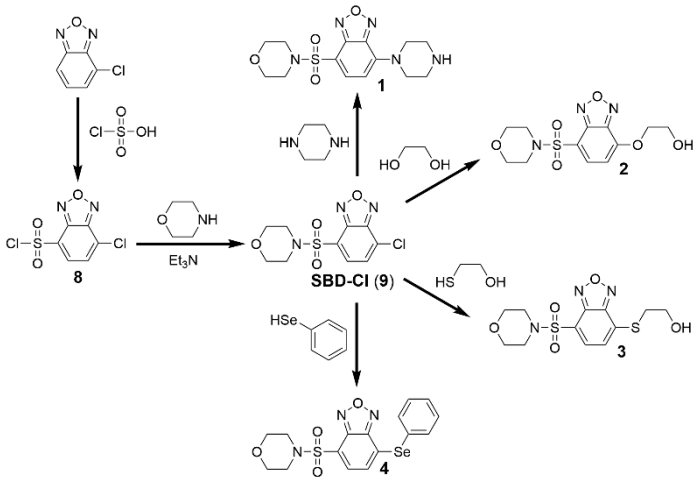
[a]State Key Laboratory of Elemento-Organic Chemistry and Department of Chemical Biology, College of Chemistry, National Pesticide Engineering Research Center, Collaborative Innovation Center of Chemical Science and Engineering, Nankai University, Tianjin, 300071, China.
[b]State Key Laboratory of Organic-Inorganic Composites and Beijing Key Lab of Bioprocess, Beijing University of Chemical Technology (BUCT), Beijing, 100029, China.
[c]Tianjin Key Laboratory on Technologies Enabling Development of Clinical Therapeutics and Diagnostics (Theranostics), School of Pharmacy, Tianjin Medical University, Tianjin, 300070, China

Table of contents

1. Reagents and instruments

All chemicals and solvents used for synthesis were purchased from commercial suppliers and applied directly in the experiment without further purification. The progress of the reaction was monitored by TLC on pre-coated silica plates (Merck 60F-254, 250 μm in thickness), and spots were visualized by UV light. Merck silica gel 60 (70-200 mesh) was used for general column chromatography purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer. Chemical shifts are reported in parts per million relative to internal standard tetramethylsilane ($Si(CH_3)_4$ = 0.00 ppm) or residual solvent peaks ($CDCl_3$ = 7.26 ppm, DMSO-d_6 = 2.50 ppm). ^{1}H NMR coupling constants (*J*) are reported in Hertz (Hz), and multiplicity is indicated as the following: s (singlet), d (doublet), dd (doublet doublet), t (triplet), q (quartet), m (multiplet). High-resolution mass spectrum (HRMS) was obtained on an Agilent 6540 UHD Accurate-Mass Q-TOFLC/MS. The UV-visible spectra were recorded on a UV-6000 UV-VIS-NIR-spectrophotometer (METASH, China). Fluorescence studies were carried out using F-280 spectrophotometer (Tianjin Gangdong Sci & Tech., Development. Co., Ltd).

2. Synthetic procedure of probes



Synthesis of 8

Compound **8** was synthesized according to a known procedure.[1]

4-Chloro-2,1,3-benzoxadiazole (2 g, 13 mmol) was slowly added to chlorosulfonic acid (20 mL) under ice bath. The reaction mixture was stirred at 0 °C for 5 min and then heated at 120 °C for 5 h. The resulting mixture was slowly poured into ice water and extracted with dichloromethane (50 mL × 3). The combined organic layer was washed with HCl (1 M, 50 mL) and brine (50 mL) and dried over Na_2SO_4. The organic layer was concentrated under reduced pressure and purified by column chromatography to give the desired product **8** as a yellow solid (2.61 g, 79.8%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 7.5 Hz, 1H), 7.65 (d, J = 7.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.1, 143.9, 134.7, 132.0, 130.8, 128.6.

Synthesis of SBD-Cl (9)

A mixture solution of morpholine (0.35 g, 4.0 mmol) and triethylamine (1.1 mL, 8.0 mmol) in dichloromethane (10 mL) was added slowly to a stirred solution of compound **8** (1.0 g, 4.0 mmol) in dichloromethane (25 mL) under ice bath. The reaction mixture was stirred at 0 °C for 15 min and then at room temperature for 1 h. The mixture was washed with diluted HCl (1 M, 50 mL x 2) and brine (50 mL x 1), and dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography with dichloromethane to give the pure desired product **SBD-Cl** (**9**) as a yellow solid (0.92 g, 75.6%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 7.4 Hz, 1H), 7.59 (d, J = 7.4 Hz, 1H), 3.76 (t, J = 8.2 Hz, 4H), 3.35 (t, J = 8.4 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.0, 145.7, 134.8, 129.2, 128.4, 126.0, 66.5, 46.1.

Synthesis of 1

A solution of piperazine (145 mg, 1.68 mmol) in dichloromethane was added slowly to a stirred solution of **9** (85 mg, 0.28 mmol) in dichloromethane (5 mL). After being stirred at room temperature for 6 h, the solvent was removed under reduced pressure, and the residue was purified by column chromatography to obtain a red oil product **1** (95 mg, 96.0%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.82 (d, J = 8.4 Hz, 1H), 6.59 (d, J = 8.4 Hz, 1H), 3.82 (t, J = 8.0 Hz, 4H), 3.60 (t, J = 8.2 Hz, 4H), 3.04 (t, J = 8.8 Hz, 4H), 2.90 (t, J = 8.0 Hz, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 147.1, 144.9, 143.1,

139.4, 106.9, 104.1, 65.5, 50.0, 45.7, 45.3. HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{14}H_{20}N_5O_4S^+$: 354.1231, found 354.1196.

Synthesis of 2

9 (100 mg, 0.33 mmol) and sodium hydroxide (40 mg, 1.0 mmol) were added to 3 mL of ethylene glycol and the reaction was stirred at 50 °C for 3 h. The mixture was poured into 10 mL diluted HCl (1 M) and extracted with ethyl acetate (20 mL x 2), and then dried over Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by column chromatography to give a pale yellow solid **2** (96 mg, 88.4%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.02 (d, J = 8.0 Hz, 1H), 7.04 (d, J = 8.0 Hz, 1H), 5.09 (t, J = 5.6 Hz, 1H), 4.38 (t, J = 8.0 Hz, 2H), 3.86 (dd, J = 9.6, 5.2 Hz, 2H), 3.61 (t, J = 8.4 Hz, 4H), 3.10 (t, J = 8.2 Hz, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.9, 146.7, 145.1, 139.3, 115.2, 106.5, 72.1, 65.5, 58.9, 45.6. HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{12}H_{16}N_3O_6S^+$: 330.0754, found 330.0750.

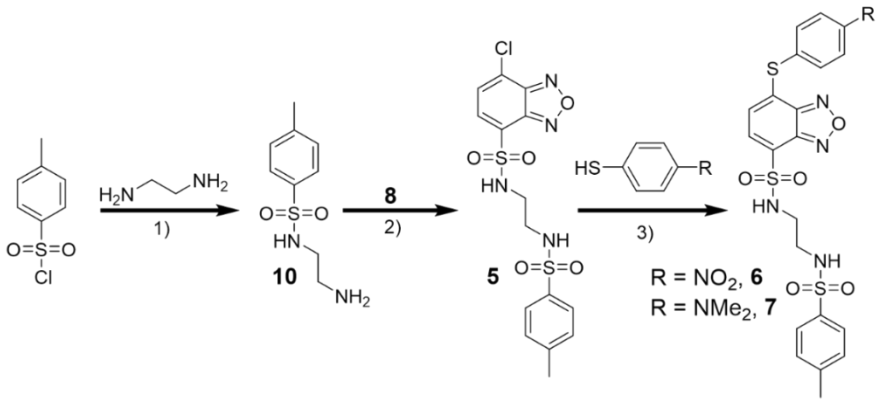
Synthesis of 3

9 (80 mg, 0.26 mmol) and 2-mercaptoethanol (62 mg, 0.78 mmol) were mixed in 5 ml dichloromethane at room temperature. *N, N'*-Diisopropylethylamine (90 μL, 0.52 mmol) was then added into the mixture. After stirred for 3 h, the solvent was removed under vacuum, and the residue was purified by column chromatography to give a yellow solid **3**. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.92 (d, J = 7.6 Hz, 1H), 7.51 (d, J = 7.5 Hz, 1H), 5.17 (t, J = 5.5 Hz, 1H), 3.77 (q, J = 6.0 Hz, 2H), 3.64-3.59 (m, 4H), 3.40 (t, J = 6.2 Hz, 2H), 3.16-3.10 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 148.8, 145.2, 136.2, 135.6, 123.1, 119.1, 65.6, 58.8, 45.5, 33.7. HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{12}H_{16}N_3O_5S_2^+$: 346.0526, found 346.0535.

Synthesis of 4

A solution of **9** (50 mg, 0.17 mmol), phenylselenol (40 mg, 0.25 mmol), and *N, N'*-diisopropylethylamine (40 μL, 0.25 mmol) in dichloromethane was stirred at room temperature for 3 h. The reaction mixture was then diluted with water and extracted into dichloromethane. The organic phase was washed with brine and dried over Na_2SO_4 to yield the crude product. Purification via column chromatography afforded

compound **1** as a pure yellow solid **4** (60 mg, 85.6%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 2H), 7.67 (d, J = 7.2 Hz, 1H), 7.56-7.49 (m, 3H), 6.84 (d, J = 7.2 Hz, 1H), 3.72 (t, J = 8.0 Hz, 4H), 3.27 (t, J = 8.0 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.3, 145.0, 137.1, 134.9, 133.8, 130.6, 126.6, 124.0, 122.4, 66.5, 46.1. HRMS (ESI): m/z $[M+Na]^+$ calculated for $C_{16}H_{15}N_3NaO_4SSe^+$:447.9841, found 447.9816.



Synthesis of 10

Compound **10** was synthesized according to a previous reported method with minor modifications.[2] A solution of *p*-toluenesulfonyl chloride (1.90 g, 10 mmol) in dichloromethane (25 mL) was added slowly to a stirred solution of ethylenediamine (6.0 g, 100 mmol) in dichloromethane (25 mL). After being stirred at 40 °C for 1.5 h, the mixture was washed twice with water (25 mL) and brine (25 mL), and dried over sodium sulfate. The solvent was removed under reduced pressure and purified by column chromatography to obtain a white solid product **10** (1.51 g, 70.6%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.3 Hz, 2H), 7.30 (d, J = 8.0 Hz, 2H), 2.97-2.93 (m, 2H), 2.80-2.76 (m, 2H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 142.5, 137.7, 129.6, 126.5, 46.2, 41.4, 20.9.

Synthesis of 5

Compound **10** (220 mg, 1.03 mmol) and triethylamine (286 μL, 2.06 mmol) in dichloromethane (15 mL) were added slowly to compound **8** (200 mg, 0.79 mmol) in dichloromethane (30 mL) under ice bath. Then, the resulted mixture was stirred for 1 h at room temperature. The reaction mixture was extracted with diluted HCl (1 M, 30 mL x 2) and brine (30 mL), and dried over Na_2SO_4 and concentrated under reduced

pressure. The residue was purified by column chromatography to give the pure desired product **5** as a yellow powder (328 mg, 73.9%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.33 (t, J = 5.6 Hz, 1H), 7.98 (d, J = 7.4 Hz, 1H), 7.89 (d, J = 7.4 Hz, 1H), 7.57 (d, J = 8.2 Hz, 2H), 7.51 (t, J = 6.0 Hz, 1H), 7.36 (d, J = 8.1 Hz, 2H), 2.99 (dd, J = 12.8, 6.4 Hz, 2H), 2.69 (dd, J = 13.3, 6.5 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.4, 145.6, 143.2, 137.6, 134.7, 131.2, 130.1, 128.3, 126.9, 125.8, 49.1, 42.7, 21.4. HRMS (ESI): m/z $[M+Na]^+$ calculated for $C_{15}H_{15}ClN_4O_5S_2Na^+$: 453.0065, found 453.0068.

Synthesis of 6

Compound **5** (42 mg, 0.07 mmol) and 4-nitro-benzenethiol (44.8 mg, 0.21 mmol) were added to 2 mL of DMF with stirring. Then, triethylamine (27.3 μL, 0.14 mmol) in DMF (1 mL) was added slowly. After being stirred at room temperature for 2 h, the solvent was removed under reduced pressure, and the residue was purified by column chromatography to obtain a yellow solid product (35.2 mg, 65.7%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.30 (t, J = 5.8 Hz, 1H), 8.27-8.20 (m, 2H), 7.94 (d, J = 7.2 Hz, 1H), 7.82-7.76 (m, 2H), 7.59 (t, J = 7.6 Hz, 3H), 7.52 (t, J = 6.0 Hz, 1H), 7.36 (d, J = 8.1 Hz, 2H), 3.01 (dd, J = 13.2, 6.4 Hz, 2H), 2.71 (dd, J = 13.4, 6.4 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.1, 147.1, 144.9, 142.8, 139.6, 137.1, 133.9, 132.1, 132.0, 129.6, 128.3, 127.8, 126.4, 124.6, 42.4, 42.2, 20.9.

Synthesis of 7

Compound **7** was prepared following similar method described for the preparation of compound **6** with using 4-(dimethylamino) benzenethiol to afford a red solid (73.3%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 7.4 Hz, 1H), 7.67 (d, J = 8.2 Hz, 2H), 7.45 (d, J = 8.8 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 6.83 (d, J = 8.4 Hz, 2H), 6.58 (d, J = 7.4 Hz, 1H), 5.58 (t, J = 6.0 Hz, 1H), 5.15 (t, J = 6.0 Hz, 1H), 3.17 (t, J = 5.6 Hz, 2H), 3.07 (s, 8H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 148.1, 144.6, 143.9, 140.8, 137.1, 136.5, 134.5, 130.0, 127.2, 122.4, 122.0, 113.8, 43.3, 40.5, 21.7. HRMS (ESI): m/z $[M+H]^+$ calculated for $C_{23}H_{26}N_5O_5S_3^+$: 548.1091; found: 548.1095.

