

## Electronic Supplementary Information

Jianfang Li, <sup>a</sup> Caixia Yin, <sup>\*a</sup> FangjunHuo, <sup>\*b</sup> Jianbin Chao, <sup>b</sup> Yongbin Zhang, <sup>b</sup> Lixi Niu<sup>c</sup>

<sup>a</sup>*Institute of Molecular Science, Shanxi University, Taiyuan, 030006, China.*

<sup>b</sup>*Research Institute of Applied Chemistry, Shanxi University, Taiyuan, 030006, China.*

<sup>c</sup>*Institute of Biotechnology, Shanxi University, Taiyuan 030006, China.*

**Figure S1:** The characterization data of the probe

**Figure S2:** The UV–vis and fluorescence titration spectra of ME and MPA

**Figure S3:** The UV–vis and fluorescence titration spectra of GSH and Cys

**Figure S4:** The detection limits of Cys and GSH

**Figure S5:** Kinetic study of the response of the probe to Hcy, Cys and GSH at 25 °C

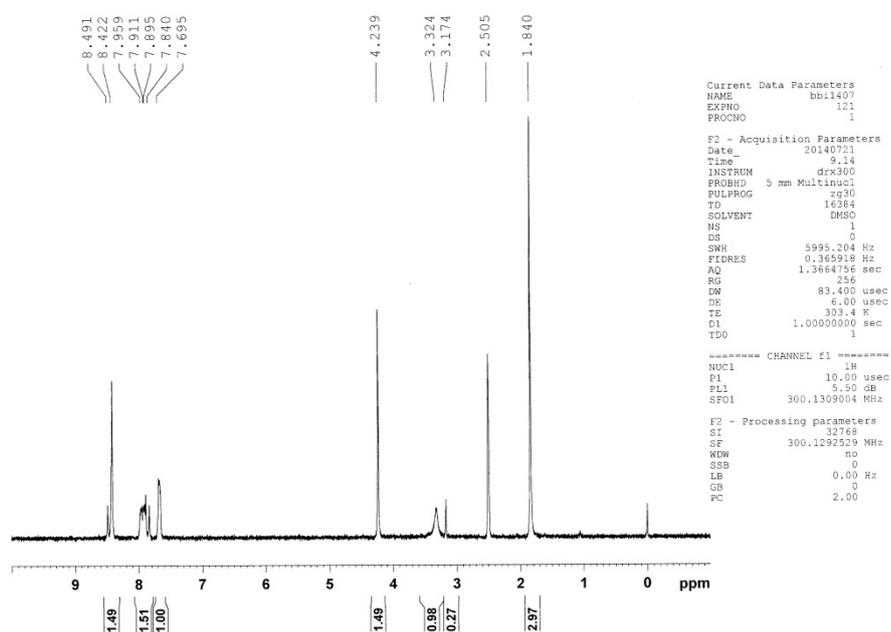
**Figure S6:** Choice of pH range for the measurements

**Figure S7:** NMR spectra of probe and probe-ME

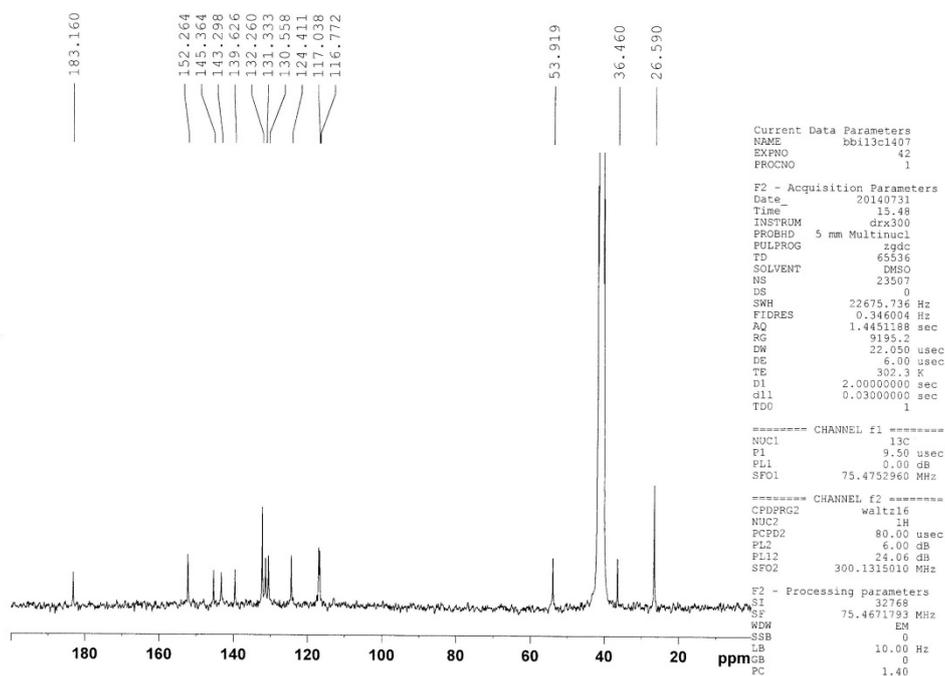
**Figure S8:** ESI-MS spectra of the probe-ME adduct

