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Electronic Supplementary Information

A novel near-infrared xanthene fluorescent probe for detection of thiophenol in vitro and in vivo

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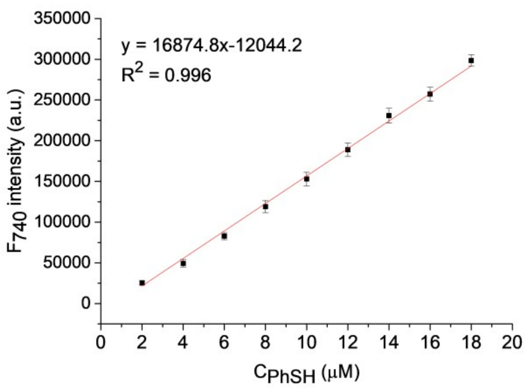

Fig. S1 Linearity between the fluorescence intensity at 740 nm versus PhSH concentration in the range of 2 −18 μM. λ_{ex} = 670 nm, λ_{em} = 740 nm.

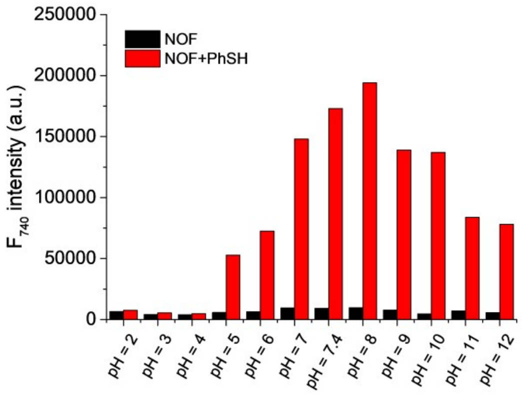

Fig. S2 The pH-dependent fluorescence response of NOF (10 μM) towards PhSH (30 μM). λ_{ex} = 670 nm, λ_{em} = 740 nm.

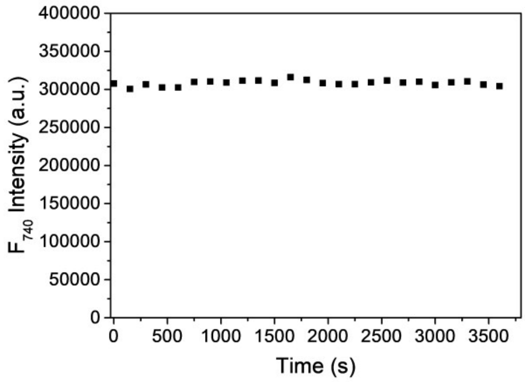

Fig. S3 Changes of fluorescence intensity of NOF irradiated at 670 nm for 60 min, λ_{em} = 740 nm.

Table S1. Comparison of representative fluorescent probes for thiophenol (PhSH)

References	λ_{ex} /nm	$\lambda_{em\ max}$/nm	Detection limit/μM	Imaging applications
Jiang, W. *et al. Angew. Chem Int. Ed.,* **2007**, 46, 8445.	465	555	2.000	Not given
Lin. W. *et al. Chem. Commun.*, **2010***,* 46, 1503.	405	494	0.0018	HeLa cells
Wang Z. *et al. Anal. Chem.,* **2012**, 84, 4915.	481	590	0.020	Not given
Yu D. *et al. Anal. Chem.,* **2014**, 86, 8835.	490	670	0.150	HeLa cells
Shao, X. *et al. Anal. Chem.,* **2015**, 87, 339.	580	633	0.037	SMMC-7721 cells
Zhang, W. *et al. J. Mater. Chem. C*, **2015**, 3, 8248.	380	517	0.0103	A549 cells
Yue Y. *et al. Anal. Chem.,* **2016**, 88, 10499.	404	536	0.026	HepG2 cells
Shang, H. et al. *Biosen. Bioelectron.*, **2017**, 95, 81.	570	625	0.363	HeLa cells Living tissues
Xiong, L. *et al. ACS Sens.,* **2017**, 2, 599.	538	645	0.0099	Not given
Zhang, D. *et al. Ind. Eng. Chem. Res.,* **2017**, 56, 9303.	490	510	0.026	MCF-7 cells
Guo S. *et al. Talanta*, **2018**, 185, 359.	595	653	0.015	HeLa Cells
Zhou S. *et al. Sens. Actuators B Chem.*, **2018**, 276, 361.	488	590	0.036	HeLa cells
Li Y. *et al. Talanta*, **2019**, 199, 355.	540	658	0.220	HeLa cells
Liu, Q. *et al. Sens. Actuators B Chem.*, **2019**, 283, 820.	543	624	0.0081	HepG2 cells HeLa cells
Xu T. *et al. ACS Sustain. Chem. Eng.,* **2020**, 8, 6413.	470	585	0.0028	Not given
Yang L. *et al. Dyes Pigments,* **2020**, 175, 108154.	574	620	0.550	Not given
This work	670	740	0.120	MCF-7 cells mice

