

Supplementary data

Novel coumarin-based sensitive and selective fluorescent probes for biothiols in aqueous solution and in living cells

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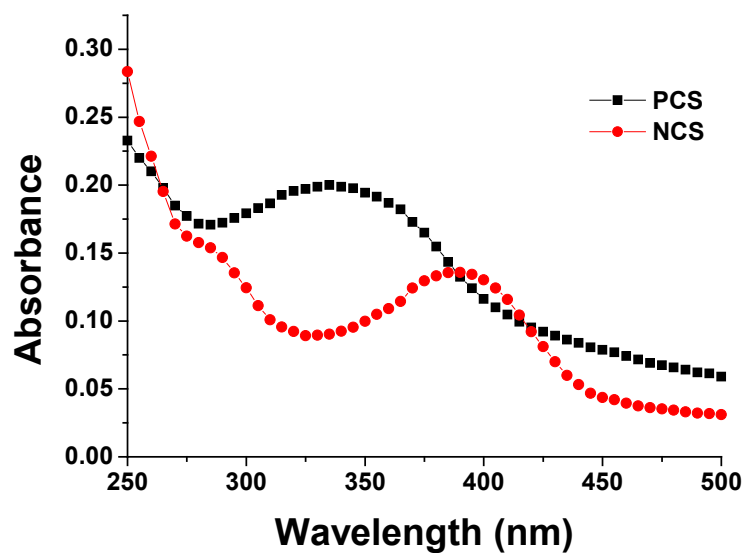


Fig. S1. The UV-Vis absorption spectra of 10 μM PCS and 10 μM NCS in 0.1 M phosphate buffer (pH 8.0) at 30 $^{\circ}\text{C}$.

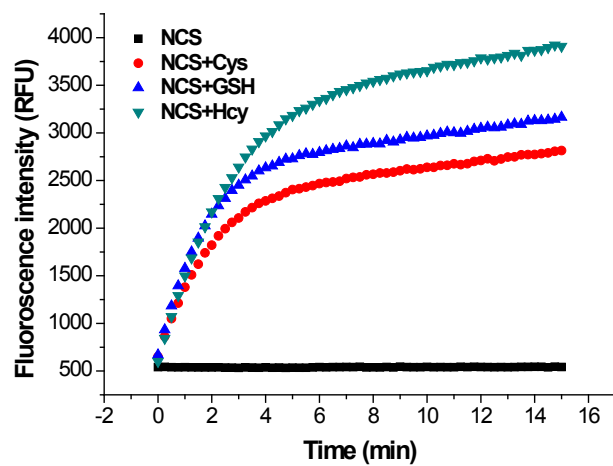


Fig. S2. Time-dependent fluorescence spectra ($\lambda_{\text{ex}} = 405 \text{ nm}$, $\lambda_{\text{em}} = 455 \text{ nm}$) of 10 μM NCS in the presence of three representative biothiols (10 μM) at 0.1 M phosphate buffer (pH 8.0) at 30 $^{\circ}\text{C}$.

