Electronic Supporting Information

Reaction–based fluorescent probe for selective and sensitive detection of thiophenols with a large stokes shift and its application in water samples

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Preparation of test solutions:

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1. Preparation of probe solution: The solution of Probe **1** was prepared in DMSO at 0.2 mM. The test solution of the Probe **1** (10 μM) in 3 mL HEPES buffer (50 Mm, pH 7.4) was prepared by placing 0.15 mL stock solution of Probe **1** (10 μM) and 0.75 mL DMSO in 2.1 mL HEPES buffer.
2. Preparation of the solutions of various tested analytes: NaF, NaCl, NaBr, NaI, $NaClO_4$, NaClO, $NaHSO_3$, Na_2SO_3, Na_2SO_4, KCl, $ZnCl_2$, $FeCl_3$, $AlCl_3$, $CuCl_2$, $HgCl_2$, $CoCl_2$ were prepared at 3 mM in distilled water. PhSH, p–NH_2–PhSH, p–CH_3–PhSH, p–NO_2–PhSH, Hcy, Cys, GSH, $(CH_3)_3SH$, $HOCH_2CH_2SH$, NaSH, Na_2S, $C_6H_5NH_2$, C_6H_5OH were prepared at 3 mM in EtOH.

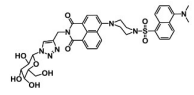
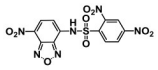
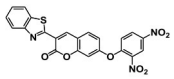
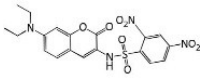
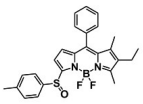
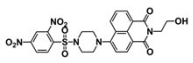
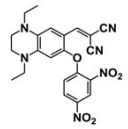
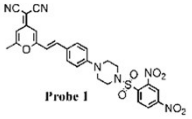
Probe	$\lambda_{ex}/\lambda_{em}$ (nm) (stokes shift)	Response speed	Detection limit	Reference
	260/414 (154)	5 s	3.8 nM	Dyes Pigms 2015; 116: 52–57
	465/555 (90)	20 min	2 μM	Chem Commun 2010; 46: 1944–1946
	461/494 (33)	30 min	1.8 nM	Chem Commun 2010, 46, 1503−1505.
	370/515 (145)	15 min	150 nM	Anal. Chem. 2014, 86, 8835 – 8841
	484/568 (84)	30 min	0.74 μM	Org Biomol Chem. 2012; 10: 4689−4691.
	380/517 (137)	3 min	10 nM	J Mater Chem C 2015, 3, 8248−8254.
	477/606 (129)	2 min	8.2 nM	J Mater Chem C 2016, 4, 4320−4326.
	454/613 (159)	15 min	8.3 nM	This work

Table S1. Comparison of determined detection limit with those of some literatures.

