Supporting Information

Dosimetric Chromogenic Probe for Selective Detection of Sulfide *via* Sol-Gel Methodology

Rameez Raza,[†] Atanu Panja,[†] Manjira Mukherjee,[†] Pabitra Chattopadhyay[¶*] and Kumaresh Ghosh[†*]

[†]*Department of Chemistry, University of Kalyani, Kalyani-741235, India. Email: ghosh_k2003@yahoo.co.in; kumareshchem18@klyuniv.ac.in Fax: +913325828282; Tel: +913325828750 Extn: 305.*
[¶]*Department of Chemistry, University of Burdwan, Burdwan-713104, West Bengal, India, E-mail: pabitracc@yahoo.com.*

Table of contents

Table S1. Results of gelation test for compounds **1** and **2**.

Solvent	1	2
DMSO	S	S
DMF	S	S
CH_3CN	S	G
THF	S	S
$CHCl_3$	S	S
2% MeOH in $CHCl_3$	S	S
DMSO-H_2O(1:1,v/v)	P	G
DMF-H_2O (1:1,v/v)	P	G
CH_3CN-H_2O (1:1,v/v)	S	G
Ethanol: H_2O (1:1, v/v)	P	G

S = solution; G = gel; P = Precipitation. Gelation tests were performed by taking 20 mg of the respective compounds in 1 ml of pure solvent or solvent mixture after ~15 min of sample preparation.

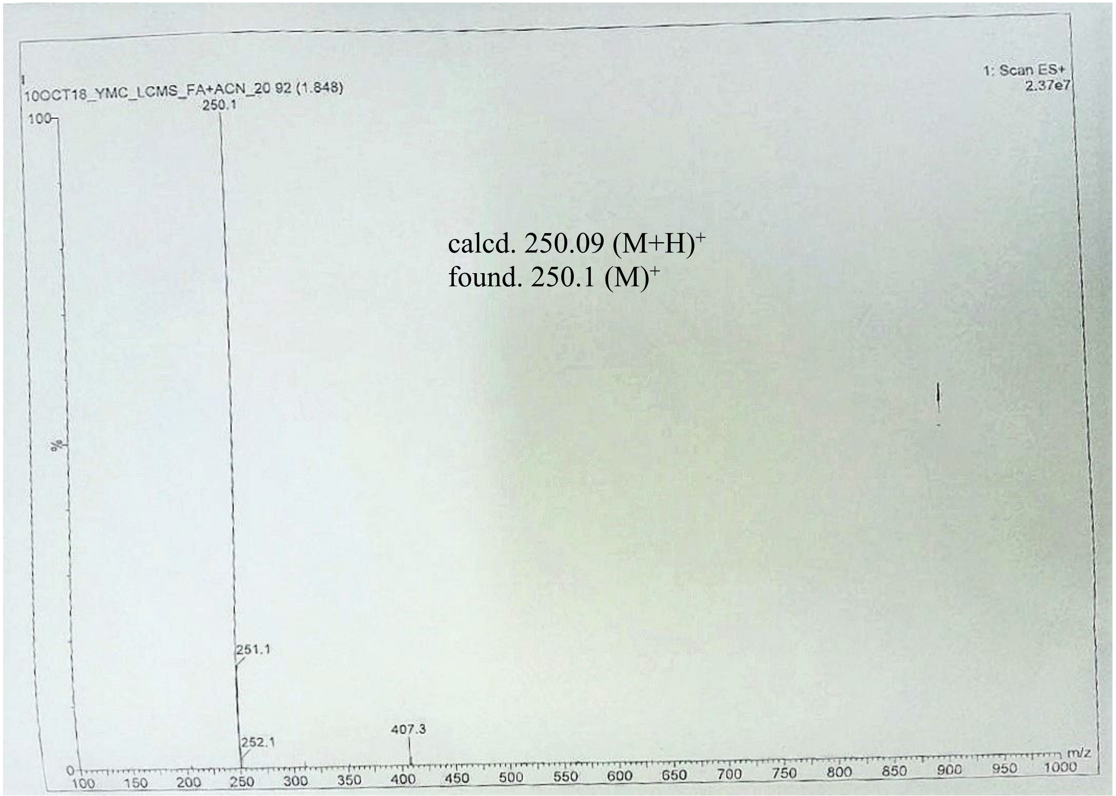


Figure S1. Mass spectra of the product obtained from the reaction of **1** with sulfide.

