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Supplementary Material

A new fluorescent probe for quick and highly selective detection of hydrogen sulfide and its application in living cells

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Fluorescence quantum yield measurement

The quantum yield of the compound was calculated according to the equation:

$$\Phi_u = \Phi_s \frac{I_u}{I_s} \times \frac{A_s}{A_u} \times (\frac{n_u}{n_s})^2$$

Φ denotes the quantum yield; I denotes the area under the fluorescence curve; A denotes the absorbance at the excitation wavelength; n denotes the refractive index of the solvent. Quinine sulfate (Φ = 0.542 in 0.1 M sulfuric acid solution) and Fluorescein (Φ = 0.79 in 0.1 M NaOH solution) was used as the reference standard.

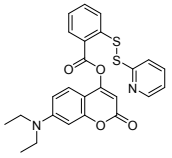
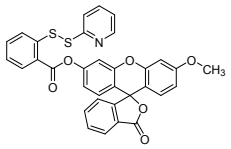
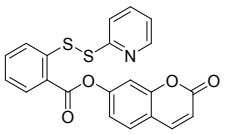
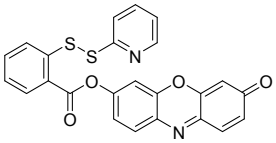
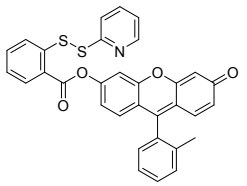
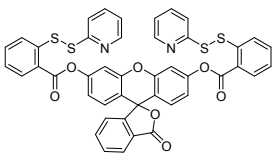
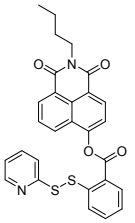
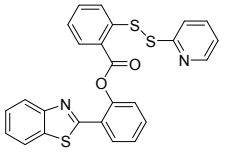
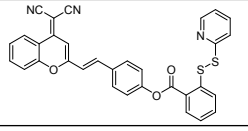
The limit of detection measurement

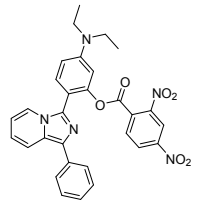
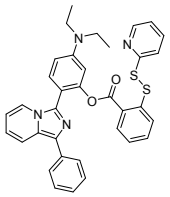
The detection limit of **NIPY-Acr** towards Cys was determined through fluorescence titration, which was measured ten times. The standard deviation of the blank solution was also measured for 15 times. After the linear slope of fluorescence intensity vs. concentrations of Cys was obtained, the detection of limit (LOD) was calculated by following equation:

$$LOD = 3\sigma/\kappa$$

Where σ denotes the standard deviation of blank measurement, κ denotes the slope of the fluorescence intensity vs. Cys concentrations.

Table S1. Comparison of fluorescent probes for H2S with correlated active group.

Probes	Fluorescence enhancement (at concentration of Na_2S)	Stokes shift	Limit of detection	Response time	Detection medium	reference
	81-fold (I403/I519) at 320 μM	53 nm	0.020±0.001 μM	35 min	PBS buffer	[1]
	130-fold at 50 μM	40 nm	60 nM	Less than 5 min	PBS buffer with 1 mM CTAB	[2,3]
	275-fold at 50 μM	71 nm	79 nM			
	68-fold at 50 μM	36 nm	47 nM			
	20-fold at 50 μM	19 nm	266 nM			
	60-fold at 50 μM	23 nm	47 nM			
	30-fold (I550/T442) at 15 μM	165 nm	0.87 μM	3 min	DMF:PBS (1:9, v/v,) with 1 mM CTAB	[4]
	30-fold at 30 μM	192 nm	0.12 μM	2 min	Tris-HCl buffer with 1mM CTAB	[5]
	*	120 nm	1.1 nM	30 min	DMSO:PBS buffer (1/1, v/v)	[6]

	273-fold at 100 μM	193 nm	0.36 μM	5 min	PBS buffer with 1.5 mM CTAB	[7]
	230-fold at 20 μM	208 nm	43 nm	1.5 min	PBS buffer with 0.5 mM CTAB	This work

*the data was not mentioned.

