

Supporting Information

Constructing fluorescent probe for specific detection of cysteine over homocysteine and glutathione based on a novel cysteine-binding group but-3-yn-2-one

Yawei Liu,^a Song Zhang,^b Xin Lv,^a Yuan-Qiang Sun,^a Jing Liu,^a and Wei Guo^{*a}

^a School of Chemistry and Chemical Engineering and Institute of Biotechnology, Shanxi University, Taiyuan 030006, China.

^b Shanxi Academy of Analytical Sciences

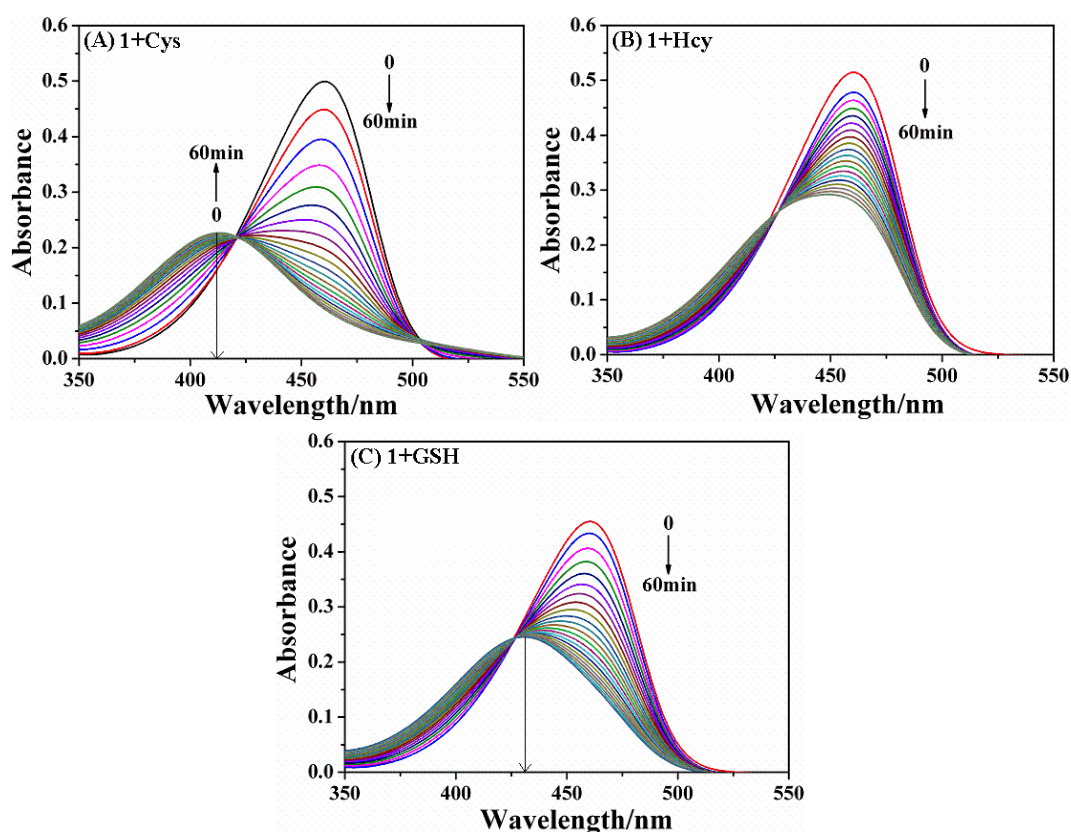


Figure S1 Time-dependent absorption spectra of **1** (10 μM) in the presence of 20 equiv of Cys (A), Hcy (B), and GSH (C) in PBS buffer (20 mM, pH 7.4) at 37 °C.