**Figure S9:** Cellular Imaging about GSH

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

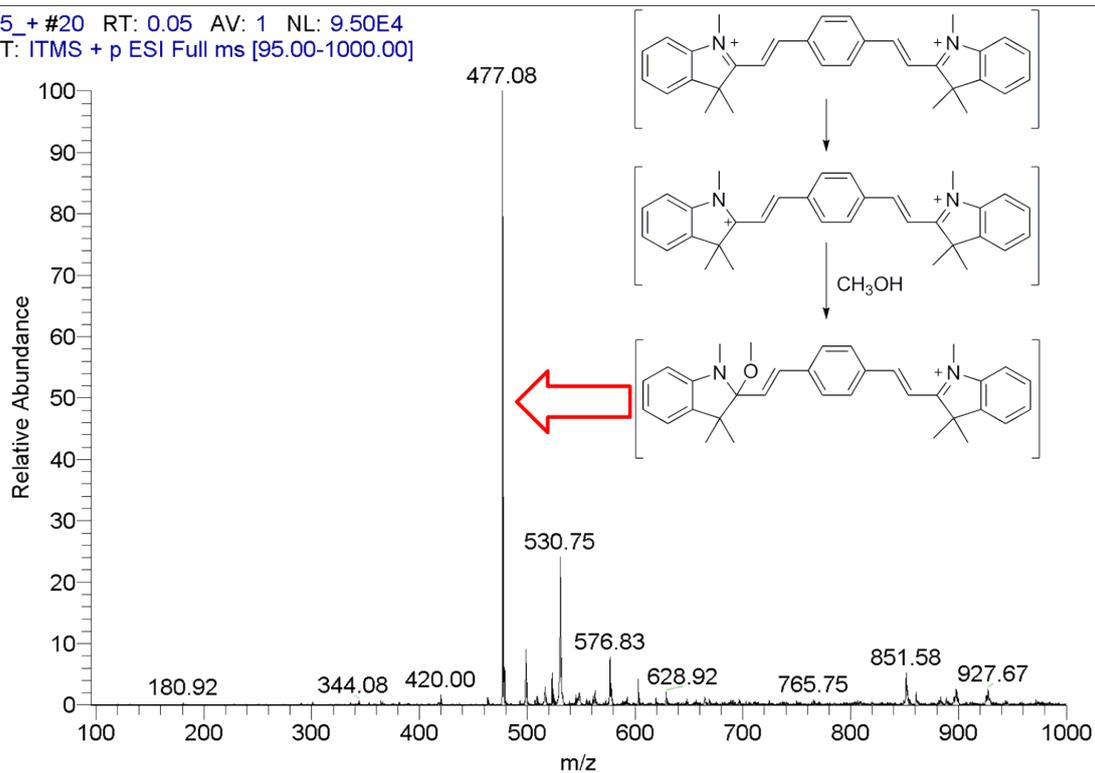


The  $^1\text{H}$  NMR (300MHz) spectra of the **probe** in DMSO



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

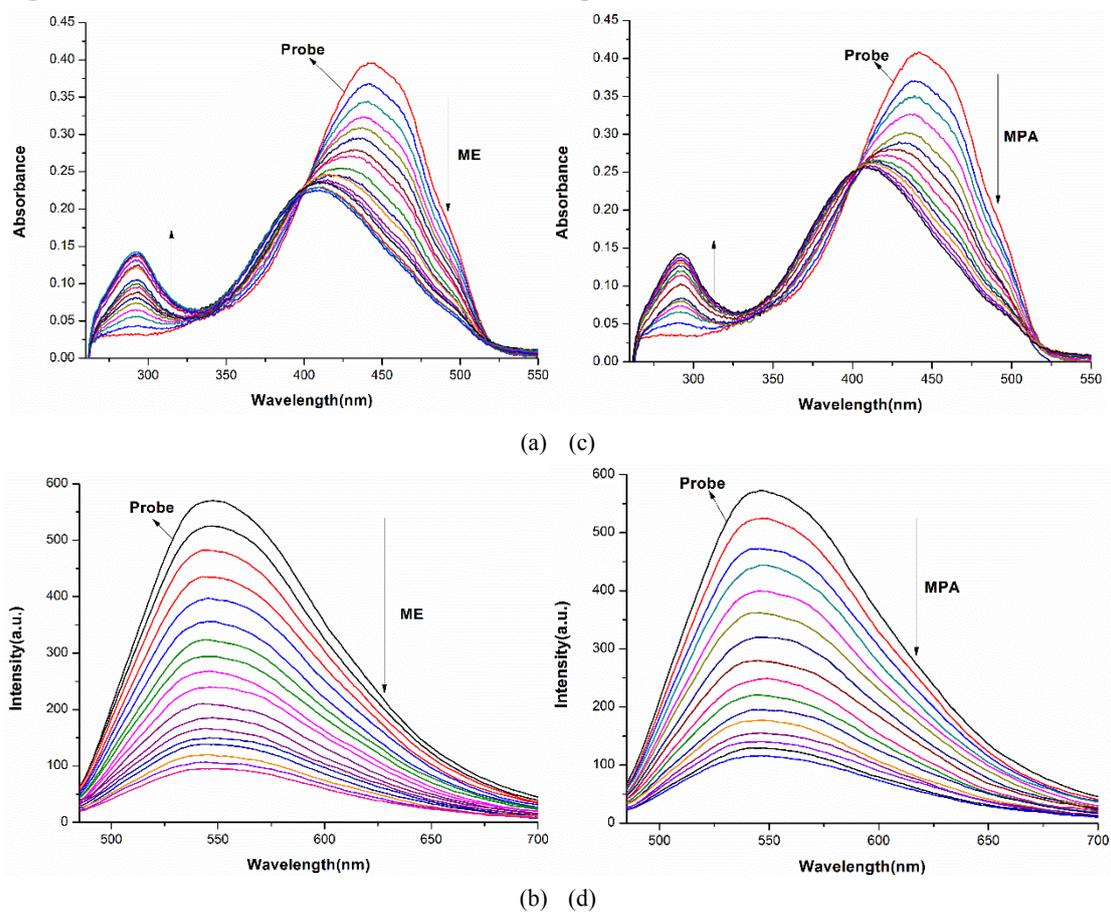
5\_+ #20 RT: 0.05 AV: 1 NL: 9.50E4  
T: ITMS + p ESI Full ms [95.00-1000.00]



ESI-MS of the probe: HRMS (ESI-TOF) m/z: [probe- 2I + CH<sub>3</sub>OH]<sup>+</sup> Calcd for C<sub>33</sub>H<sub>37</sub>N<sub>2</sub>O 477.29, Found 477.08