1 J. Kang, F. Huo and C. Yin, *Dyes and Pigments*, 2017, **146**, 287–292.

2 Liu Chunrong, Pan Jia, Li Sheng, Zhao Yu, Wu Lisa Y., Berkman Clifford E., Whorton A. Richard and Xian Ming, *Angewandte Chemie International Edition*, 2011, **50**, 10327–10329.

3 B. Peng, W. Chen, C. Liu, E. W. Rosser, A. Pacheco, Y. Zhao, H. C. Aguilar and M. Xian, *Chemistry – A European Journal*, 2014, **20**, 1010–1016.

4 C. Zhang, G. Zhang, L. Feng and J. Li, *Sensors and Actuators B: Chemical*, 2015, **216**, 412–417.

5 Z. Xu, L. Xu, J. Zhou, Y. Xu, W. Zhu and X. Qian, *Chem. Commun. (Cambridge, U. K.)*, 2012, **48**, 10871–10873.

6 J. Men, X. Yang, H. Zhang and J. Zhou, *Dyes and Pigments*, 2018, **153**, 206–212.

7 S. Chen, H. Li and P. Hou, *Sensors and Actuators B: Chemical*, 2018, **256**, 1086–1092.

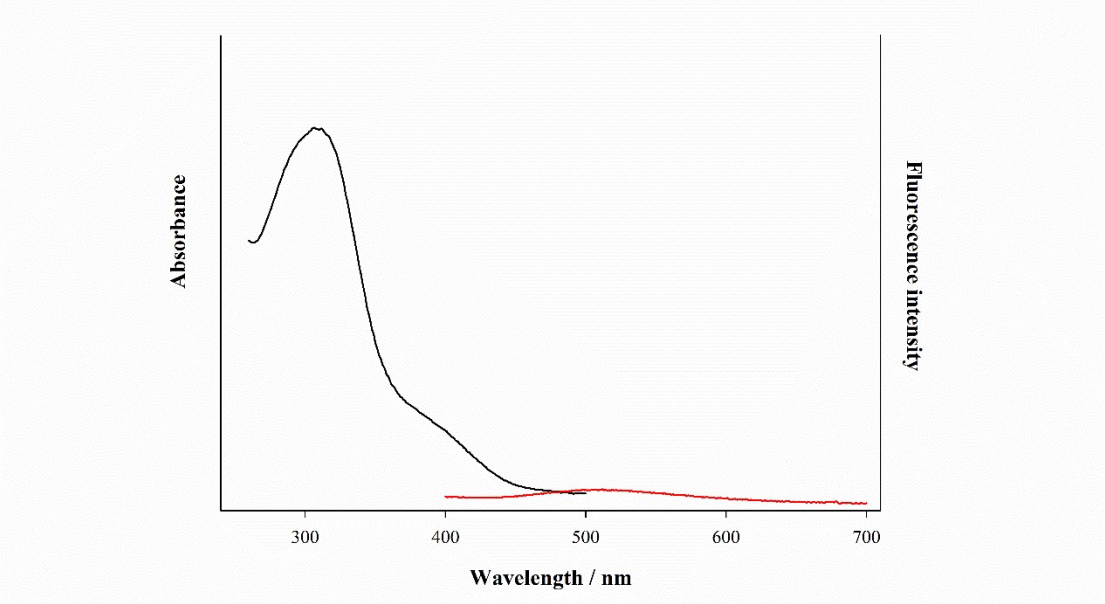


Figure S 1. Fluorescence (the red line) and absorption (the black line) spectra of **NIPY-PBA** (10 μM) in PBS buffer (50 mM, pH 7.4, containing 0.5 mM CTAB).

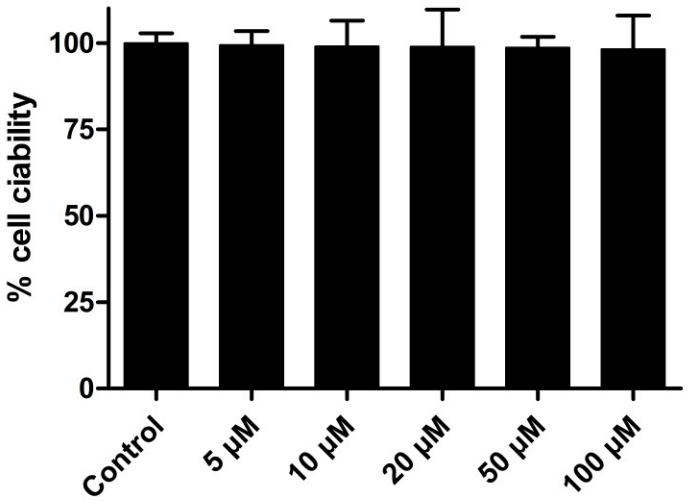


Figure S2. Cytotoxicity studies of **NIPY-PBA** (5 μM; 10 μM; 20 μM; 50 μM; 100 μM) for A549 cells.