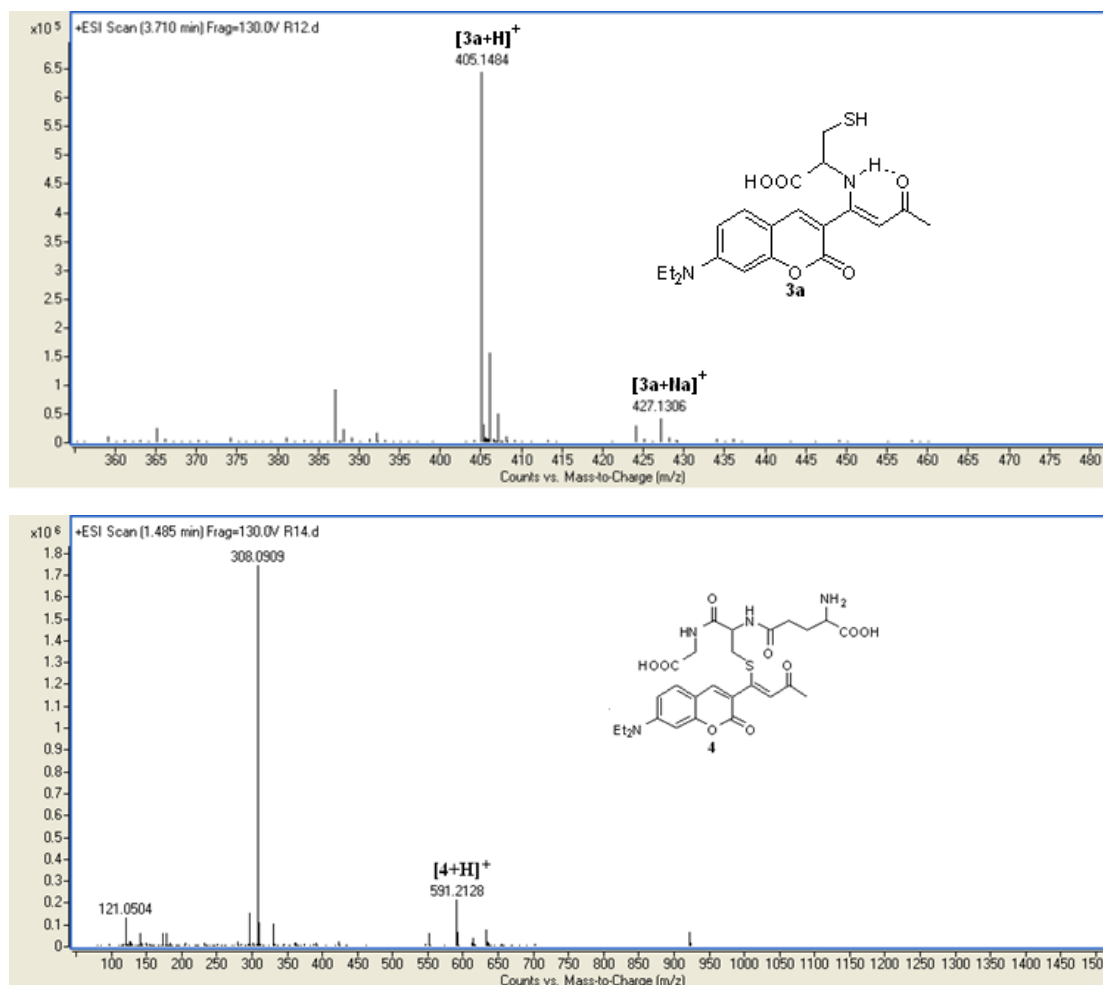


Figure S2 HRMS charts of **1** treated with excess of Cys (above) or GSH (below).

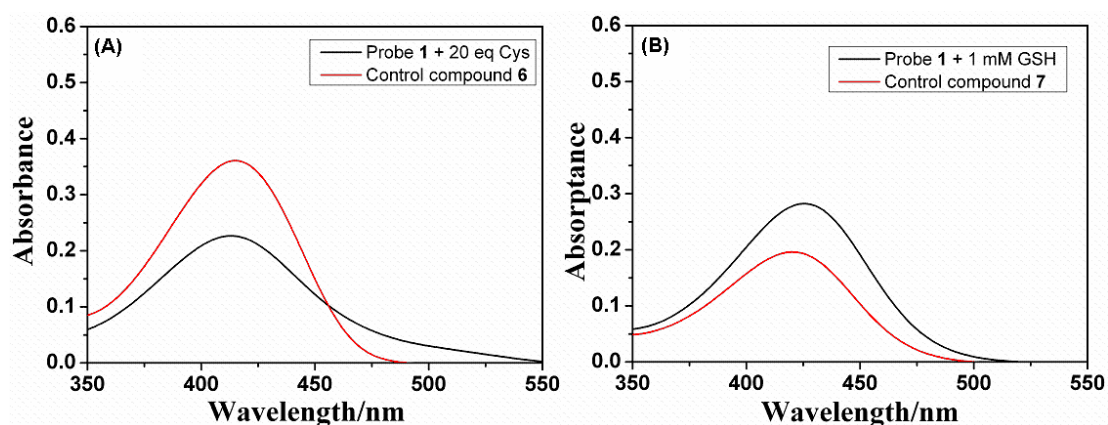


Figure S3 Absorption spectrum of **1** (10 μ M) upon addition of 20 equiv of Cys (A) (or Hcy (B)) vs that of control compound **6** (**7**).

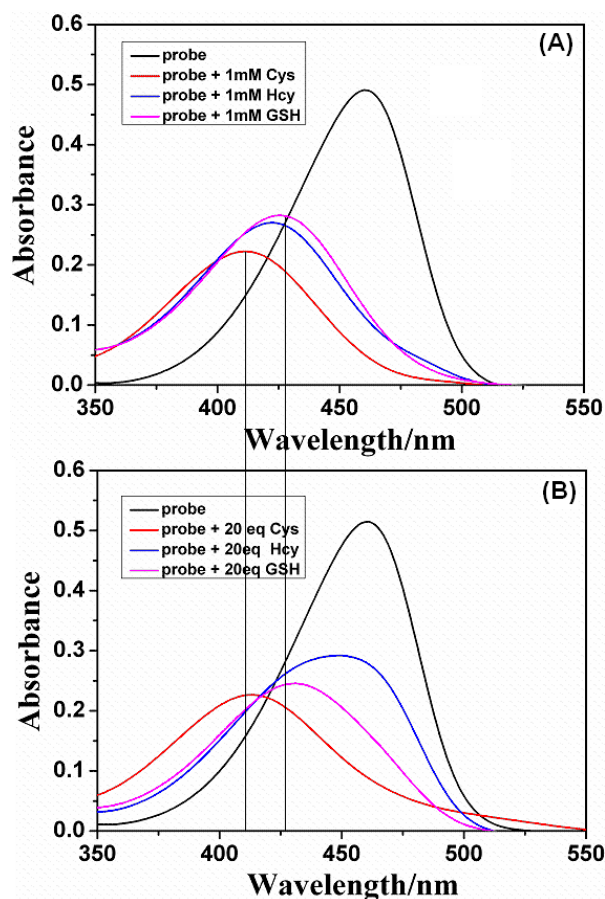


Figure S4 Absorption spectra of **1** (10 μM) treated with 1 mM (above) and 0.2 mM (20 equiv, below) of Cys, Hcy, and GSH, respectively, in PBS buffer (20 mM, pH 7.4) at 37 °C after 60 min.