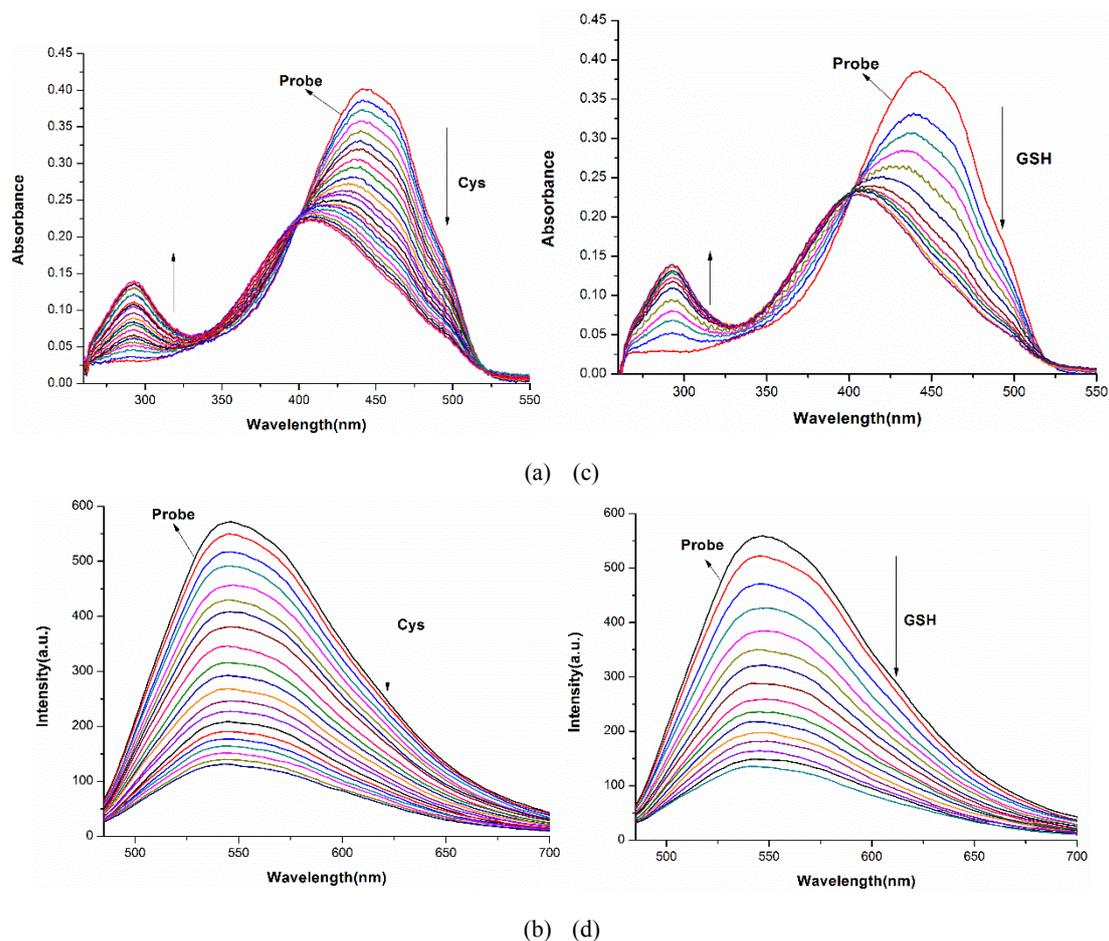
Note: Probe 1 loses two I<sup>-</sup> in the process of ionize, and form a molecule with two positive charges which is easily to capture a methanol molecule. Therefore, we observed the peak is 477.08 m/z on the ESI-MS.

**Figure S2:** The UV-vis and fluorescence titration spectra of ME and MPA



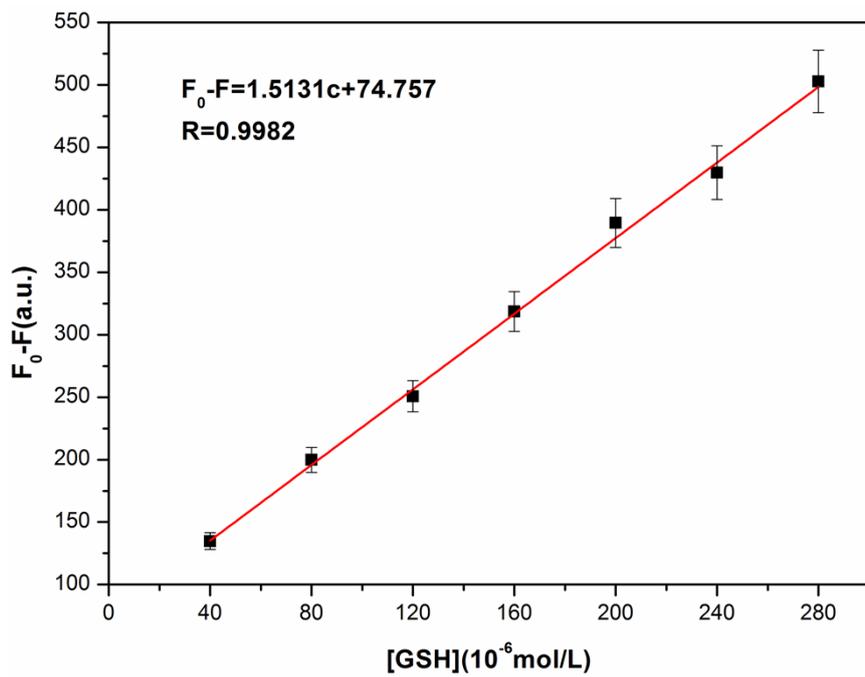
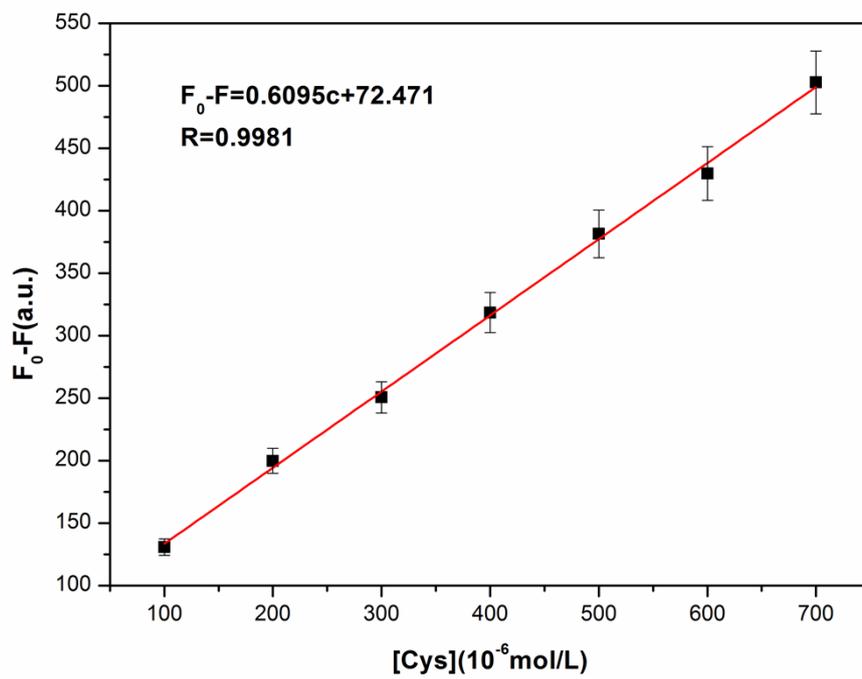
**Figure S2:** (a) UV-vis spectra of the probe ( $5 \mu\text{M}$ ) with ME (2-Mercaptoethanol) ( $110 \mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) (b) Fluorescence spectra of probe ( $15 \mu\text{M}$ ) with ME ( $440 \mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) ( $\lambda_{\text{ex}} = 450 \text{ nm}$ , slit: 5.0 nm/5.0 nm) (c) UV-vis spectra of the probe ( $5 \mu\text{M}$ ) with MPA (Mercaptopropionic Acid) ( $100 \mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) (d) Fluorescence spectra of probe ( $15 \mu\text{M}$ ) with MPA ( $360 \mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) ( $\lambda_{\text{ex}} = 450 \text{ nm}$ , slit: 5.0 nm/5.0 nm).