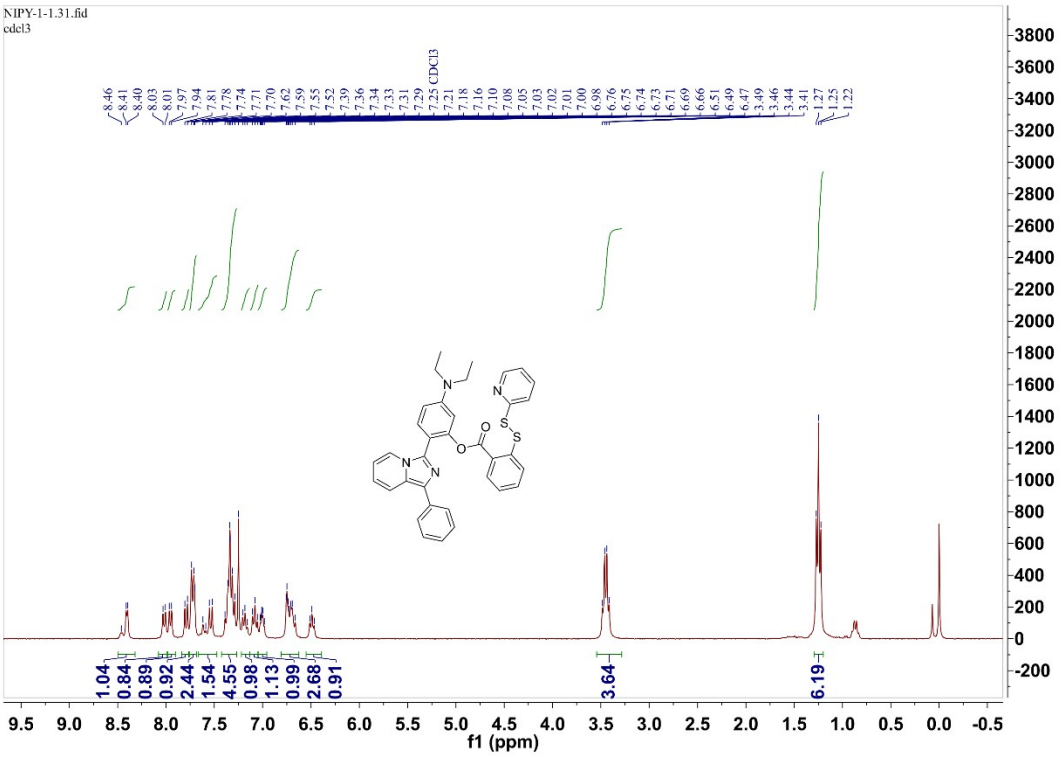


Figure S3. ^{1}H NMR spectrum of the probe **NIPY-PBA**.

