Supplementary Information

For

A squaraine-based red emission off-on chemosensor for biothiols and its application in living cells imaging

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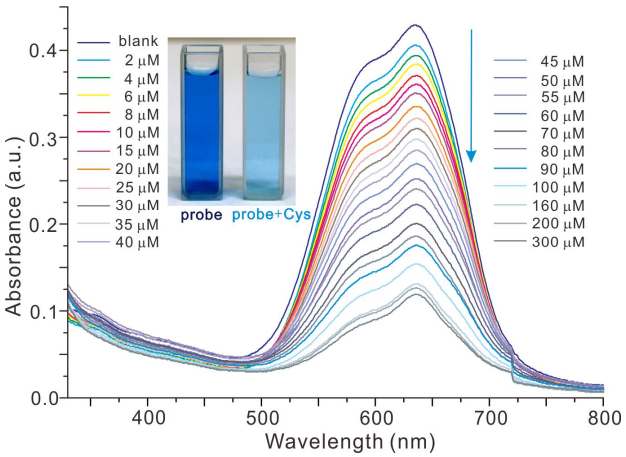

Fig. S1 Absorption spectra of compound **1** (10 μM) upon addition of increasing concentration of Cys. Inset shows naked-eye visible images of **1** (10 μM) in the absence and presence of 300 μM Cys. Conditions: acetonitrile-PBS buffer (20 mM, pH 7.0) solution (1 : 9, v/v, rt).

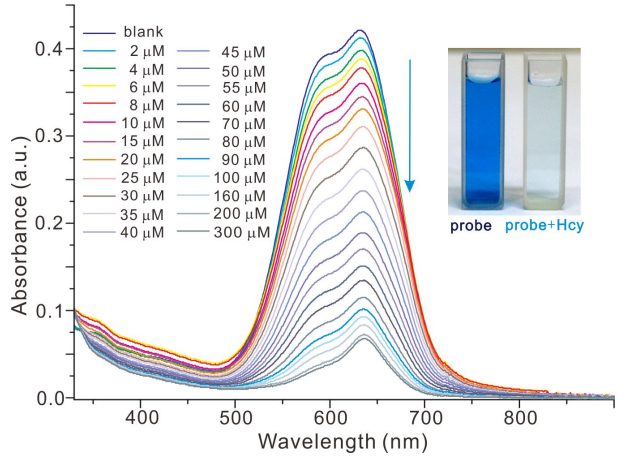

Fig. S2 Absorption spectra of compound **1** (10 μM) upon addition of increasing concentration of Hcy. Inset shows naked-eye visible images of **1** (10 μM) in the absence and presence of 300 μM Hcy. Conditions: acetonitrile-PBS buffer (20 mM, pH 7.0) solution (1 : 9, v/v, rt).

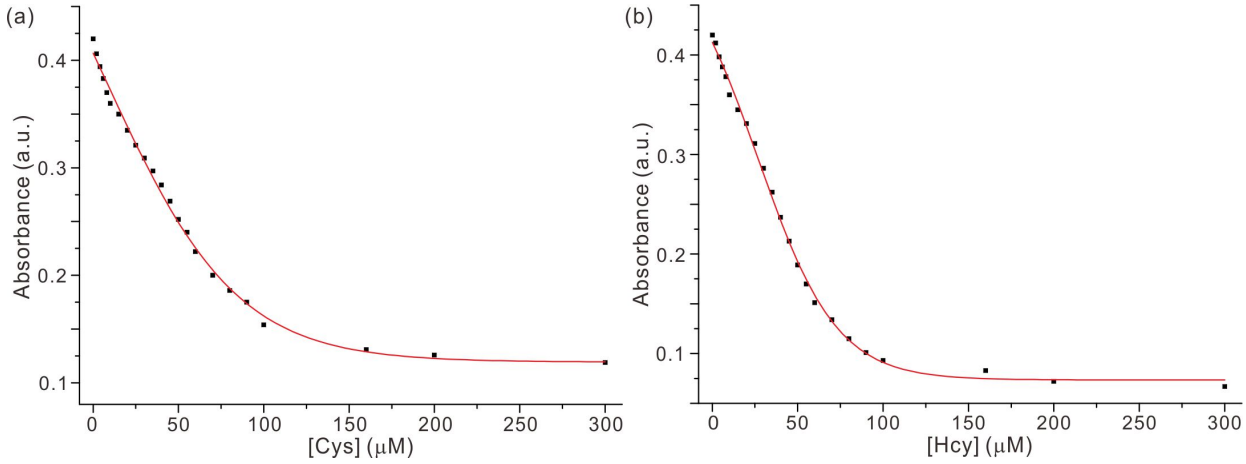

Fig. S3 Absorbance changes of probe **1** against [Cys] (a) and [Hcy] (b).

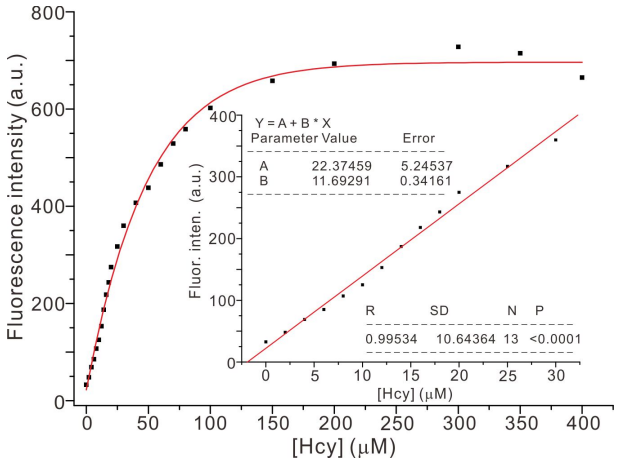

Fig. S4 Fluorescence response of probe **1** (10 μM) at 656 nm upon reacting with Hcy (0 – 400 μM). Inset shows the linear plot of fluorescence intensity at 656 nm of **1** (10 μM) upon addition of Hcy (0 – 30 μM).