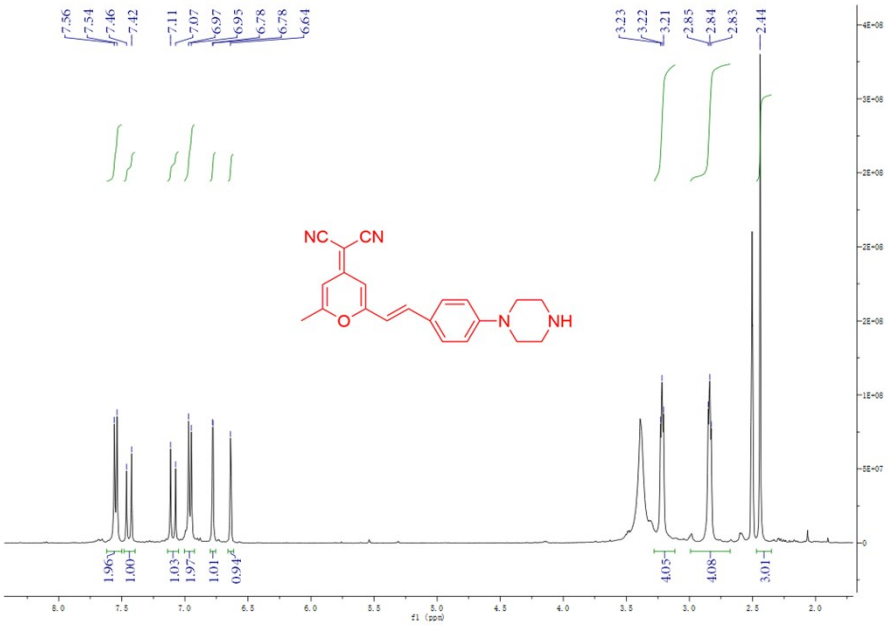


Fig. S1. ^{1}H NMR spectrum of compound **2** in DMSO-d_6

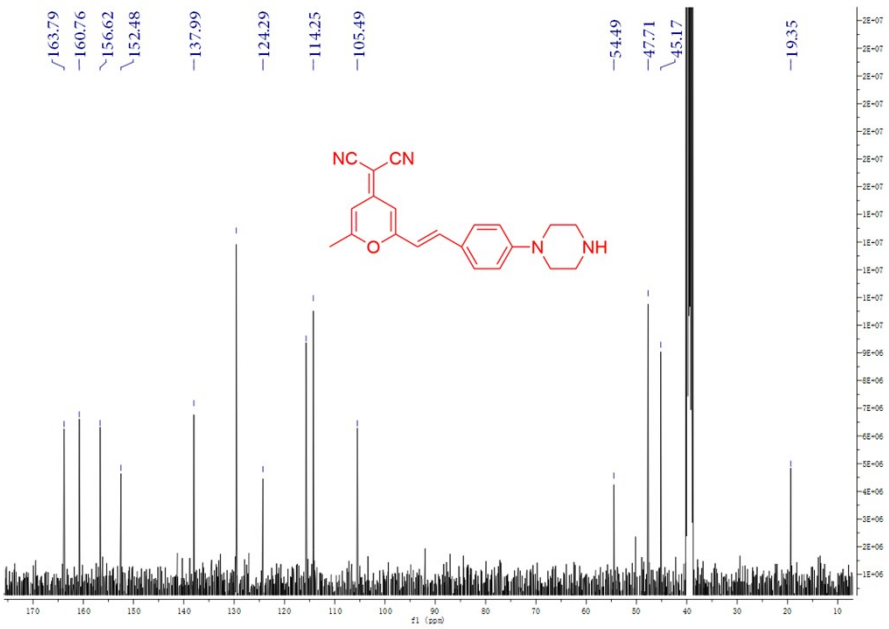


Fig. S2. ^{13}C NMR spectrum of compound **2** in DMSO-d_6

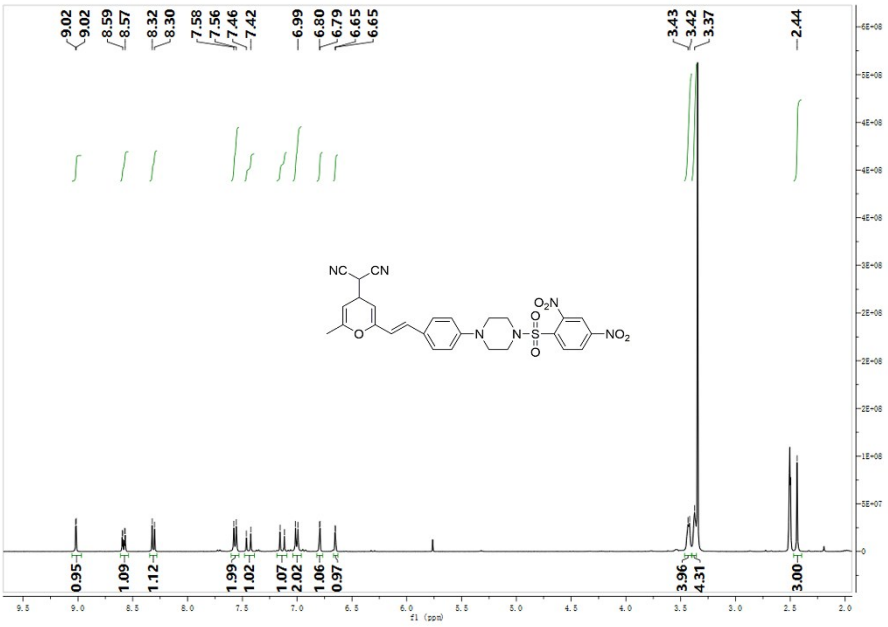


