

Electronic Supplementary Information

§ Tao Liu, ^a Fangjun Huo,^{*b} Caixia Yin,^{*a} § JianFang Li, ^a Lixi Niu ^c

^aInstitute of Molecular Science, Shanxi University, Taiyuan, 030006, China.

^b Research Institute of Applied Chemistry, Shanxi University, Taiyuan, 030006, China.

^c Institute of Biotechnology, Shanxi University, Taiyuan 030006, PR China.

E-mail: yincx@sxu.edu.cn; huofj@sxu.edu.cn

Figure S1: The characterization data of the probe

Figure S2: The UV–vis and fluorescence titration spectra of Cys and GSH

Figure S3: The UV–vis and fluorescence titration spectra of ME and MPA

Figure S4: The UV–vis and fluorescence titration spectra of probe when all kinds of analytes added

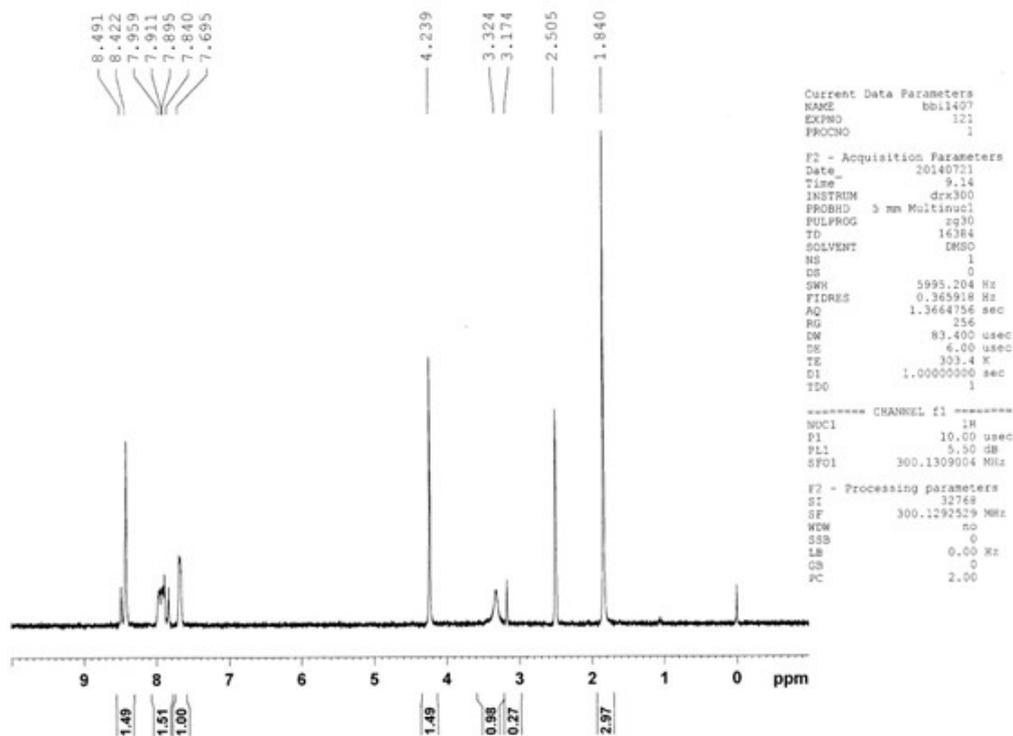
Figure S5: The detection limits of Cys

Figure S6: Kinetic study of the response of the probe to Hcy and Cys at 25 °C

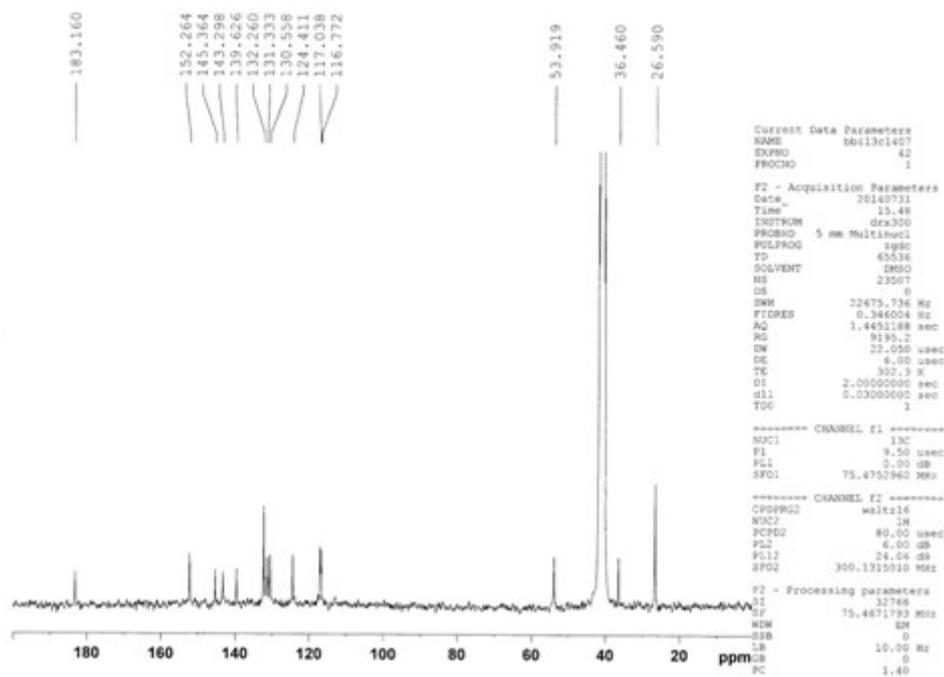
Figure S7: Choice of pH range for the measurements

Figure S8: ESI-MS spectra of the probe-ME adduct

Figure S1: 1D ^1H NMR, ^{13}C NMR, ESI-MS, and crystal structure spectra of the probe.

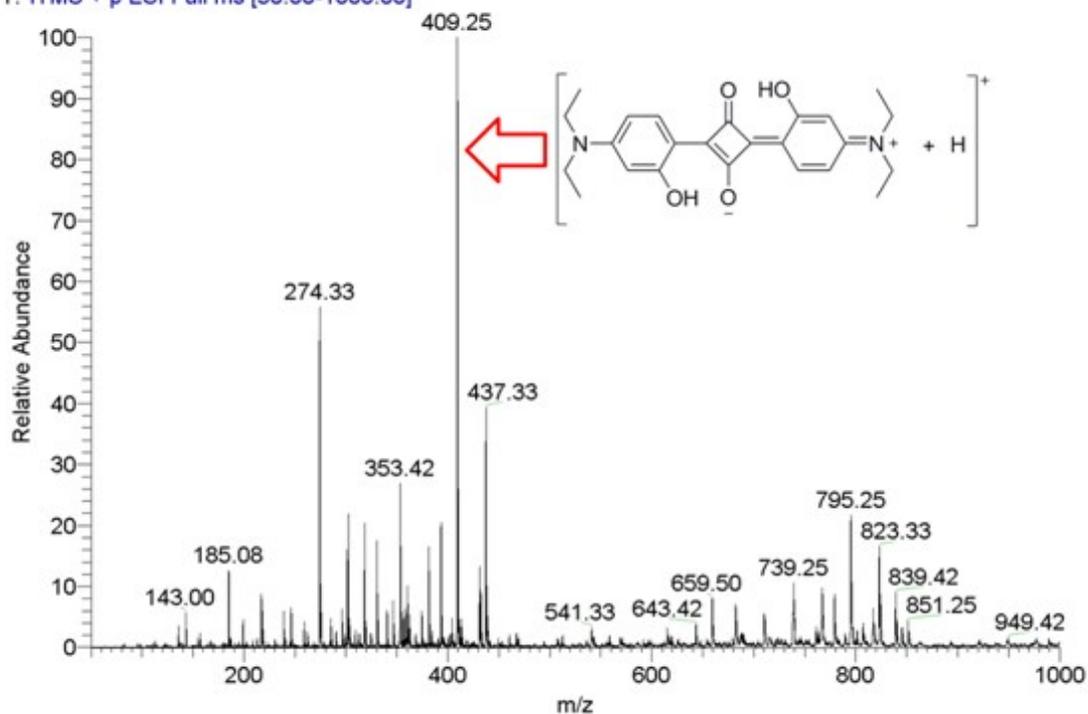


The ^1H NMR (300MHz) spectra of the **probe** in DMSO



The ^{13}C NMR (75 MHz) spectra of the **probe** in DMSO

10_+ #96 RT: 0.24 AV: 1 NL: 7.14E4
T: ITMS + p ESI Full ms [50.00-1000.00]