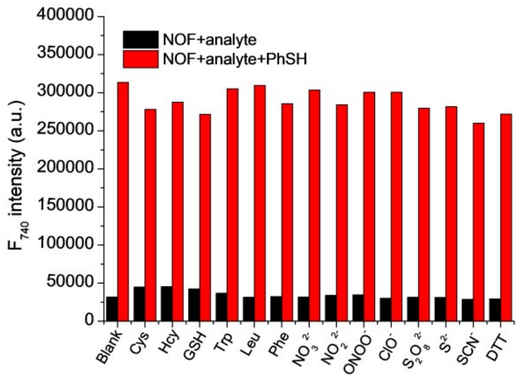

Fig. S4 Fluorescence intensity of NOF (10 μM) in the presence of various analytes. Black bars represent the addition of a single analyte (50 μM). Red bars represent the subsequent addition of thiophenol (30 μM) to the mixture. λ_{ex} = 670 nm, λ_{em} = 740 nm.

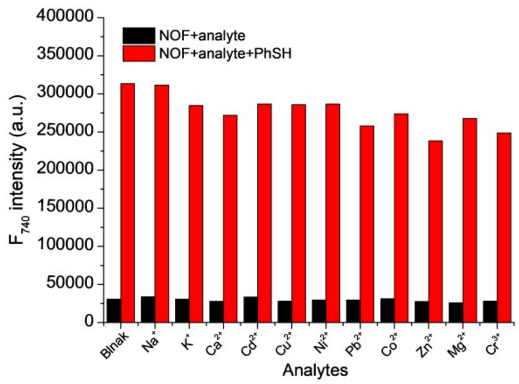

Fig. S5 Fluorescence intensity of NOF (10 μM) in the presence of various metal ions. Black bars represent the addition of a single metal ion (50 μM). Red bars represent the subsequent addition of thiophenol (30 μM) to the mixture. λ_{ex} = 670 nm, λ_{em} = 740 nm.

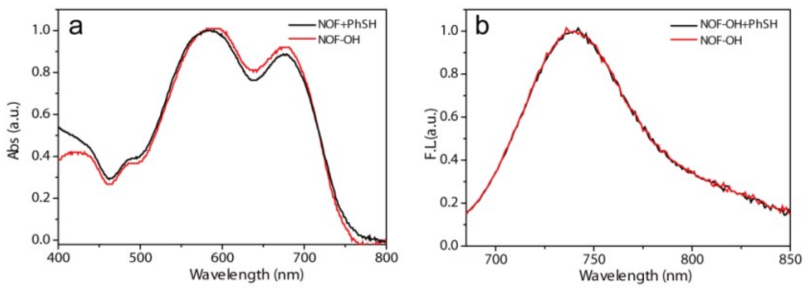

Fig. S6 (a) Absorption and (b) fluorescence spectra of NOF and the product of NOF reacted with PhSH. λ_{ex} = 670 nm, $\lambda_{em\ max}$= 740 nm.

