Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information (SI)

A fluorescent probe for benzenethiols and its application on test paper, in water samples and living cells

Wenying Zhang,[a] Xingjiang Liu,[b] Hongyan Zhang,[c] Chengcheng Feng,[a] Chunxia Liu,[a] Mingming Yu,[a]* Liuhe Wei[a] and Zhanxian Li[a]*

[a] College of Chemistry and Molecular Engineering, Zhengzhou University

[b] College of Chemistry and Chemical Engineering, Central South University, Changsha, Hunan 410083, China

[c] Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, 100190, China

Corresponding Author

*Fax: 86 371-67781205. E-mail: yumm@zzu.edu.cn; lizx@zzu.edu.cn.

Figures

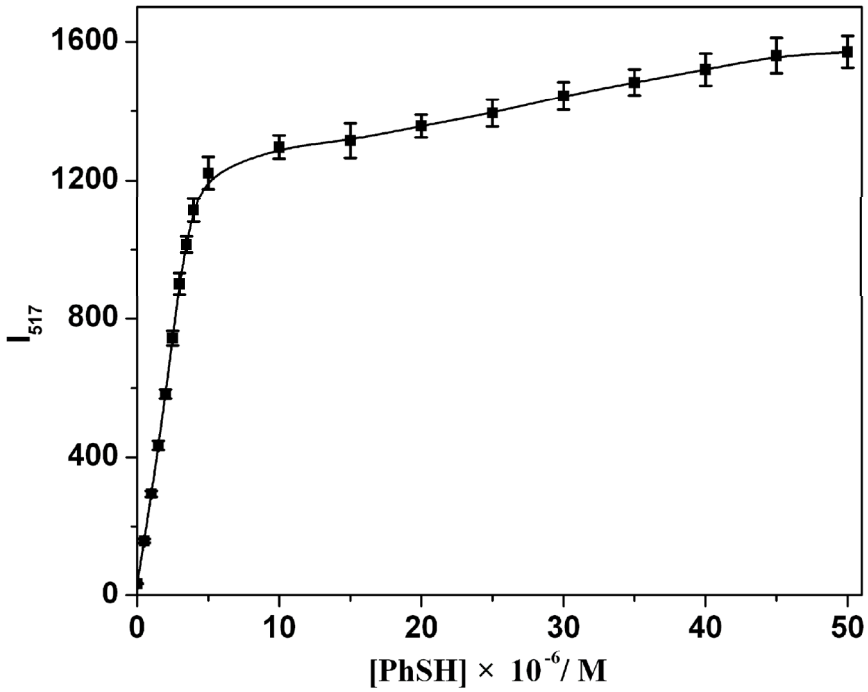

Fig. S1 Emission intensity of compound **1** (5.0 × 10^{-6} M, V_{water}:$V_{ethanol}$ = 7:3) at 517 nm (black square) as a function of addition of benzenethiol ethanol solution.

