Supporting Information

A Highly Selective Ratiometric Fluorescent Probe for Biothiol and Imaging in Live Cells

Baozhen Gao[a], Lixia Cui[a], Yong Pan[b], Guomei Zhang[a], Ying Zhou[a], Caihong Zhang[a,*], Shaomin Shuang[a], Chuan Dong[a,*]

Table of Contents:

*Corresponding authors: E-mail: chzhang@sxu.edu.cn (C. Zhang); Tel: +86 351 7010588; Fax: +86 351 7018613
*Corresponding authors: E-mail: dc@sxu.edu.cn (C. Dong); Tel: +86 351 7010588; Fax: +86 351 7018613

1. ^{1}H NMR, ^{13}CNMR and MS spectra of probe

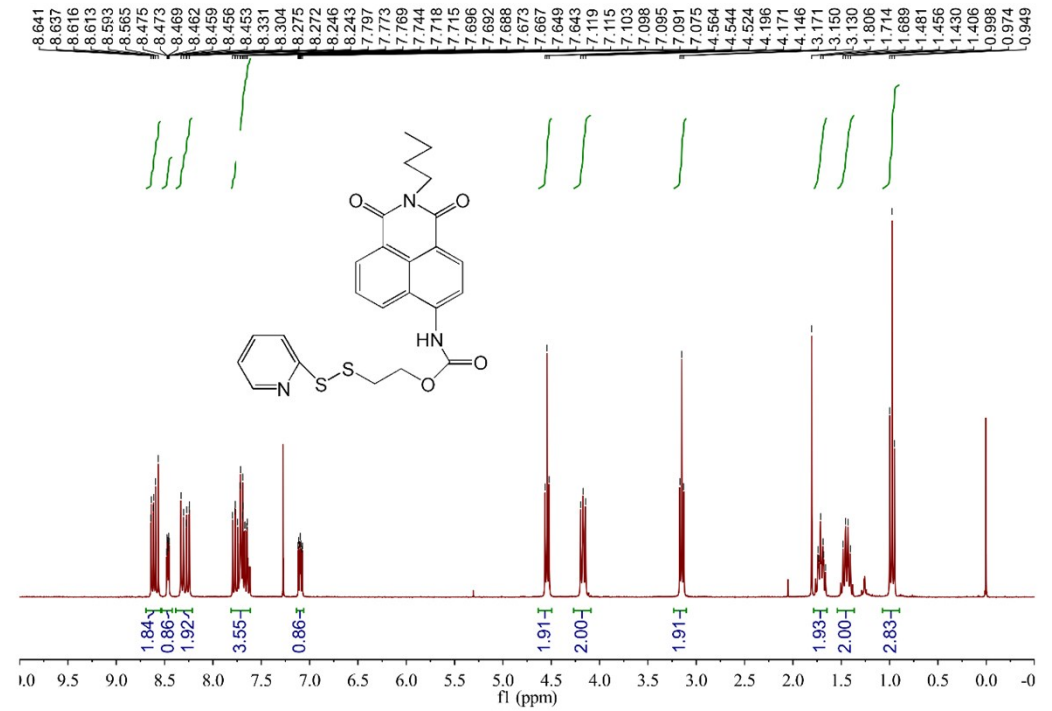

Fig.S1(a) The ^{1}HNMR spectrum of probe.