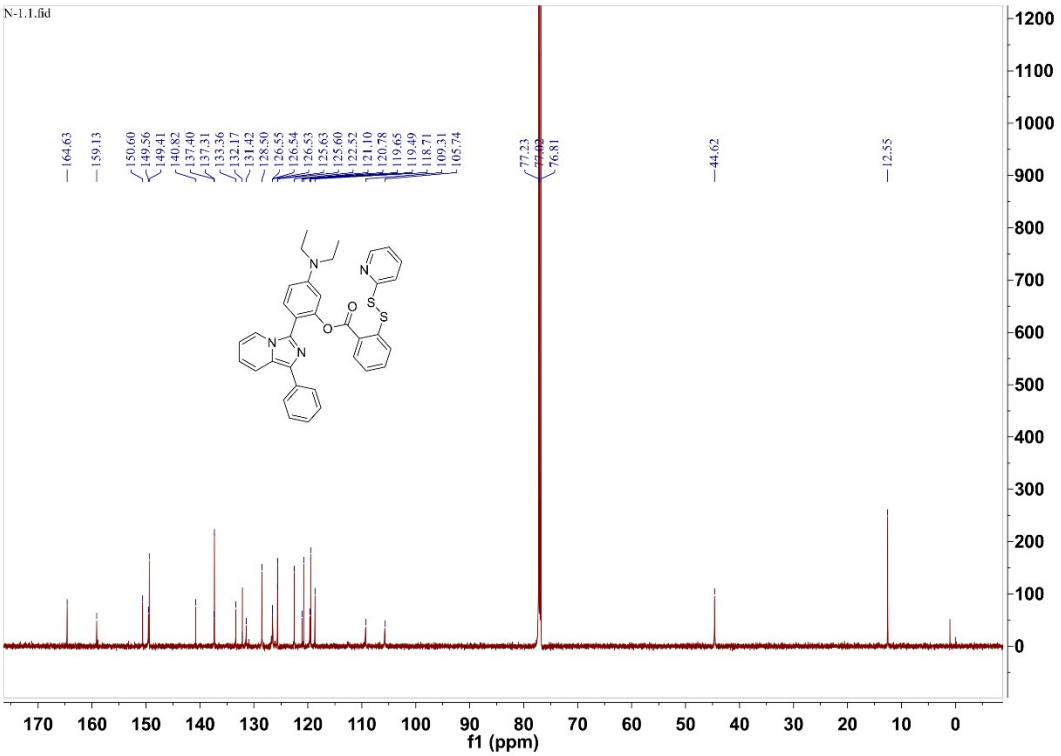


Figure S4. ^{13}C NMR spectrum of the probe **NIPY-PBA**.

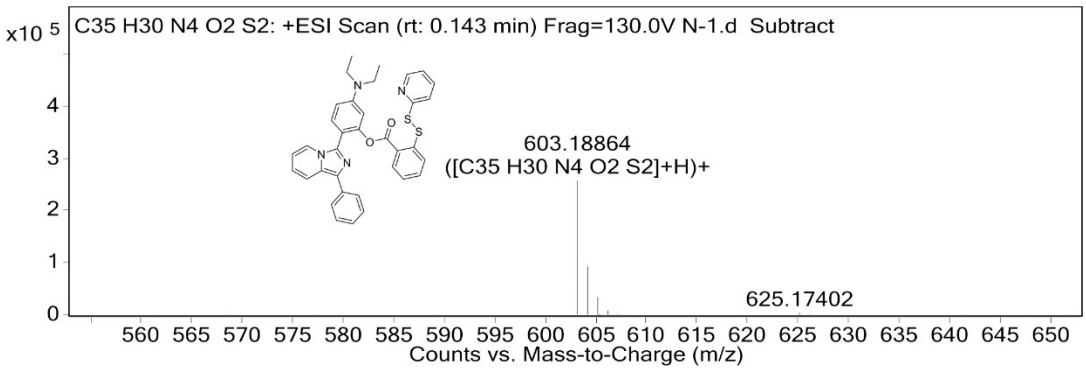


Figure S5. HRMS spectrum of the probe **NIPY-PBA**.