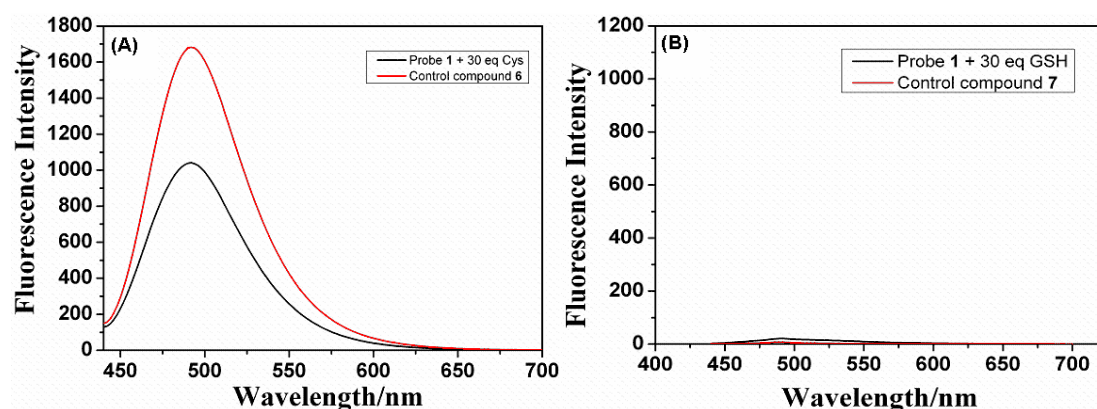


Figure S5 (A) Fluorescence spectrum of probe **1** (5 μM) treated with 30 equiv. of Cys vs that control compound **6**. (B) Fluorescence spectrum of probe **1** (5 μM) treated with 30 equiv. of GSH vs that control compound **7**.

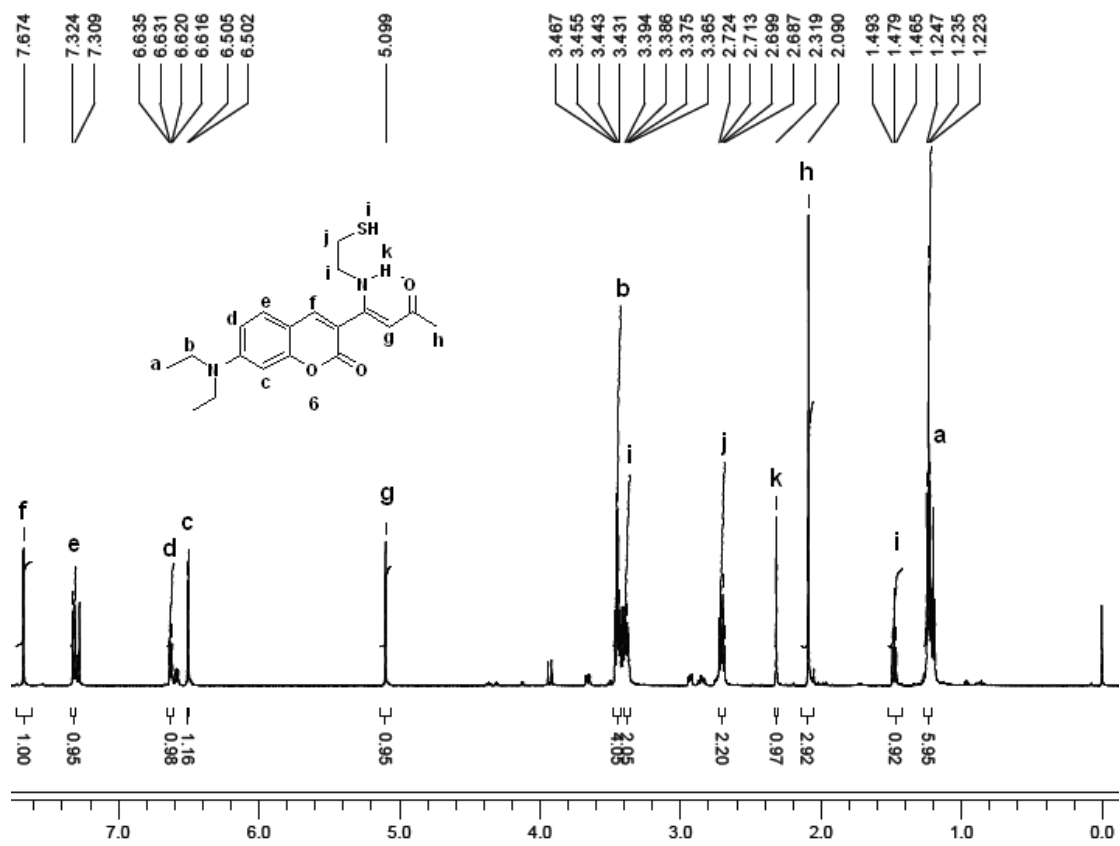
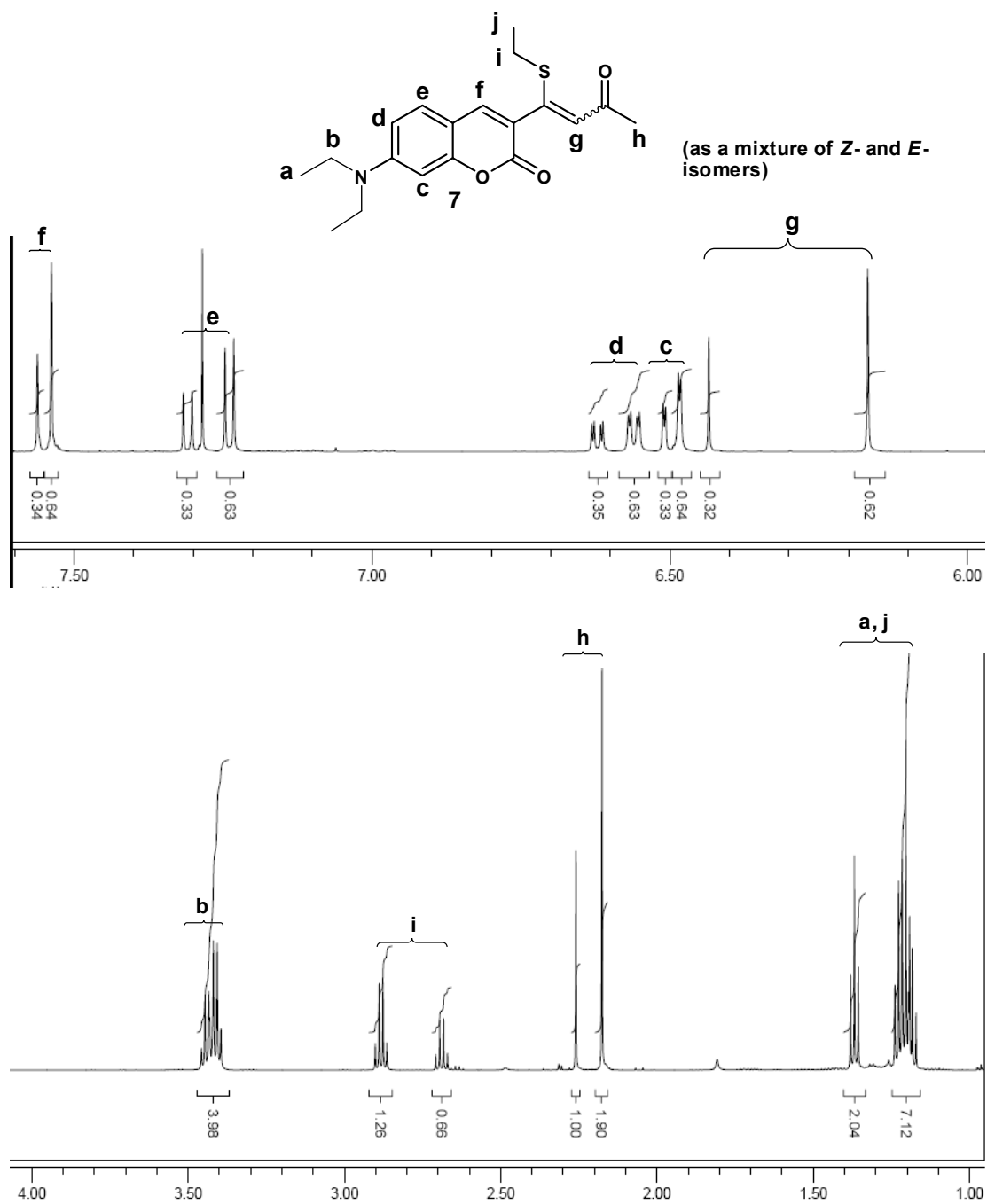


