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 (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.
**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).

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m/z calcd for $\text{C}_{32}\text{H}_{36}\text{N}_{2}\text{NaO}_{12}^+$ 663.2166

Fig. S18 HRMS of 1.

m/z calcd for $\text{C}_{38}\text{H}_{38}\text{N}_{4}\text{NaO}_{18}^+$ 893.1800
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