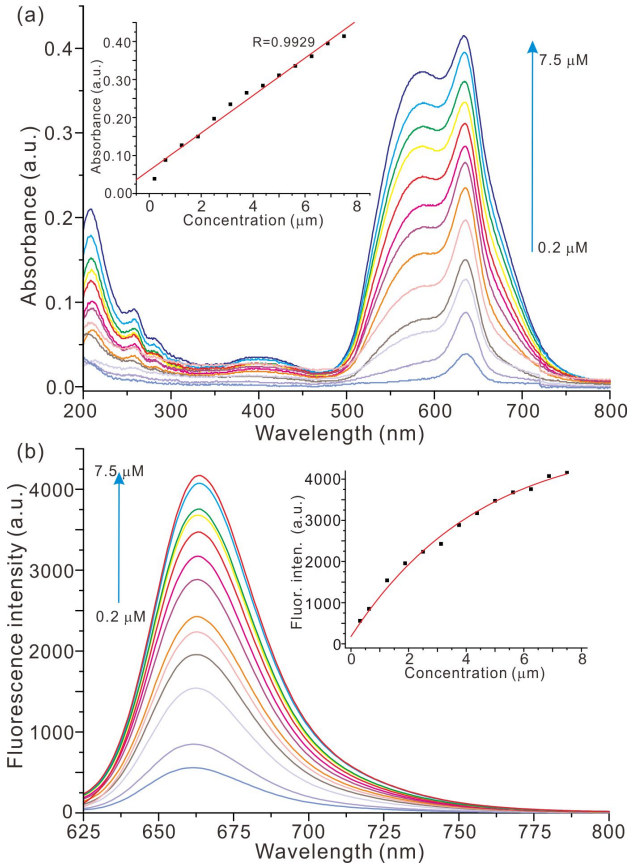

Fig. S5 (a) Absorption spectra of compound **4** at different concentrations in acetonitrile-redistilled water solution (1:9, v/v, rt). Inset shows absorbance values of compound **4** of different concentration at 635 nm; (b) Emission spectra of compound **4** at different concentrations in acetonitrile-redistilled water solution (1:9, v/v, rt). Inset shows fluorescence intensities of compound **4** of different concentration at 656 nm.

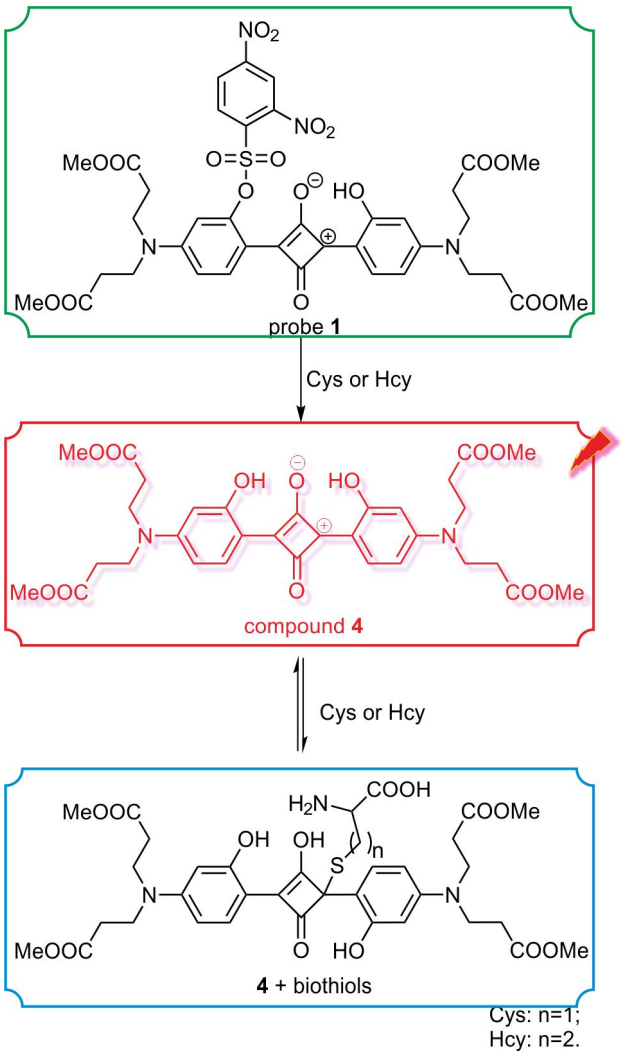

Fig. S6 The proposed simplified reaction mechanism of probe **1** with Cys or Hcy.