Figure S6 ¹H NMR charts of **6** (CDCl₃, 600 MHz).



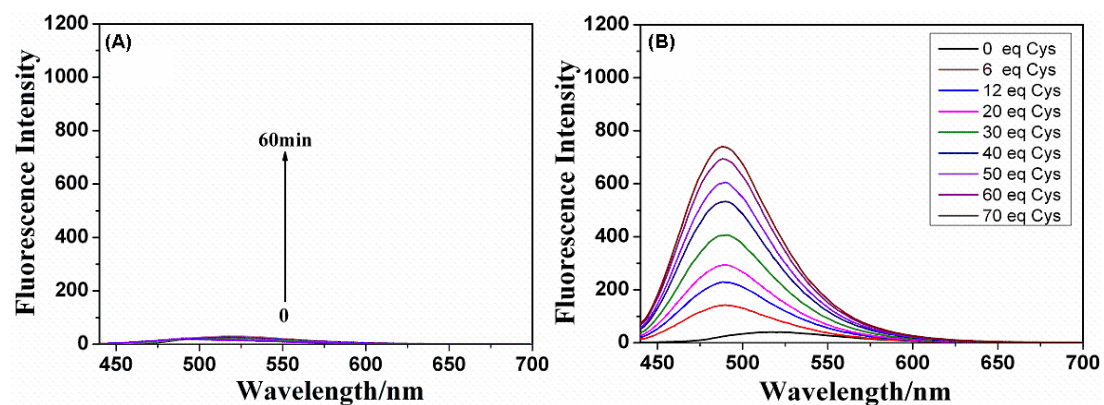


Figure S8 (A) Time-dependent fluorescence spectra of probe **1** (5 μM) treated with 1 mM of GSH. (B) Fluorescence spectra of probe **1** treated with the mixtures of GSH (1 mM)/Cys (0–70 equiv).