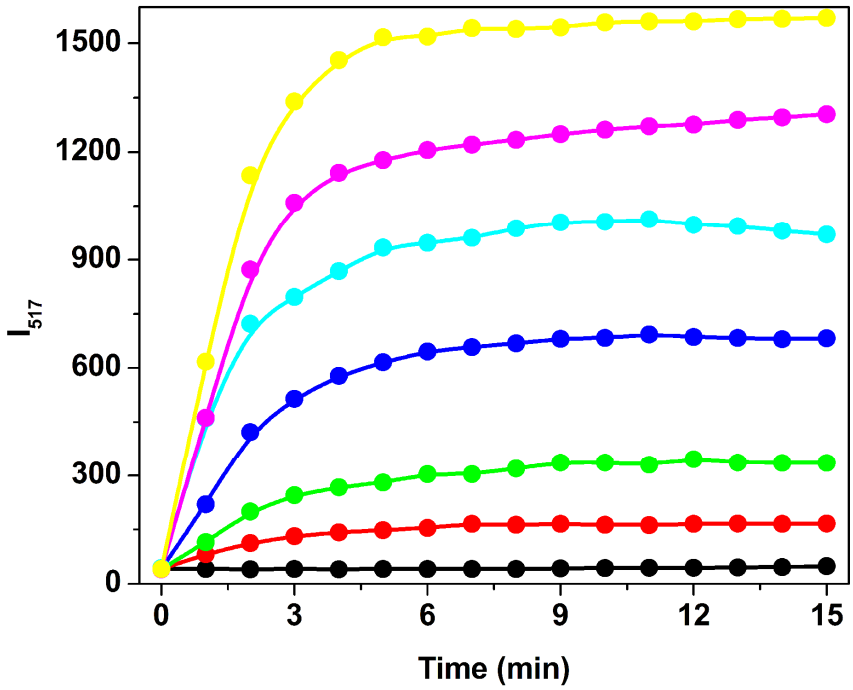

Fig. S2 Kinetic curves of probe **1** (5.0 × 10^{-6} M, V_{water}:$V_{ethanol}$ = 7:3) at 517 nm with benzenethiol at different concentrations (the concentrations of benzenethiol are 0, 5.0 × 10^{-7} M, 1.0 × 10^{-6} M, 2.5 × 10^{-6} M, 5.0 × 10^{-6} M, 7.5 × 10^{-6} M, and 1.0 × 10^{-5} M from down to up). The excitation wavelength was 380 nm.

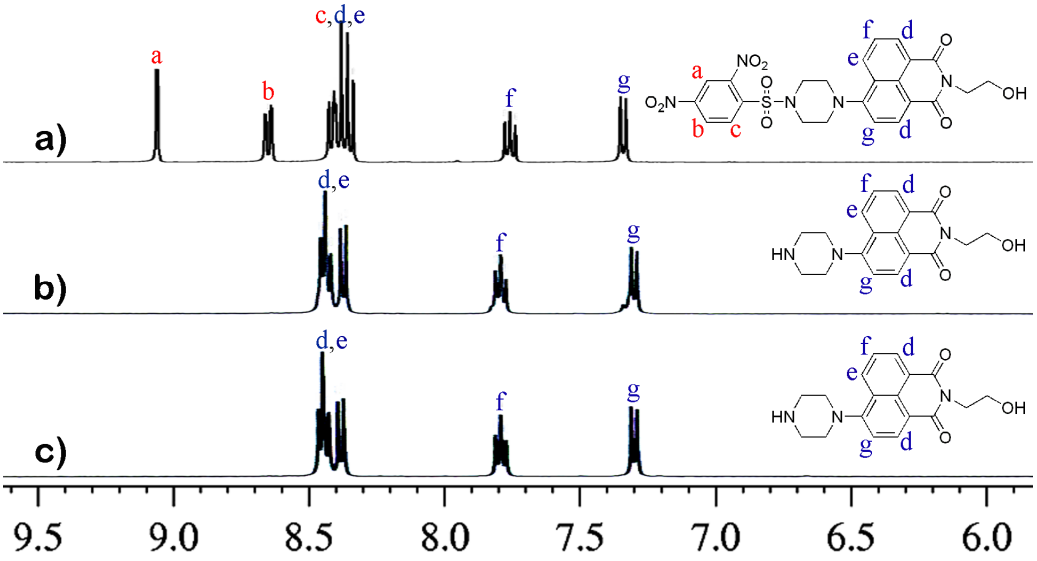

Fig. S3 Partial ^{1}H NMR spectra of **1** upon addition of benzenethiol in DMSO-d_6. (a) Only probe **1**, (b) the isolated product after probe **1** reacted with benzenethiol in mixture of water and ethanol, (c) the reference compound **2**.