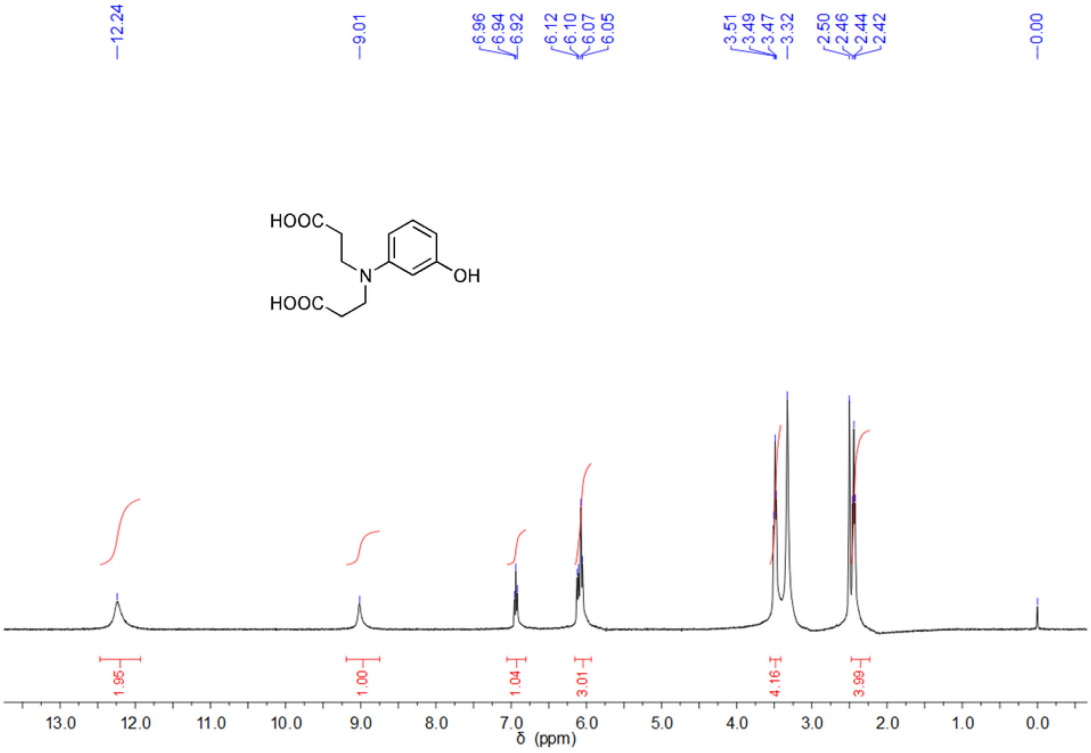

Fig. S7 ^{1}H NMR (400 MHz) of **2** in DMSO-d_6.

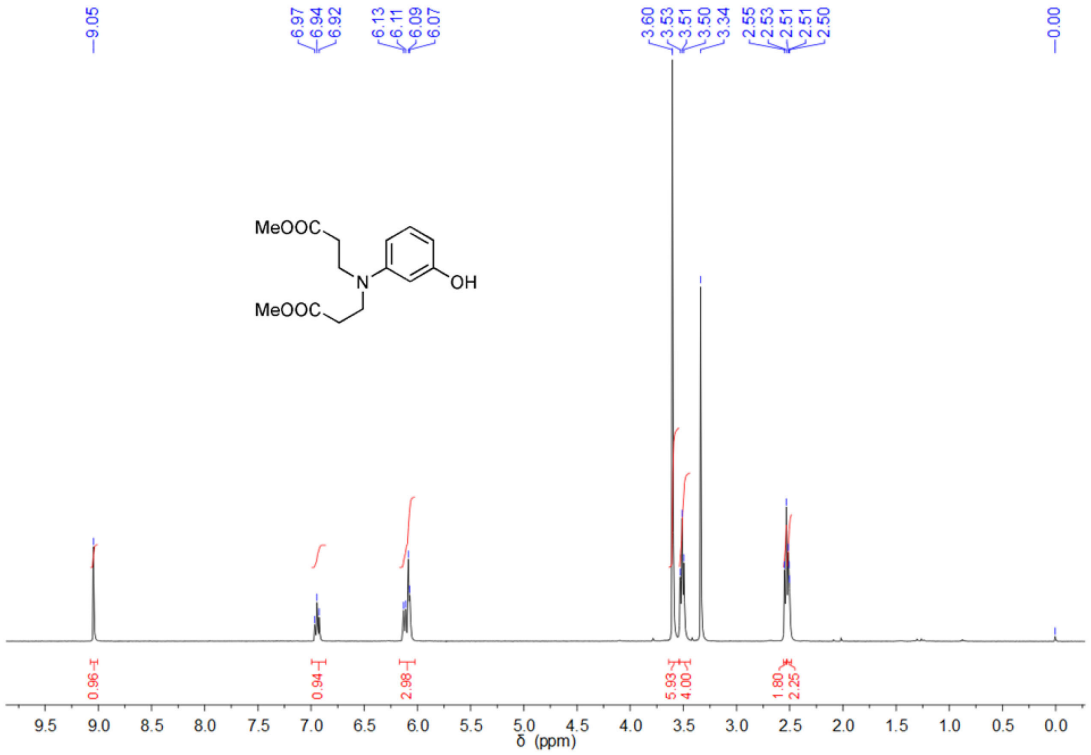

Fig. S8 ^{1}H NMR (400 MHz) of **3** in DMSO-d_6.