Fig. S3. ^{1}H NMR spectrum of Probe **1** in DMSO-d_6

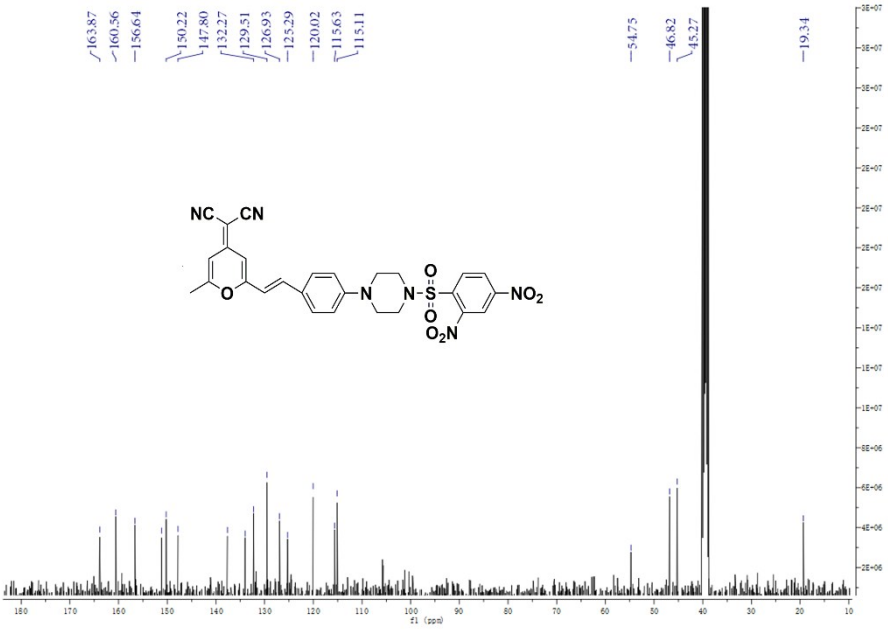


Fig. S4. ^{13}C NMR spectrum of Probe **1** in DMSO-d_6

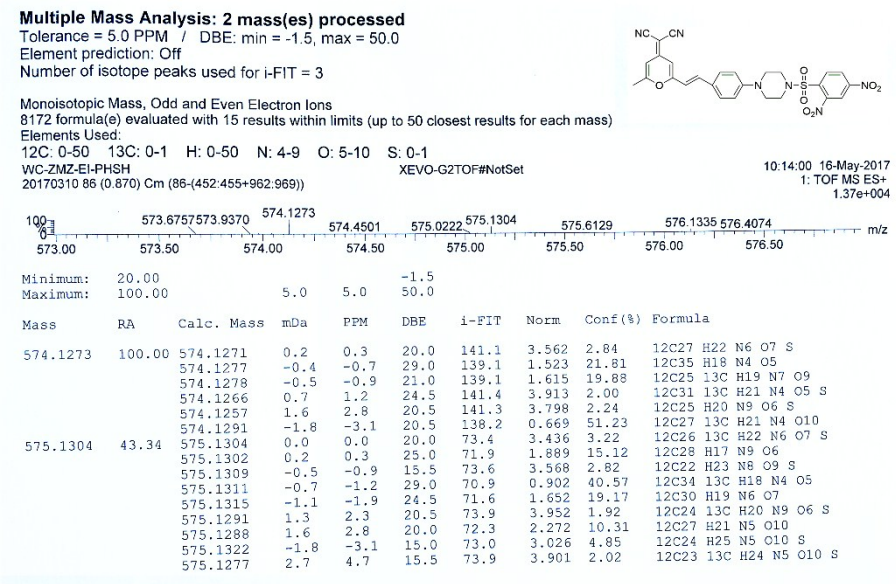


Fig. S5. HRMS spectrum of Probe **1**.