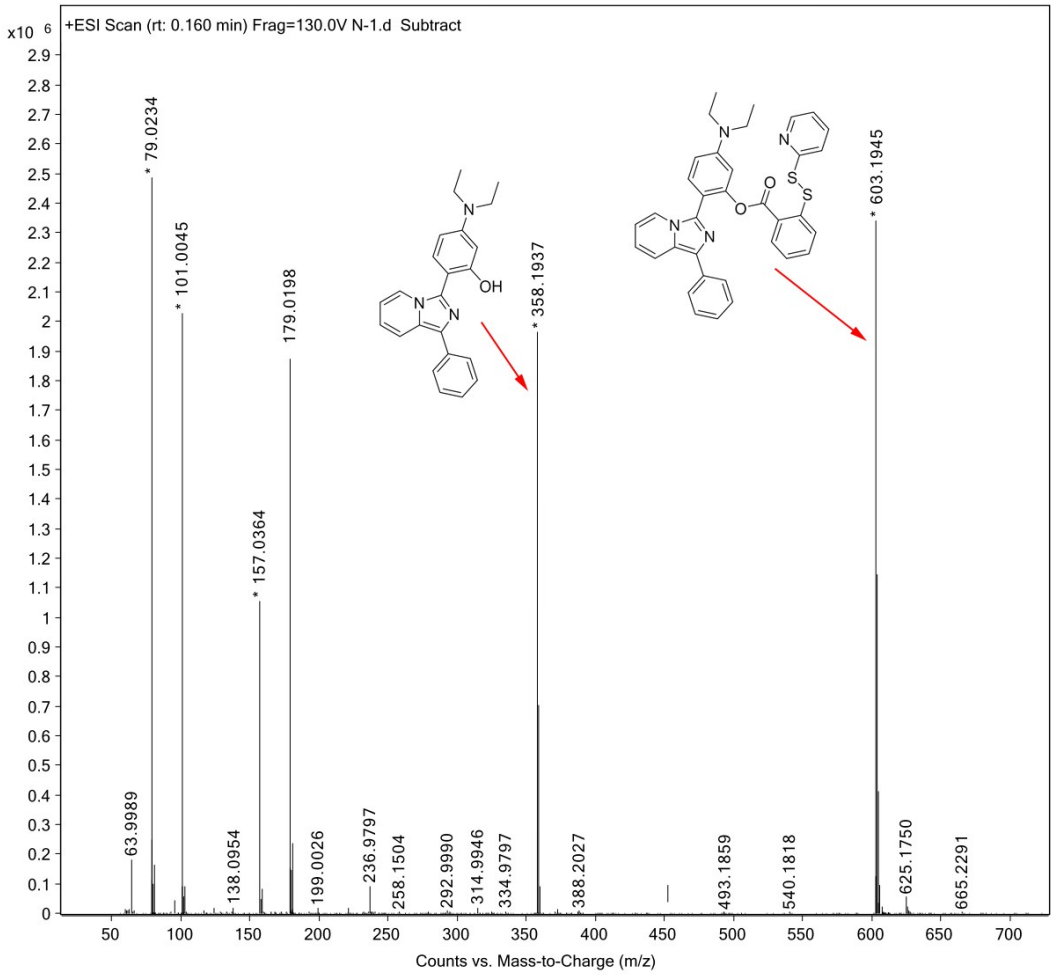


Figure S6. HRMS spectrum of the reaction product of the probe **NIPY-PBA** with Na_2S.