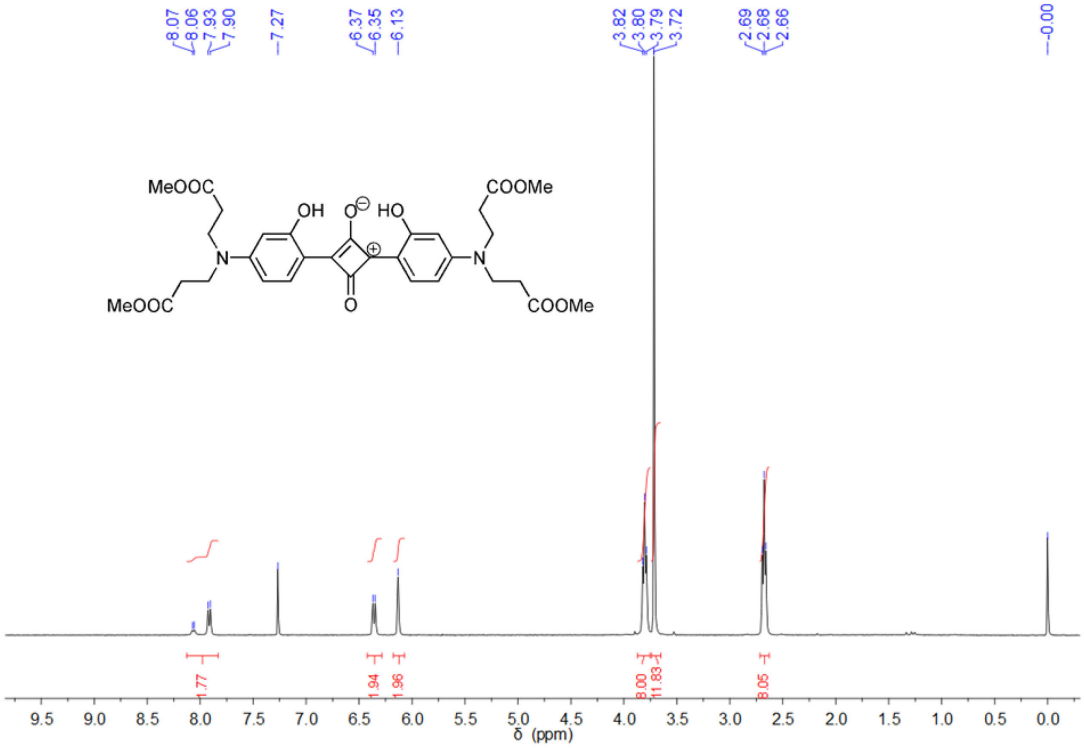

Fig. S9 ^{1}H NMR spectra (400 MHz) of **4** in $CDCl_3$.

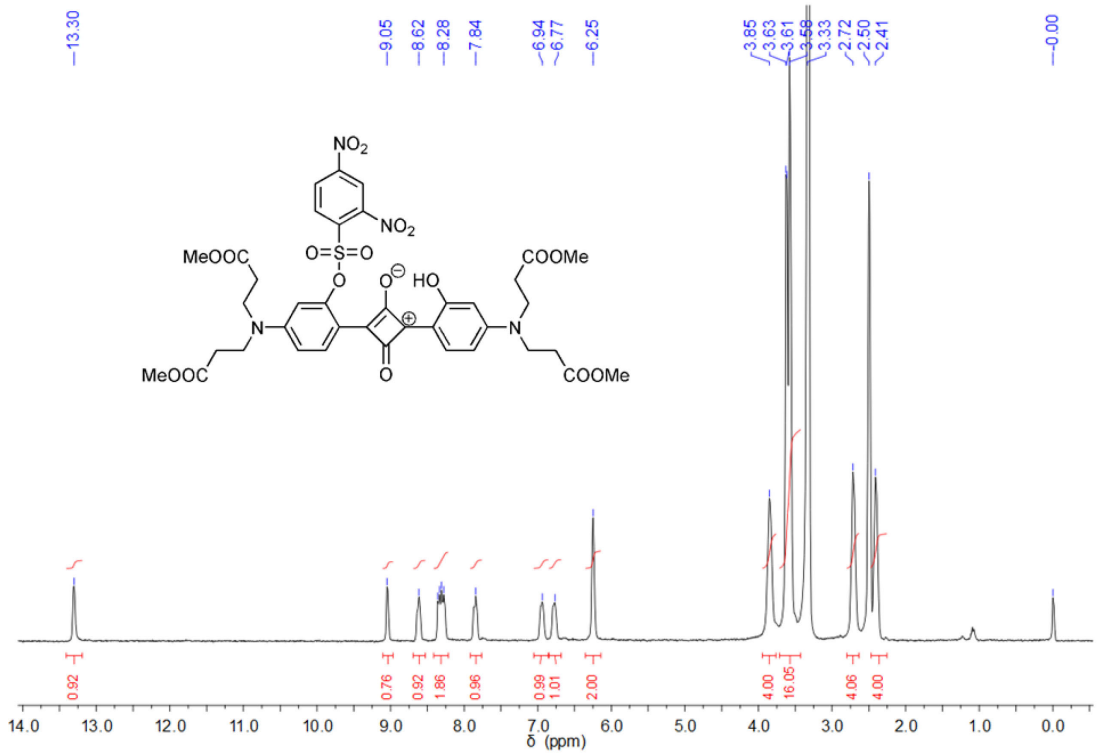

Fig. S10 ^{1}H NMR (300 MHz) of **1** in DMSO-d_6.

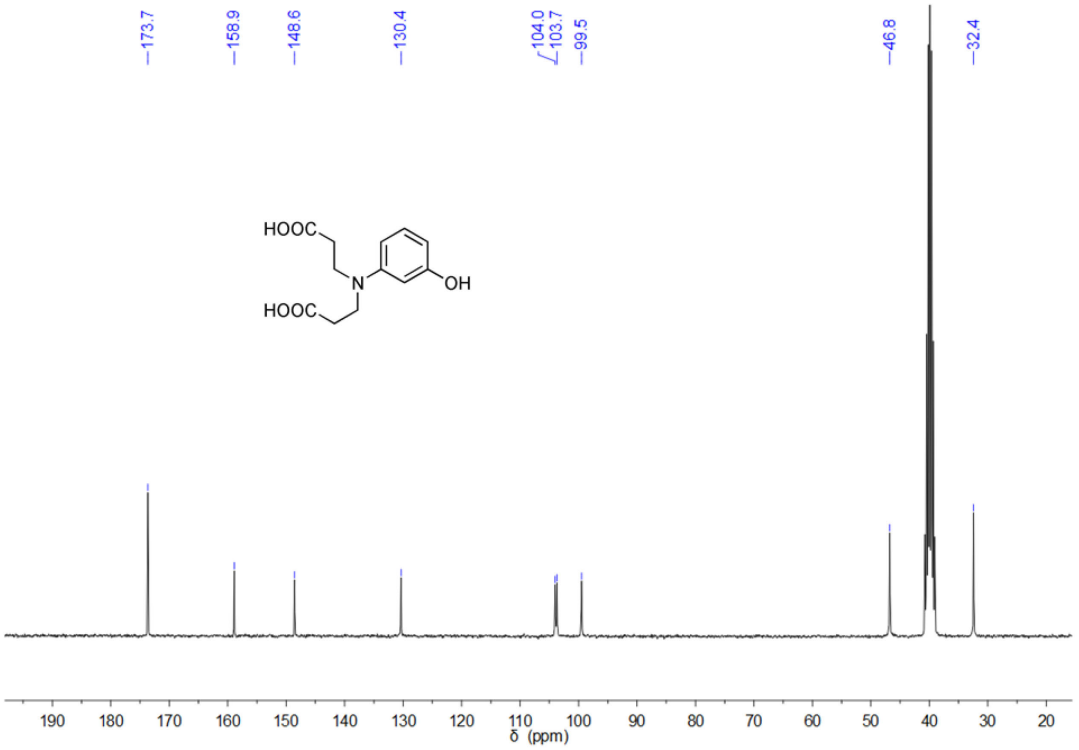

Fig. S11 ^{13}C NMR (75 MHz) of **2** in DMSO-d_6.