.

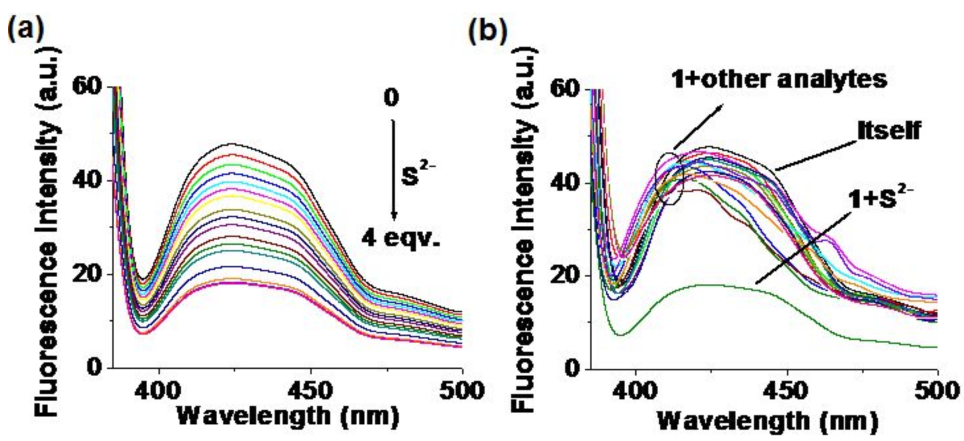


Figure S2. Change in fluorescence intensity (λ_{ex} = 370 nm) of **1** (c = 2.50 x 10^{-5} M) upon addition of 4 equiv. amount (a) sulfide and (b) different analytes (c = 1.0 x 10^{-3} M) in DMSO-H_2O (1:1, v/v).

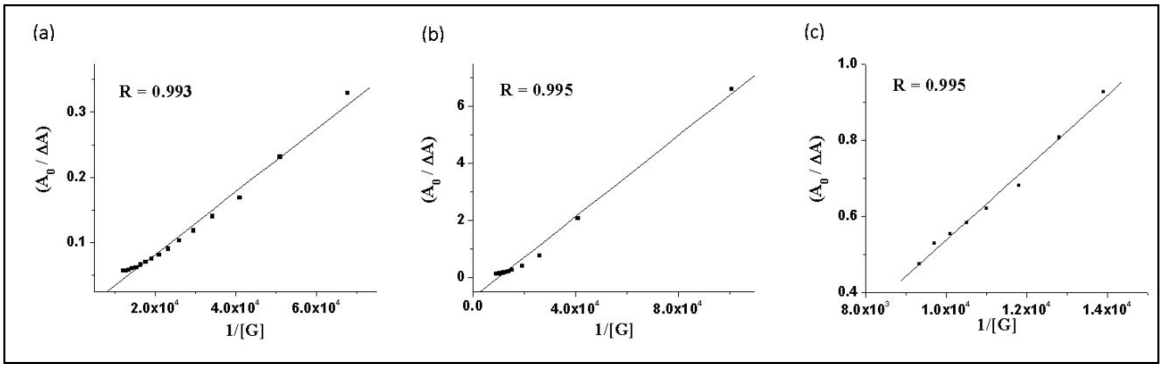


Figure S3. Benesi–Hilderband plots of **1** (c = 2.50 x 10-5 M) for sulfide in (a) 1:1 DMSO-H_2O (v/v) , (b) 1:3 DMSO-H_2O (v/v) and (c) 1:5 DMSO-H_2O (v/v**).**