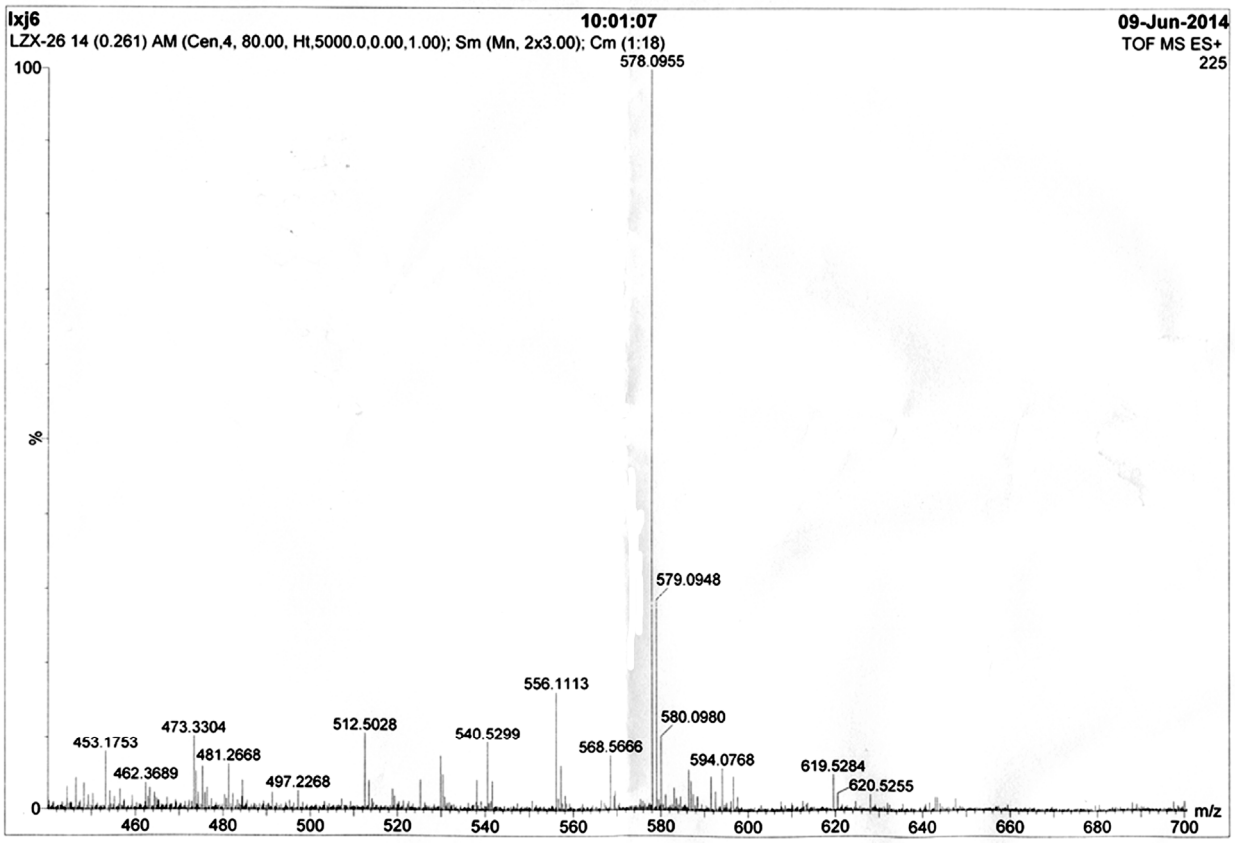

Fig. S4 TOF mass spectra of **1**.