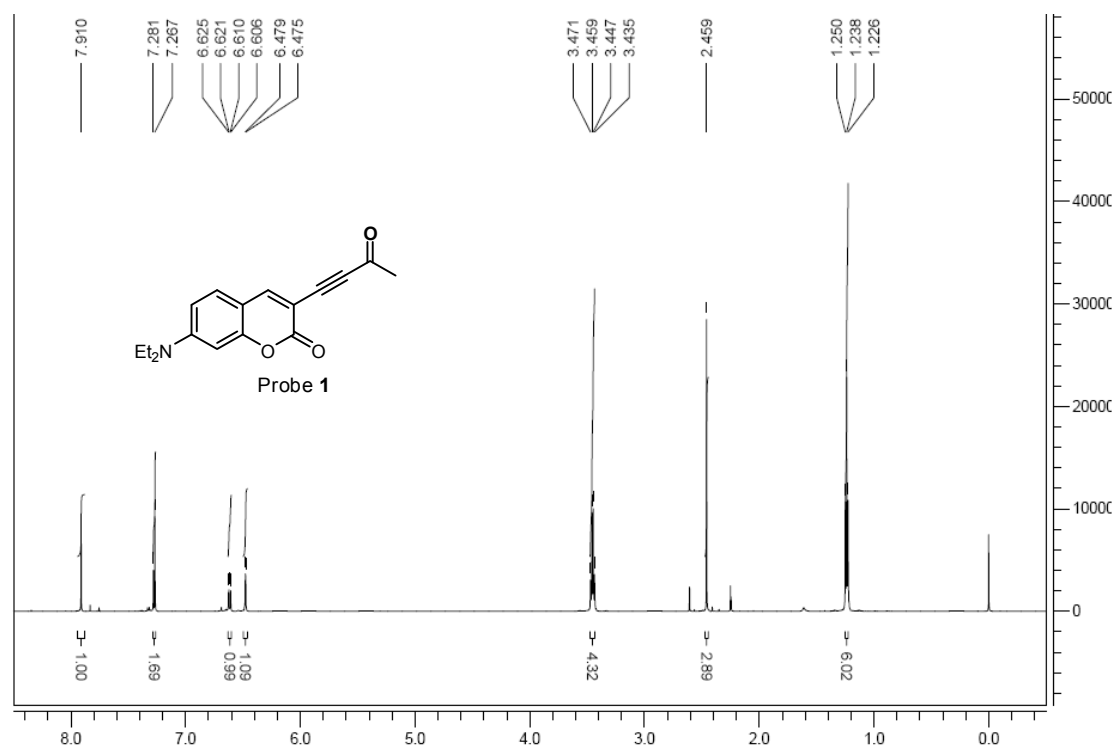


Figure S9 ¹H NMR charts of probe **1** (CDCl₃, 600 MHz).

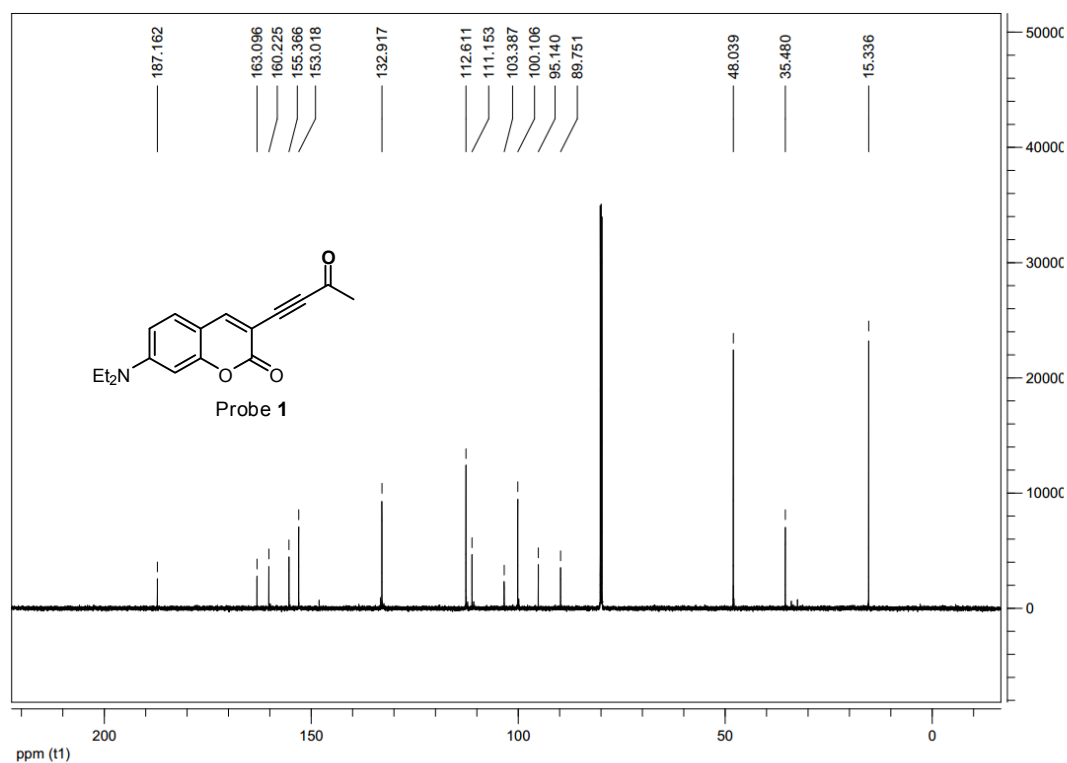


Figure S10 ^{13}C NMR charts of probe **1** (CDCl_3 , 150 MHz).

| Sample | Formula (M) | Ion Formula | Measured m/z | Calc m/z | Diff (ppm) |
|----------------|--|--|--------------|----------|------------|
| Probe 1 | $\text{C}_{17}\text{H}_{17}\text{N}\text{O}_3$ | $\text{C}_{17}\text{H}_{18}\text{N}\text{O}_3$ | 284.1284 | 284.1281 | -0.91 |