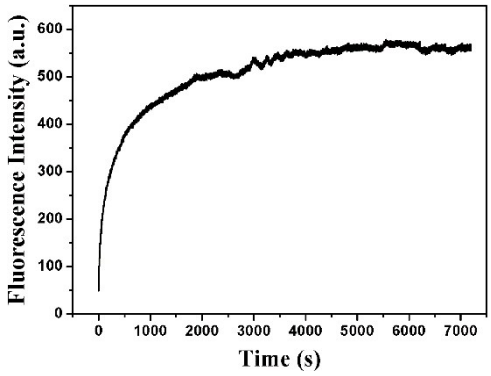


Fig. S6. Time course of Probe **1** (10 μM) upon addition of thiolphenol (20 μM) in DMSO–HEPES (V/V = 3 : 7, 50 mM, pH 7.4) solution. Slit width: 3/5 nm. λ_{ex} = 454 nm.

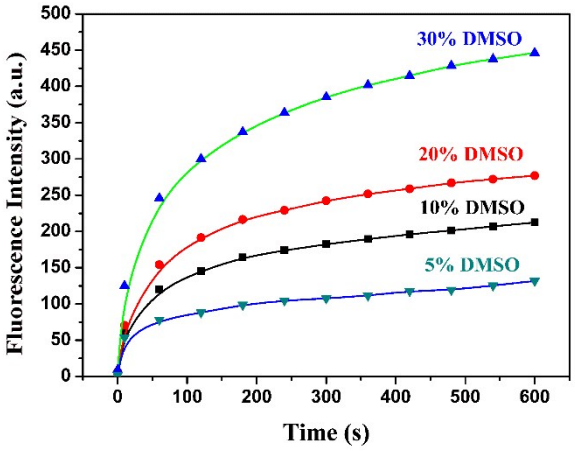


Fig. S7. Time dependent fluorescence spectra of Probe **1** (10 μM) in the present of PhSH (50 μM) in different DMSO/HEPES buffer solution (30/70, 20/80, 10/90, 5/95, pH = 7.4, 50 mM). λ_{ex} = 454 nm.

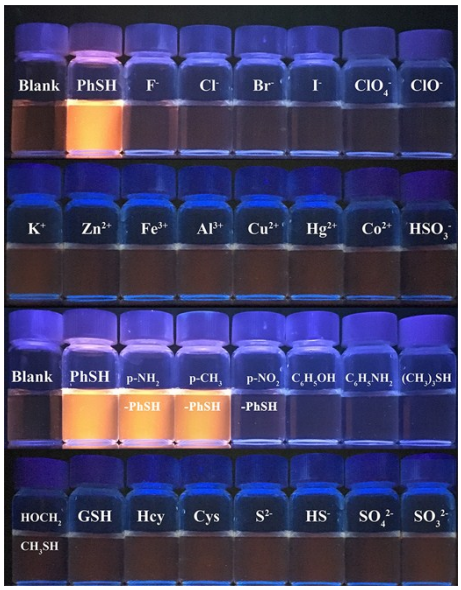


Fig. S8. Color changes of Probe **1** upon addition of different species under UV light (365 nm).