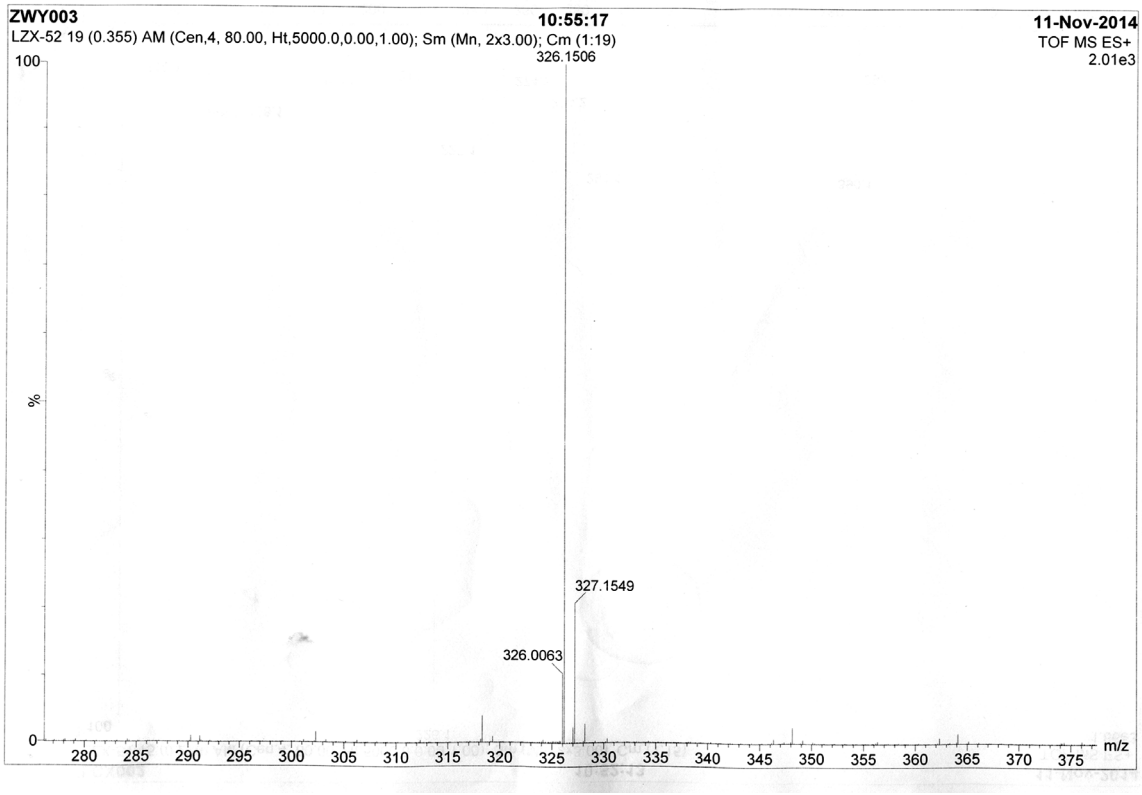

Fig. S5 TOF mass spectra of the product from the reaction of **1** with benzenethiol.