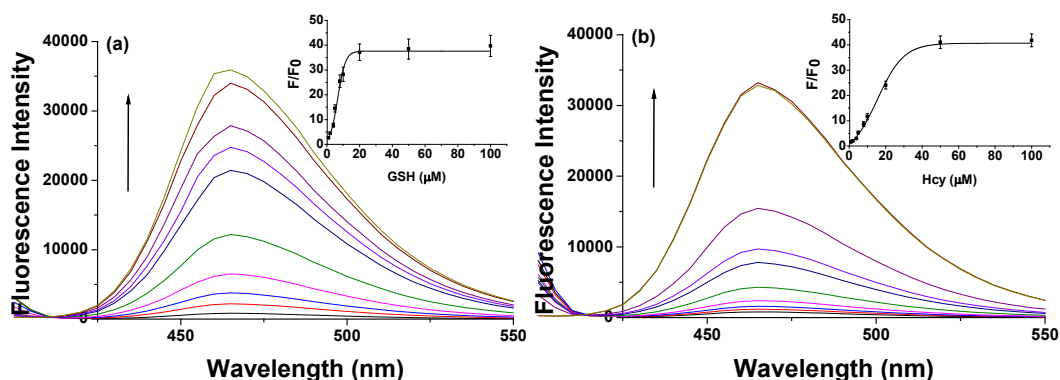


Fig. S3. Fluorescence spectra ($\lambda_{\text{ex}} = 390 \text{ nm}$, $\lambda_{\text{em}} = 510 \text{ nm}$) of $10 \mu\text{M}$ PCS in the presence of various concentrations of GSH (a) and Hcy (b) at 0.1 M phosphate buffer (pH 8.0) at $30 \text{ }^\circ\text{C}$ after 30 min incubation. Inset: relative fluorescence intensity depending on the concentrations of GSH (a) or Hcy (b).

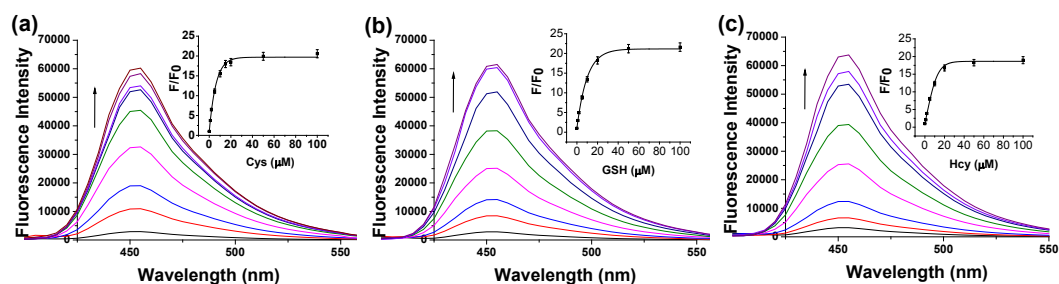


Fig. S4. Fluorescence spectra of $10 \mu\text{M}$ NCS ($\lambda_{\text{ex}} = 405 \text{ nm}$, $\lambda_{\text{em}} = 455 \text{ nm}$) in the presence of various concentrations of Cys (a), GSH (b) and Hcy (c) at 0.1 M phosphate buffer (pH 9.0) at $30 \text{ }^\circ\text{C}$ after 30 min incubation. Inset: relative fluorescence intensity depending on the concentrations of Cys (a), GSH (b) or Hcy (c).

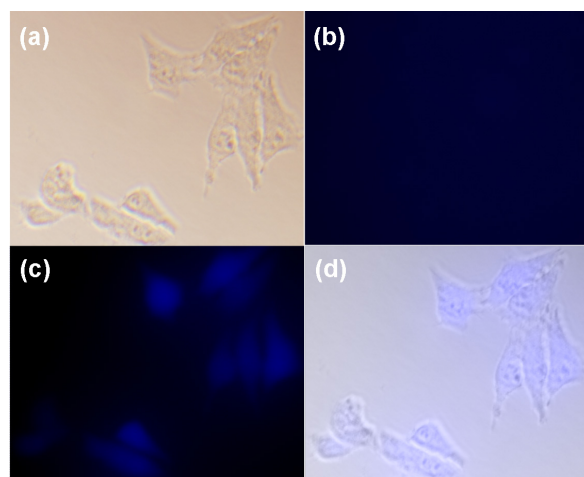


Fig. S5. (a) Brightfield image of HeLa cells. (b) Fluorescence microscopy images of HeLa cells pretreated with N-methylmaleimide (500 μM) for 30 min at 37 $^{\circ}\text{C}$ and then incubated with NCS (20 μM) after incubation for 30 min. (c) Image of HeLa cells after treatment with 20 μM NCS for 30 min at 37 $^{\circ}\text{C}$. (d) Merged image of (a) and (c).