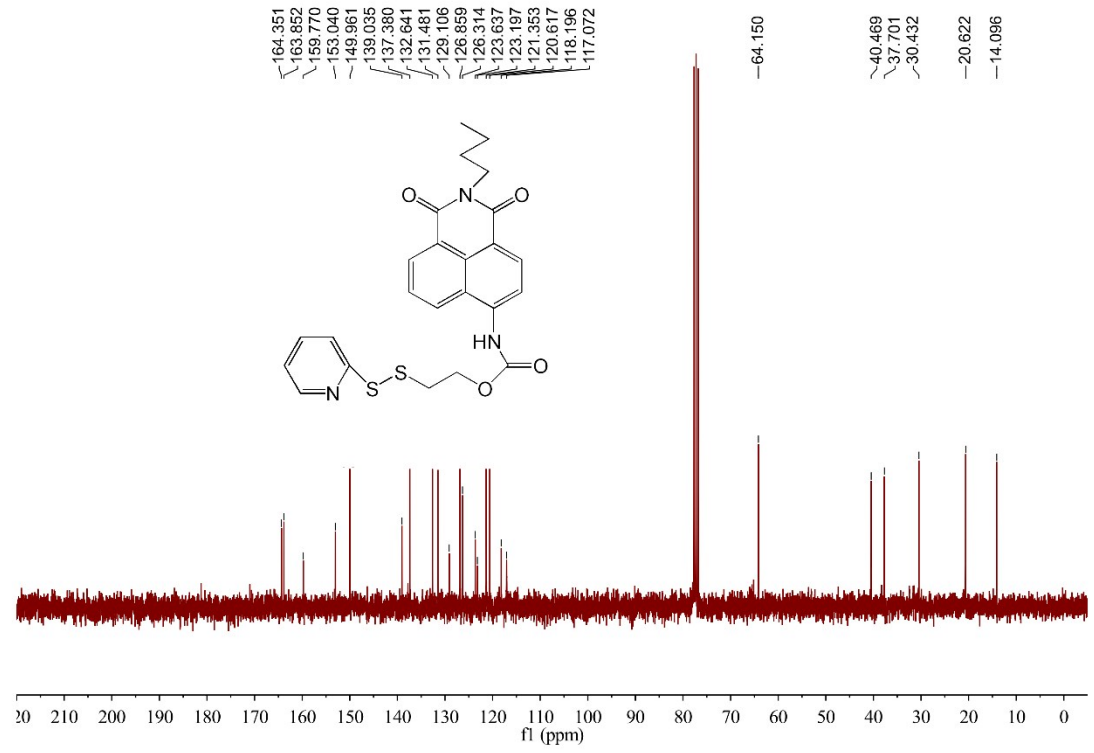

Fig.S1(b) The ^{13}CNMR spectrum of probe.

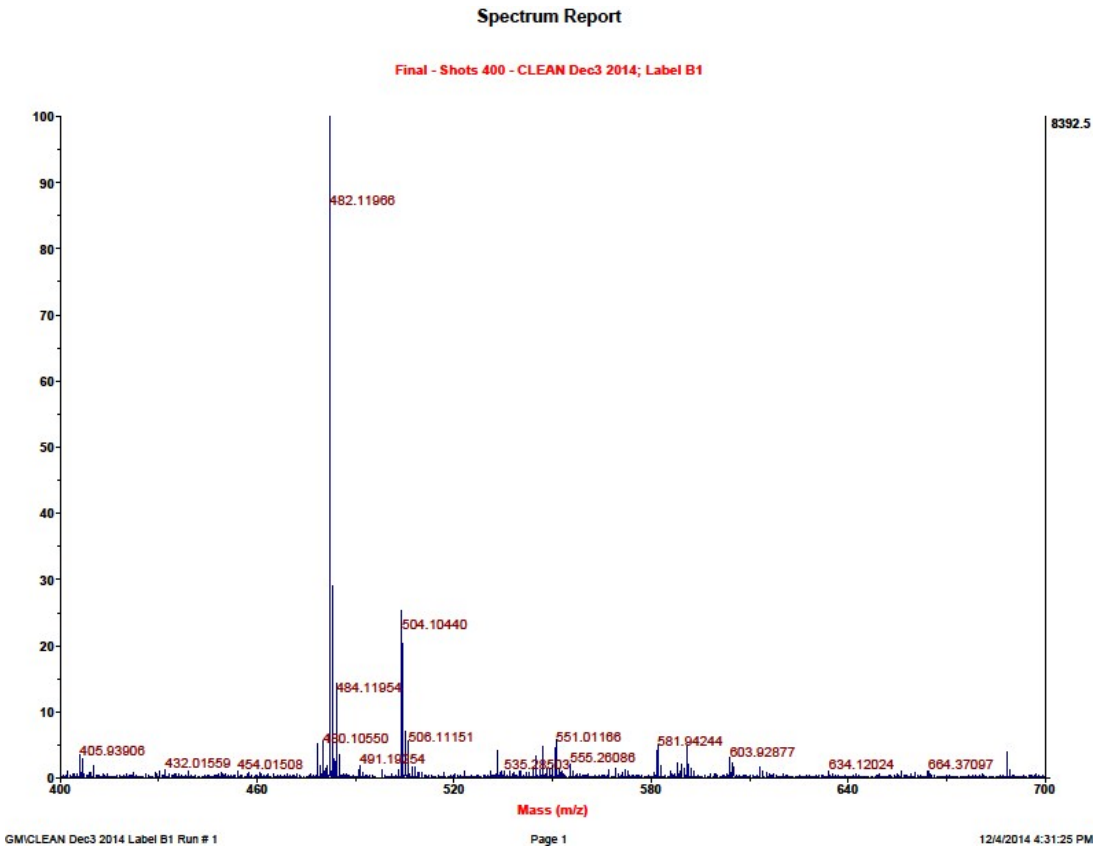

Fig.S1(c) The MS spectrum of probe.