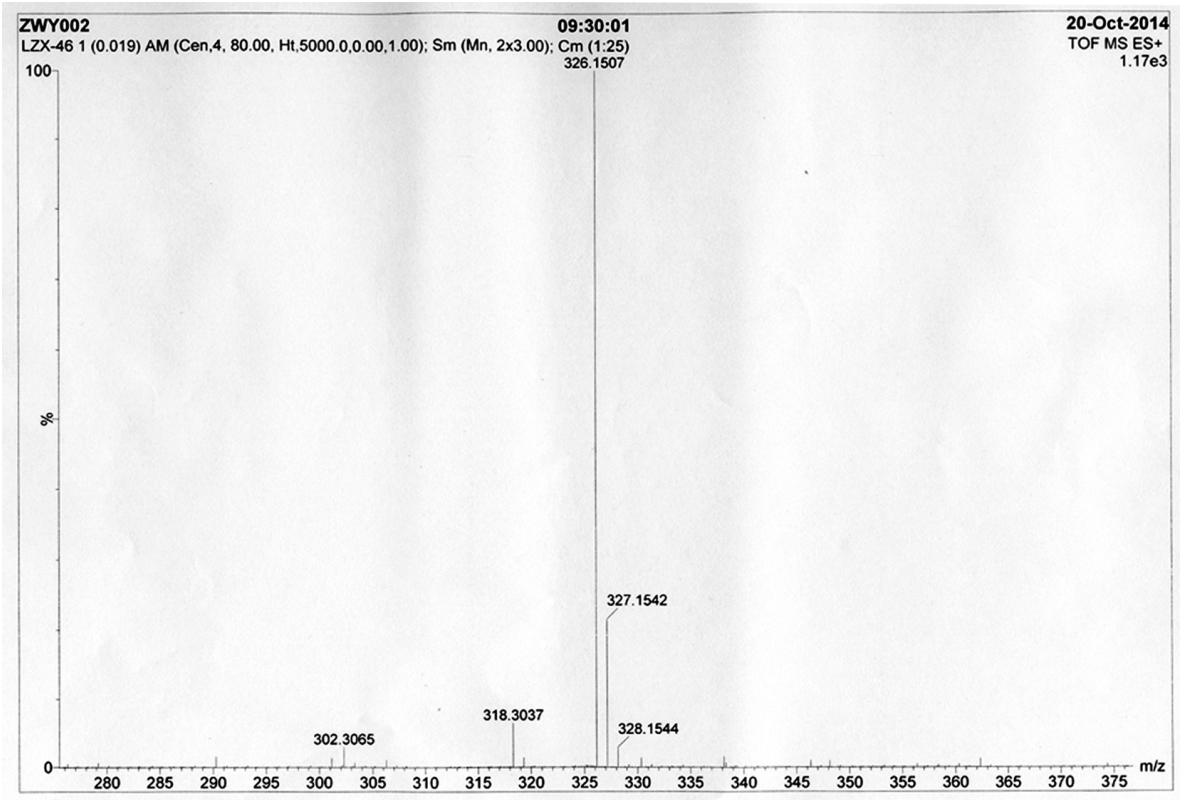

Fig. S6 TOF mass spectra of the product from compound **2**.

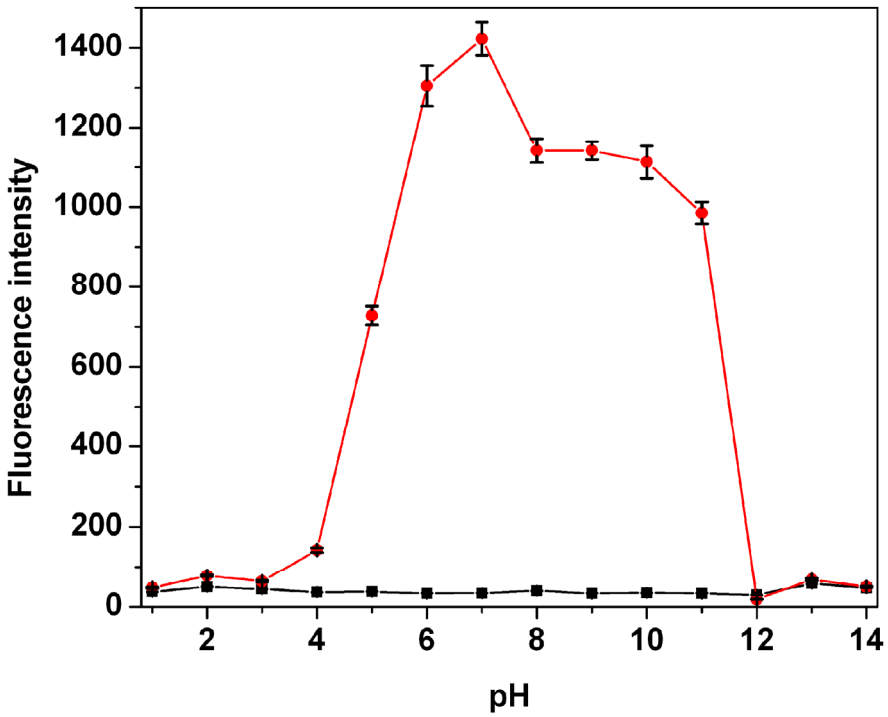

Fig. S7 Fluorescence intensity change of **1** (5.0×10^{-6} M, V_{water}:$V_{ethanol}$ = 7:3) before and after addition of benzenethiol with different pH.