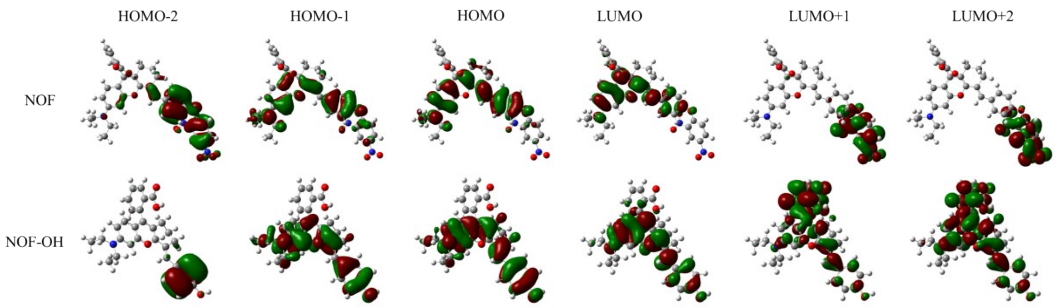

Fig. S7 Representations of the frontier molecular orbitals (MOs) for the S_0 geometry of NOF and NOF-OH as determined at the DFT//B3LYP/6-31G* level.

Table S2 Frontier molecular orbital energies (in eV) calculated at the DFT//B3LYP/6-31G* level.

Sample	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	GAP
NOF	-9.57	-8.81	-8.18	-5.60	-4.58	-4.24	2.58
NOF-OH	-9.56	-8.73	-8.06	-5.54	-3.88	-3.82	2.52

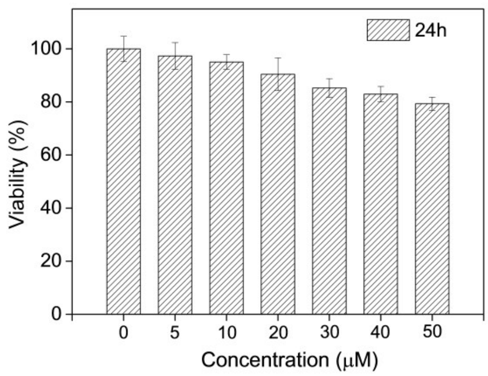

Fig. S8 Viable cells after treatment with indicated concentrations of probe NOF after 24 hours, the cell viability was observed via MTT assay.

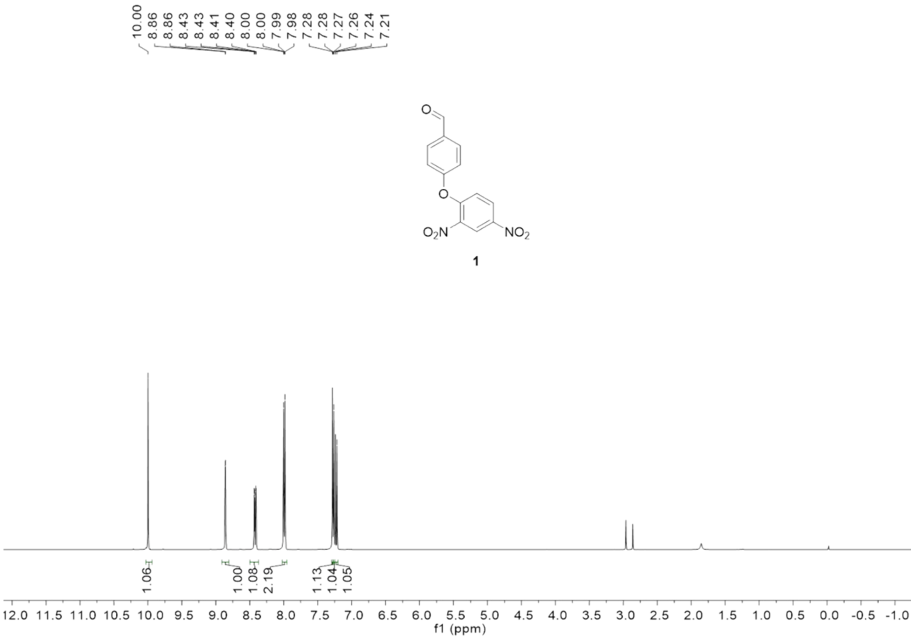

Fig. S9 ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 1.