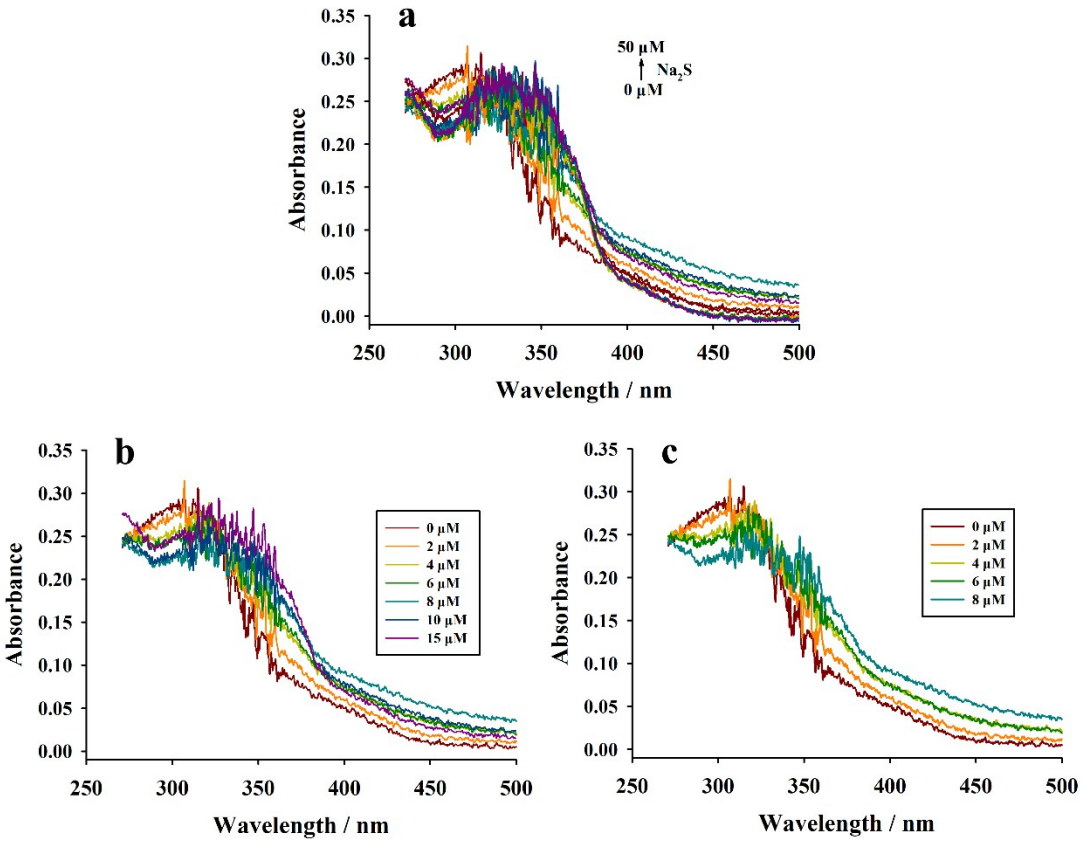


Figure S7. The UV-vis titration spectra of **NIPY-PBA** (10 μM) to different concentration of H_2S (a-c: 0-50 μM; 0-15 μM; 0-8 μM).

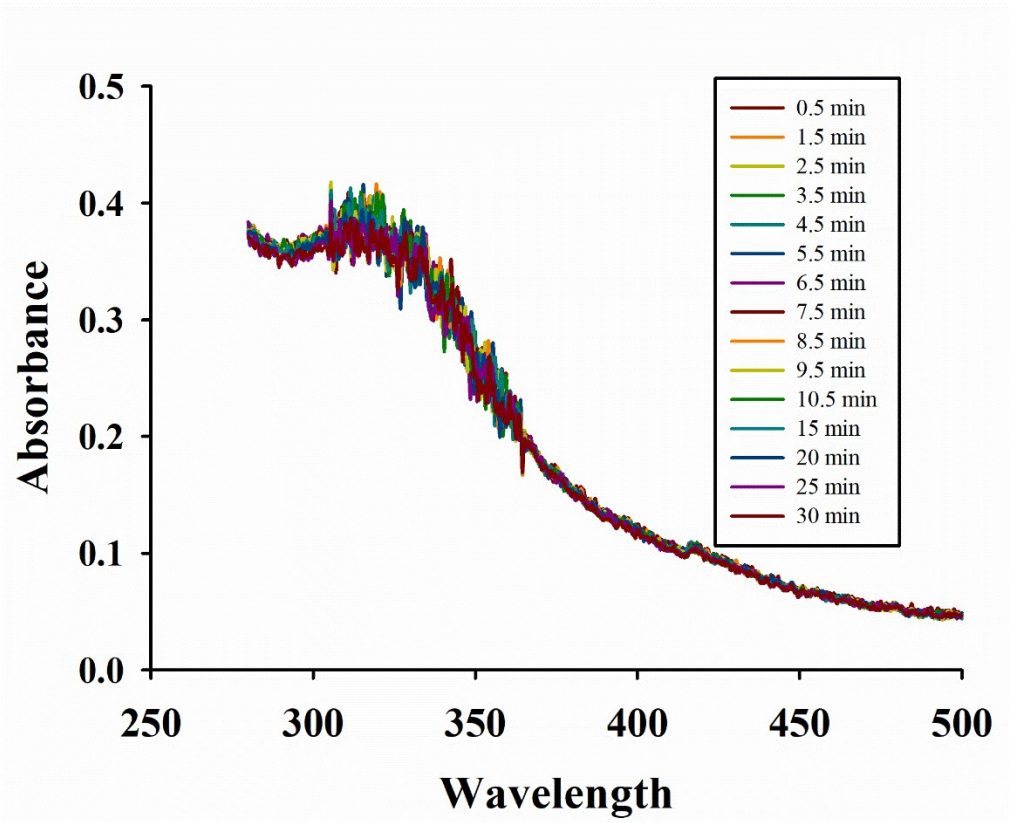


Figure S8. Time-dependent absorption changes of NIPY-PBA (10 μM) towards H_2S (20 μM) in the PBS buffer (50 mM, pH 7.4, containing 1 mM CTAB).