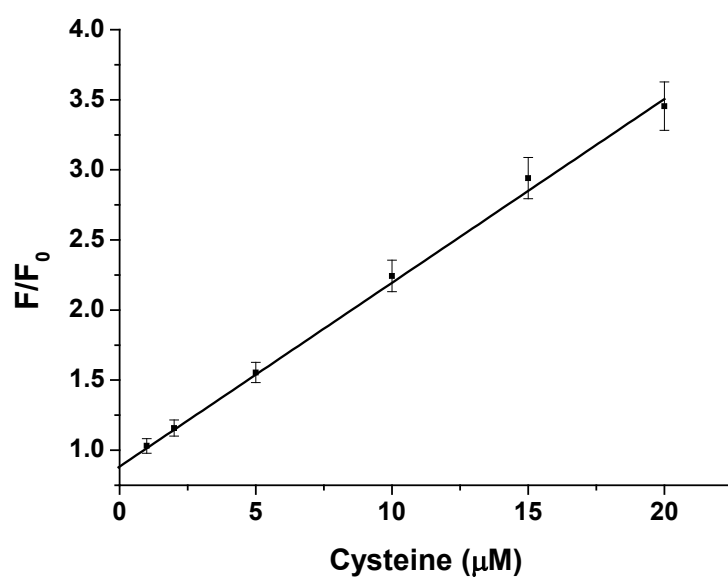


Fig. S6. Standard addition method used for the determination of total biothiols in human serum, using Cys as reference. The concentration of biothiols was determined from the intersection of the straight line with the X axis.

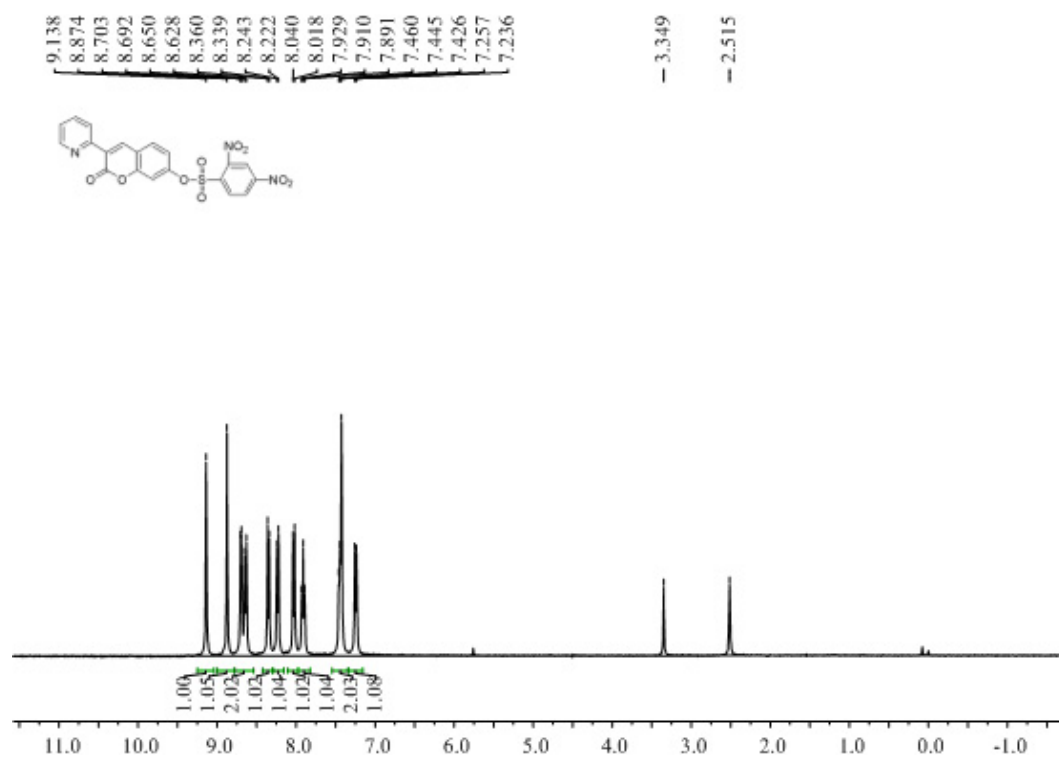


Fig. S7. $^1\text{H-NMR}$ spectra of compound PCS in $\text{DMSO-}d_6$.