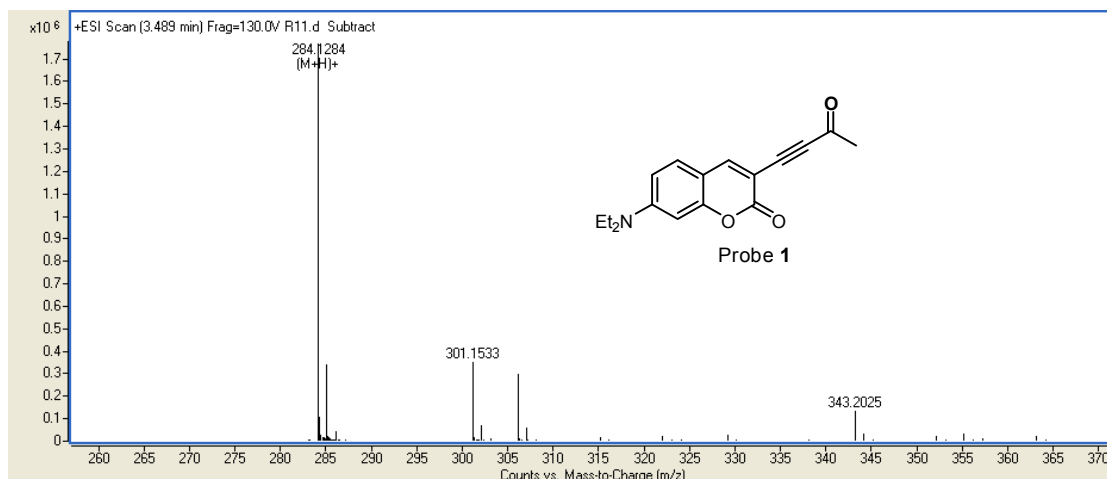


Figure S11 HRMS charts of probe **1**.

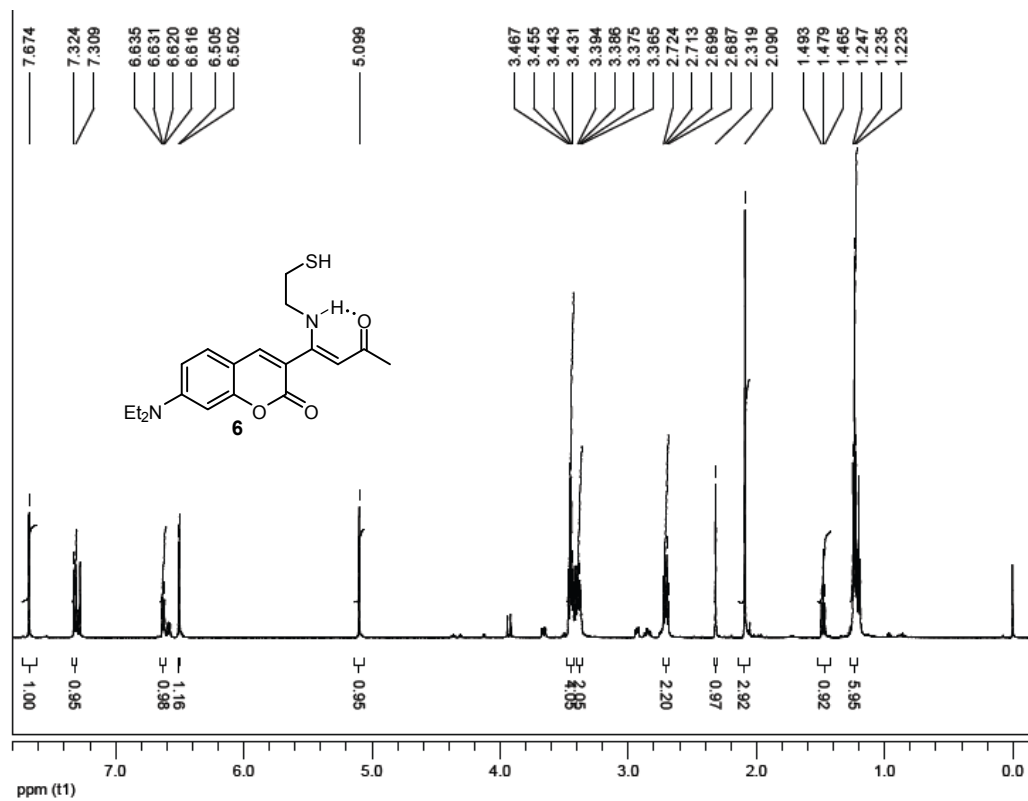


Figure S12 ^1H NMR charts of **6** (CDCl_3 , 600 MHz).