**Figure S3:** The UV–vis and fluorescence titration spectra of GSH and Cys

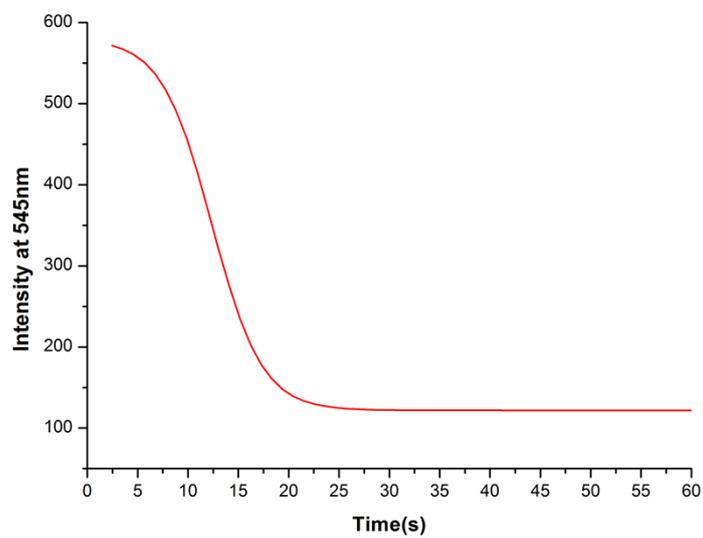


(c) **Figure S3:**(a) UV–vis spectra of the probe (5  $\mu\text{M}$ ) with Cys(375 $\mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) (b)Fluorescence spectra of probe (15 $\mu\text{M}$ ) with Cys (700 $\mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) ( $\lambda_{\text{ex}}$  = 450 nm, slit: 5.0 nm/5.0 nm) (c) UV–vis spectra of the probe (5  $\mu\text{M}$ ) with GSH (90 $\mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) (d) Fluorescence spectra of probe (15 $\mu\text{M}$ ) with GSH (280 $\mu\text{M}$ ) in HEPES: DMF = 1:1 (V/V pH=7.0) ( $\lambda_{\text{ex}}$  = 450nm, slit: 5.0 nm/5.0 nm).