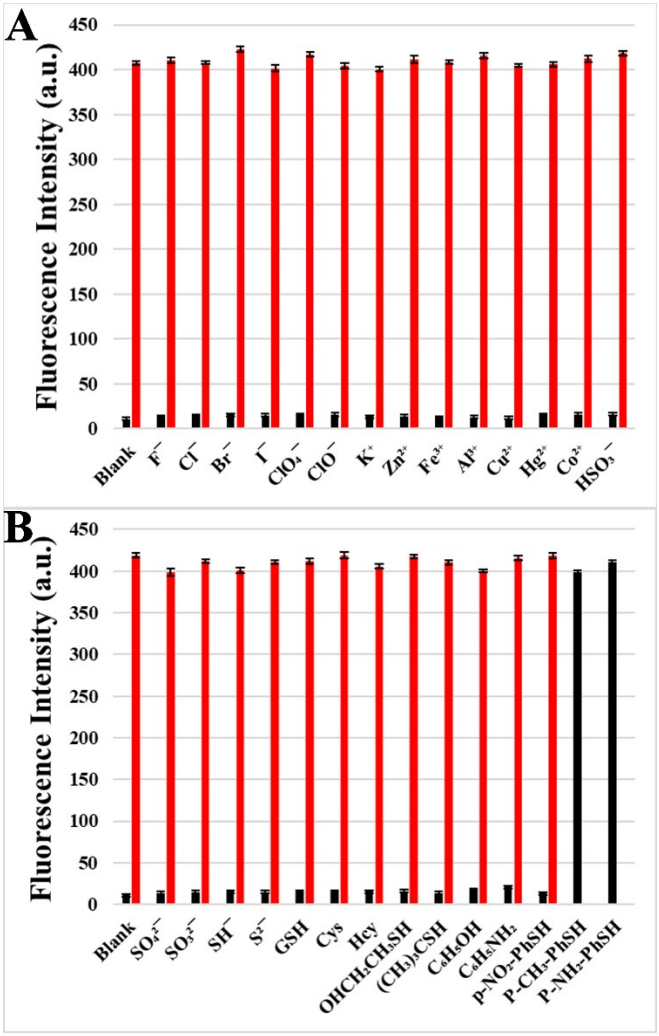


Fig. S9. Fluorescence responses of Probe **1** (10 μM) at 613 nm toward thiolphenol (20 μM) in the presence of some competitive species (100 μM) in DMSO–HEPES (V/V = 3 : 7, 50 mM, pH 7.4) solution. λ_{ex} = 454 nm.

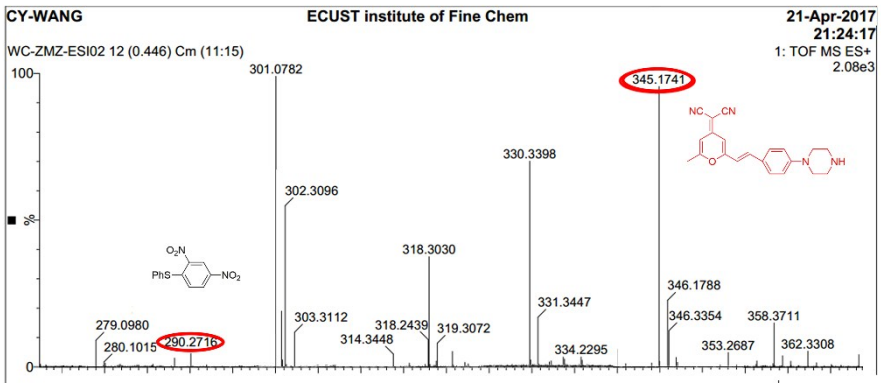


Fig. S10. HRMS spectrum of the reaction between Probe **1** and PhSH.

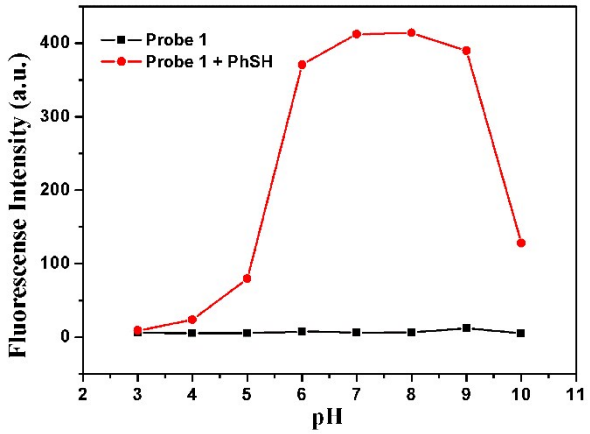


Fig. S11. Effect of pH on the fluorescence intensity at 613 nm of Probe **1** (10 μM) in DMSO–HEPES (V/V = 3 : 7, 50 mM, pH 7.4) solution with (●) and without (■) PhSH (20 μM). λ_{ex} = 454 nm.