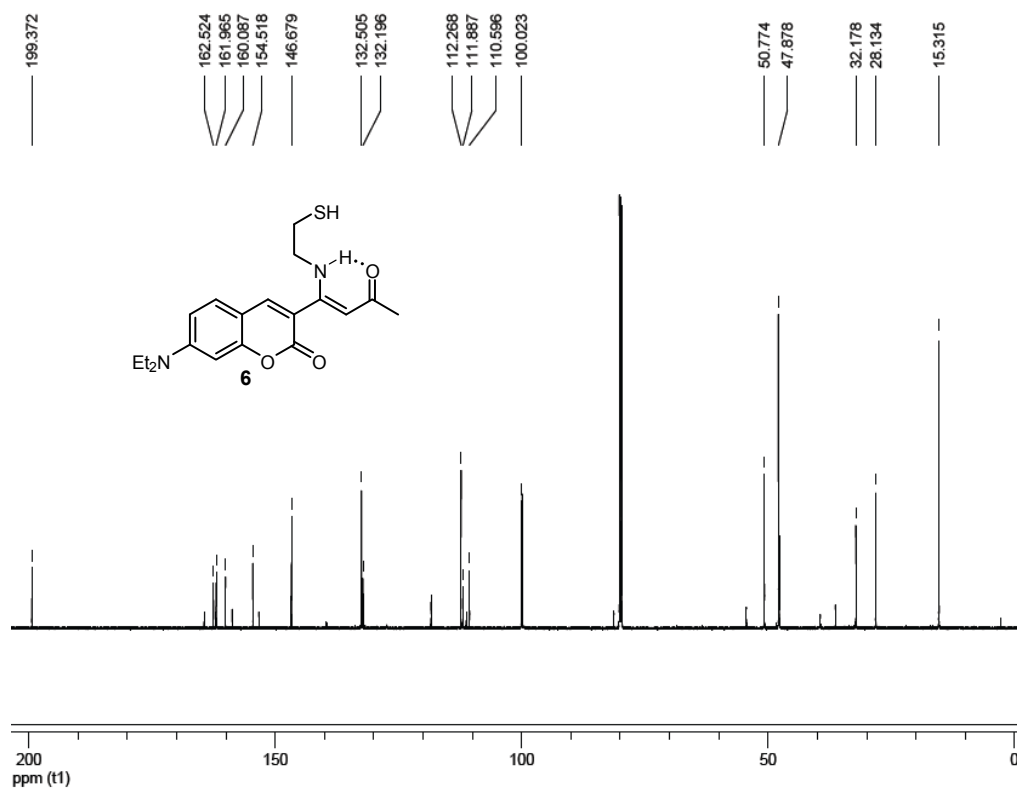


Figure S13 ^{13}C NMR charts of **6** (CDCl_3 , 150 MHz).

1_140311133832 #246 RT: 4.09 AV: 1 NL: 1.82E7
T: FTMS + p ESI Full ms [50.00-2000.00]

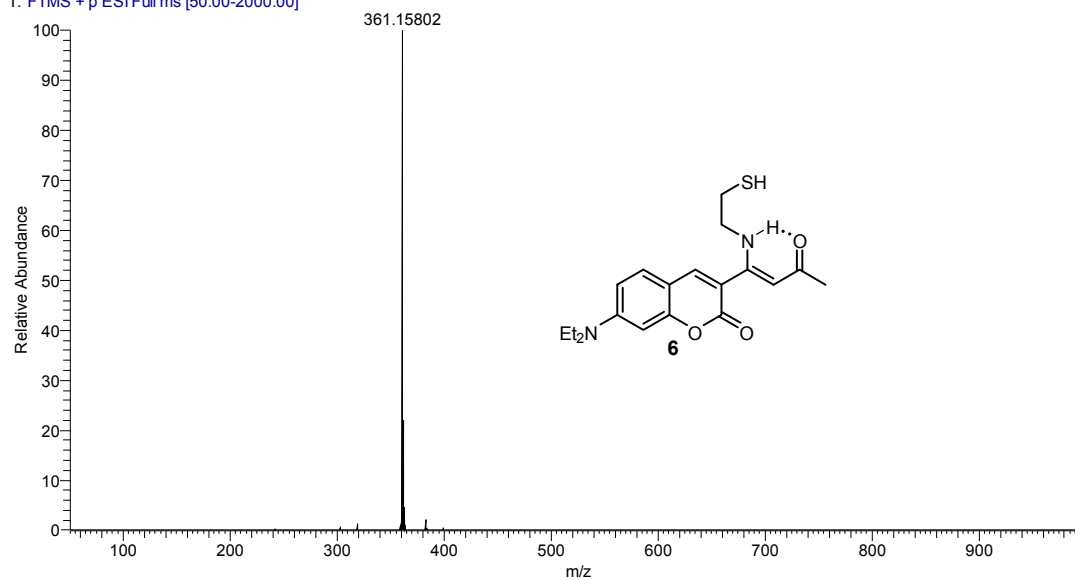


Figure S14 HRMS charts of 6.