3. General procedure for spectroscopic studies

All measurements were performed in degassed phosphate buffer (PBS, 50 mM, pH 7.4, containing 30% DMSO). Compounds were dissolved into DMSO to prepare the stock solutions with a concentration of 1-10 mM. Various stock solutions (20 mM) of different analytes were prepared in PBS buffer. Appropriate amount of bio-relevant species was added to separate portions of the probe solution and mixed thoroughly. The reaction mixture was shaken uniformly before spectra were measured. All measurements were performed in a 3 mL corvette with 2 mL solution at room temperature and all fluorescence spectra were obtained by excitation at 420 nm. For the selectivity experiment, fluorescence spectra of probe **7** (10 μM) toward different species with or without GSH in PBS buffer were monitored after 1 h incubation at room temperature. GSH was 1 mM and all other species were 100 μM. For the determination of the detection limit, probe **7** (10 μM) was incubated with various concentrations of GSH (0.1-1.0 mM) for 1 h before recording the emission profiles. The detection limit was calculated with the 3σ/k method.[3]

4. HPLC measurement

For the HPLC studies, a mixture of probe **1**, **2**, **3** or **4** (200 μM) and GSH (1 mM or 10 mM) in PBS (50 mM, pH = 7.4; 30% DMSO) was analyzed by HPLC at different reaction time. Conditions: Agilent Technologies HPLC LC-10F; C_{18} column with 4.6 mm x 250 mm; buffer A: 0.1% (v/v) trifluoroacetic acid in water; buffer B: methanol. flow 1.0 mL/min; The elution conditions were: 0-2 min, buffer B: 5-60%; 2-23 min, buffer B: 60-85%; 23-25 min, buffer B: 85-5%. The detection wavelength: 400 nm for **1**, **3**, or **4**; 360 nm for probe **2**.

HPLC analysis of probe **7** treated with different biothiols was performed by Agilent Technologies HPLC LC-1260 Infinity II using C_{18} column with 4.6 mm x 250 mm. Buffer A: 0.1% (v/v) trifluoroacetic acid in water; buffer B: methanol; flow: 1.0 mL/min. The elution conditions were: 0-3 min, buffer B: 5-40%; 3-15 min, buffer B:

40-75%; 15-25 min, buffer B: 75-95%; 25-30 min, buffer B: 95-5%. The detection wavelength for HPLC is 254 nm.

5. Cell culture and MTT assay

FHC and HeLa cell lines were purchased from the Cell Bank of the Chinese Academy of Sciences (Shanghai, China). The cells were cultured in RPMI 1640 and DMEM medium, respectively, with 10% fetal bovine serum and 1% penicillin/streptomycin under standard cell culture conditions at 37 °C in a humidified CO_2 incubator. The cytotoxicity of probes **5** and **7** was evaluated via a 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay by using the FHC cells. Briefly, the FHC cells were transferred to the 96-well plate and cultured for 12 h before experiments. After that, the culture medium was replaced with fresh one and the FHC cells were incubated with different concentrations of probe **5** or **7** (0, 5, 10, 25, 50, 75 and 100 μM) for 24 h. Then, 5 mg/mL MTT in PBS (20 μL) was added to each well and incubated for another 4 h. Finally, the medium was replaced with 150 μL of DMSO to dissolve the purple formazan crystals. The absorbance intensity in each well was detected at 490 nm by a microplate spectrophotometer (SpectraMax M2E (Molecular Device, Inc.)).

6. Bioimaging

The feasibility of probe **7** to detect GSH in live cells was evaluated by fluorescence imaging. The HeLa cells were transferred to the 24-well plate and cultured for 12 h before the experiments. After that, the culture medium was replaced with fresh one, and the cells were pretreated with or without the thiol blocking reagent *N*-ethylmaleimide (NEM, 1 mM) for 30 min, and treated with probe **7** (20 μM) at 37 °C for another 30 min, and then with ER-Tracker Red (1.0 μM) at 37 °C for 15 min. After incubation, the cells were quickly washed for three times with PBS, and fixed with 4% paraformaldehyde solution at 37 °C for 5 min. A confocal microscope

(Olympus FV1000) with a 100 × objective lens was used for imaging. Emission for probe **7** was collected at 500-580 nm with 405 nm excitation, and emission for ER-Tracker Red was collected at 570-670 nm with 561 nm excitation.

7. References

1. T.-K. Liu, P.-Y. Hsieh, Y.-D. Zhuang, C.-Y. Hsia, C.-L. Huang, H.-P. Lai, H.-S. Lin, I.-C. Chen, H.-Y. Hsu and K.-T. Tan, *ACS Chem. Biol.*, 2014, **9**, 2359-2365.
2. K. N. Hearn, T. D. Nalder, R. P. Cox, H. D. Maynard, T. D. M. Bell, F. M. Pfeffer and T. D. Ashton, *Chem. Commun.*, 2017, **53**, 12298-12301.
3. J. Radford-Knoery and G. A. Cutter, *Anal. Chem.*, 1993, **65**, 976-982.

8. Supplementary figures

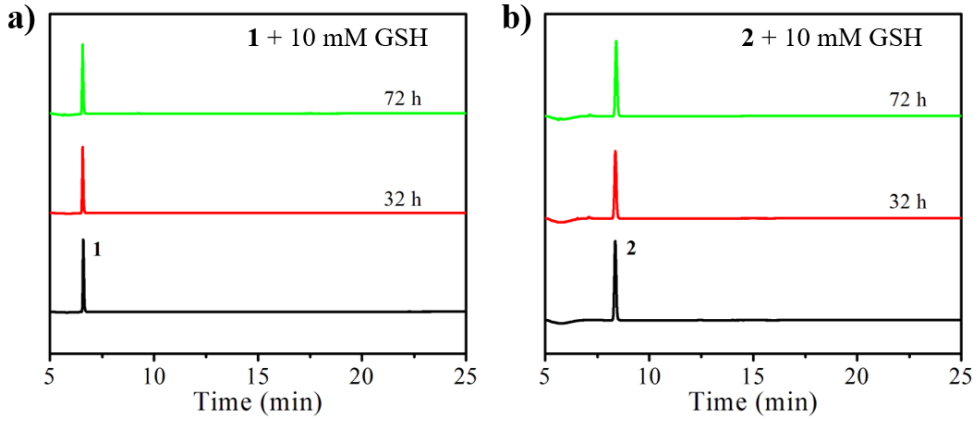


Fig. S1 Time-dependent HPLC traces for 200 μM probes **1** (a) and **2** (b) in the presence of 10 mM GSH in PBS buffer (pH 7.4, containing 30% DMSO).

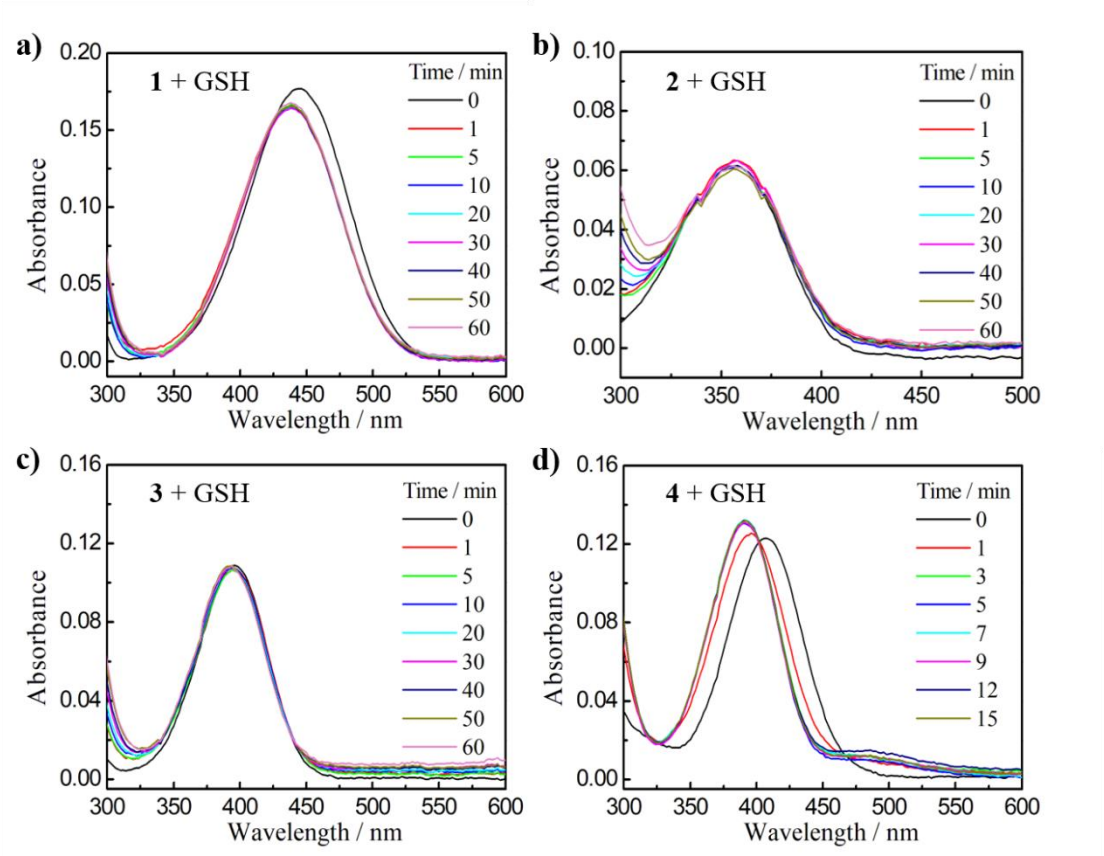


Fig. S2 Time-dependent absorbance spectra of (a) 10 μM **1** and 10 mM GSH; (b) 10 μM **2** and 10 mM GSH; (c) 10 μM **3** and 10 mM GSH; (d) 10 μM **4** and 1.0 mM GSH in PBS buffer (pH 7.4).

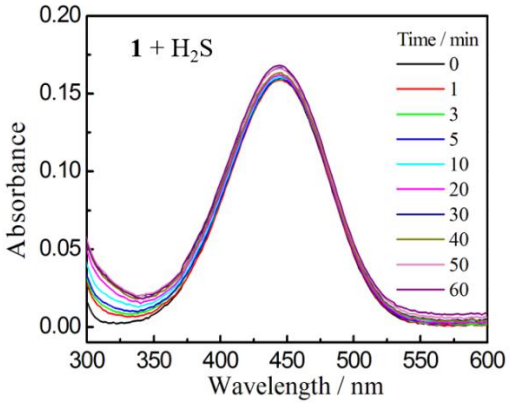


Fig. S3 Time-dependent of UV-vis spectra of **1** (10 μM) and H_2S (0.25 mM).

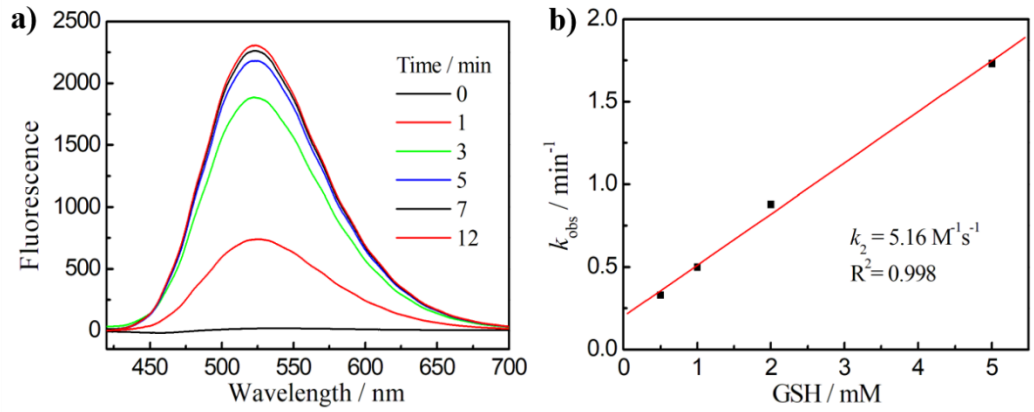


Fig. S4 (a) Time-dependent emission spectra (Ex. at 400 nm) of the probe **4** (10 μM) toward 1 mM GSH in PBS buffer (pH 7.4). (b) The linear relationship between concentrations of GSH and k_{obs} values to produce the reaction rate k_2.

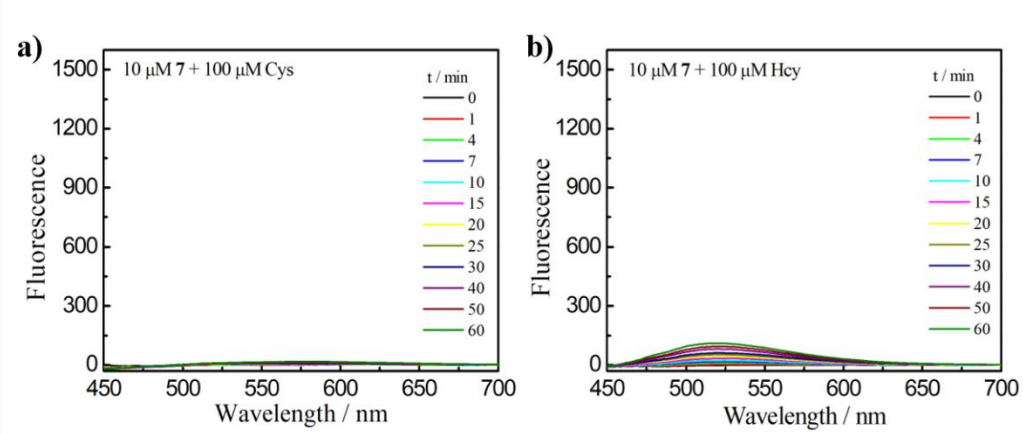


Fig. S5 Time-dependent fluorescence spectra of **7** (10 μM) toward 100 μM Cys (a) or Hcy (b).

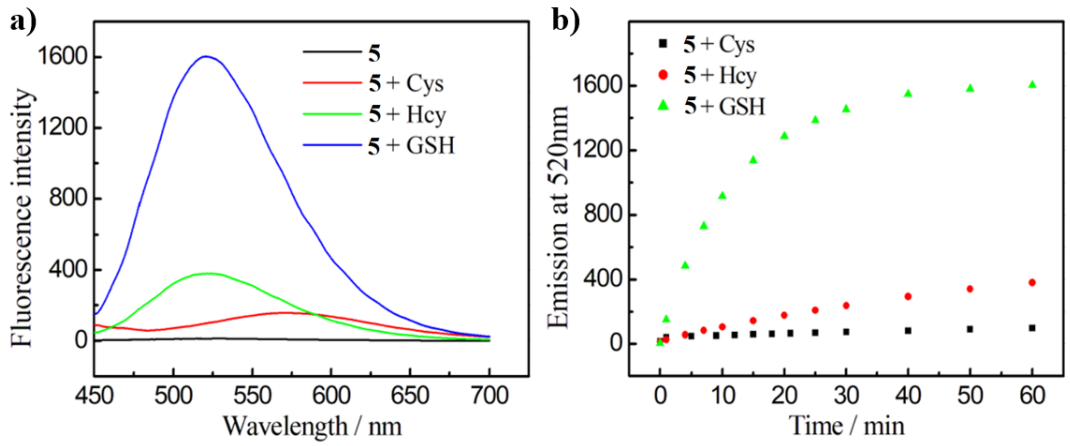


Fig. S6 (a) Fluorescent spectra of 10 μM probe **5** (a) and their reaction with Cys (100 μM), Hcy (100 μM) or GSH (2 mM) for 1 h. (b) Time-dependent emission intensities of 10 μM **5** toward these biothiols.