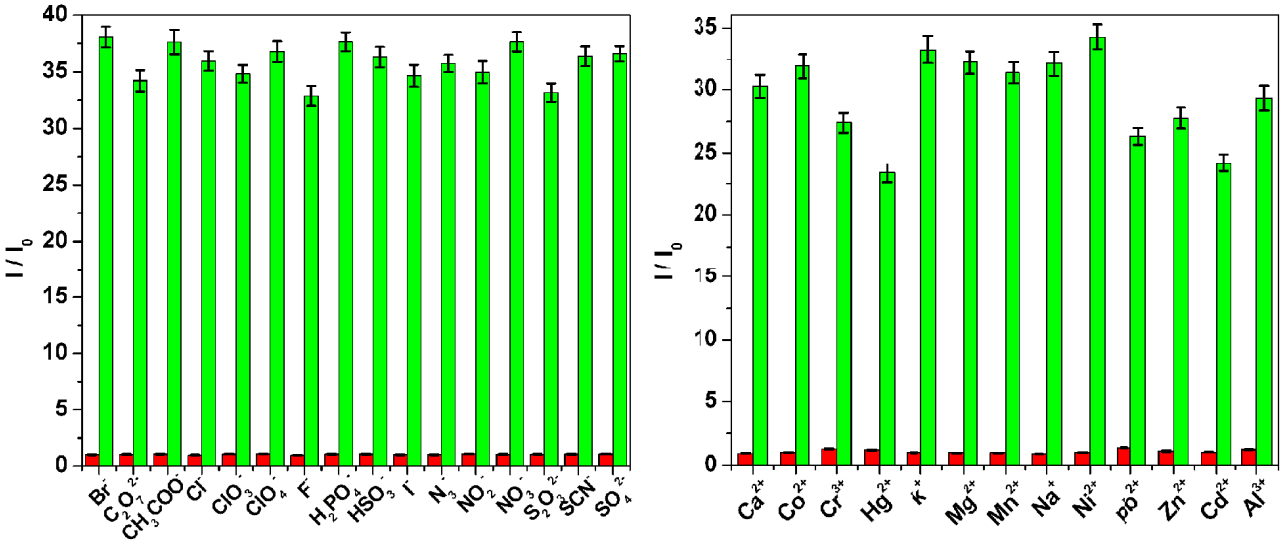

Fig. S8 Fluorescence responses of **1** (5.0×10^{-6} M, V_{water}:$V_{ethanol}$ = 7:3) upon addition of 10 equiv. of different anions (left, red bars) and 10 equiv. of metal ions (right, red bars). Fluorescence changes of the mixture of **1** and benzenethiol after addition of 2 equiv of anions (left, green bars) and 2 equiv of metal ions (right, green bars). The excitation wavelength was 380 nm. I_0 represents the emission intensity at 517 nm in the fluorescence spectroscopy of compound **1**. I represents the emission intensity at 517 nm in the fluorescence spectroscopy of compound **1** after addition of the species to the solution of **1** (red bars) and of the mixture of **1** and benzenethiol after addition of an excess of the species (green bars). The anions and metal ions used were Br^-, $Cr_2O_7^{2-}$, Cl^-, ClO_3^-, ClO_4^-, F^-, $H_2PO_4^-$, HSO_3^-, NO_2^-, NO_3^-,

$S_2O_3^{2-}$, SCN^-, SO_4^{2-}, Ca^{2+}, Co^{2+}, Cr^{3+}, Hg^{2+}, K^+, Mg^{2+}, Mn^{2+}, Na^+, Ni^{2+}, Pb^{2+}, Zn^{2+}, Cd^{2+}, and Al^{3+}.