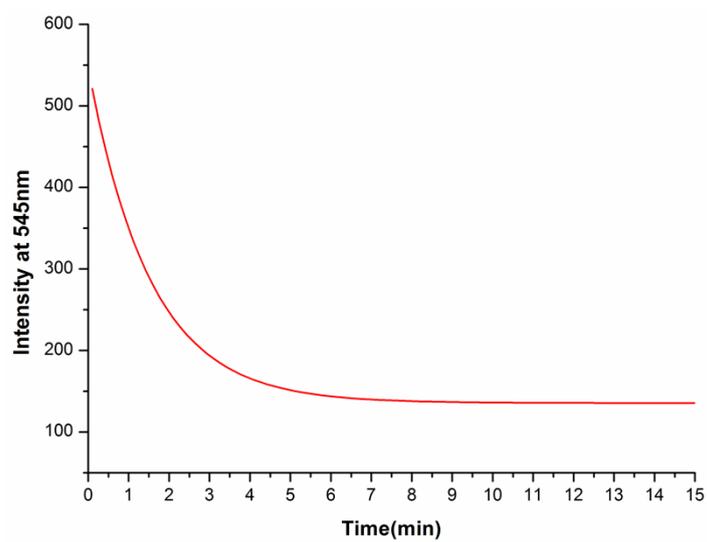
**Figure S4:**The detection limits of Cys and GSH



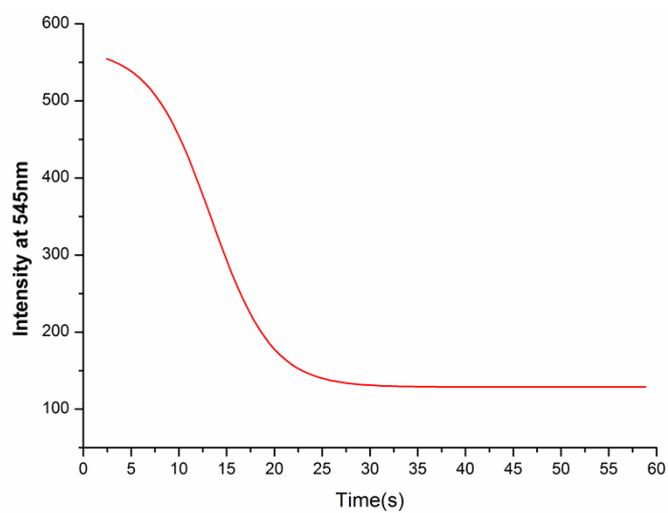
**Figure S5:** Kinetic study of the response of the probe to Hcy, Cys and GSH at 25 °C



(a)



(b)



(c)

Figure S5: Time-dependent fluorescence of probe at 545 nm in the presence of 1 equiv Hcy (a), GSH (b) and Cys (c).