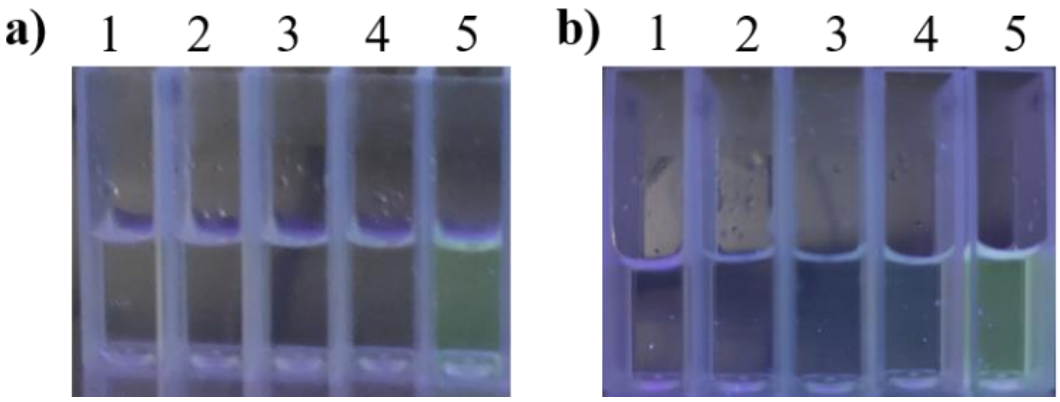


Fig. S7 The photo under 365 nm UV light of **7** (10 μM) and its reaction with thiols for 1 h (a) and 24 h (b) in PBS buffer. From 1 to 5: probe **7** only, probe **7** and 100 μM Cys, probe **7** and 100 μM Hcy, probe **7** and 100 μM GSH, probe **7** and 1 mM GSH, respectively.

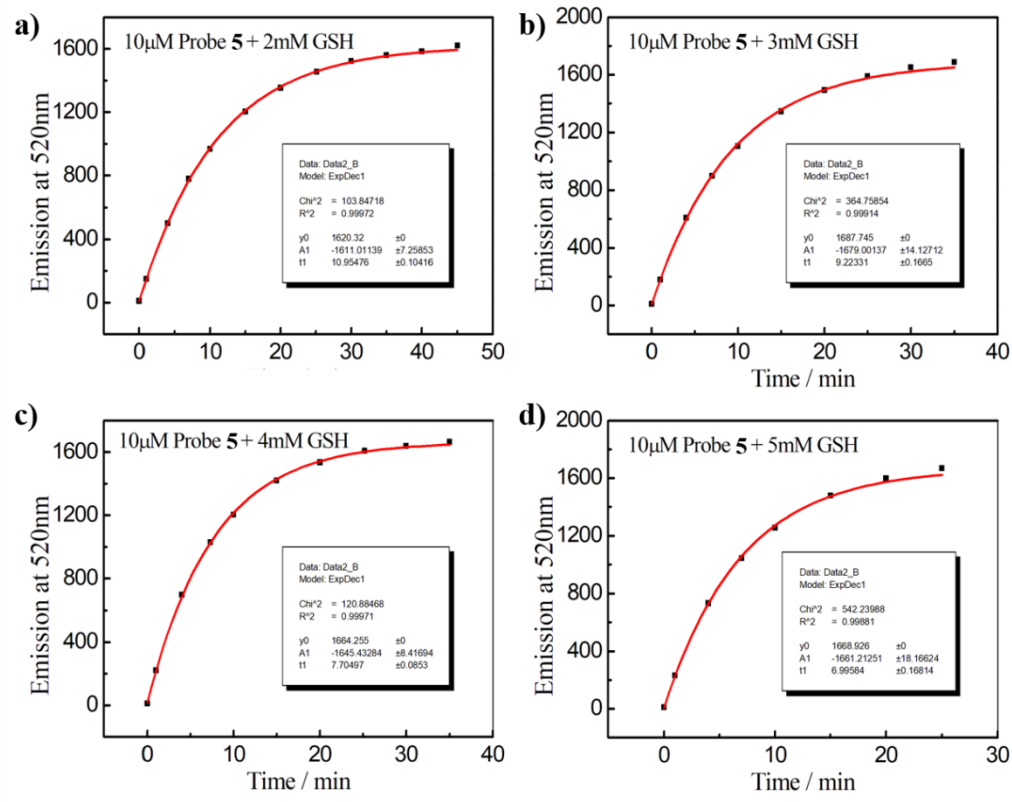


Fig. S8 Time-dependent fluorescence intensities of probe **5** (10 μM) in the presence of different concentrations of GSH.

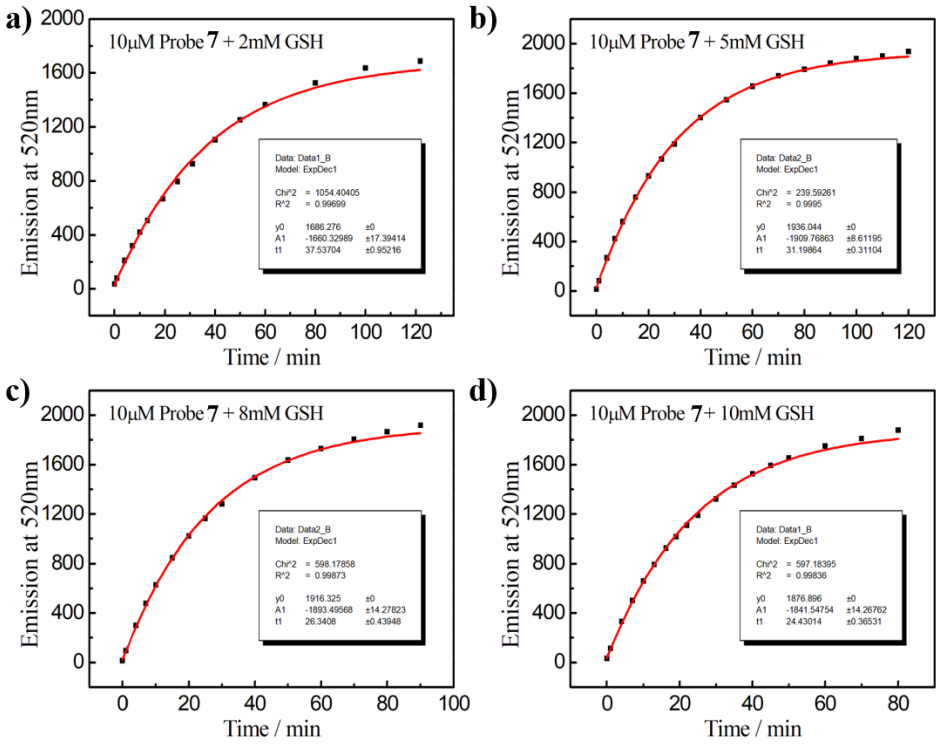


Fig. S9 Time-dependent fluorescence intensities of probe **7** (10 μM) in the presence of different concentrations of GSH.

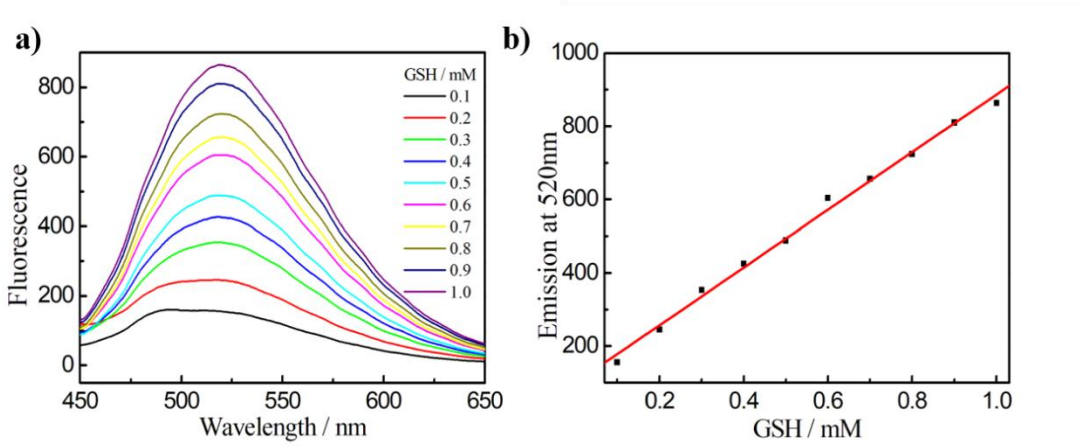


Fig. S10 (a) The fluorescence changes of probe **7** (10 μM) in the presence of various concentrations of GSH. λ_{ex} = 420 nm. (b) The linear relationship between concentrations of GSH and emission at 520 nm. The detection limit was calculated to be 2.1 μM.

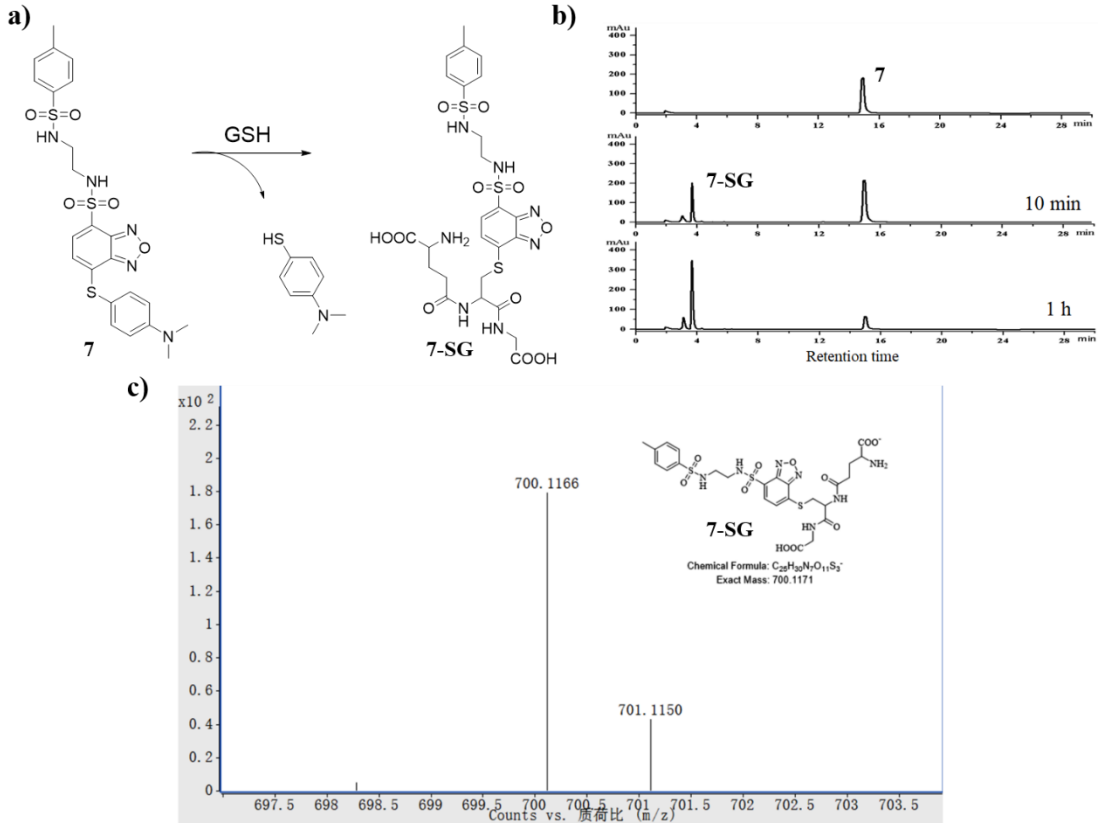


Fig. S11 (a) Reaction of probe **7** with GSH. (b) Time-dependent HPLC traces of probe **7** (10 μM) and GSH (2 mM). (c) HRMS spectrum of probe **7** (50 μM) incubated with GSH (2 mM) in PBS overnight.