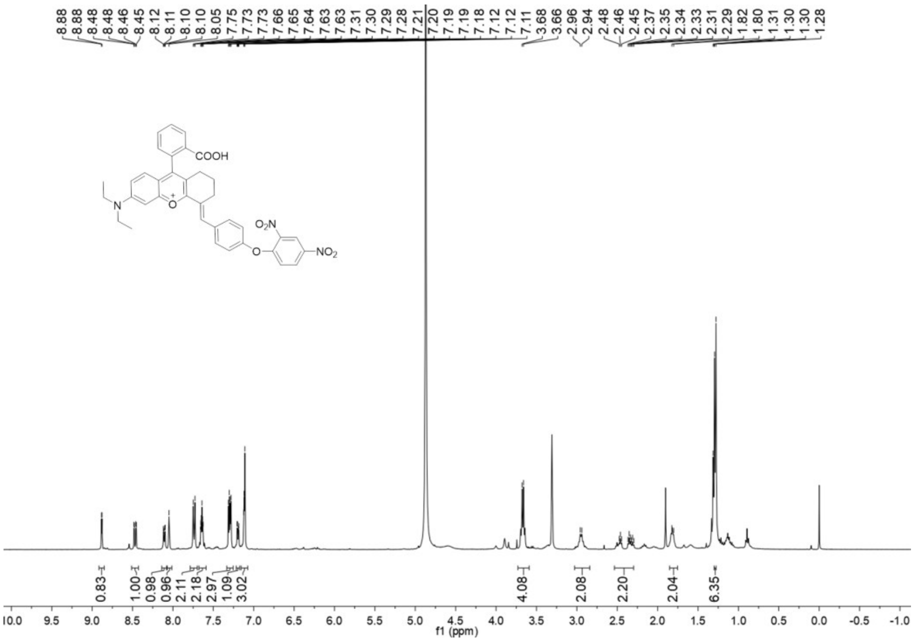

Fig. S10 ^{1}H NMR (400 MHz, CD_3OD) spectrum of NOF.

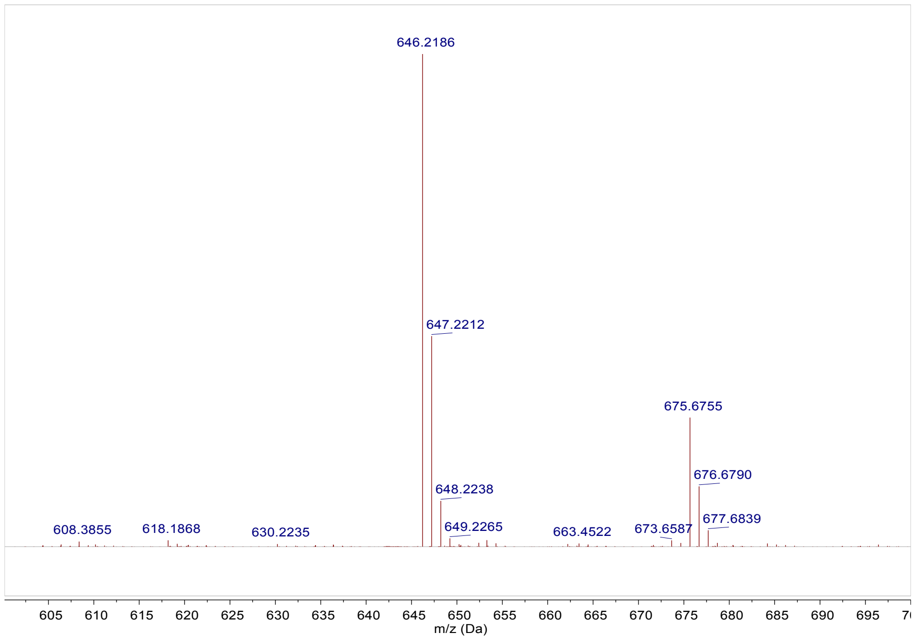

Fig. S11 HR-MS of NOF.