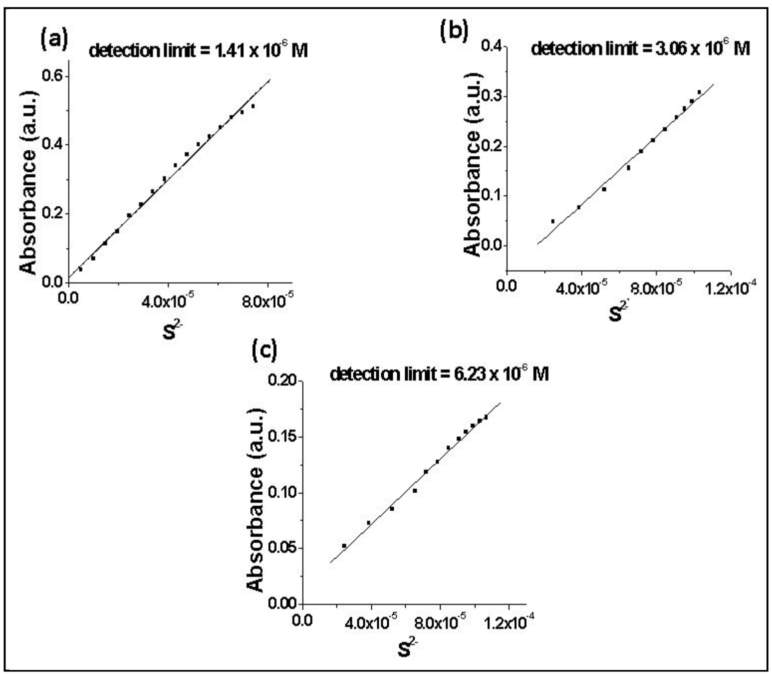
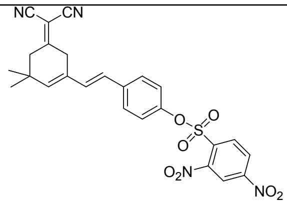
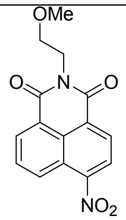
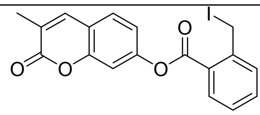
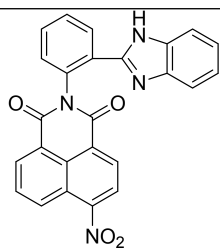
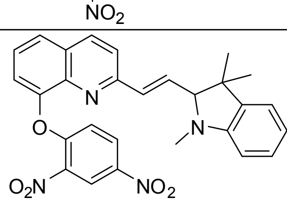
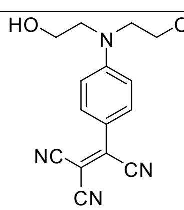
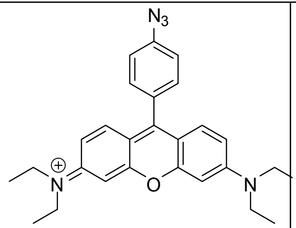
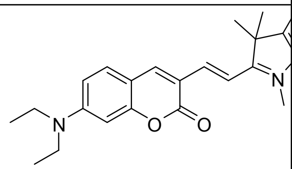
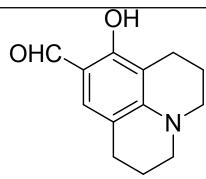
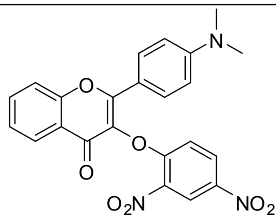
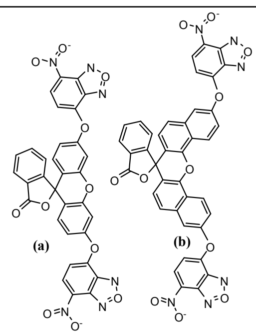
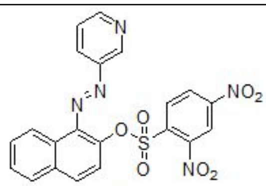


Figure S4. Calculation of detection limits of **1** (c = 2.50 x 10-5 M) for sulfide in (a) 1:1 DMSO-H_2O (v/v), (b) 1:3 DMSO-H_2O (v/v) and (c) 1:5 DMSO-H_2O (v/v).

Table S2. Reported structures for sulfide sensing in solution phase.

Entry	Structure of compounds	Gel phase detection	Sensing mechanism	solvent	Detection limit (M)	Ref.
1.		No	Fluorescence enhancement	PBS buffer	5.3×10^{-7} M.	1
2.		No	Fluorescence enhancement	aqueous buffer (50 mM PIPES)	5.0×10^{-6} M	2
3.		No	Fluorescence enhancement	PBS buffer (10 mM, pH 7.4, containing 1 mM CTAB)	30nM	3
4.		No	Fluorescence enhancement	DMSO-H_2O(1:3)	24.2×10^{-7} M	4
5.		No	Fluorescence enhancement	DMSO-H_2O(1:2 V/V)	1.08×10^{7} M	5
6.		No	Colorimetric sensing	aqueous buffer solution	10^{-10}mM	6