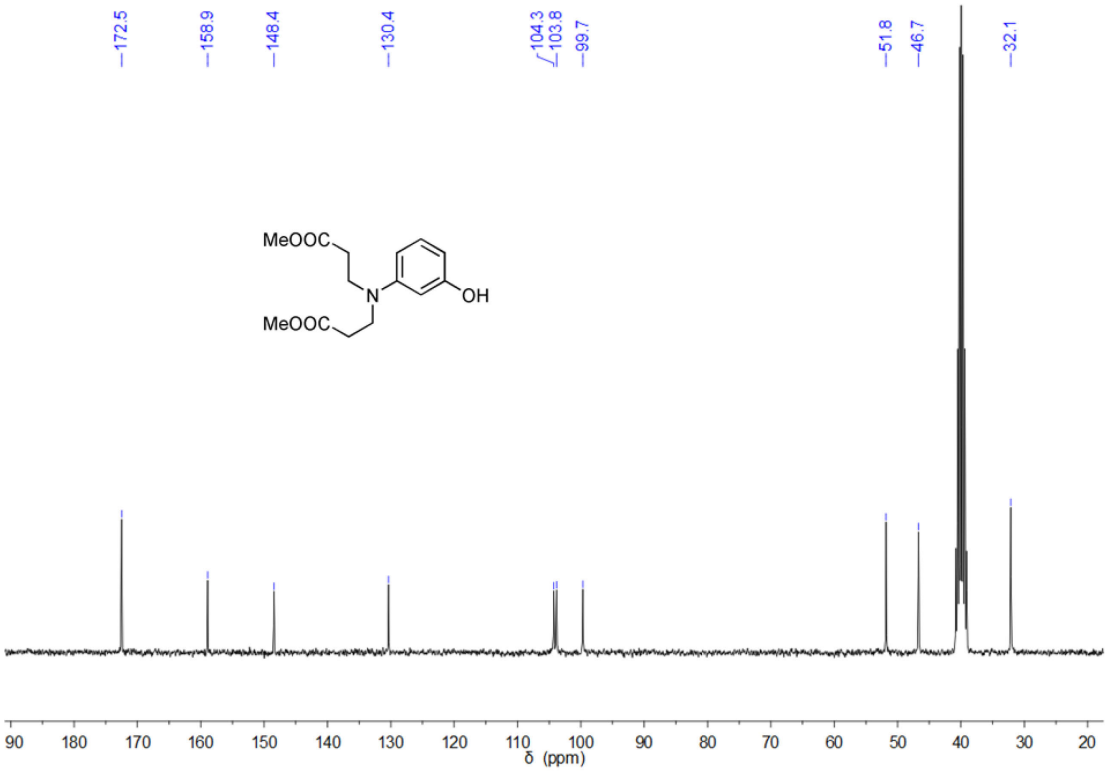

Fig. S12 ^{13}C NMR (75 MHz) of **3** in DMSO-d_6.

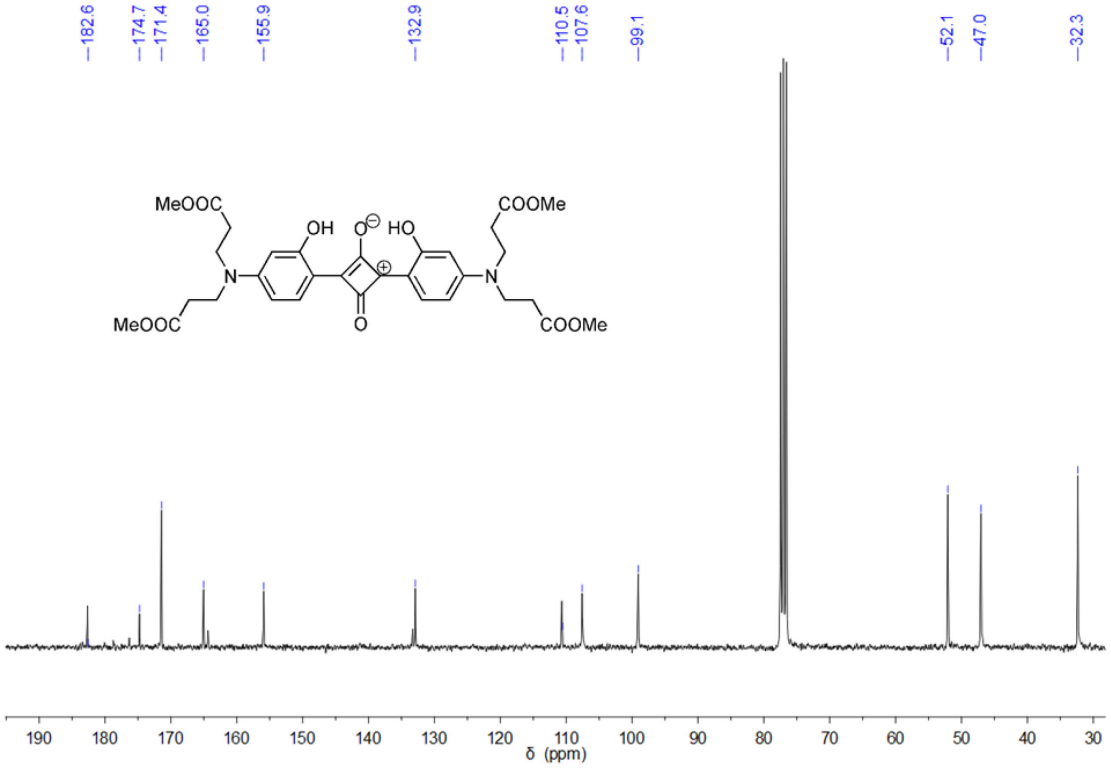

Fig. S13 ^{13}C NMR (75 MHz) of **4** in $CDCl_3$.