2. ^{1}H NMR of N-butyl-4-amino-1,8-naphthalimide

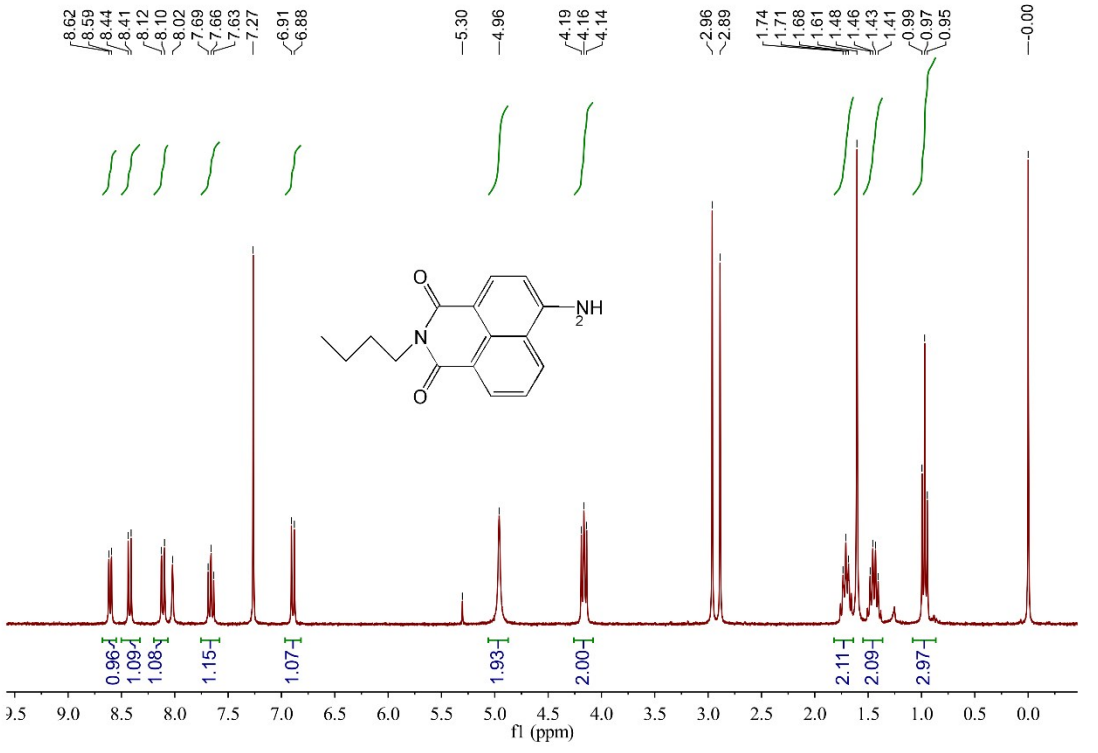

Fig.S2 The ^{1}HNMR spectrum of N-butyl-4-amino-1,8-naphthalimid

3. Ratiometric responses towards Cys

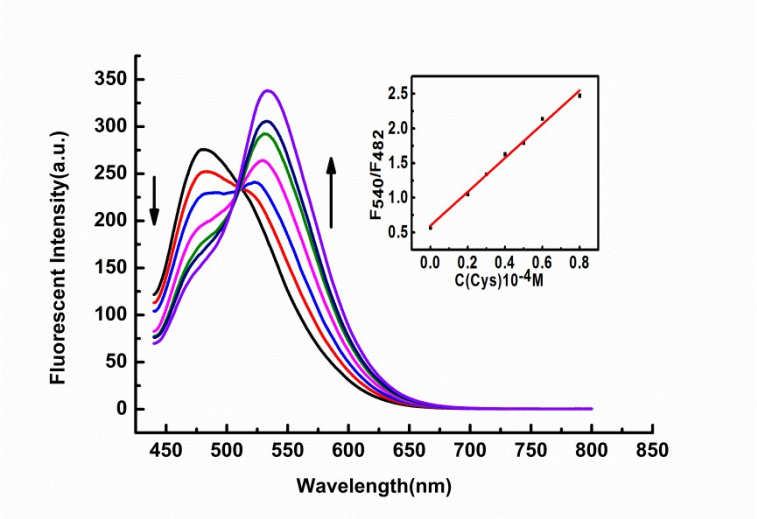

Fig.S3 The emission spectra of probe (1 μM) in 50 mM PBS buffer (pH 7.4, 10% DMF) with different concentrations of Cys (0, 20, 30, 40, 50, 60, 80, 90, 100μM) for 90 min at 25 °C, λex=420 nm. Insert is the concentration of Cys dependence of the ratiometric fluorescence signal (F_{540}/F_{482}), the concentrations of Cys is 0-80μM.