ESI-MS of the probe: HRMS (ESI-TOF) m/z: [probe + H]⁺ Calcd for C₂₄H₂₈N₂O₄ 409.21, Found 409.25, the data was measured with GCT-MS (Waters) instrument.

Figure S2: The UV-vis and fluorescence titration spectra of Cys and GSH

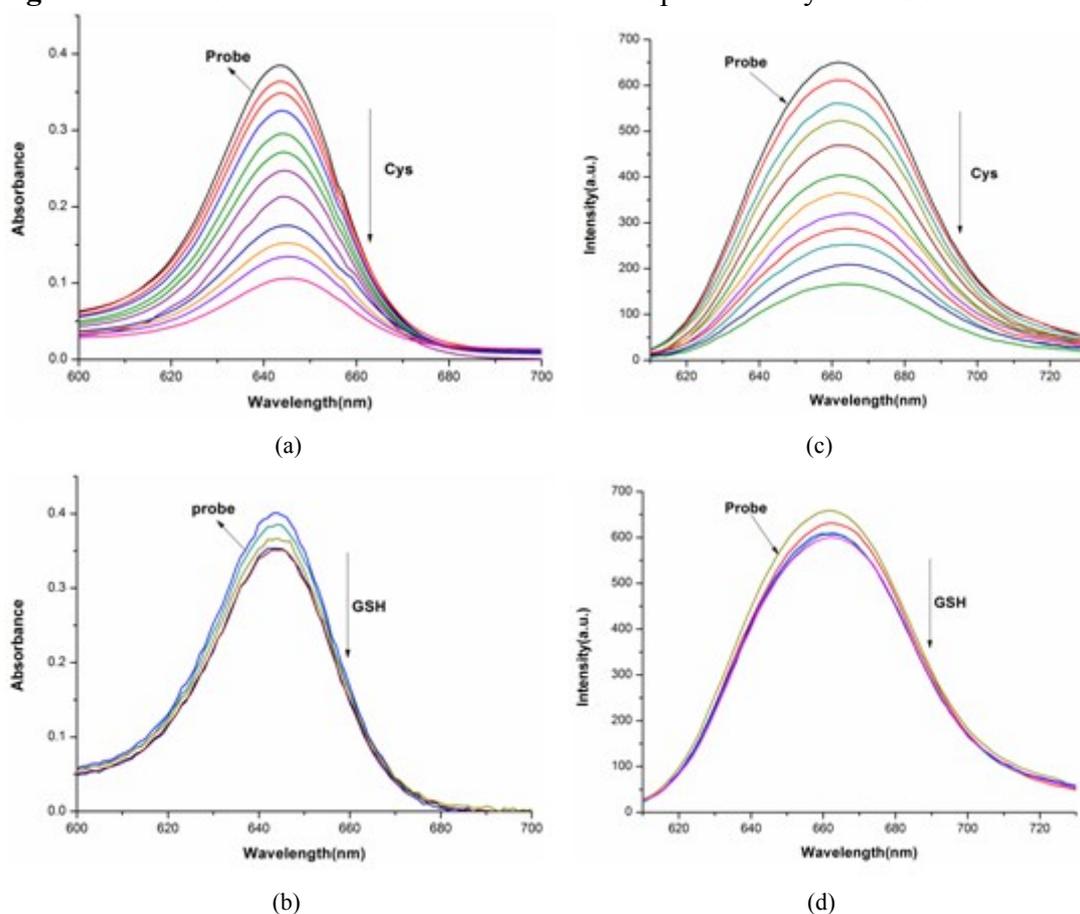


Figure S2: Left: UV-vis spectra of the probe (35 μM) with Cys (200 μM)(a) and GSH (75 μM) (b) in CH_3CN -HEPES buffer (10 mM, pH 9.0, 1 : 1, v/v). Right: Fluorescence spectra of probe (5 μM) with Cys (200 μM) (c) and GSH (40 μM) (d) in CH_3CN -HEPES buffer (10 mM, pH 9.0, 1 : 1, v/v) ($\lambda_{\text{ex}} = 575\text{nm}$, slit: 5.0 nm/5.0 nm).