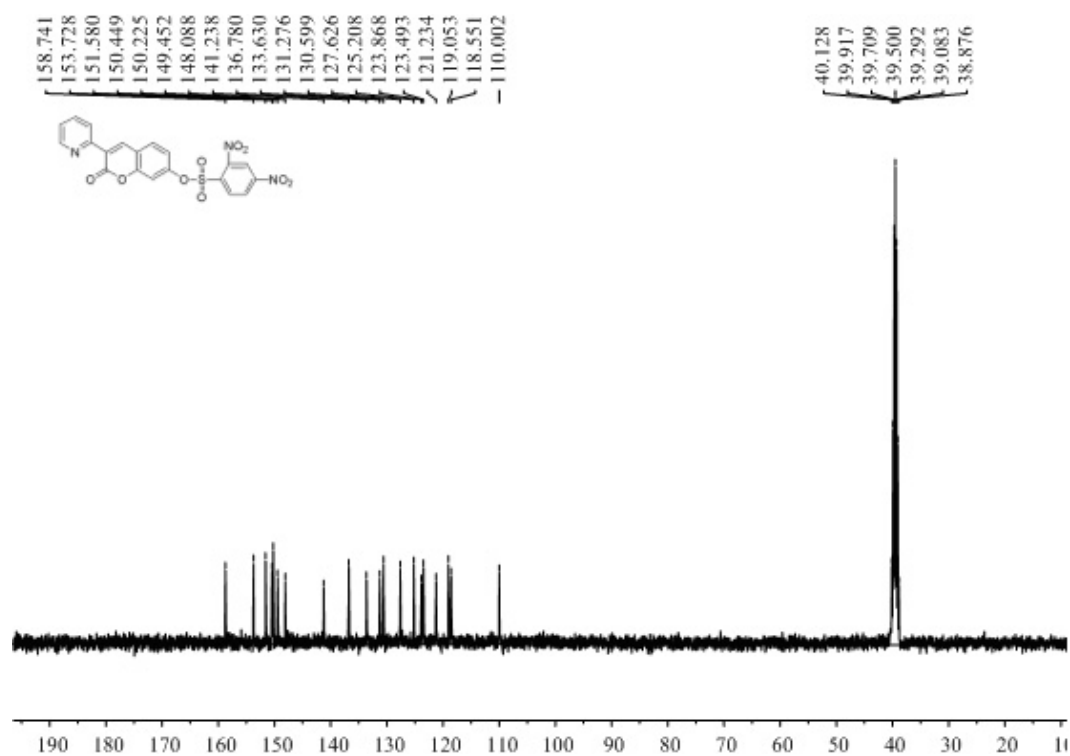


Fig. S8. $^{13}\text{C-NMR}$ spectra of compound PCS in $\text{DMSO-}d_6$

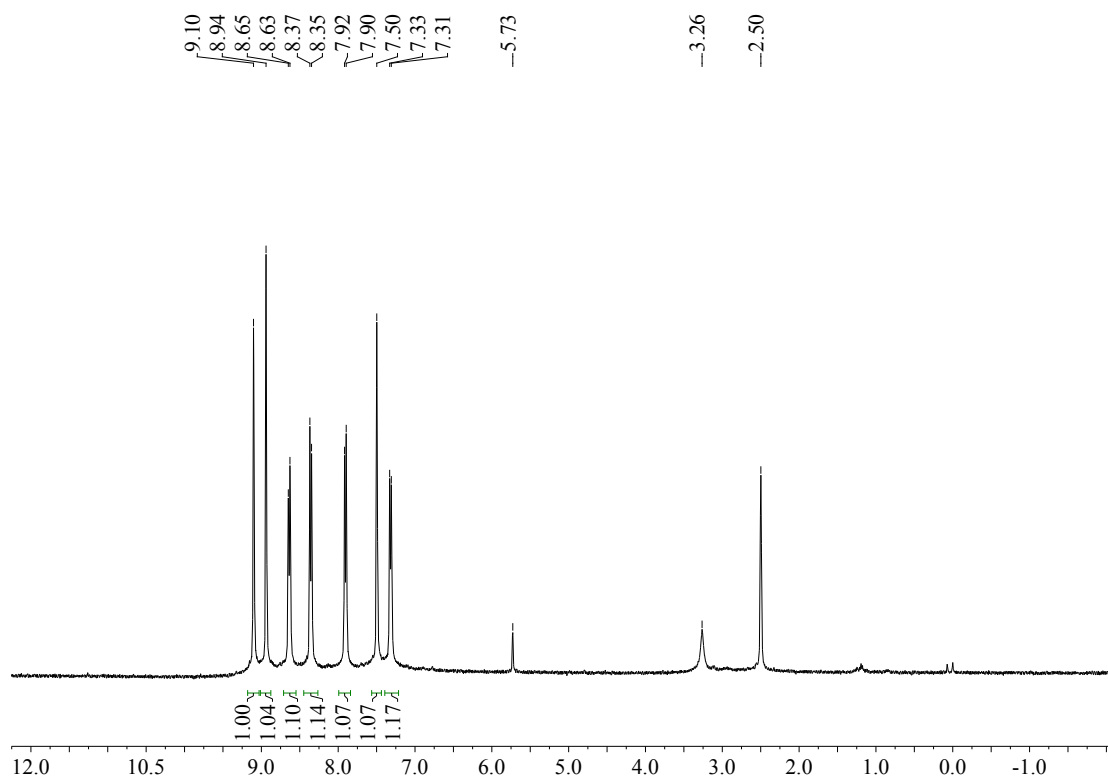