4. Ratiometric responses towards Hcy

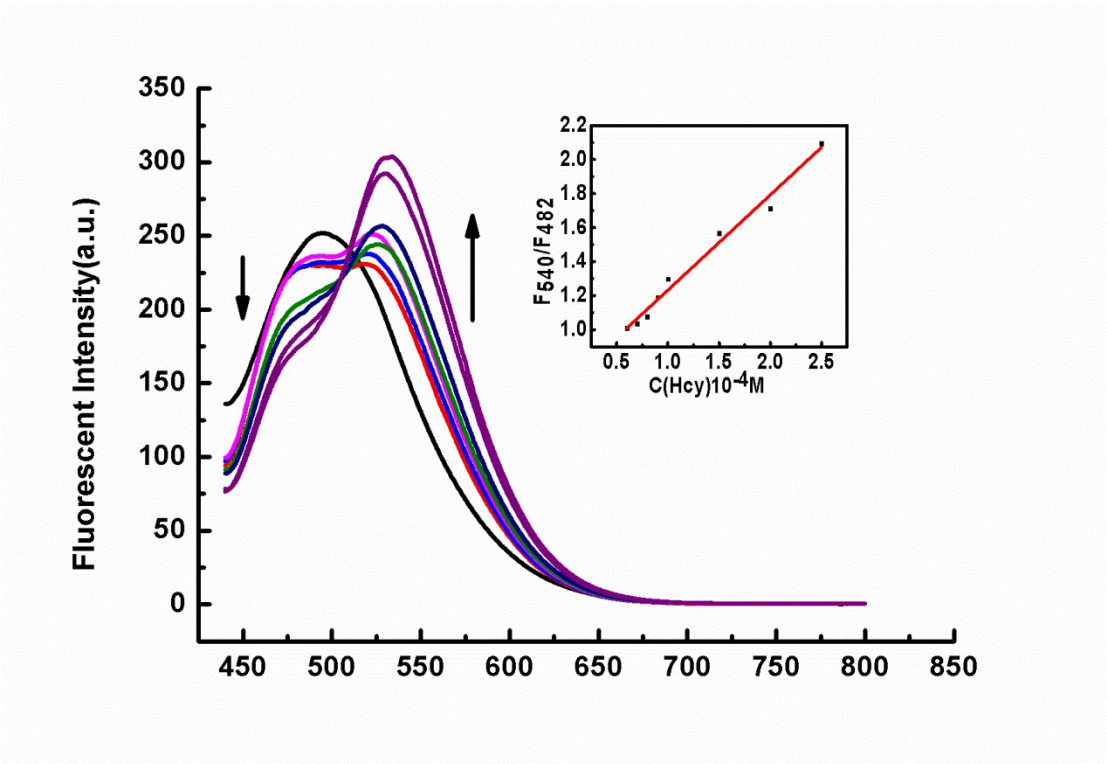

Fig.S4 The emission spectra of probe (1 μM) in 50 mM PBS buffer (pH 7.4, 10% DMF) with different concentrations of Hcy (0, 60, 70, 80, 90, 100, 150, 200, 250μM) for 90 min at 25 °C, λex=420 nm. Insert is the concentration of Hcy dependence of the ratiometric fluorescence signal (F_{540}/F_{482}), the concentrations of Hcy is 60-250μM