Figure S6: Choice of pH range for the measurements

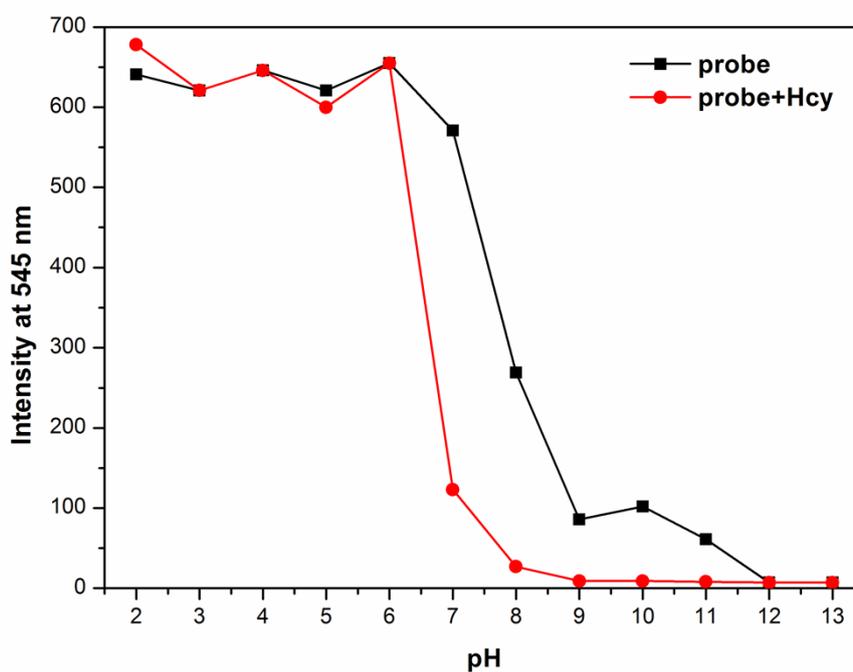
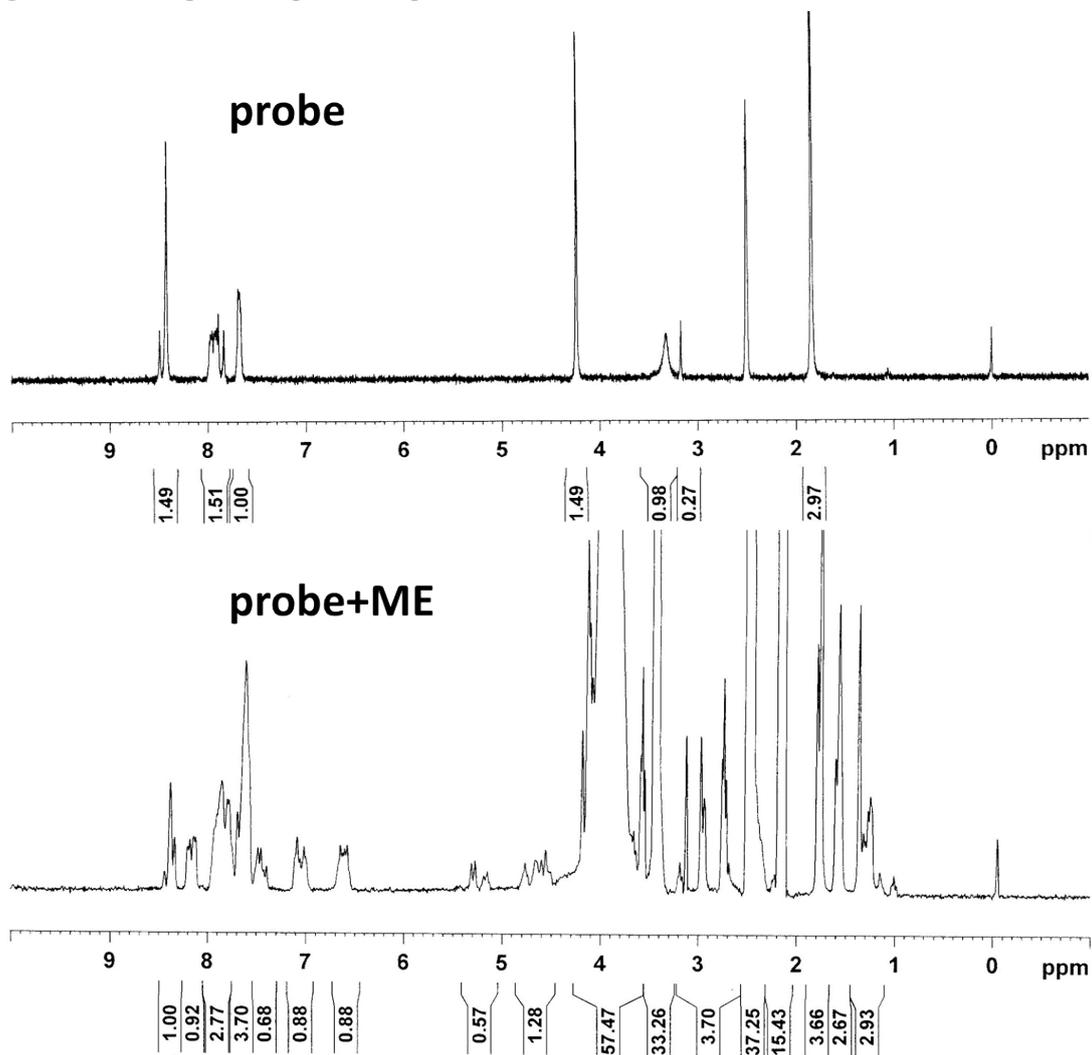