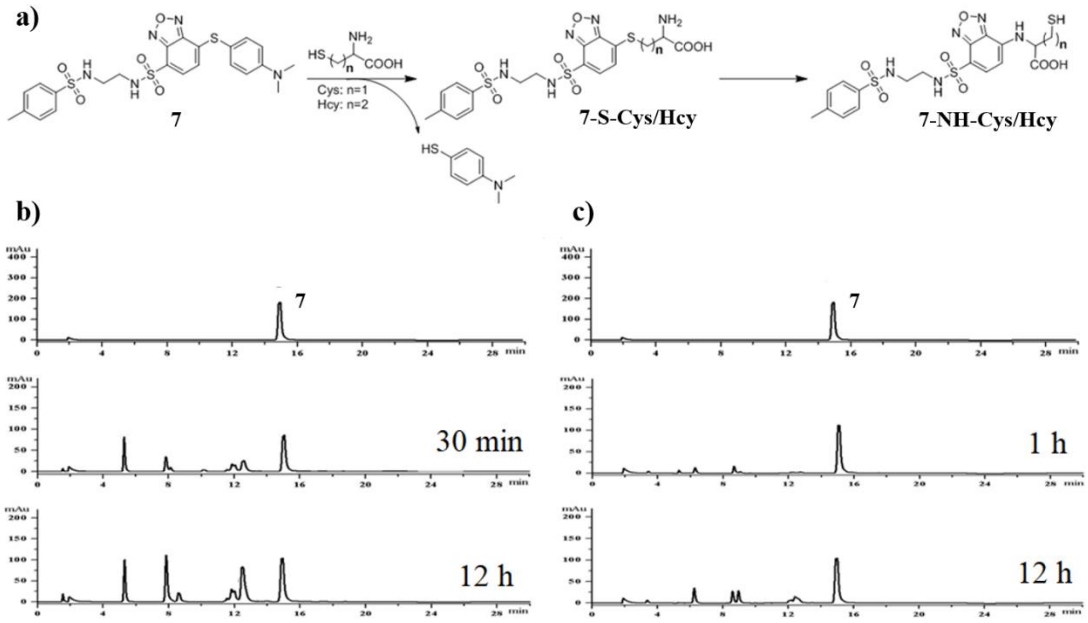
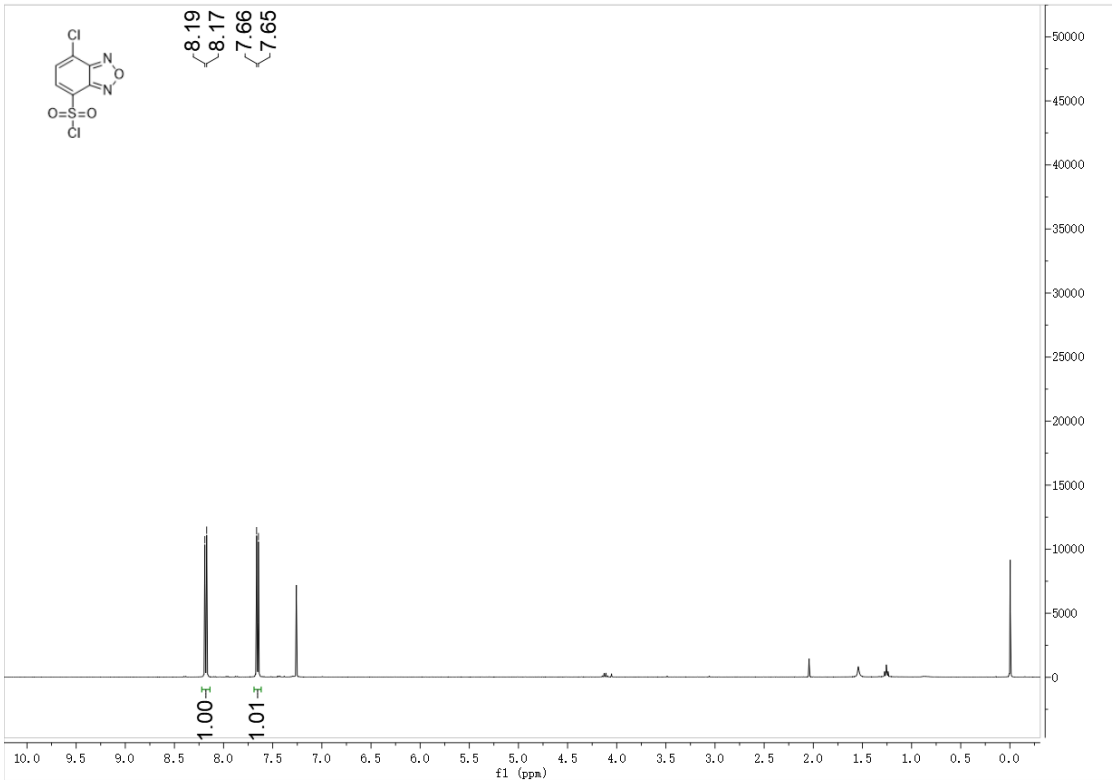
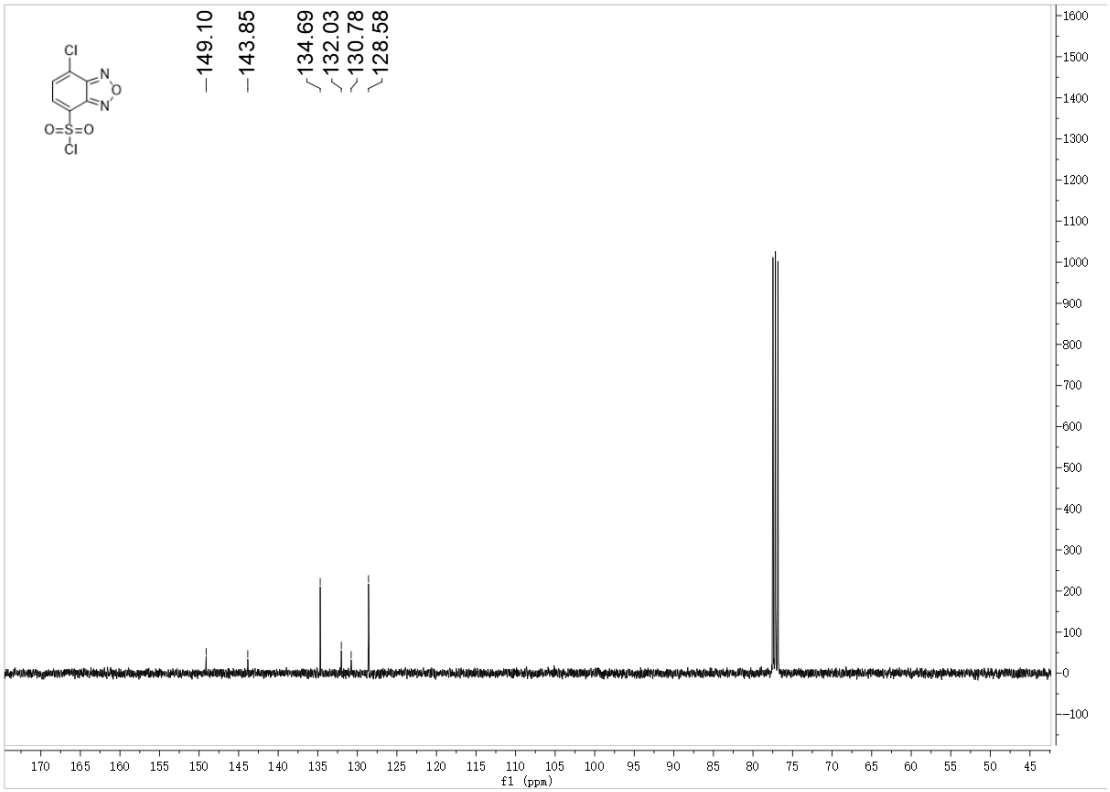
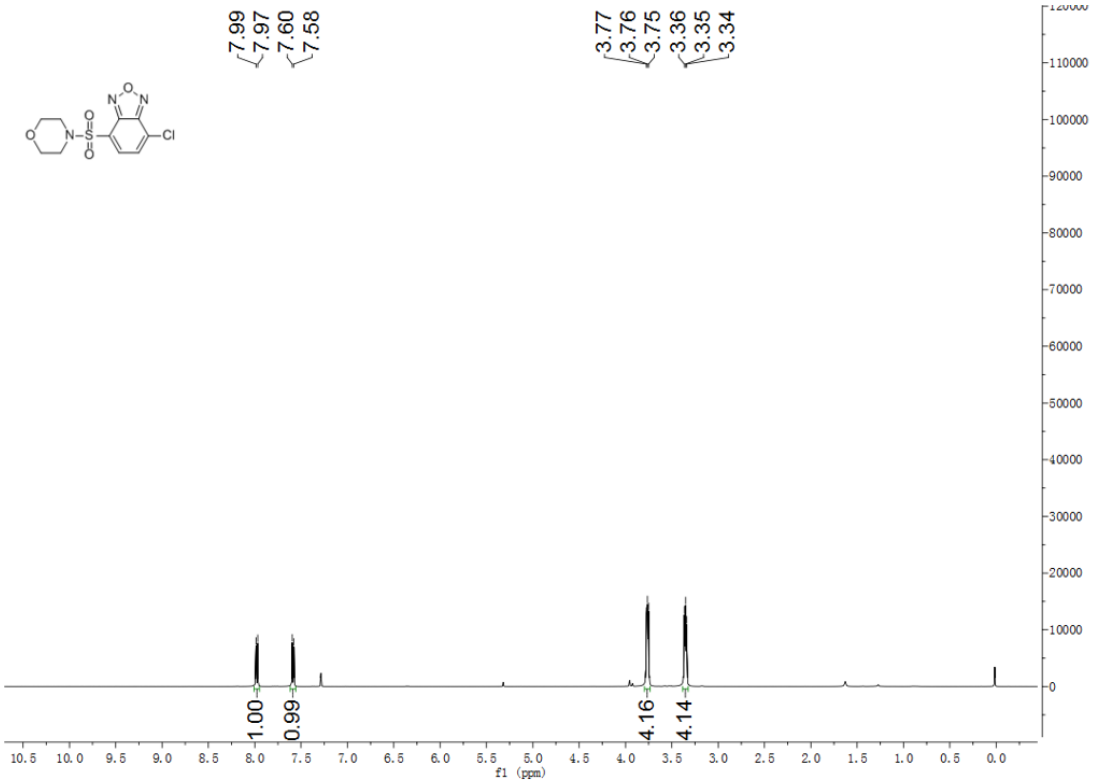


Fig. S12 (a) Reactions of probe **7** with Hcy and Cys. (b, c) Time-dependent HPLC traces of **7** (10 μM) treated with (b) Hcy (200 μM) or (c) Cys (200 μM).

8. Supplementary NMR and HRMS spectra



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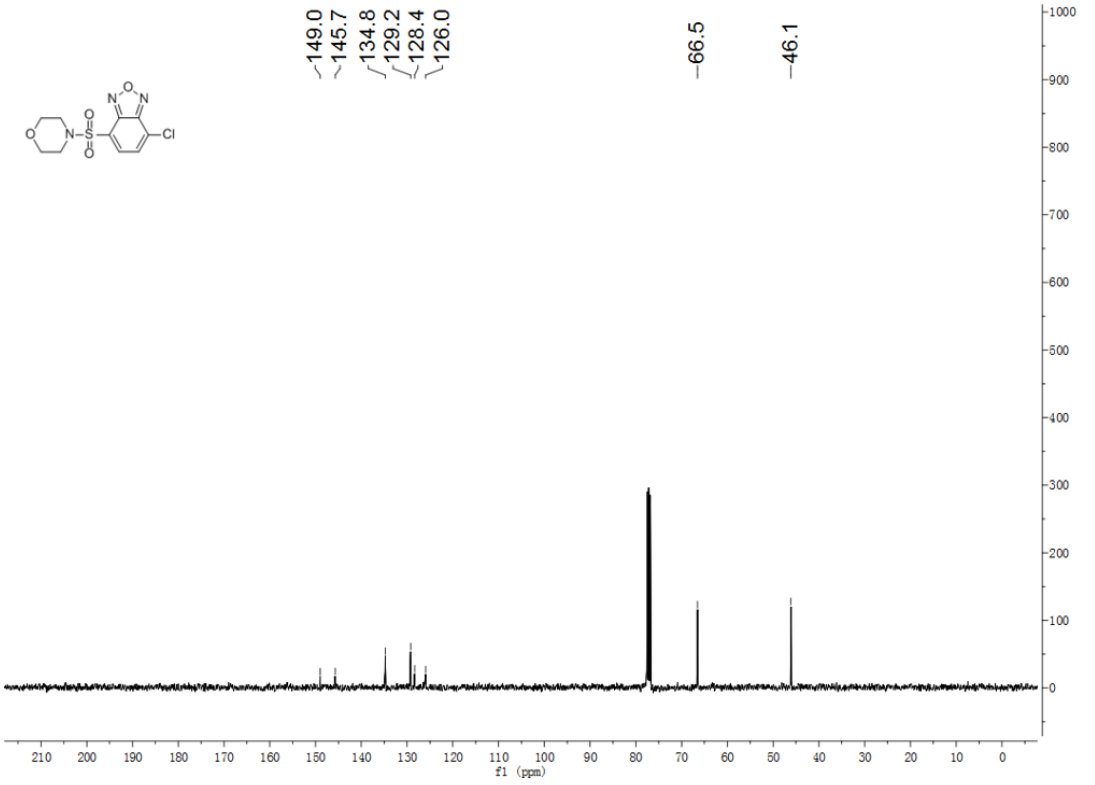
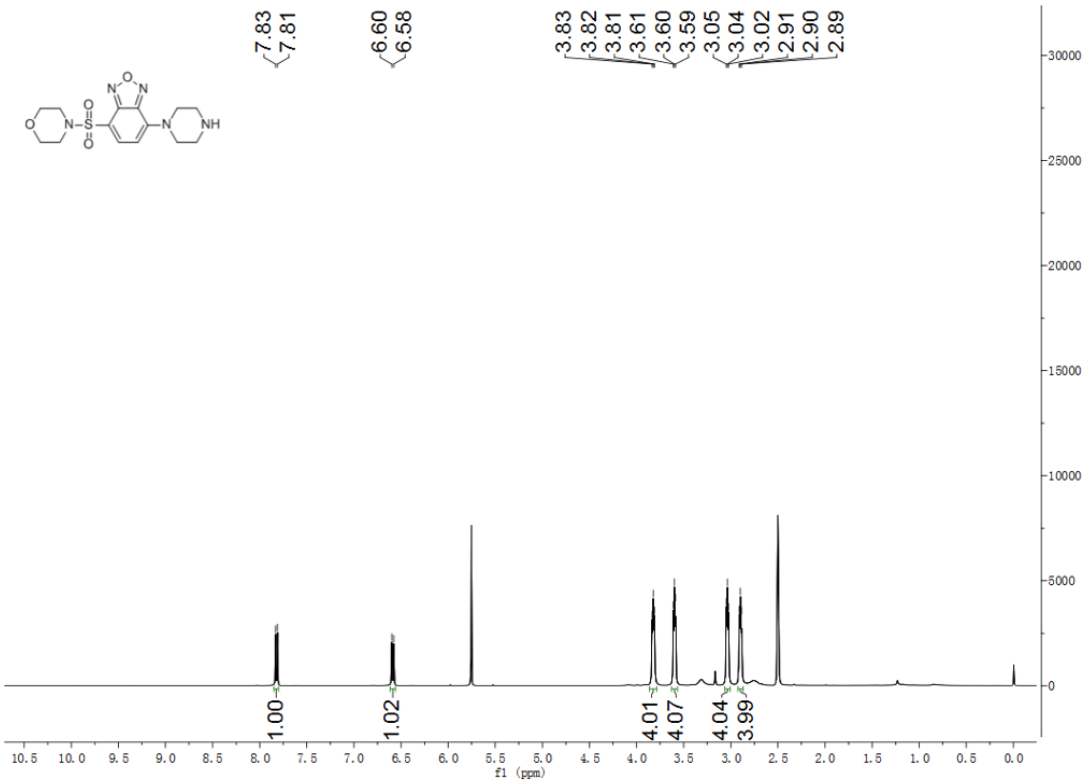
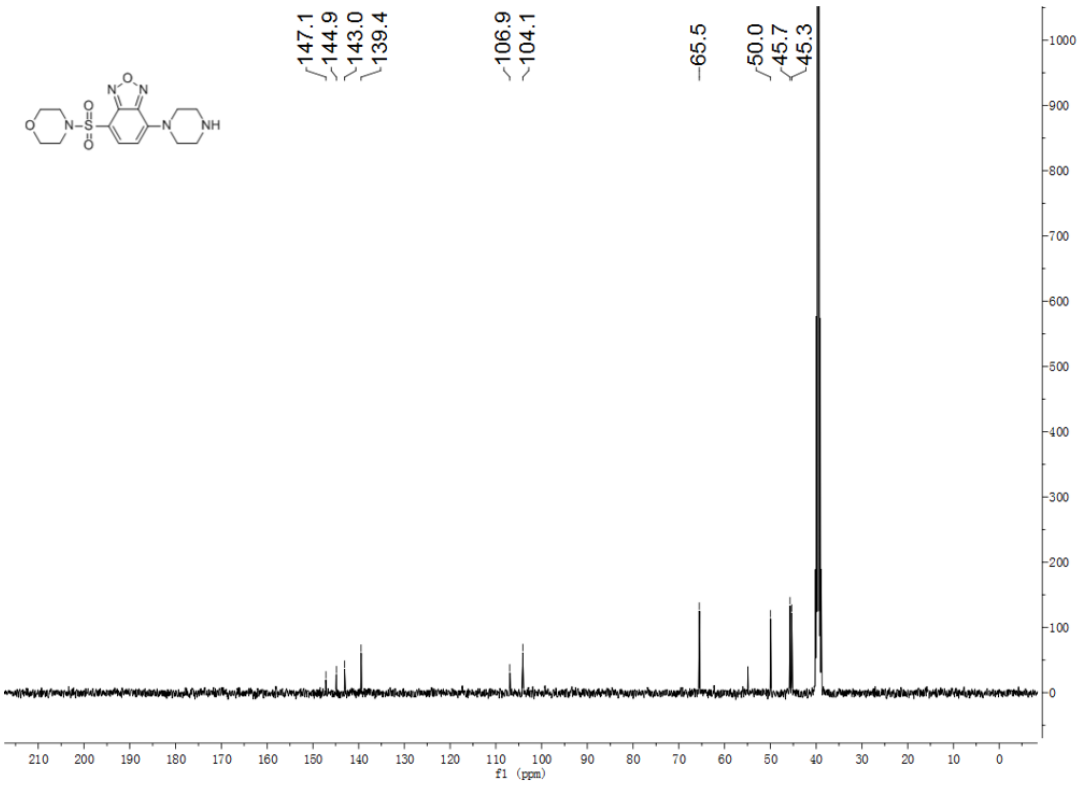
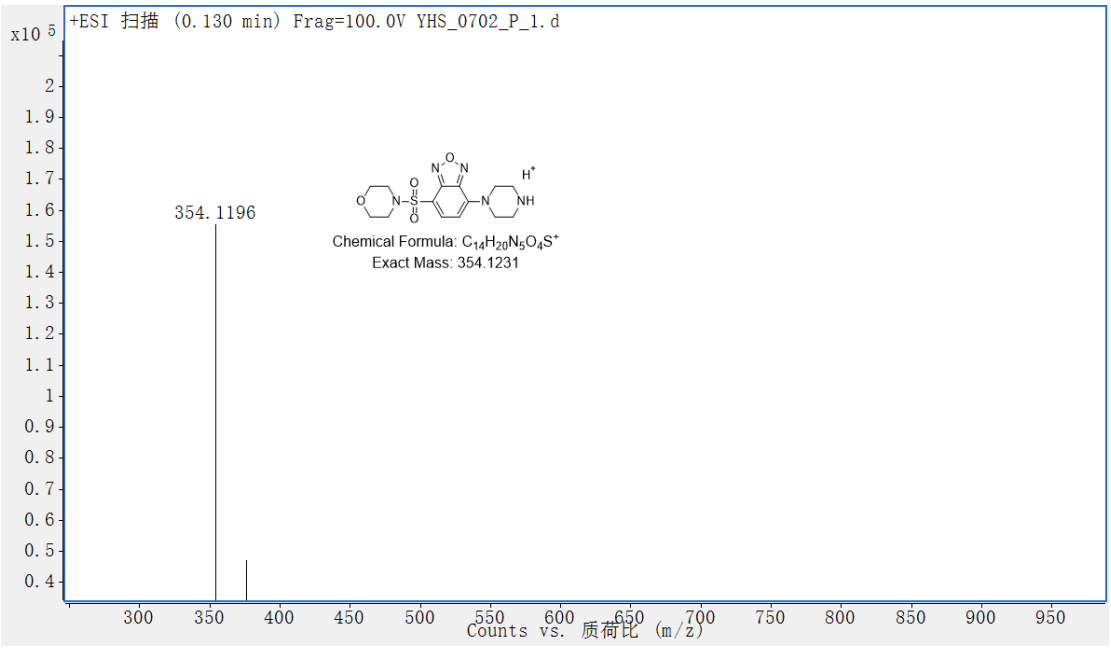
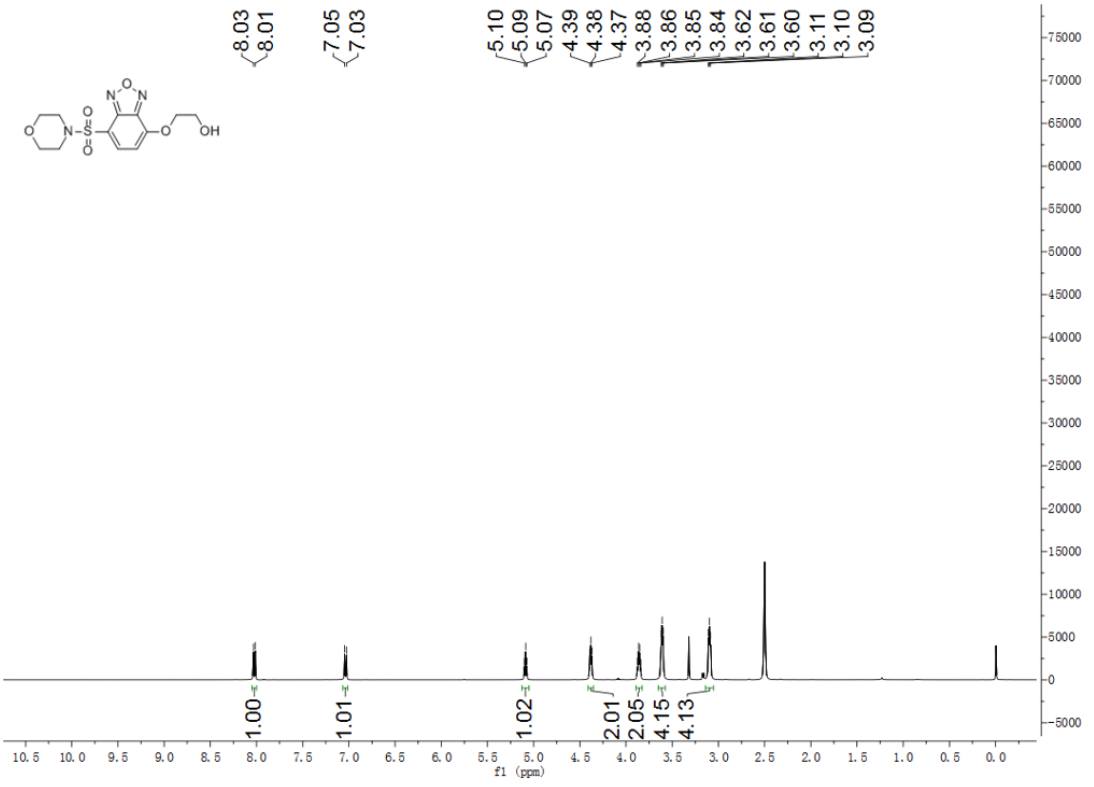
3.35
3.34
1.00
0.99
4.16
4.14
f1 (ppm)