7.		No	Fluorescence quenching	DMF/phosphate buffer (6:4,v/v)	0.25 mM	7
8.		No	Fluorescence quenching	CH_3OH-HEPES (10mM,pH-7.4)	14 nm ($14x10^{-8}$ M)	8
9.		No	Fluorescence enhancement	aqueous HEPES buffer (10 mmol/L, pH 7.0)	$9.37x10^{-6}$ M	9
10.		No	Fluorescence enhancement	PBS buffer (20 mM, pH 7.4) containing 20% DMSO (v/v)	0.13 μM ($0.13x10^{-6}$ M)	10
11.		No	Fluorescence enhancement	PBS buffer (20 mM, pH = 7.4).	0.4 μM ($0.4x10^{-6}$ M) [Detection limit for a] 16 μM ($16x10^{-6}$ M) [Detection limit for b]	11
This work	 **1**	Yes (sol-to-gel transition)	Visual sensing through sol-to-gel phase transition. Colorimetric response	DMSO-H_2O (1:1, v/v)	1.41 $x10^{-6}$ M	-

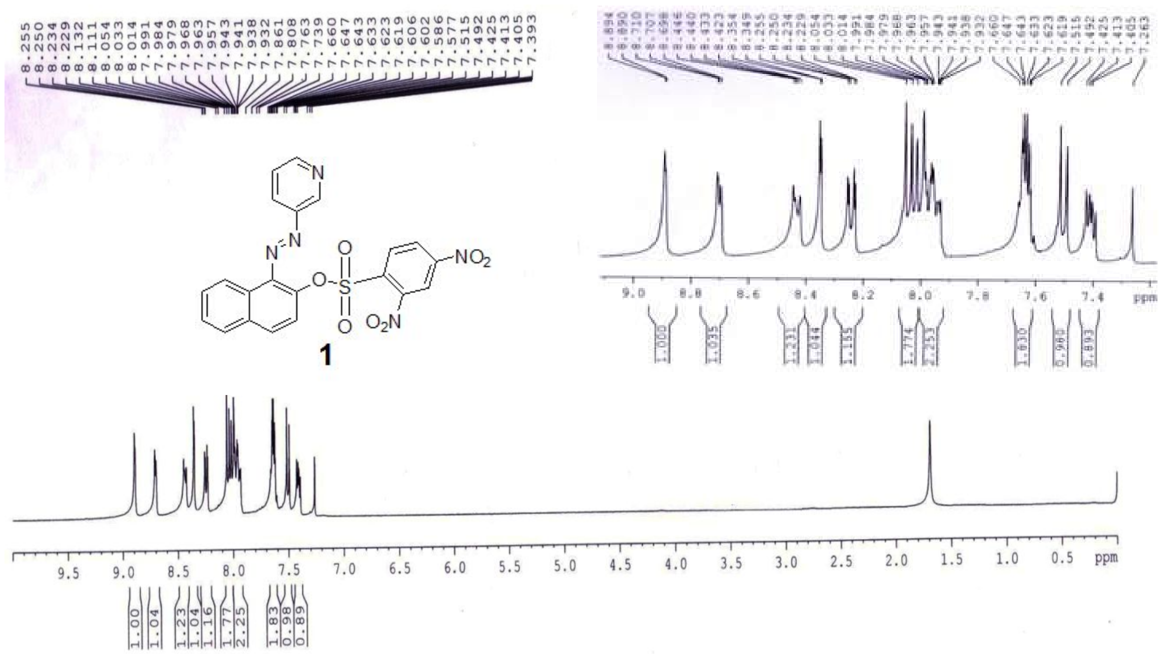


Figure S5. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **1**.