Fig. S9. $^1\text{H-NMR}$ spectra of compound NCS in $\text{DMSO-}d_6$

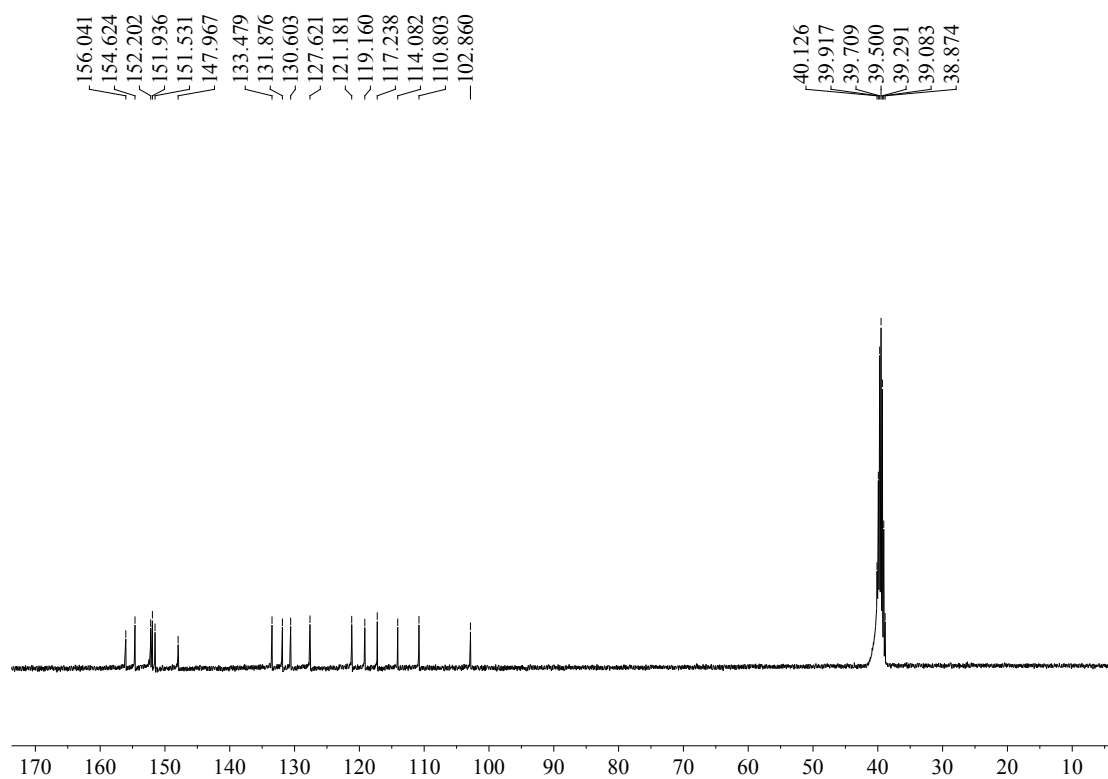


Fig. S10. $^{13}\text{C-NMR}$ spectra of compound