Figure S3: The UV-vis and fluorescence titration spectra of ME and MPA

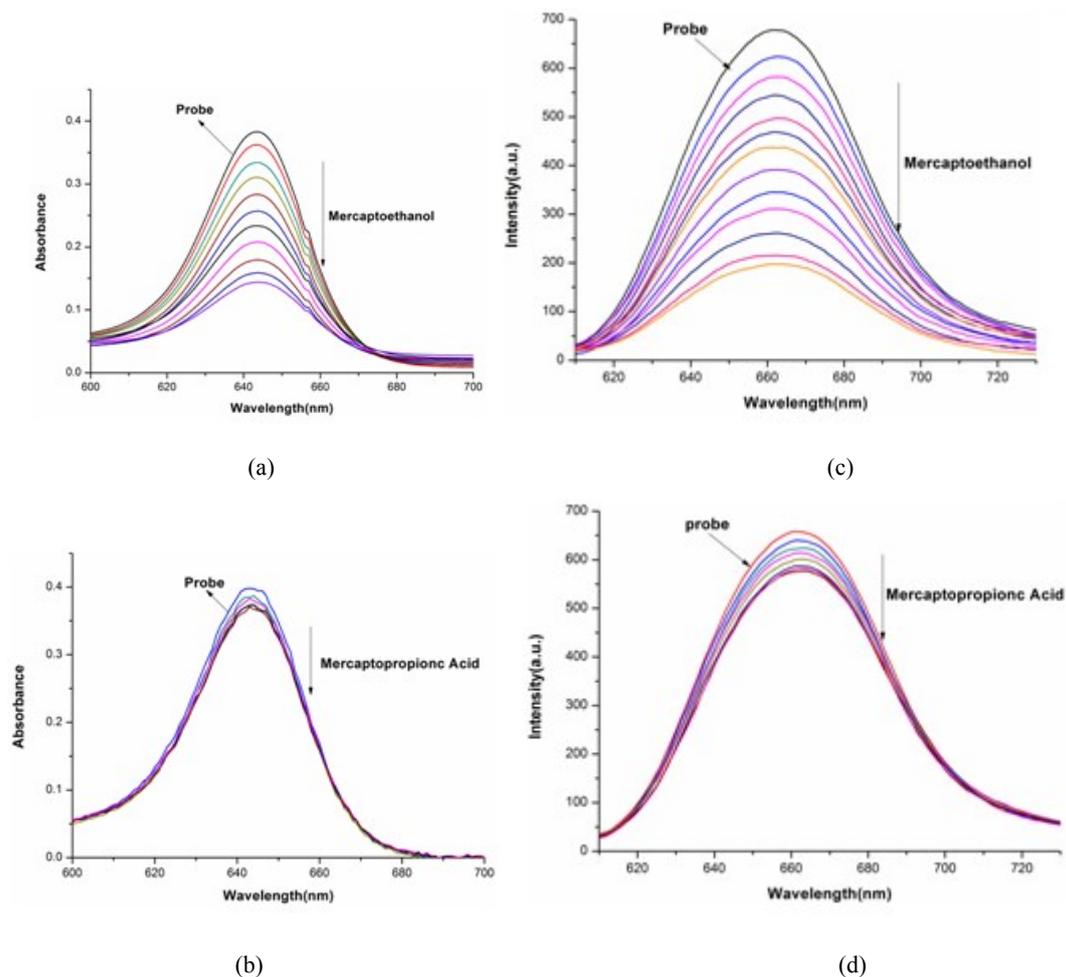


Figure S3: Left: UV-vis spectra of the probe (35 μM) with ME(2-Mercaptoethanol)(80 μM) (a) and MPA (Mercaptopropionic Acid) (80 μM) (b) in CH_3CN -HEPES buffer (10 mM, pH 9.0, 1 : 1, v/v). Right: Fluorescence spectra of probe (5 μM) with ME (50 μM) (c) and MPA (50 μM) (d) in CH_3CN -HEPES buffer (10 mM, pH 9.0, 1 : 1, v/v) ($\lambda_{\text{ex}} = 575 \text{ nm}$, slit: 5.0 nm/5.0 nm)