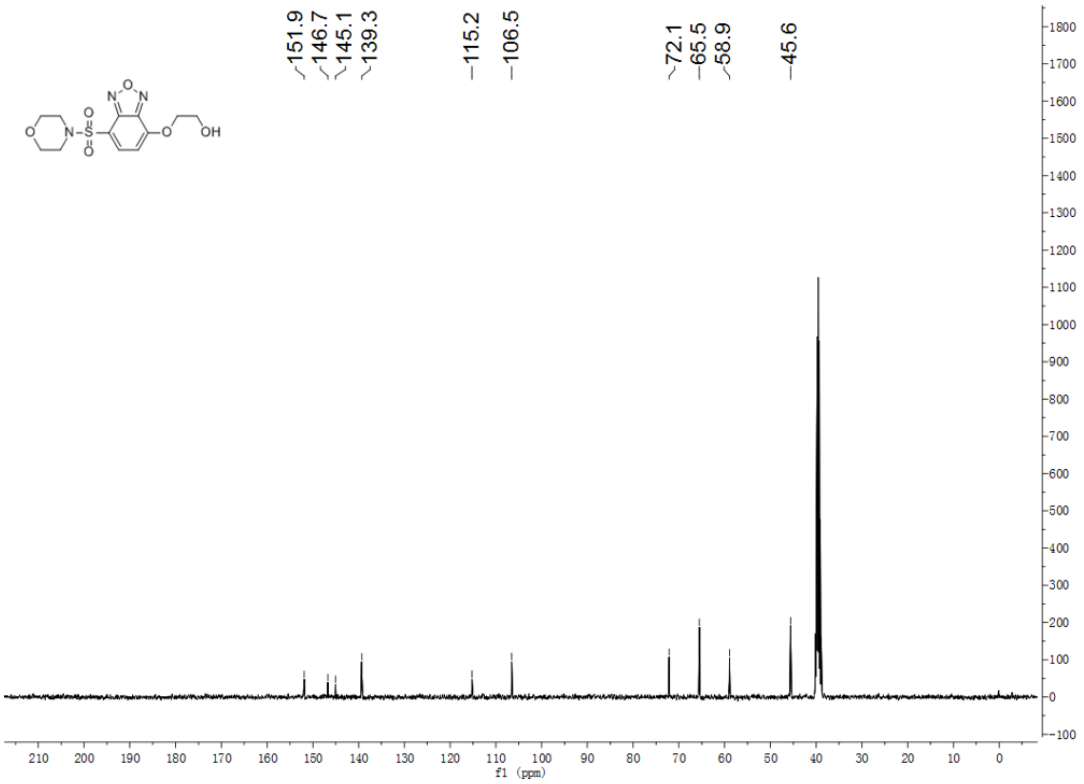

149.0
145.7
134.8
129.2
128.4
126.0
66.5
46.1
f1 (ppm)

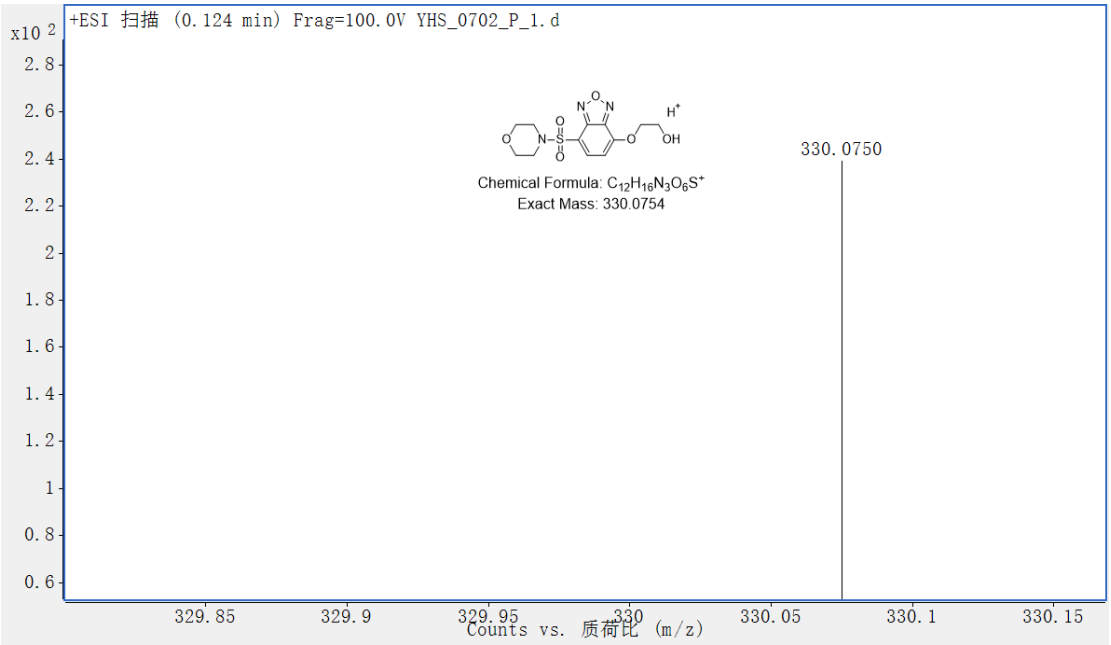

7.83
7.81
6.60
6.58
3.83
3.82
3.81
3.61
3.60
3.59
3.05
3.04
3.02
2.91
2.90
2.89
1.00
1.02
4.01
4.07
4.04
3.99
f1 (ppm)

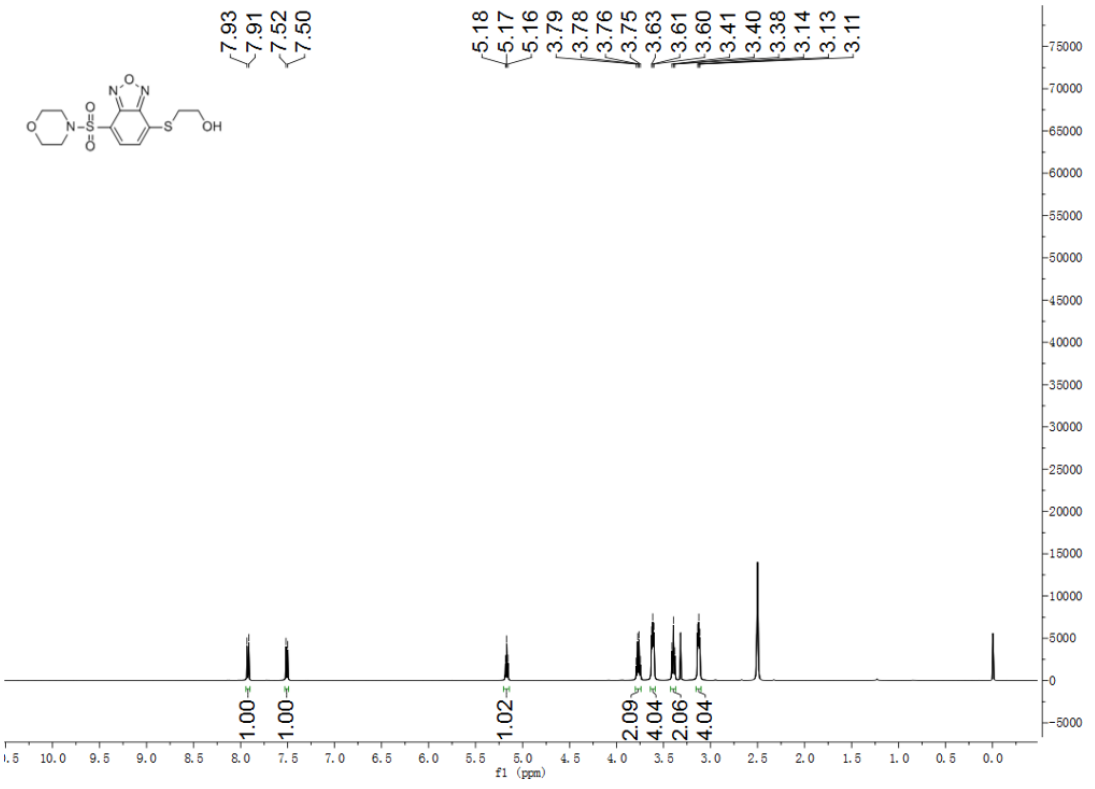

147.1
144.9
143.0
139.4
106.9
104.1
65.5
50.0
45.7
45.3
f1 (ppm)