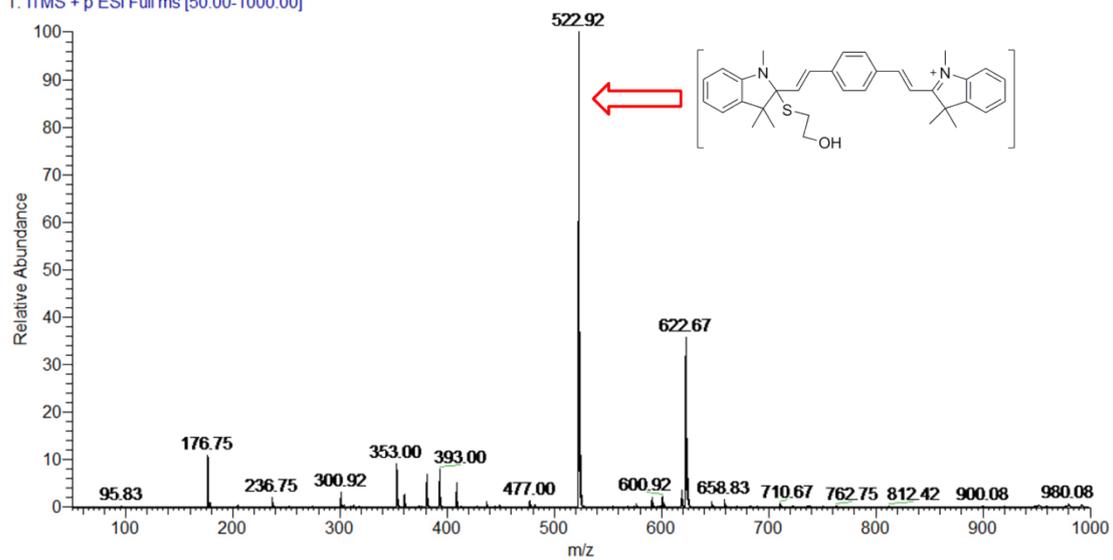
Figure S6: The fluorescence intensity of probe at 545 nm in the absence and presence of Hcy under different pH (15  $\mu$ mol/L probe in HEPES: DMF = 1:1 (V/V pH=7.0);  $\lambda_{\text{ex}}$  = 450 nm; Slit: 5nm/5 nm).

**Figure S7:** NMR spectra of probe and probe-ME

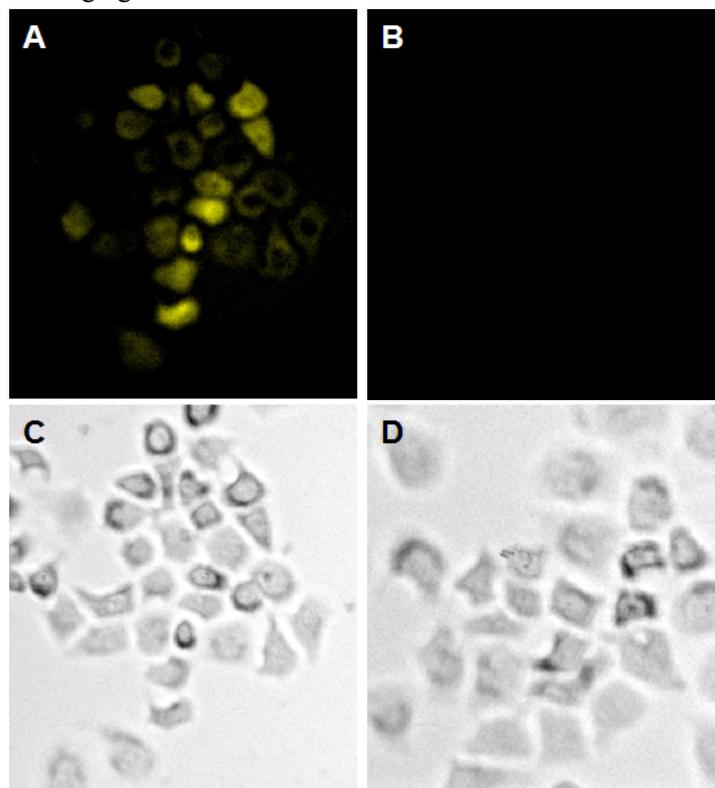


**Figure S8:** ESI-MS spectra of the probe-ME adduct

1+ 141017174007 #17 RT: 0.06 AV: 1 NL: 1.97E4  
T: ITMS + p ESI Full ms [50.00-1000.00]



**Figure S9:** Cellular Imaging about GSH



**Figure S9:** Confocal fluorescence images of HepG2 cells: (A) Fluorescence image of HepG2 cells incubated with 15  $\mu\text{mol/L}$  probe after pretreated with NEM (20 $\mu\text{mol/L}$ ) for 30 min at 37°C and its bright field image (C). (B) Fluorescence image of HepG2 cells incubated with 15  $\mu\text{mol/L}$  probe and 200  $\mu\text{mol/L}$  GSH for 30 min at 37°C and its bright field image (D).