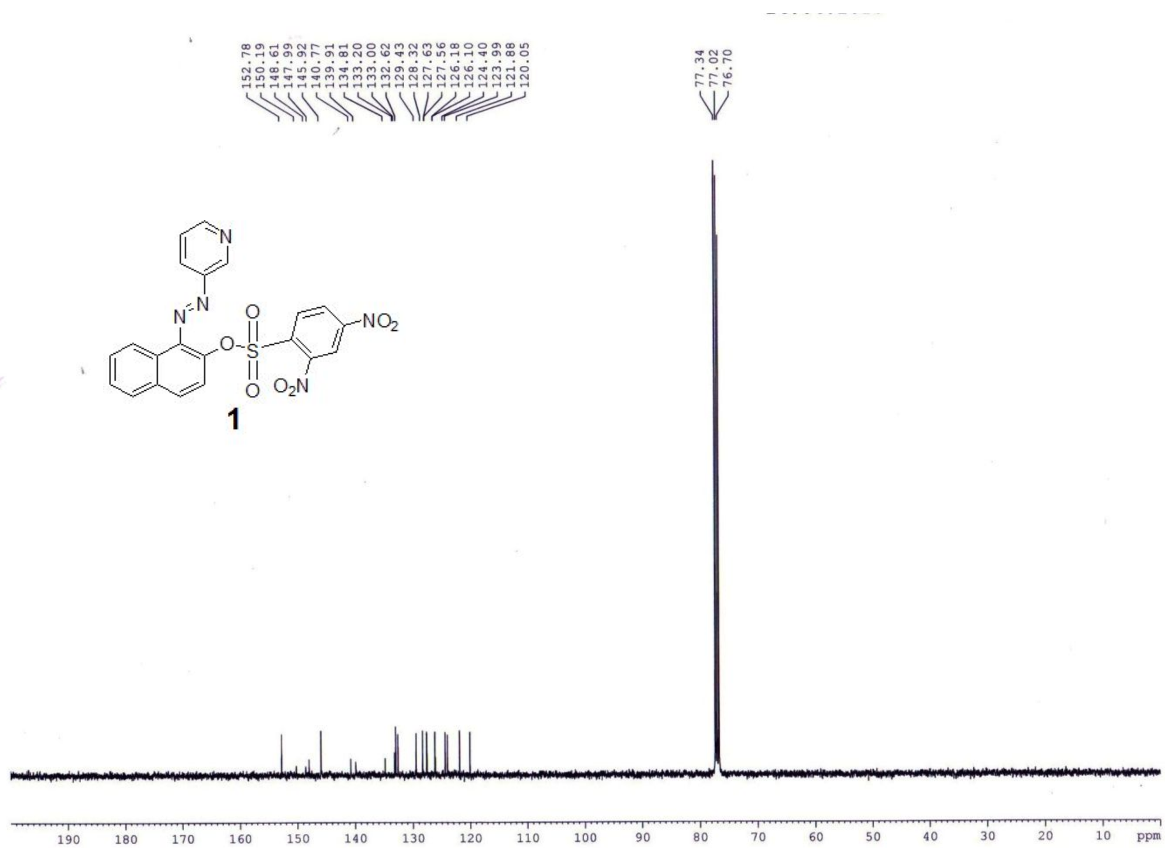


Figure S6. ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **1**.