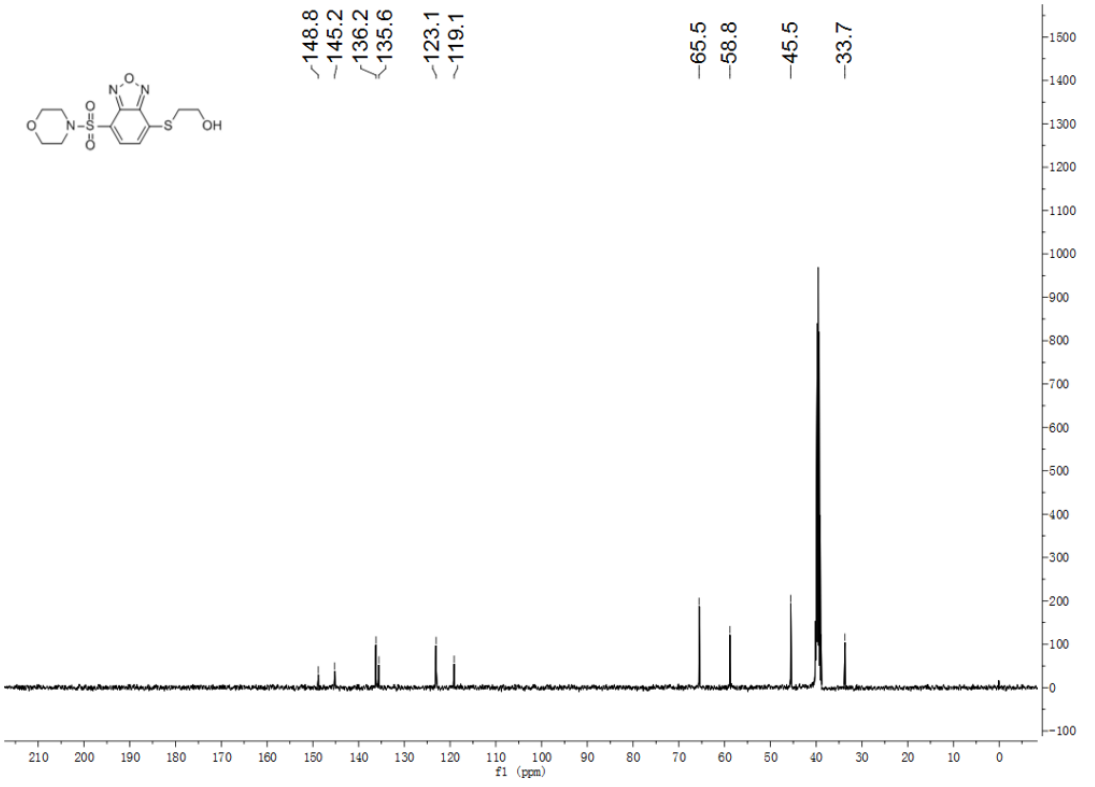

+ESI 扫描 (0.130 min) Frag=100.0V YHS_0702_P_1.d
x10 5
354.1196
Chemical Formula: C14H20N5O4S+
Exact Mass: 354.1231
Counts vs. 质荷比 (m/z)

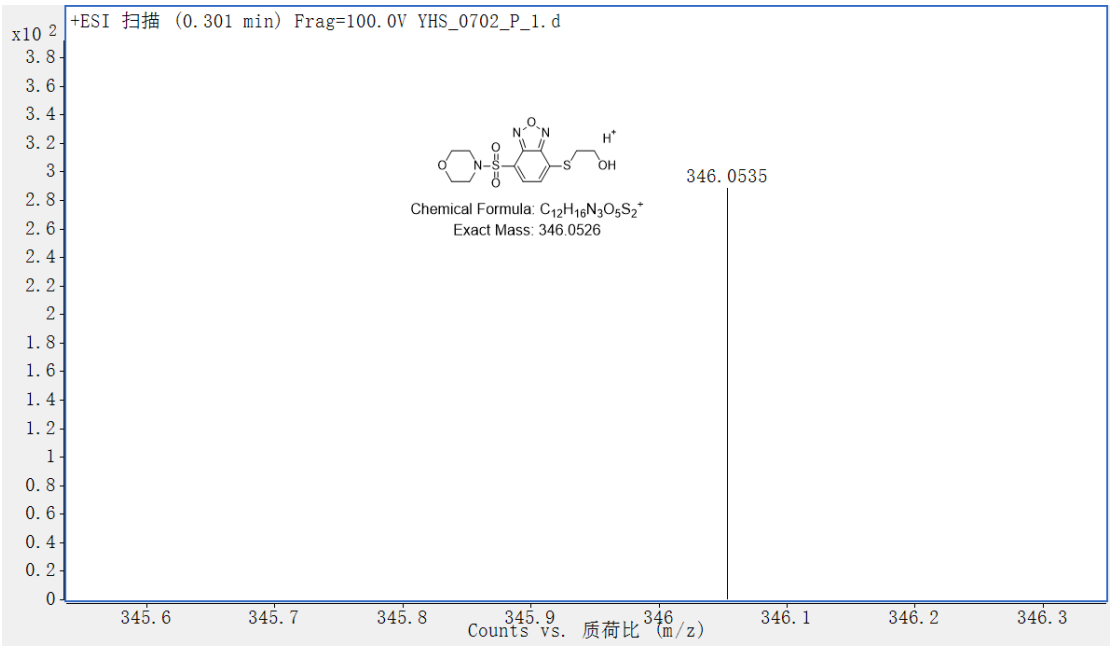

8.03
8.01
7.05
7.03
5.10
5.09
5.07
4.39
4.38
4.37
3.88
3.86
3.85
3.84
3.62
3.61
3.60
3.11
3.10
3.09
OH
1.00
1.01
1.02
2.01
2.05
4.15
4.13
f1 (ppm)

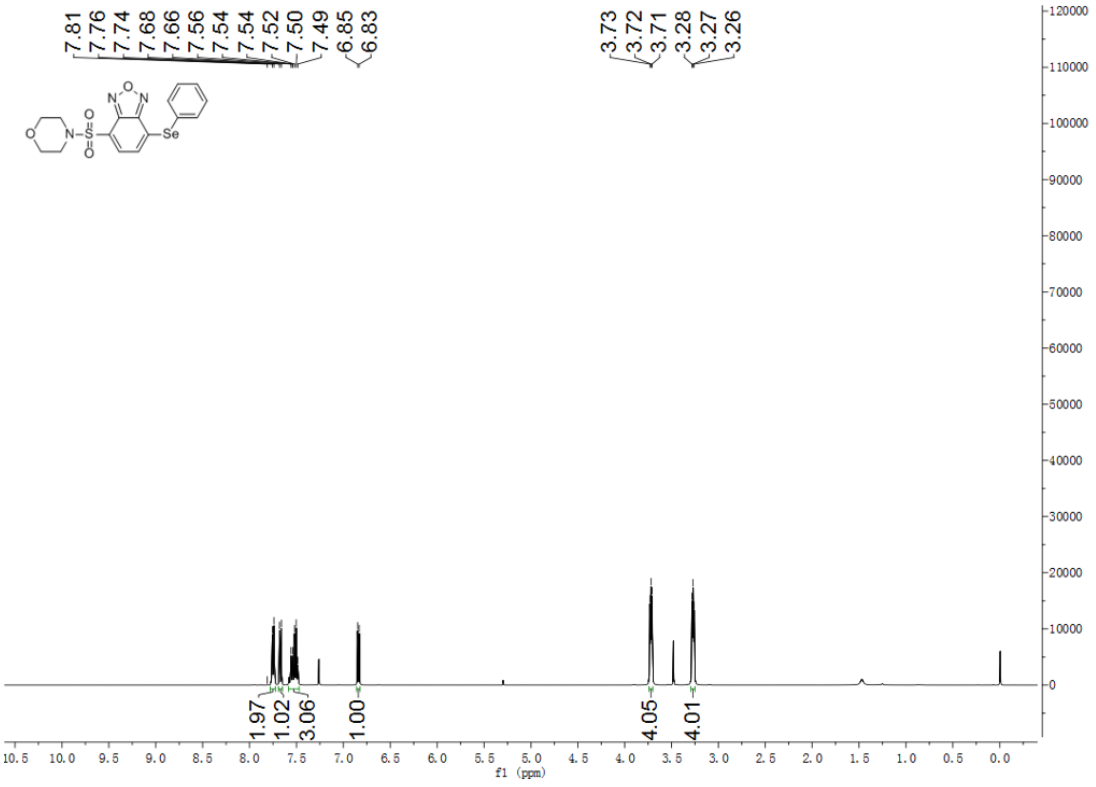

151.9
146.7
145.1
139.3
115.2
106.5
72.1
65.5
58.9
45.6
f1 (ppm)

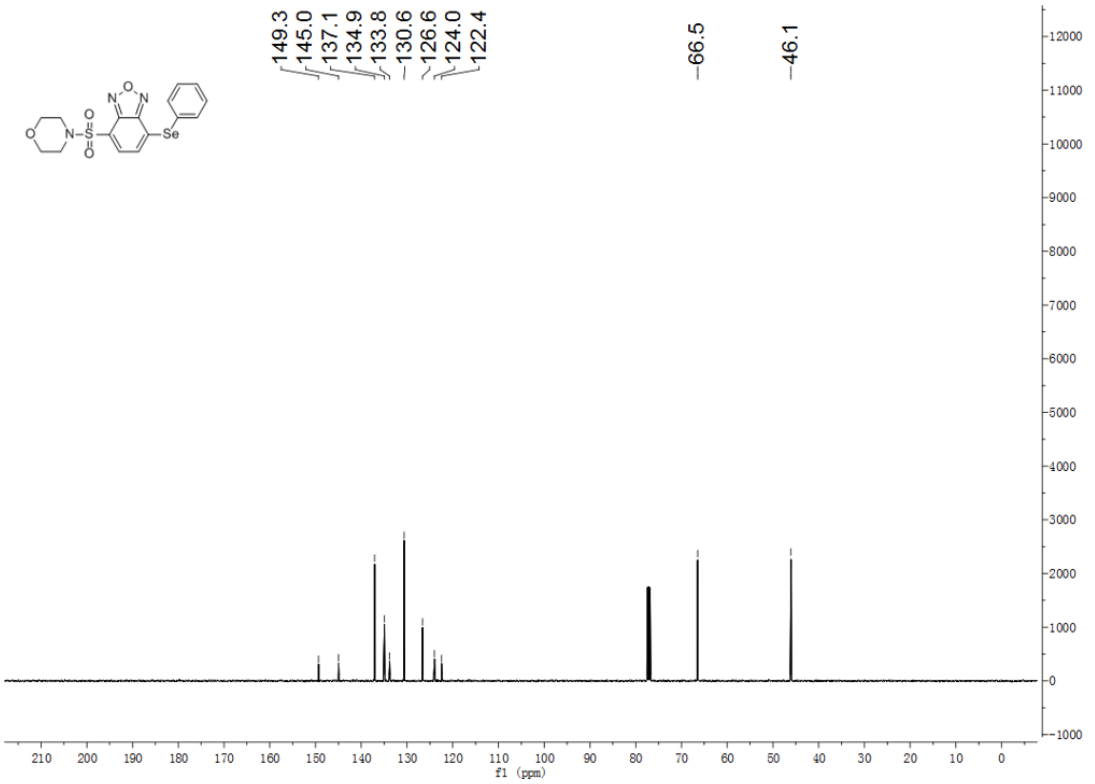

+ESI 扫描 (0.124 min) Frag=100.0V YHS_0702_P_1.d
x10 2
330.0750
Chemical Formula: C12H16N3O6S+
Exact Mass: 330.0754
Counts vs. 质荷比 (m/z)

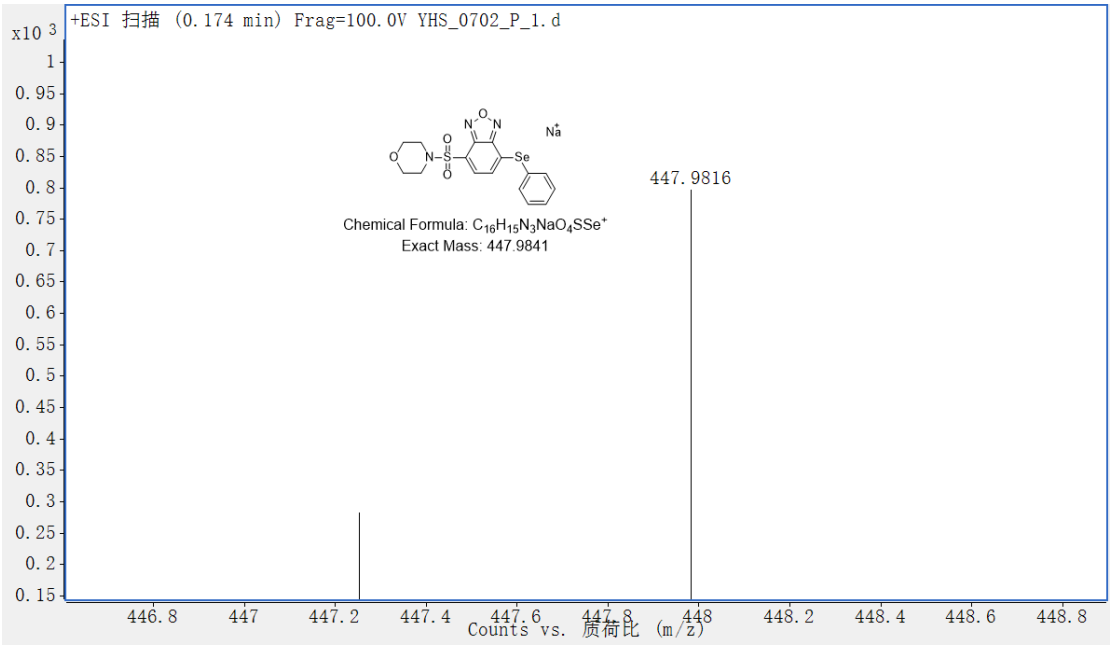

7.93
7.91
7.52
7.50
5.18
5.17
5.16
3.79
3.78
3.76
3.75
3.63
3.61
3.60
3.41
3.40
3.38
3.14
3.13
3.11
1.00
1.00
1.02
2.09
4.04
2.06
4.04
f1 (ppm)