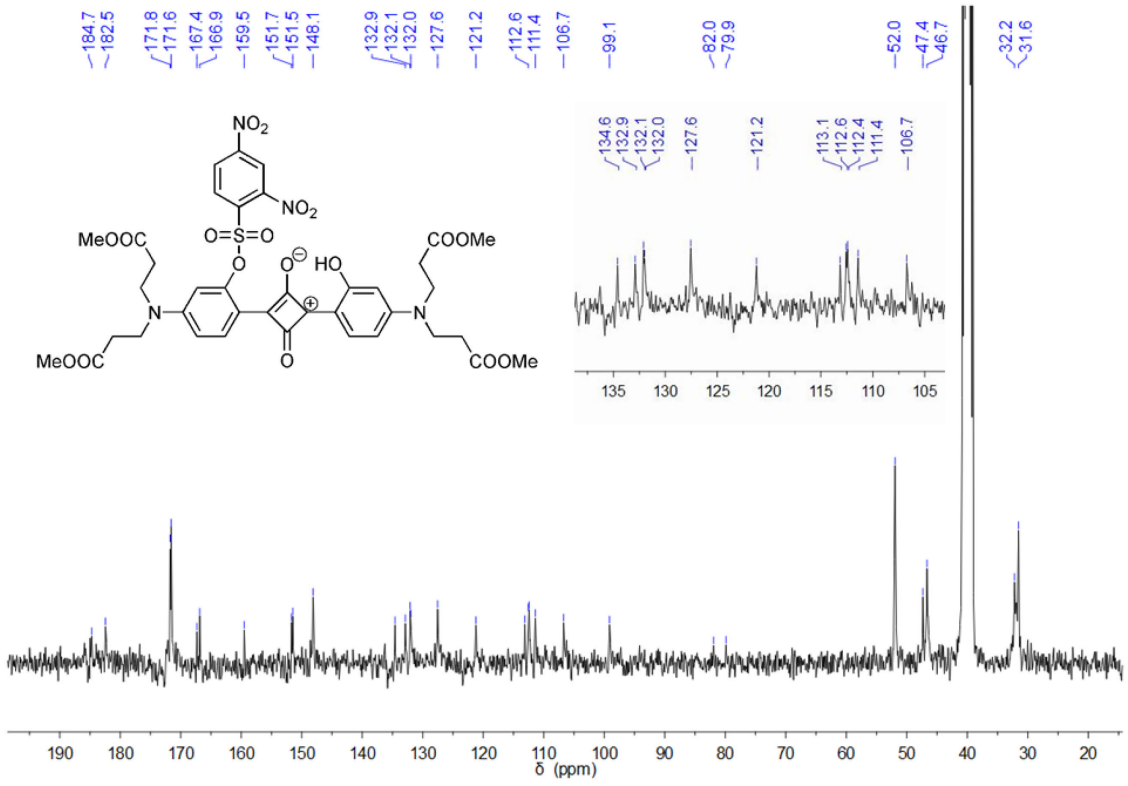

Fig. S14 ^{13}C NMR (75 MHz) of **1** in DMSO-d_6.

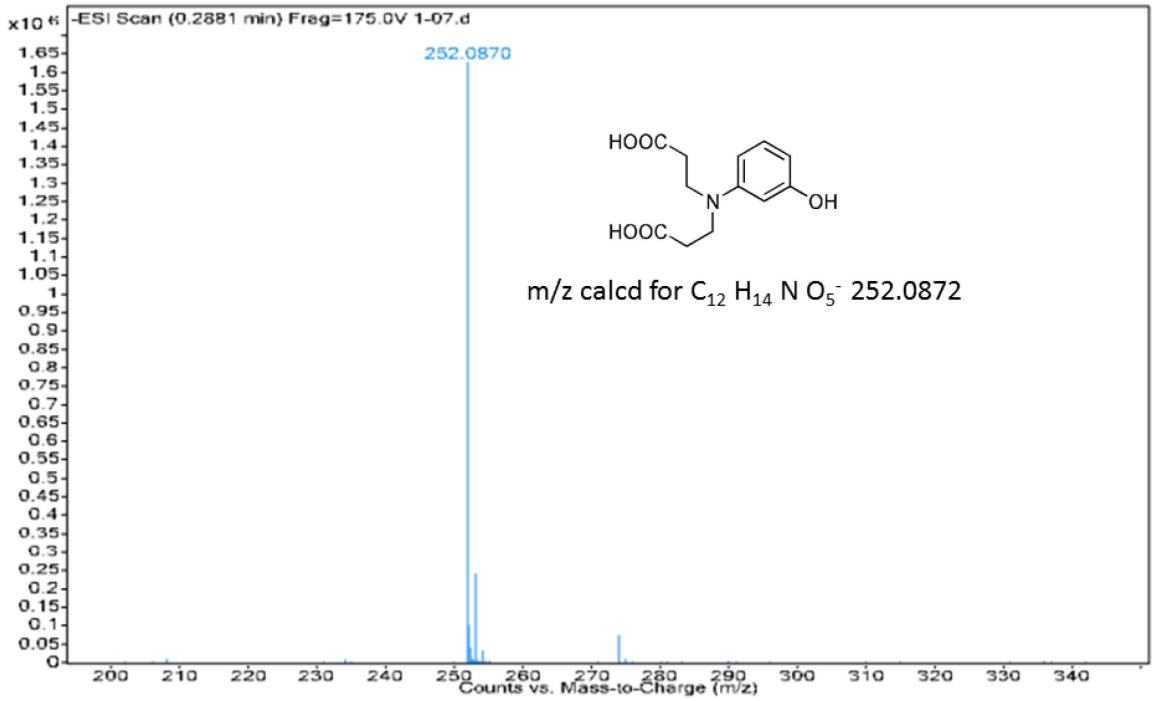

Fig. S15 HRMS of **2**.