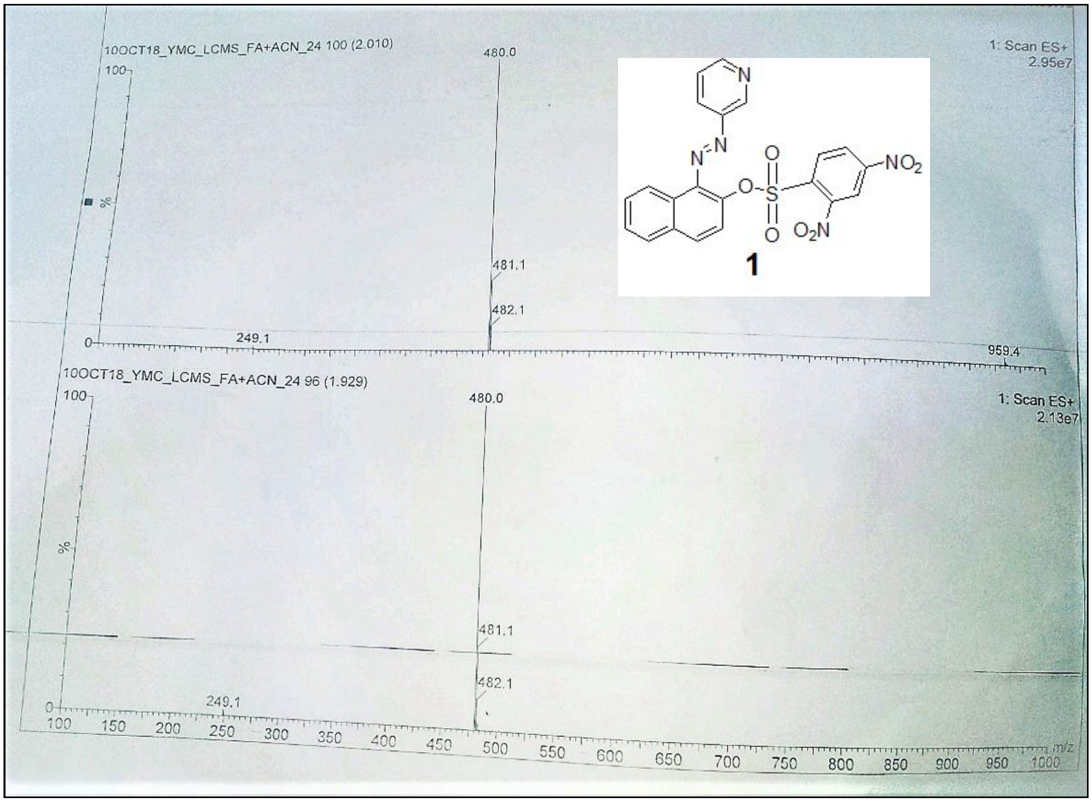


Figure S7. Mass spectrum of compound **1**.

References:

1.Huo, F.; Zhang, Y.; Ning, P.; Meng, X.; Yin, C. A novel isophorone-based red-emitting fluorescent probe for selective detection of sulfide anions in water for *in vivo* imaging**.** *J. Mater. Chem*. B. **2017**, *5*, 2798-2803.

2. Montoya, L. A.; Pluth, M. D. Selective turn-on fluorescent probes for imaging hydrogen sulfide in living cells. *Chem. Commun.* **2012***, 48,* 4767–4769.

3. Yang, Y.; Liu, Y.; Yang, L.; Liu, J.; Li, K.; Luo. S. A coumarin-based colorimetric fluorescent probe for hydrogen sulfide. *J. Chem. Sci.* **2015**, *127,* 359–363

4.Lohar, S.; Maji, A.; Pal S.; Mukhopadhyay, S. K.; Nag, D.; Demitri, N.; Chattopadhyay, P. Naphthalimide based turn on fluorosensor for aqueous sulfide ions for staining in living cells. *ChemistrySelect.* **2017**, *2*, 9977-9983.

5. Guria, U. N.; Maiti, K.; Ali, S. S.; Samanta, S. K.; Mandal, D.; Sarkar, R.; Datta, P.; Ghosh, A. K.; Mahapatra, A. K. Reaction-based bi-signaling chemodosimeter probe for selective detection of hydrogen sulfide and cellular studies. *New J. Chem*. **2018,** *42*, 5367-5375.

6. Zhao, Y.; Zhu, X.; Kan, H.; Wang, W.; Zhu, B.; Dua, B.; Zhangb, X. A highly selective colorimetric chemodosimeter for fast and quantitative detection of hydrogen sulfide. Analyst. **2012**, *137*, 5576-5580.

7. Cheng, J.; Song, J.; Niu, H.; Tang, J.; Zhang, D.; Zhaoac,Y.; Ye, Y. A new rosamine-based fluorescent chemodosimeter for hydrogen sulfide and its bioimaging in live cells. *New J. Chem.* **2016**, *40*, 6384-6388.

8. Yang Y.; Yina C.;Huob F.; Zhang Y. and Chao J. A ratiometric colorimetric and fluorescent chemosensor for rapid detection hydrogen sulfide and its bioimaging. *Sensors and Actuators B*. **2014**, 50, 596

9. Yang Y.; Yin C.; Huo F.; Chu Y.; Tong H.; Chao J.; Cheng F. and Zheng. A. pH-sensitive fluorescent salicylaldehyde derivative for selective imaging of hydrogen sulfide in living cells. *Sensors and Actuators B*. **2013**, 186, 212.

10. Liu Y. and Feng G. A visible light excitable colorimetric and fluorescent ESIPT probe for rapid and selective detection of hydrogen sulphide. *Org. Biomol. Chem.* **2014**, 12, 438-445.

11. Wei C.; Zhu Q., Liu W.; Chen W.; Xi Z. and Yi L. NBD-based colorimetric and fluorescent turn-on probes for hydrogen sulphide. *Org. Biomol. Chem.* **2014**, 12, 479-485.