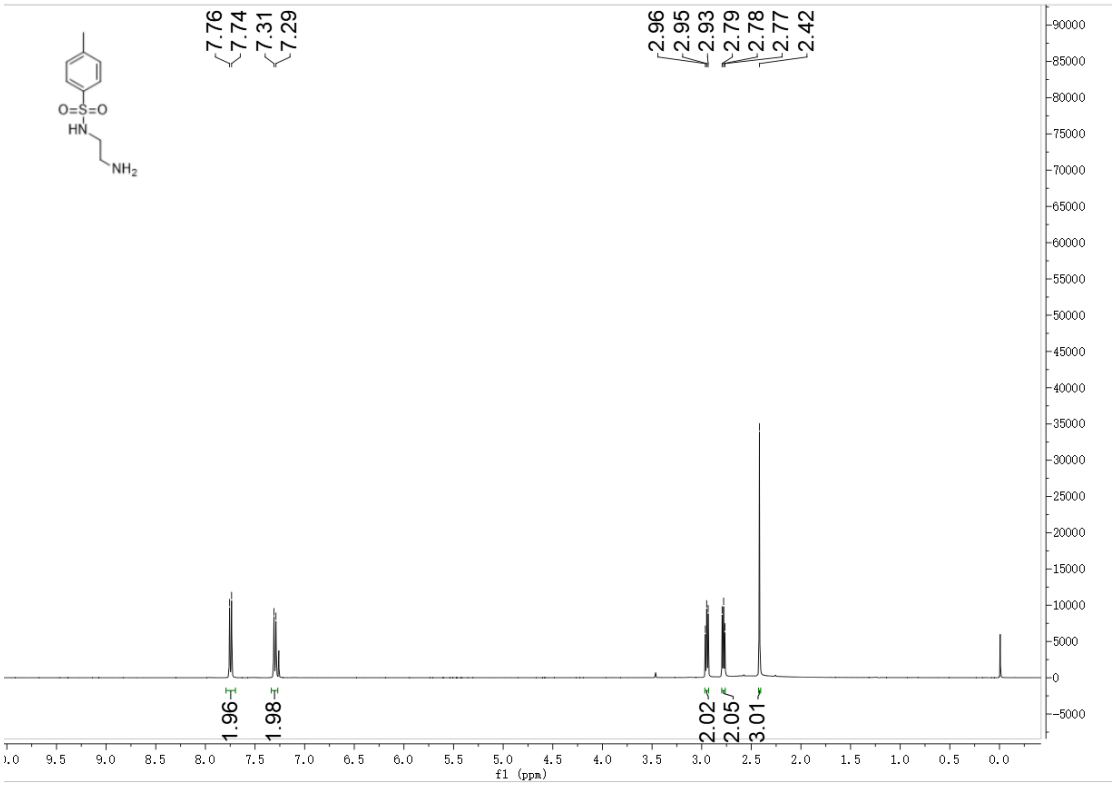

148.8
145.2
136.2
135.6
123.1
119.1
65.5
58.8
45.5
33.7
f1 (ppm)

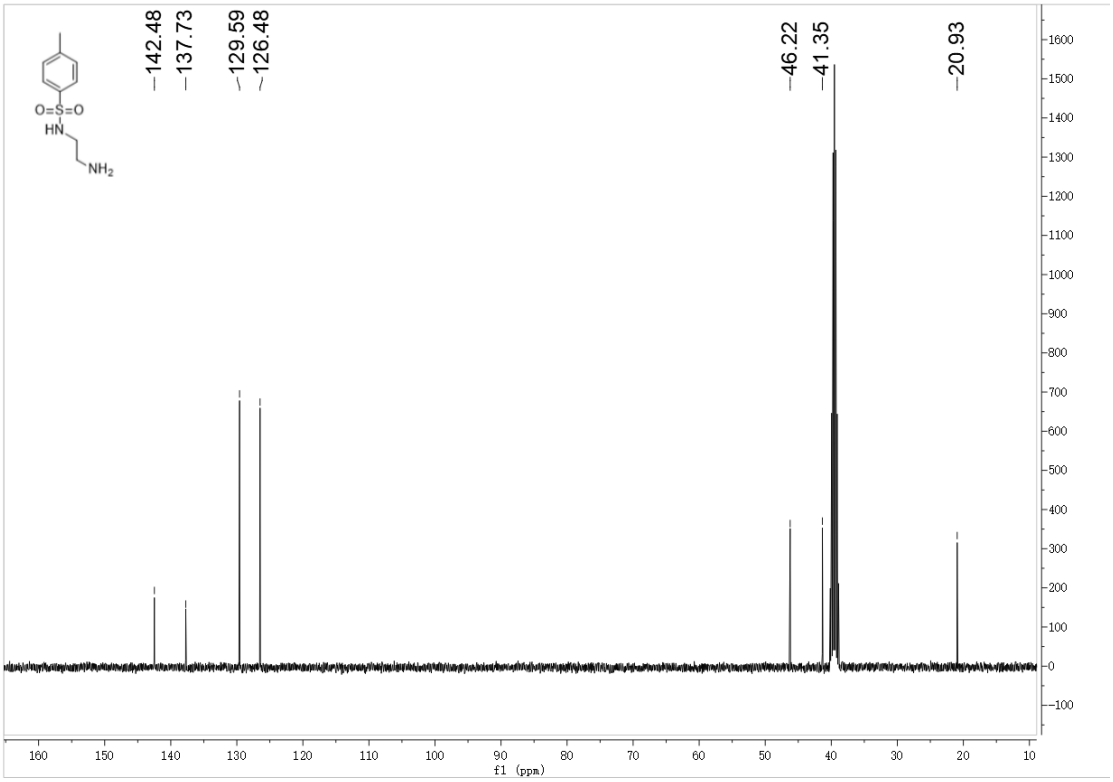

+ESI 扫描 (0.301 min) Frag=100.0V YHS_0702_P_1.d
x10 2
346.0535
Chemical Formula: C12H16N3O5S2+
Exact Mass: 346.0526
Counts vs. 质荷比 (m/z)

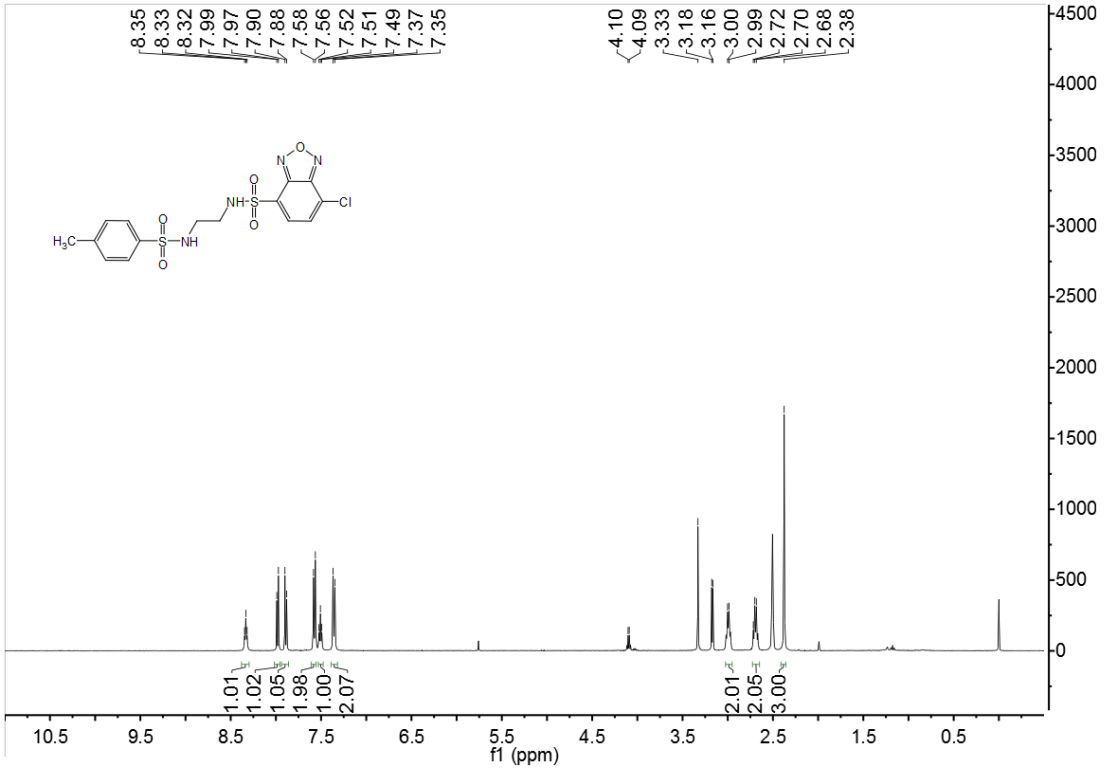

7.81
7.76
7.74
7.68
7.66
7.56
7.54
7.54
7.52
7.50
7.49
6.85
6.83
3.73
3.72
3.71
3.28
3.27
3.26
1.97
1.02
3.06
1.00
4.05
4.01
f1 (ppm)

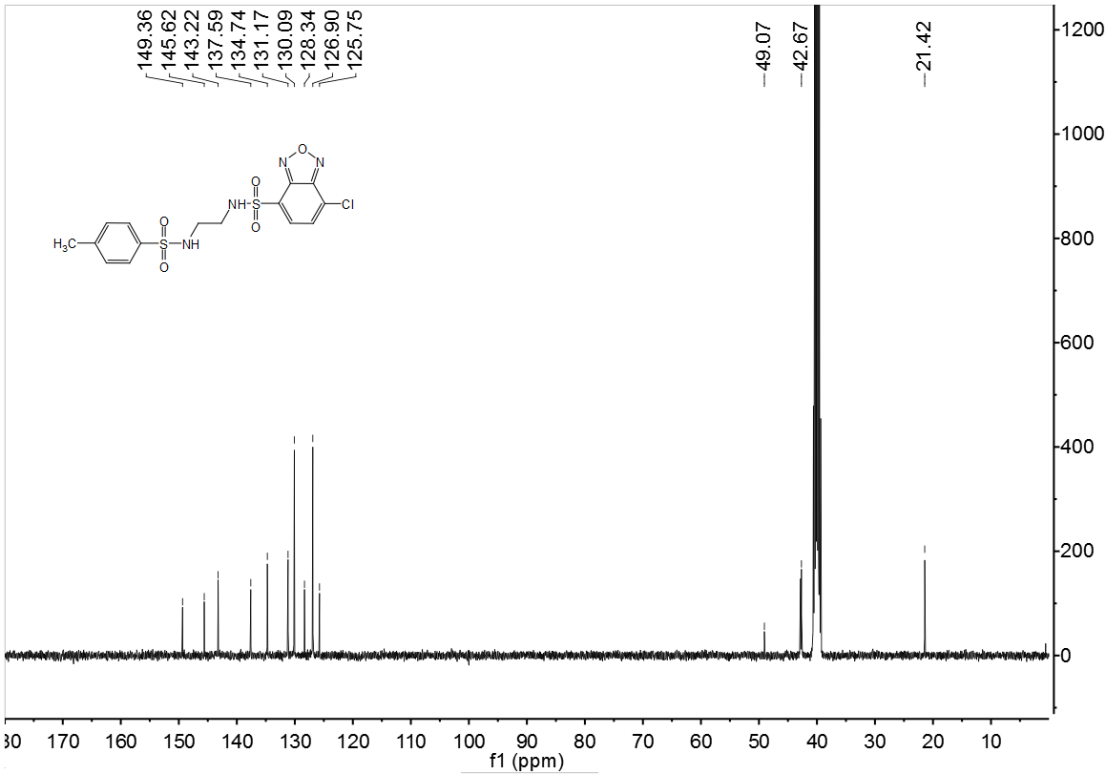

149.3
145.0
137.1
134.9
133.8
130.6
126.6
124.0
122.4
66.5
46.1
f1 (ppm)

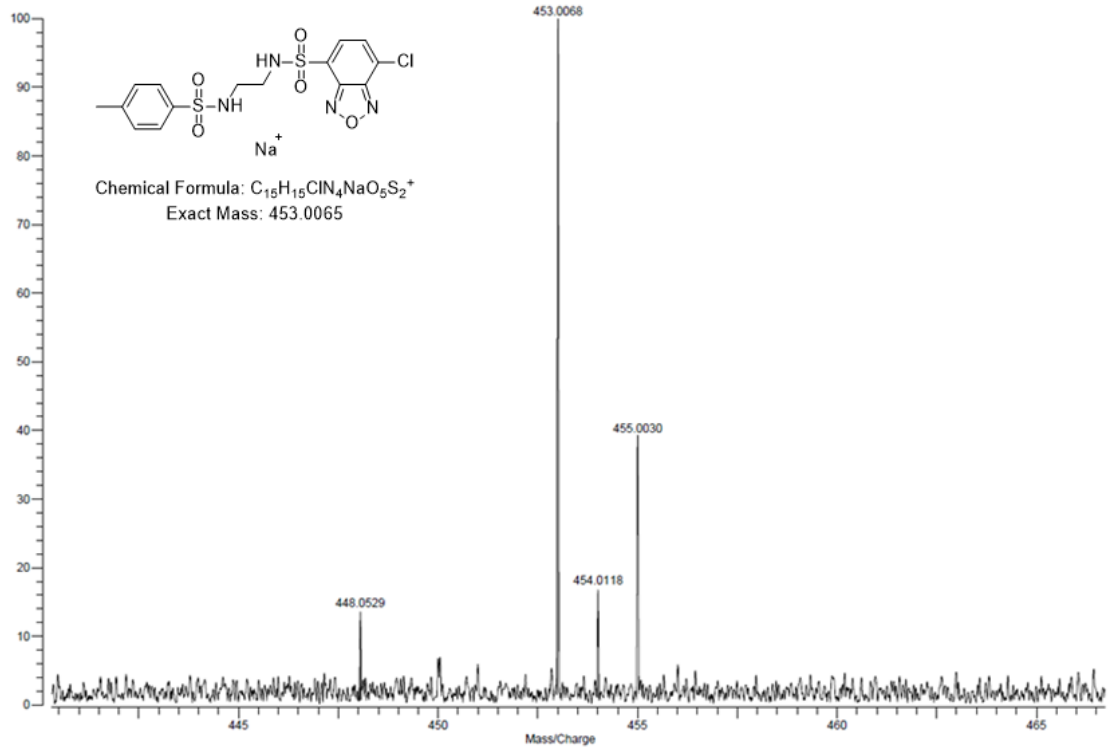

+ESI 扫描 (0.174 min) Frag=100.0V YHS_0702_P_1.d
x10 3
Chemical Formula: C16H15N3NaO4SSe+
Exact Mass: 447.9841
447.9816
Counts vs. 质荷比 (m/z)