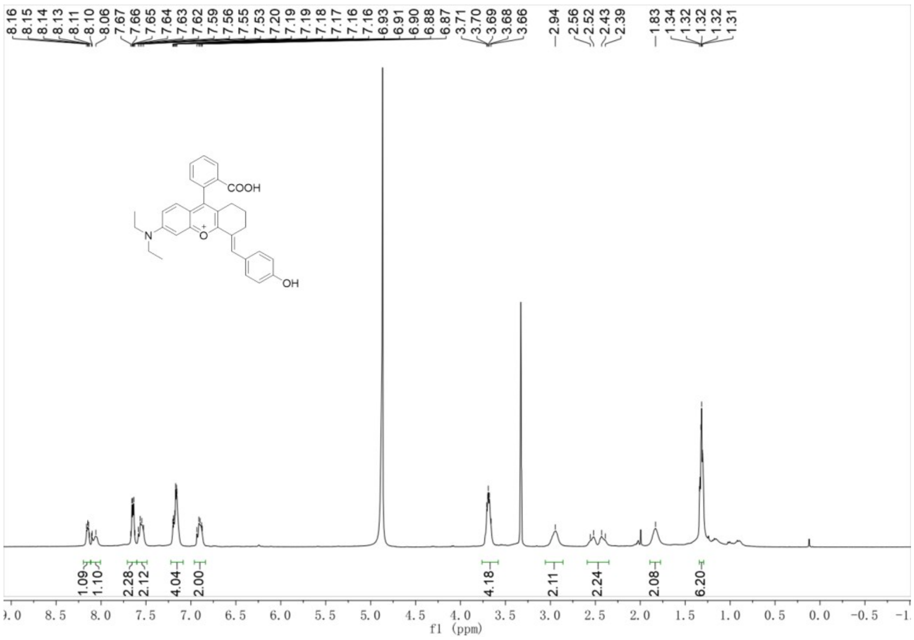

Fig. S12 ^{1}H NMR (400 MHz, CD_3OD) spectrum of NOF-OH.

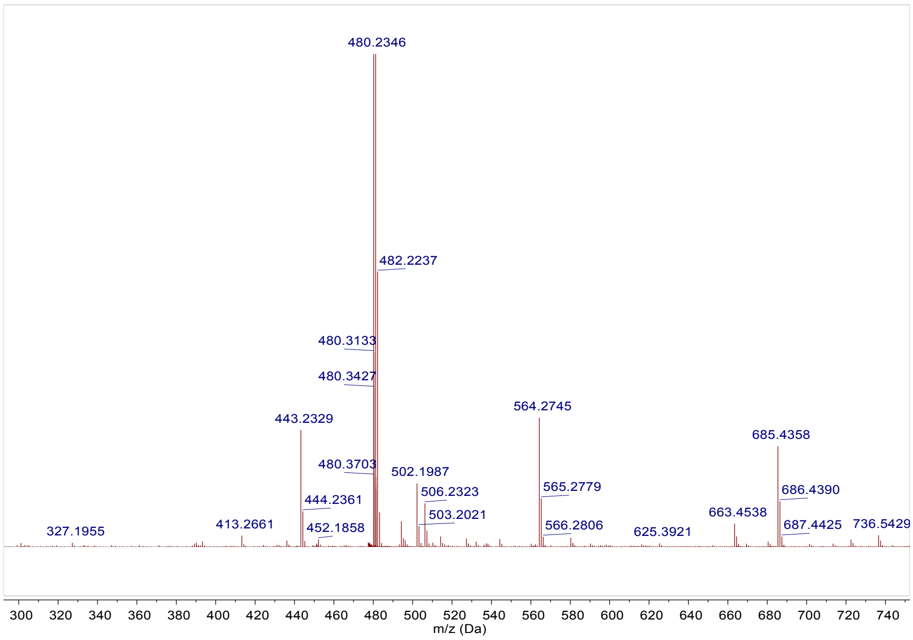

Fig. S13 HR-MS of NOF-OH.