5. Time-dependent fluorescence spectral changes of probe with biothinols.

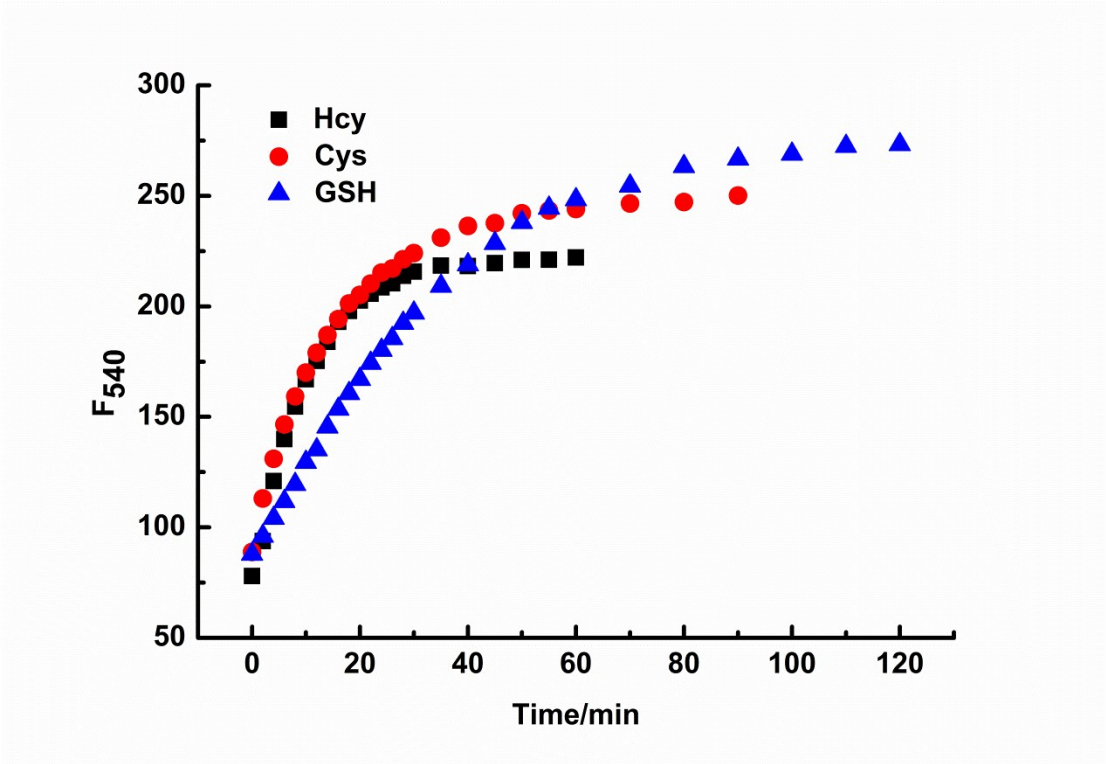

Fig.S5 Time-dependent fluorescence enhancements of probe (1 μM) in 50 mM PBS buffer (pH 7.4, 10% DMF) to GSH, Cys and Hcy (1 mM). (λex/em = 420/540 nm)

6. The effects of pH.

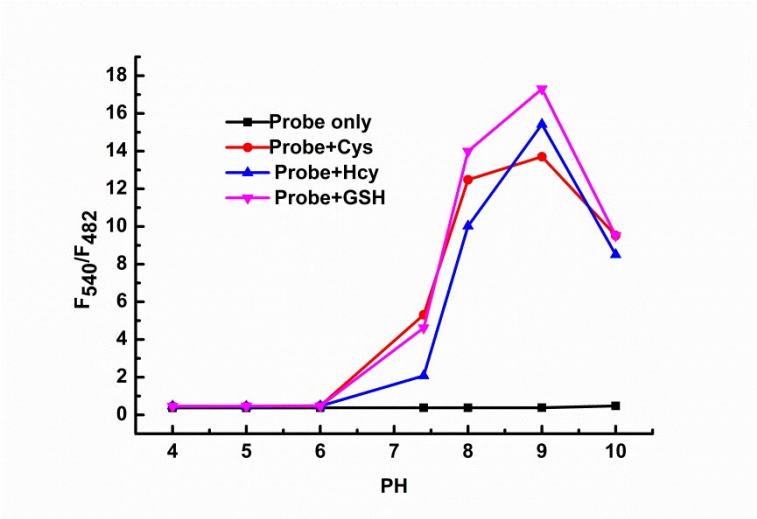

Fig.S6 pH-dependent ratiometric fluorescence changes of probe (1 μM) in 50 mM PBS buffer (pH 7.4, 10% DMF) to GSH, Cys and Hcy (1 mM). (λex = 420 nm)

7. Determination of quantum yield.

The quantum yield of probe 1 was determined according to the following equation:

$$\Phi f_{sample} = \Phi f_{standard} \times (I_{sample} / I_{standard}) \times (A_{standard} / A_{sample}) \times (n_{sample} / n_{standard})^2$$

Where Φ is quantum yield; I is integrated area under the uncorrected emission spectra; A is absorbance at the excitation wavelength; n denotes the refractive index of the solvent. 7-hydroxycoumarin (Φ_f = 0.76, excited at 330nm in 0.1 M pH 7.4 sodium phosphate buffer) as the standard. [1]

8. References

[1] K. Setsukinai, Y. Urano, K. Kikuchi, T. Higuchi, T. Nagano, J. Chem. Soc.Perkin Trans. 2, 2000, 2453–2457.