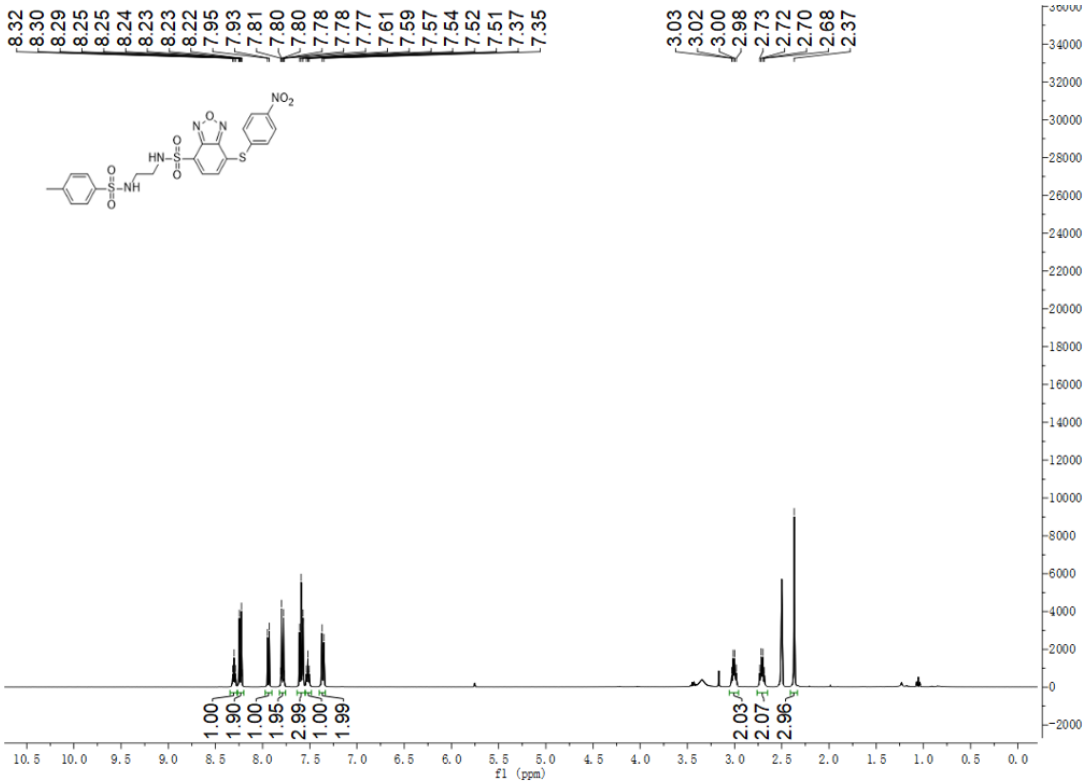

7.76
7.74
7.31
7.29
2.96
2.95
2.93
2.79
2.78
2.77
2.42
1.96
1.98
2.02
2.05
3.01
f1 (ppm)

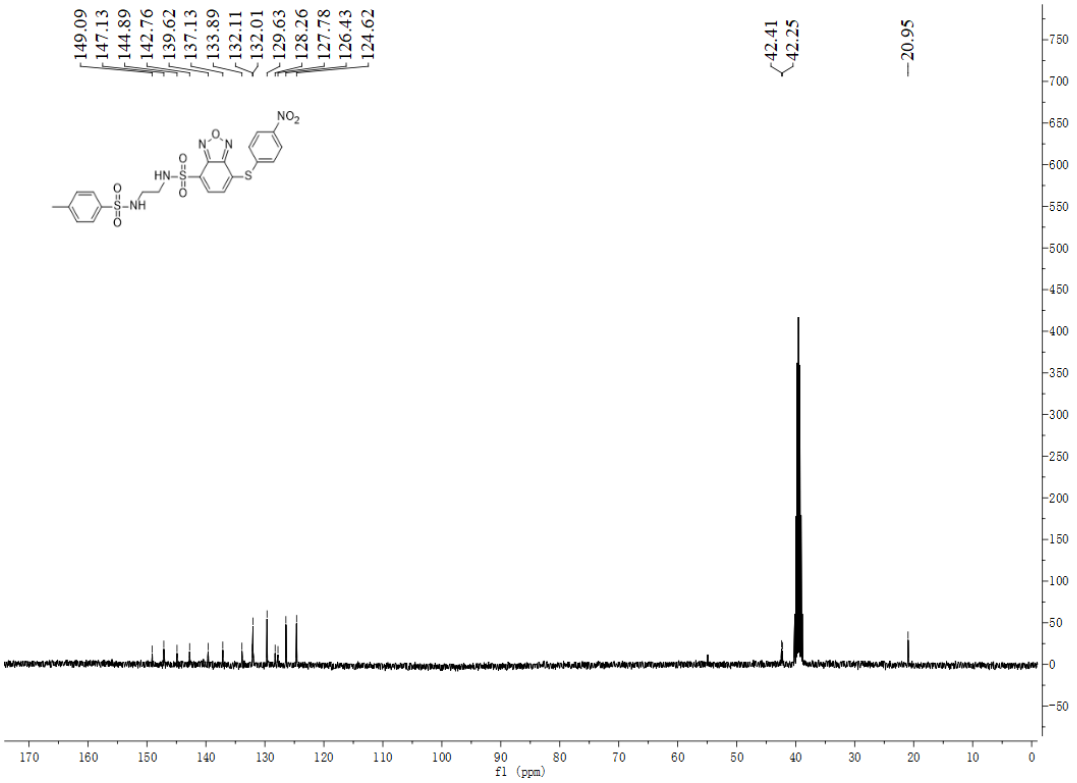

142.48
137.73
129.59
126.48
46.22
41.35
20.93
f1 (ppm)

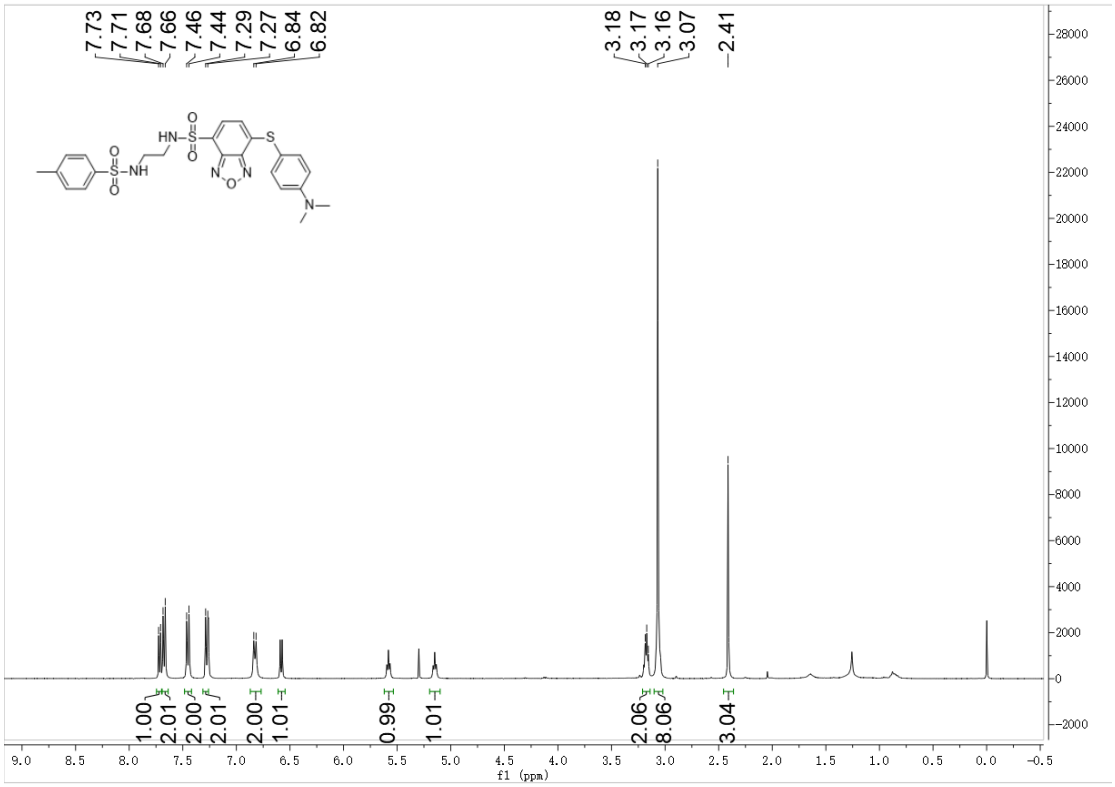

8.35
8.33
8.32
7.99
7.97
7.90
7.88
7.58
7.56
7.52
7.51
7.49
7.37
7.35
4.10
4.09
3.33
3.18
3.16
3.00
2.99
2.72
2.70
2.68
2.38
1.01
1.02
1.05
1.98
1.00
2.07
2.01
2.05
3.00
f1 (ppm)

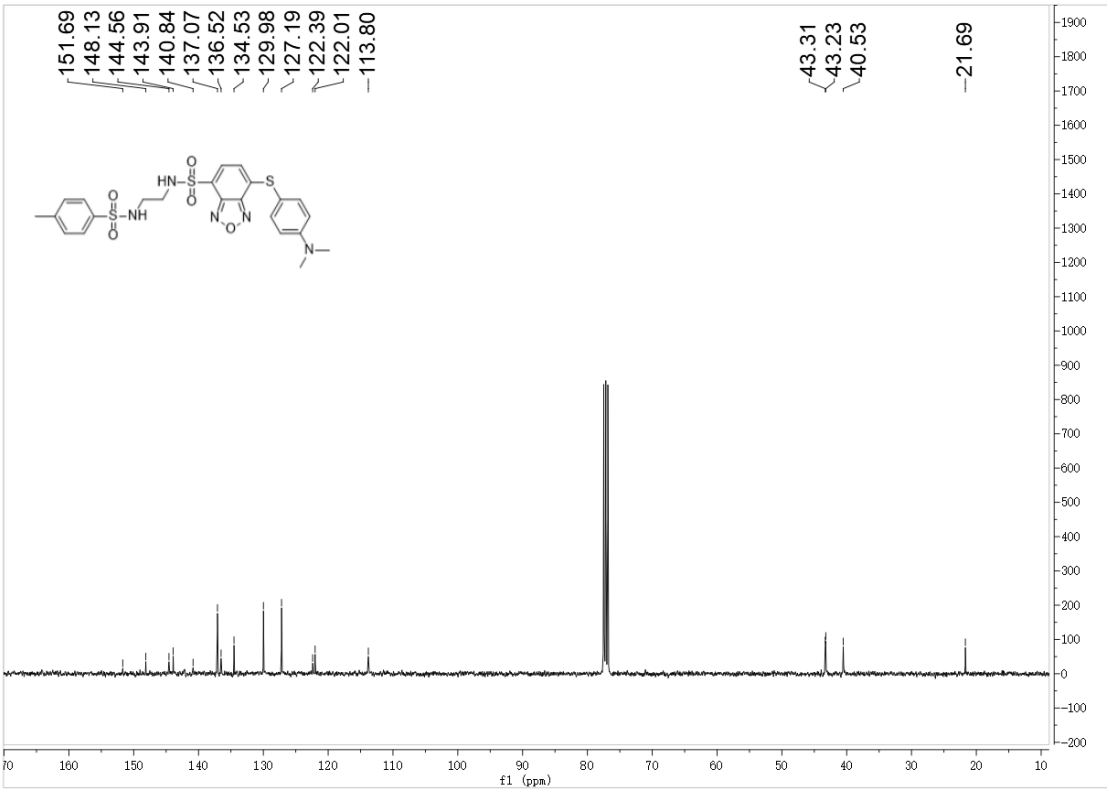

149.36
145.62
143.22
137.59
134.74
131.17
130.09
128.34
126.90
125.75
49.07
42.67
21.42
f1 (ppm)

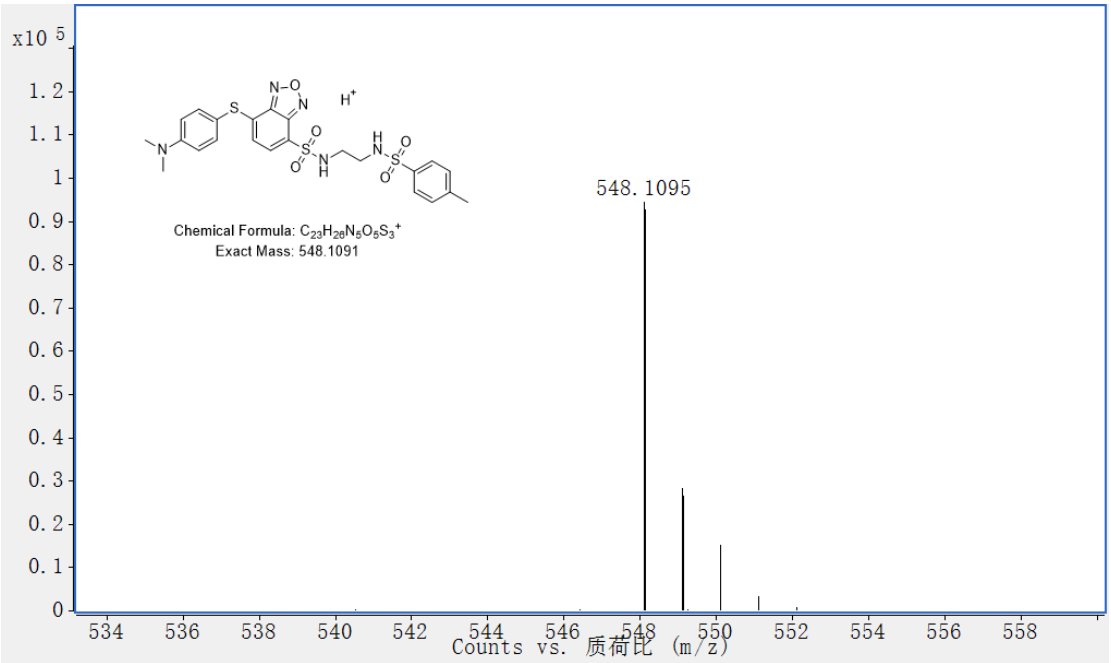

453.0068
455.0030
454.0118
448.0529
Mass/Charge
Chemical Formula: C15H15ClN4NaO5S2+
Exact Mass: 453.0065


8.32
8.30
8.29
8.25
8.25
8.24
8.23
8.23
8.22
7.95
7.93
7.81
7.80
7.80
7.78
7.78
7.77
7.61
7.59
7.57
7.54
7.52
7.51
7.37
7.35
3.03
3.02
3.00
2.98
2.73
2.72
2.70
2.68
2.37
f1 (ppm)


149.09
147.13
144.89
142.76
139.62
137.13
133.89
132.11
132.01
129.63
128.26
127.78
126.43
124.62
42.41
42.25
20.95
NO2
HN
NH
f1 (ppm)


7.73
7.71
7.68
7.66
7.46
7.44
7.29
7.27
6.84
6.82
3.18
3.17
3.16
3.07
2.41
HN
NH
N
1.00
2.01
2.00
2.01
2.00
1.01
0.99
1.01
2.06
8.06
3.04
f1 (ppm)


151.69
148.13
144.56
143.91
140.84
137.07
136.52
134.53
129.98
127.19
122.39
122.01
113.80
43.31
43.23
40.53
21.69
f1 (ppm)


x10 5
548.1095
Chemical Formula: C23H26N5O5S3+
Exact Mass: 548.1091
Counts vs. 质荷比 (m/z)