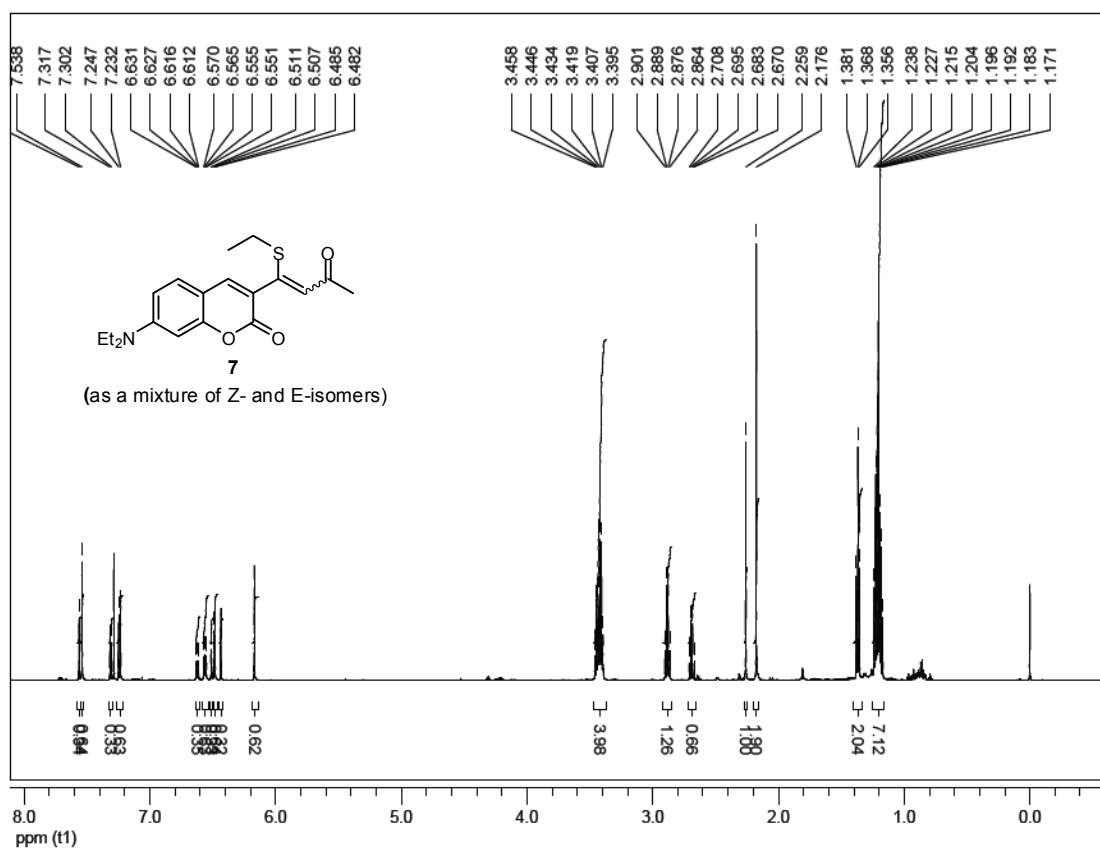


Figure S15 ¹H NMR charts of 7 (CDCl₃, 600 MHz).

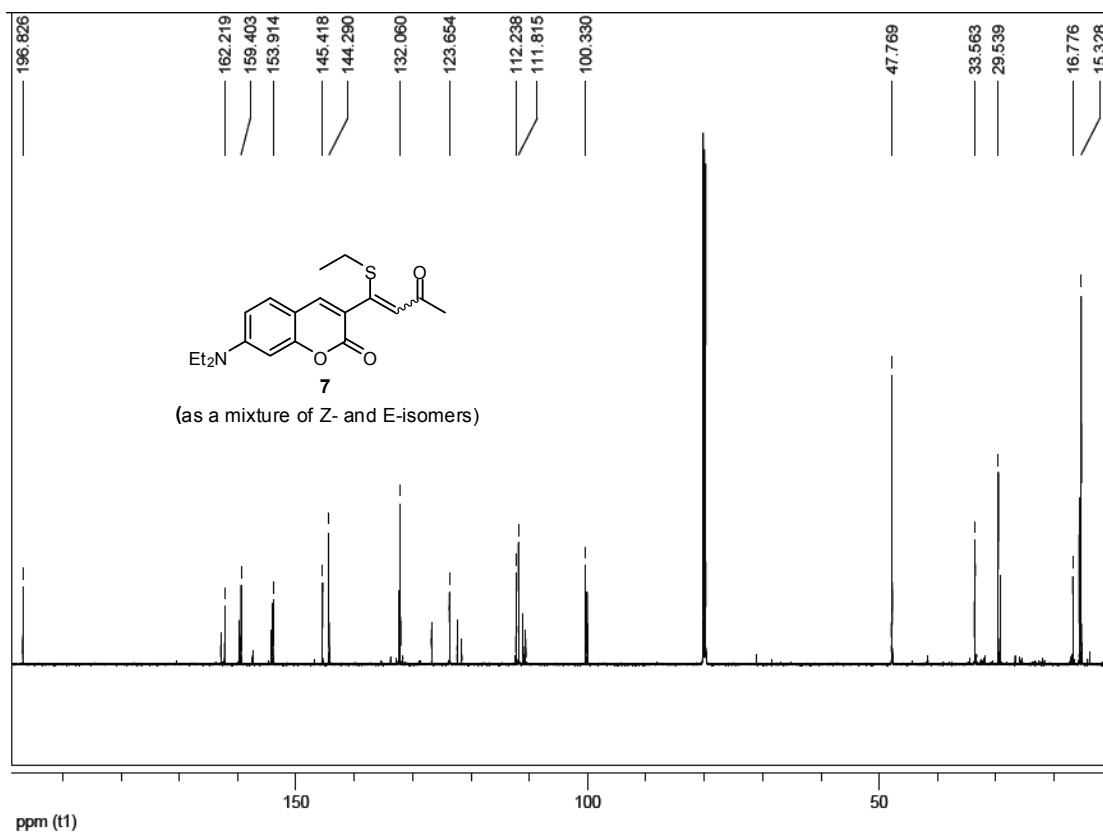


Figure S16 ^{13}C NMR charts of **7** (CDCl_3 , 150 MHz).

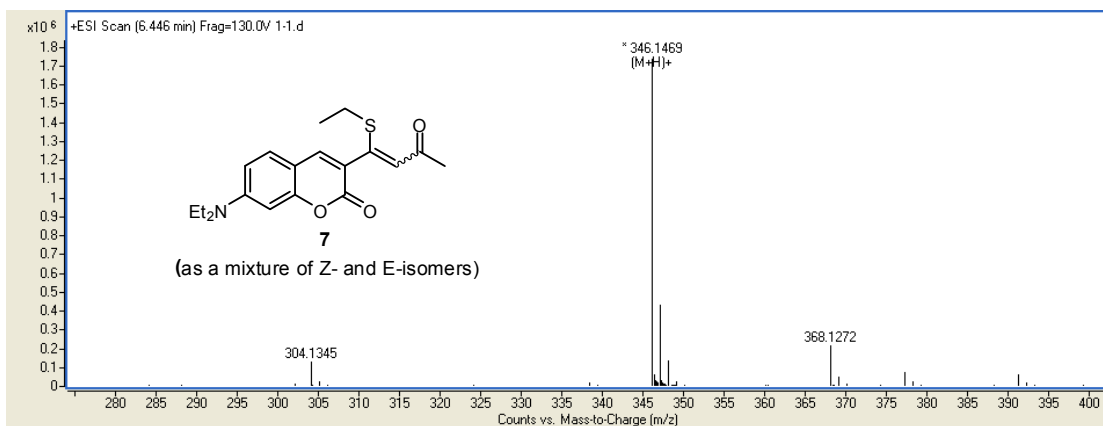


Figure S17 HRMS charts of **7**.