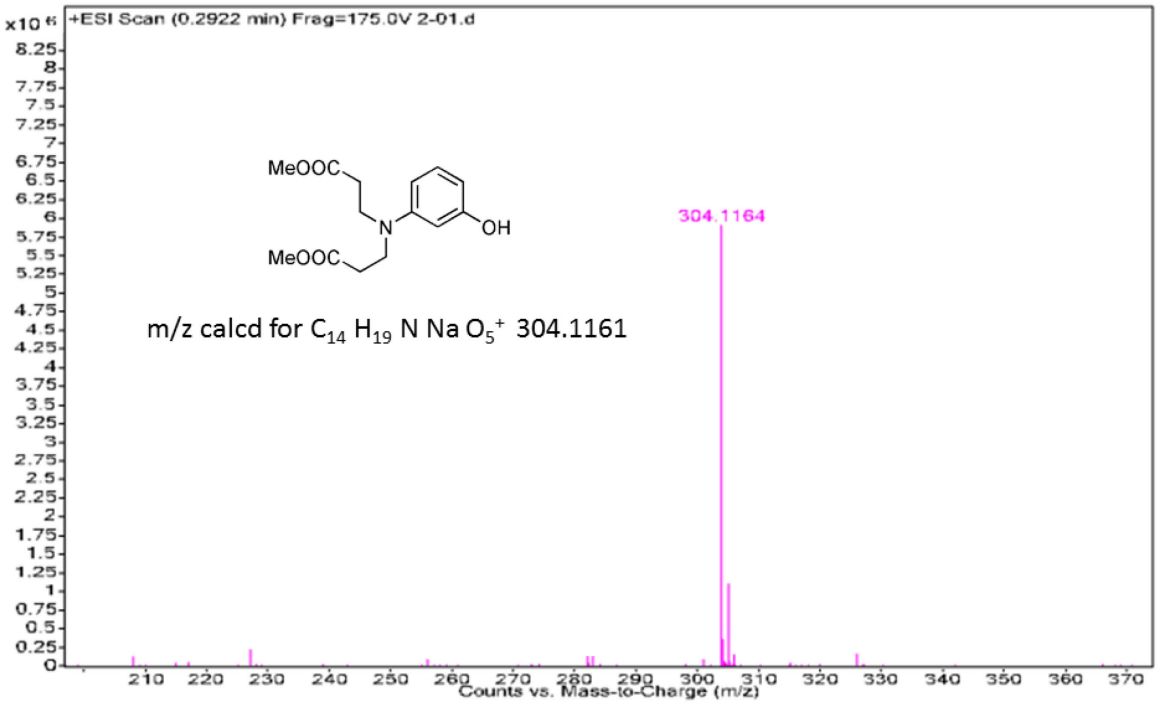

Fig. S16 HRMS of **3**.

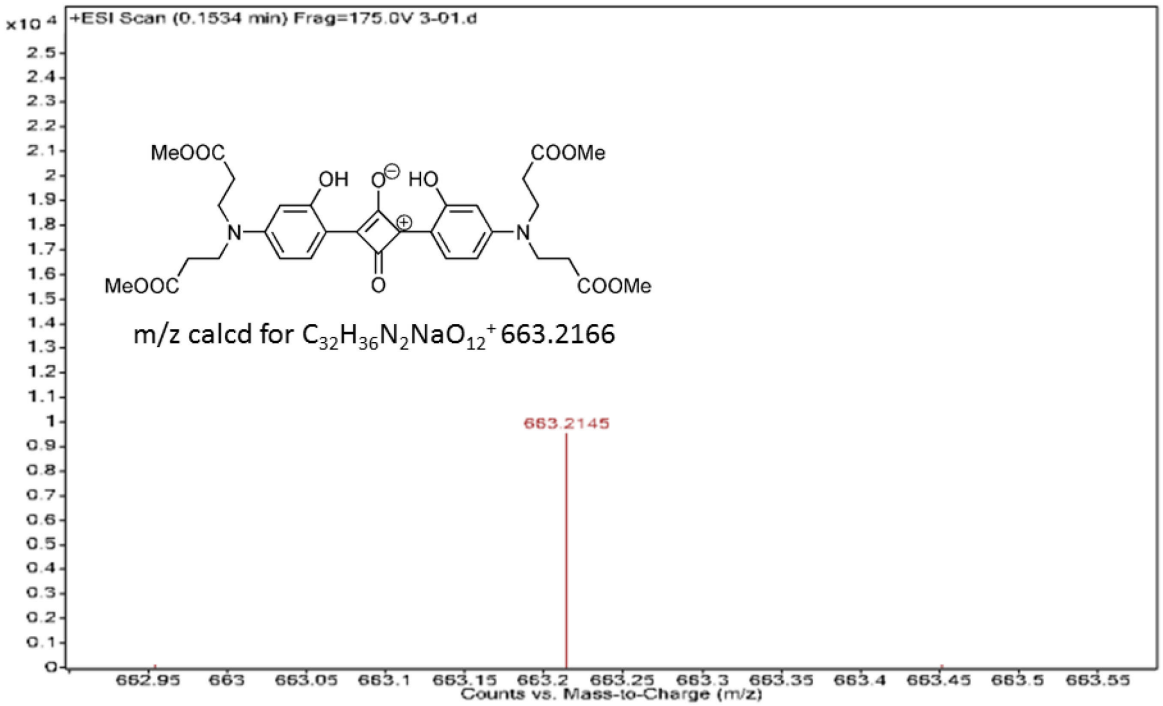

Fig. S17 HRMS of **4**.