Figure S4: The UV-vis and fluorescence titration spectra of probe when all kinds of analytes added

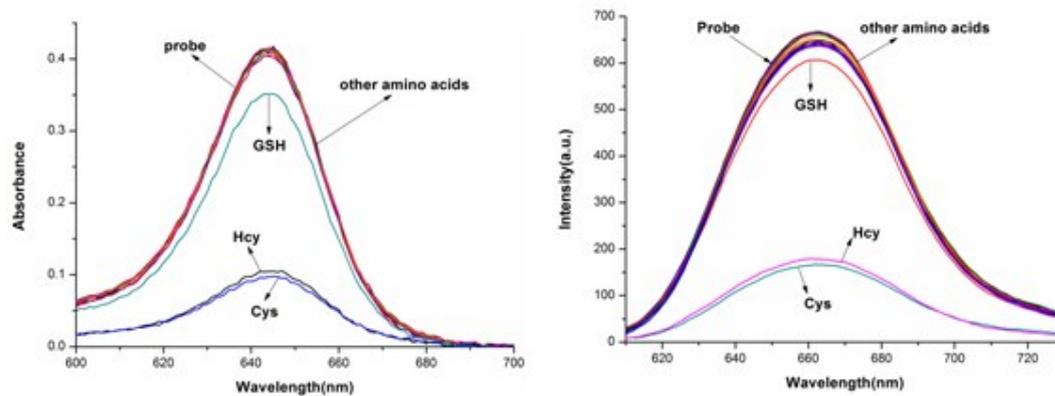


Figure S4: The selectivity of probe 1 for (Ala, Arg, Asp, Gln, Glu, Gly, His, Ile, Leu, Lys, Met, Phe, Pro, Ser, Thr, Tyr, Trp and Val).