NCS in $\text{DMSO-}d_6$.

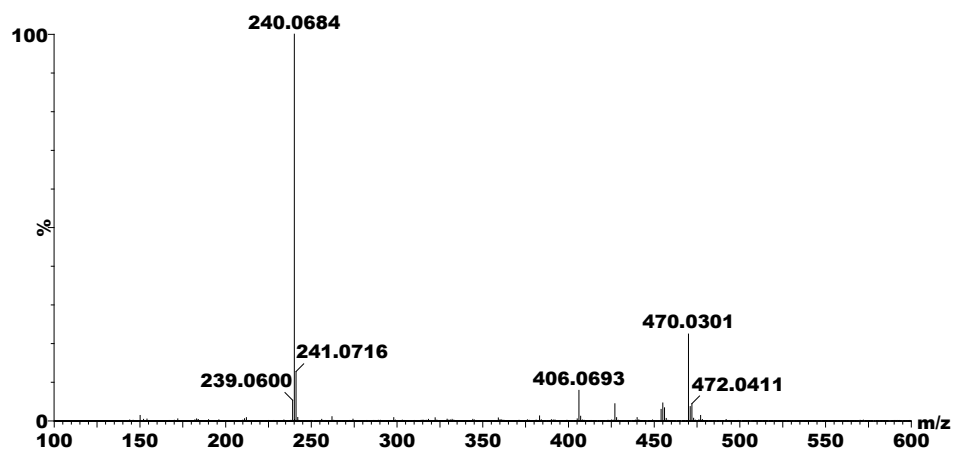


Fig. S11. HRMS of PCS

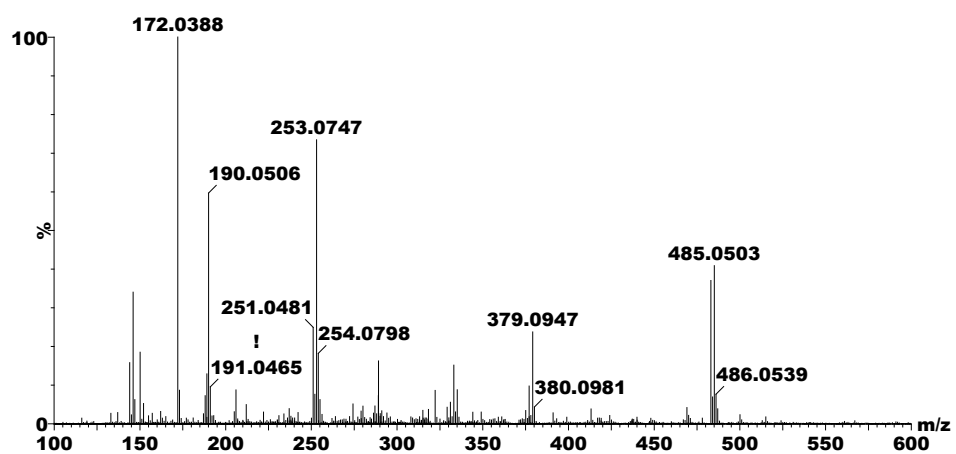


Fig. S12. HRMS of NCS