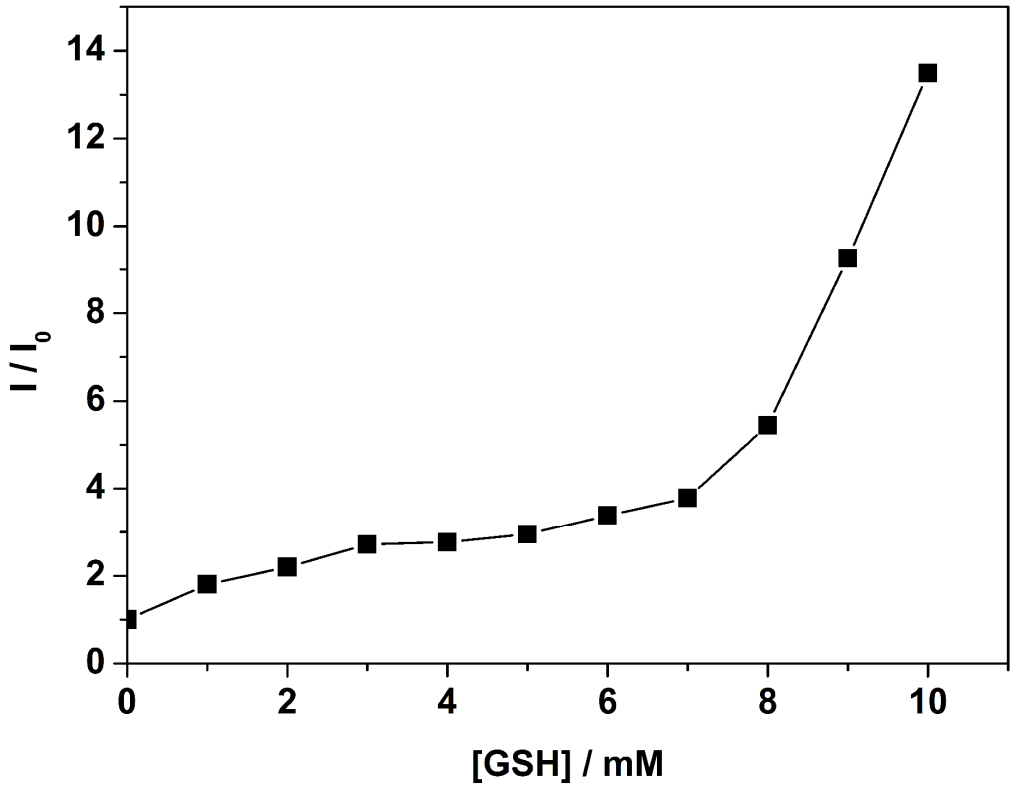

Fig. S9 Fluorescence intensity of probe **1** (5.0×10^{-6} M, V_{water}:$V_{ethanol}$ = 7:3) changes with the concentration of GSH from 1 to 10 mM. The excitation wavelength was 380 nm and the reaction time was 3 min.

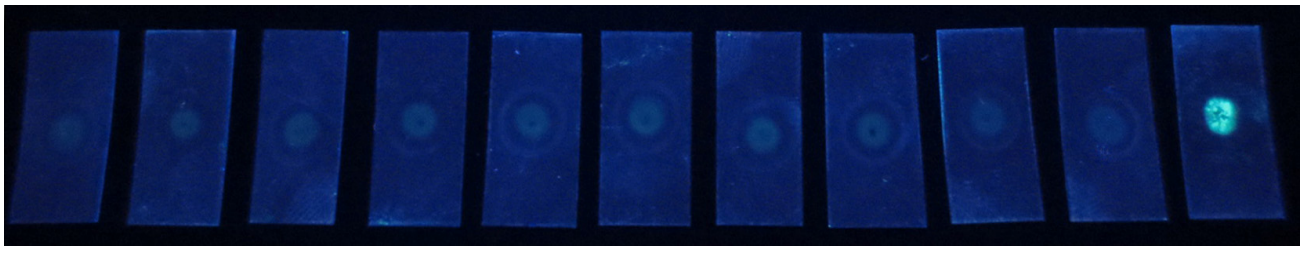

Fig. S10 Images of test papers for the selectivity of benzenethiol upon addition of 10 mM of various species (From left to right, the species used were KI, NaN_3, PhOH, $PhNH_2$, Gly, Ala, Cys, GSH, and PhSH.) in aqueous solutions of **1** (5.0×10^{-5} M, V_{water} : $V_{ethanol}$ = 7:3) under a UV lamp (365 nm).

Table S1 Determination of benzenethiol concentrations in water samples.

sample	benzenethiol spiked (μM)	benzenethiol recovered (μM)	Recovery (%)
Tap water	0	not detected	
	0.5	0.53±0.07	106
	1	0.96±0.06	96
	1.5	1.43±0.05	95
	2	2. 04±0.12	102
	2.5	2.53±0.05	101
	3	3.19±0.02	106
	3.5	3.43±0.10	98
	4	3.95±0.01	99
pond	0	not detected	
	0.5	0.45±0.04	91
	1	1.02±0.04	102
	1.5	1.53±0.06	102
	2	2.08±0.11	104
	2.5	2.48±0.02	99
	3	3.17±0.02	106
	3.5	3.51±0.07	100
	4	3.94±0.05	98
Eyebrow lake	0	not detected	
	0.5	0.45±0.02	90
	1	0.99±0.11	99
	1.5	1.43±0.06	96
	2	1.94±0.04	97
	2.5	2.51±0.12	100
	3	3.12±0.13	104
	3.5	3.39±0.04	97
	4	4.00±0.06	100