Figure S5: The detection limits of Cys

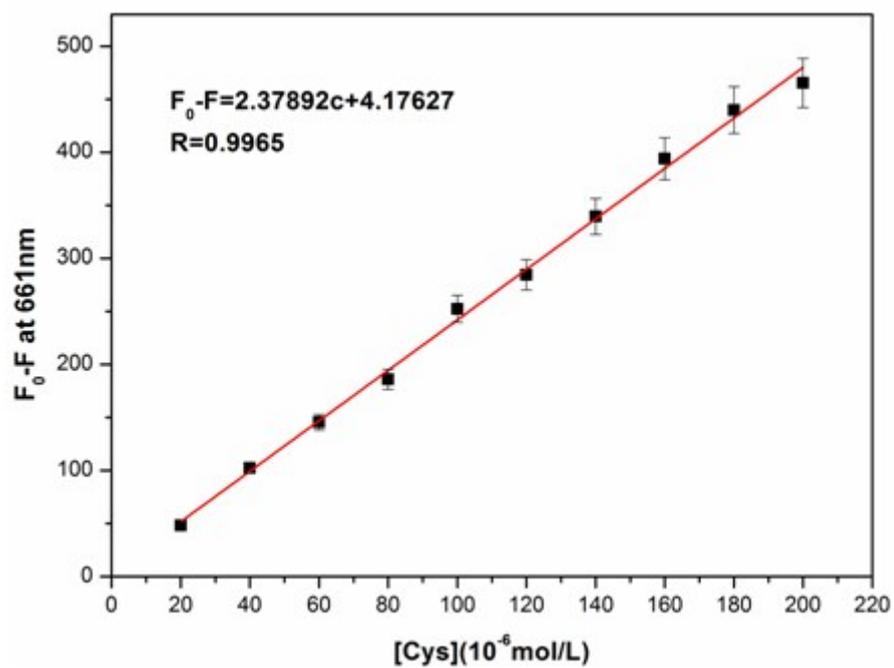
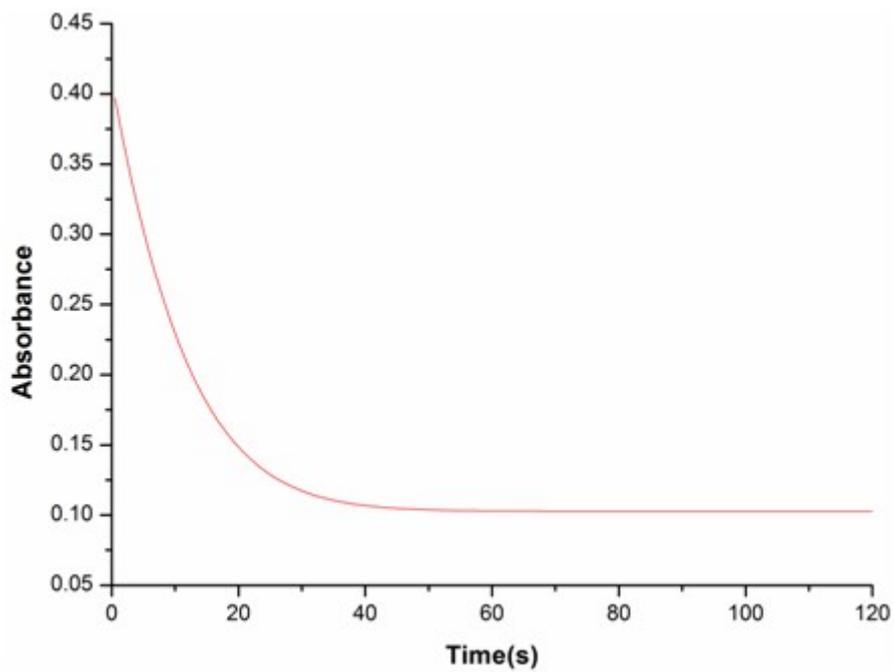
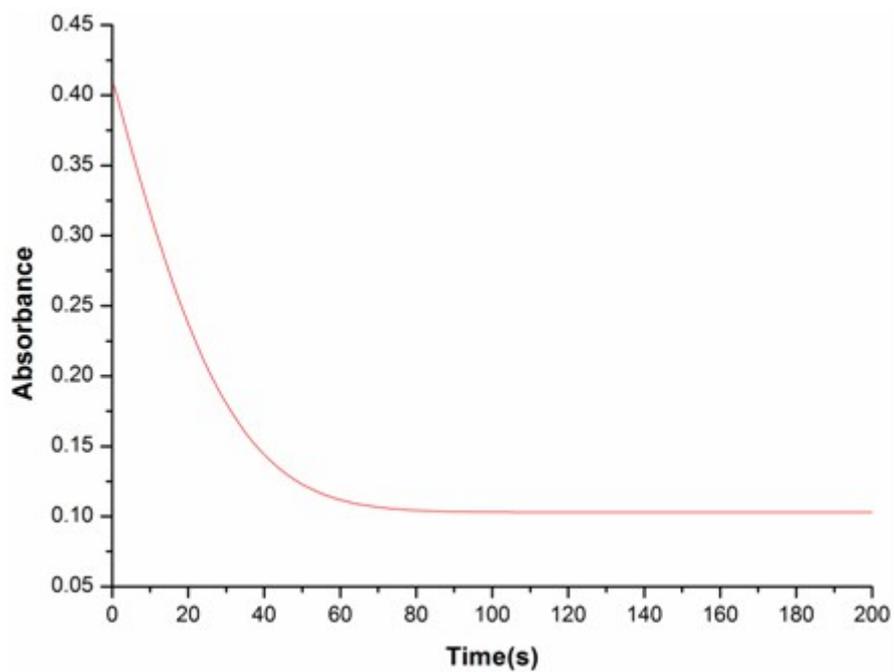


Figure S6: Kinetic study of the response of the probe to Hcy and Cys at 25 °C



(a)



(b)

Figure S6: Time-dependent absorbance of probe at 645 nm in the presence of 10 equiv. Hcy (a) and Cys (b).