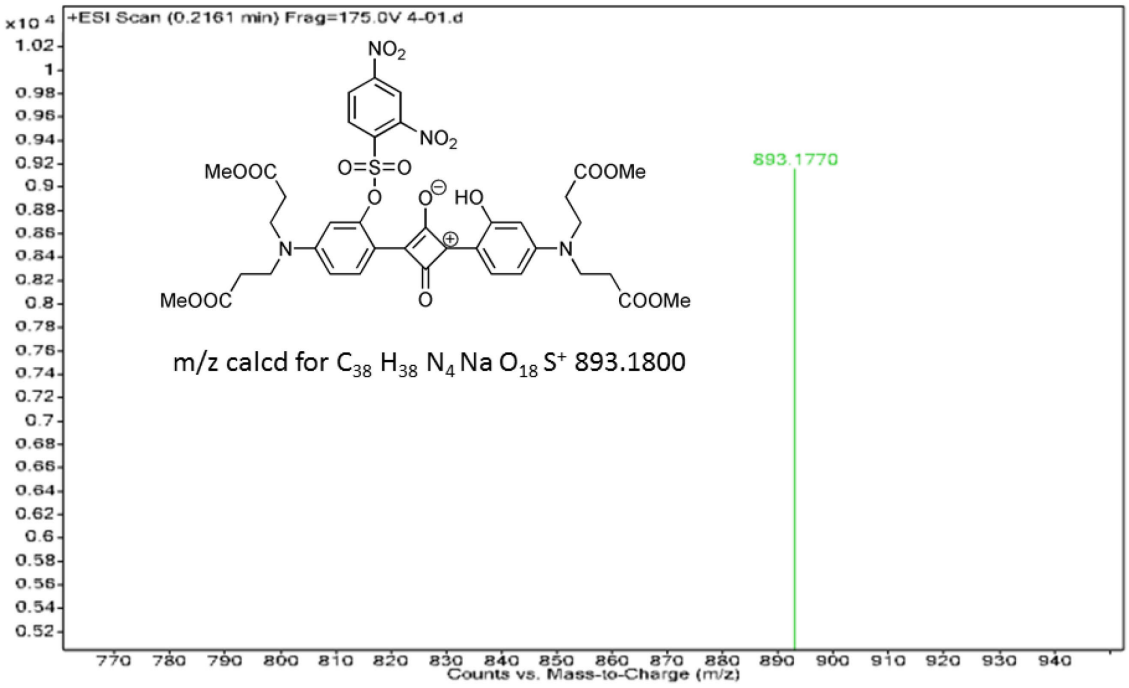

Fig. S18 HRMS of **1**.

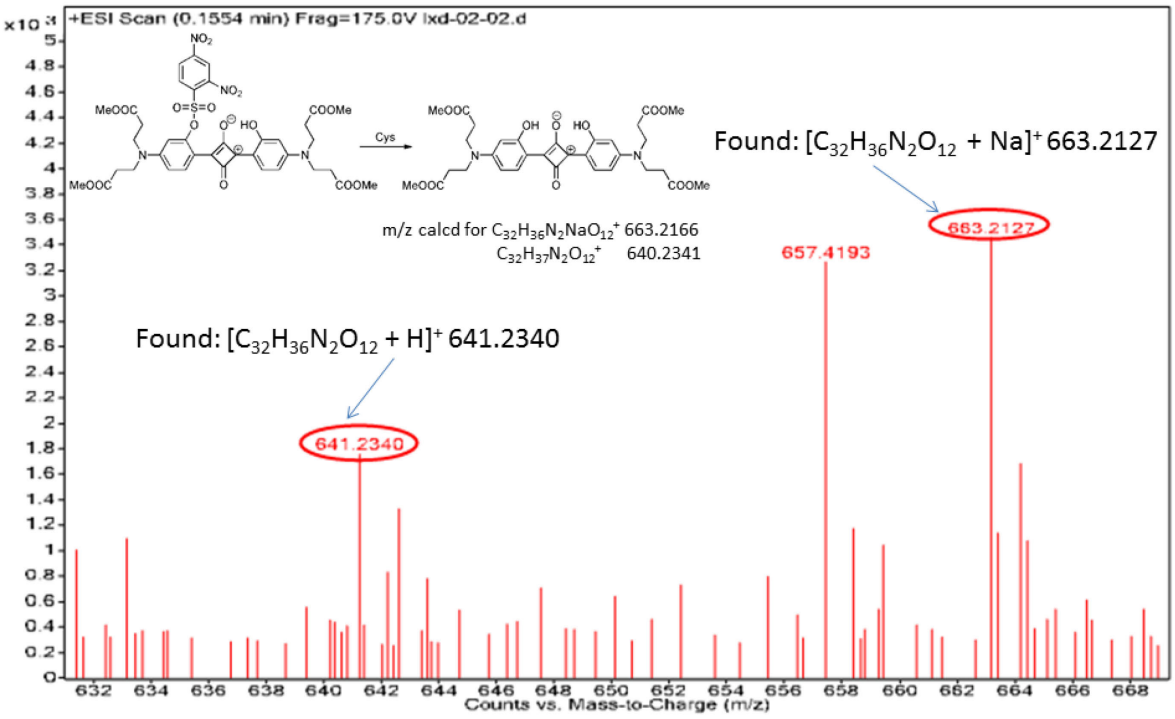

Fig. S19 HRMS of probe **1** reacting with Cys (5 equiv.) in acetonitrile - distilled water (1 : 9, v/v) at room temperature.