Figure S7: Choice of pH range for the measurements

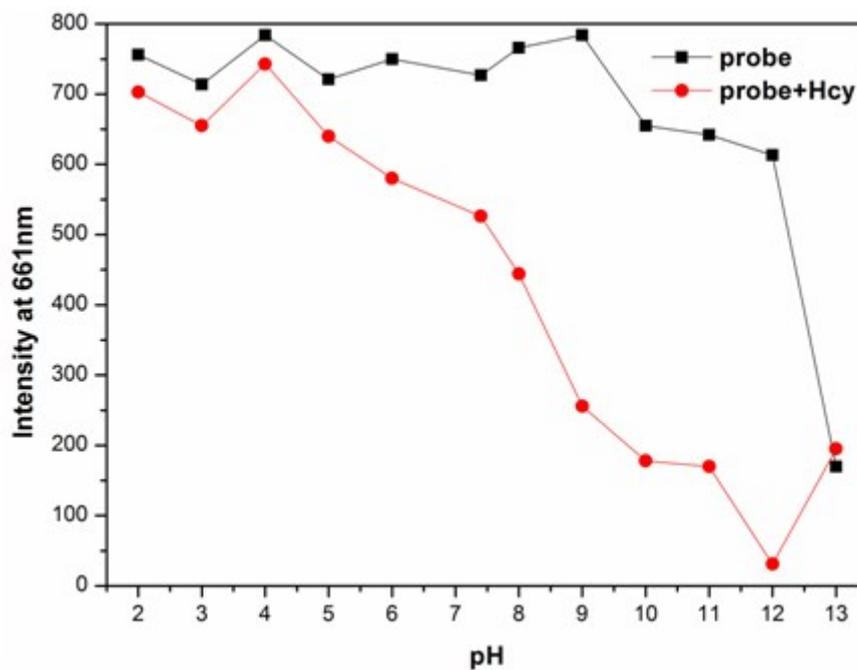
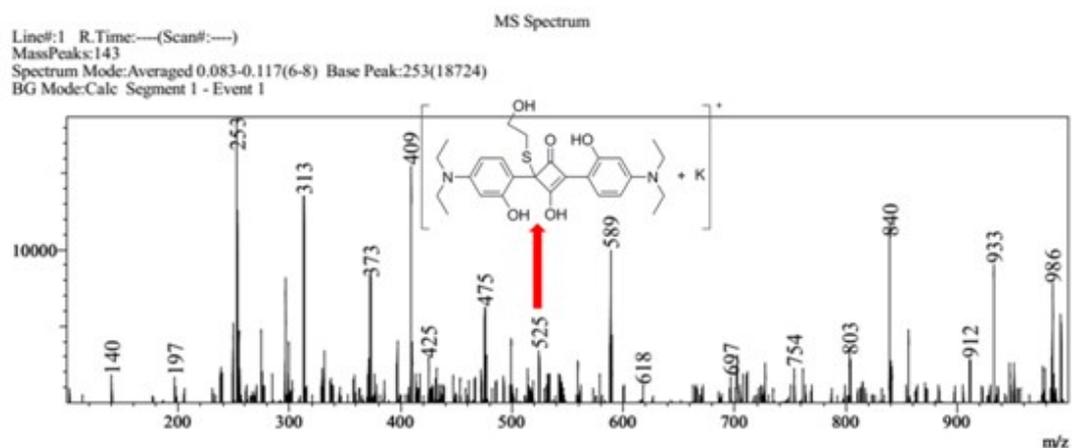


Figure S7: The fluorescence intensity of probe at 661 nm in the absence and presence of Hcy under different pH (5 $\mu\text{mol/L}$ probe in CH_3CN -HEPES buffer (10 mM, pH 9.0, 1 : 1, v/v) ($\lambda_{\text{ex}} = 575$ nm; Slit: 5nm/5 nm).

Figure S8: ESI-MS spectra of the probe-ME adduct



ESI-MS of the probe: m/z : $[\text{probe} + \text{ME} + \text{K}]^+$ Calcd for $\text{C}_{26}\text{H}_{34}\text{KN}_2\text{O}_5\text{S}$ 525.18, Found 525. The data was measured with LCMS-8030 (Shimadzu) instrument.