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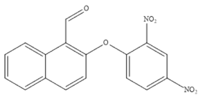
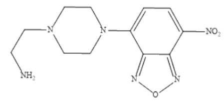
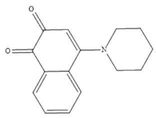
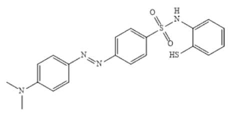
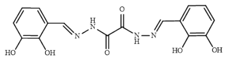
Supporting Information

A colorimetric chemosensor for sulfide in a near-perfect aqueous solution: Practical application using test kit

Seong Youl Lee, Cheal Kim*

Department of Fine Chemistry and Department of Interdisciplinary Bio IT Materials, Seoul National University of Science and Technology, Seoul 139-743, Korea. Fax: +82-2-973-9149; Tel: +82-2-970-6693; E-mail: chealkim@seoultech.ac.kr

Table S1. Examples of various S^{2-} chemosensors with colorimetric test strip

Sensor	Detection limit (μM)	Binding constant	Interference	Percent of water in solution (%)	Method of detection	Concentration of sensor/S^{2-} in test strip (μM)	Reference
	1.67	No data	None	50	Fluorescence, Colorimetric	20 / 200	1
	46.97	5.0×10^2	None	99.9	Colorimetric	3000 / 50	2
	0.77	No data	No data	50	Fluorescence, Colorimetric	20 / 100	3
	28.4	No data	No data	99.9	Colorimetric	100 / 2000	4
	28.7	1.0×10^2	None	99.9	Colorimetric	100 / 30	This work

References

1 A. K. Das, S. Goswami, C. K. Quah and H. Fun, *New J. Chem.*, 2015, **39**, 5669-5675.

2 J. J. Lee, Y. S. Kim, E. Nam, S. Y. Lee, M. H. Lim and C. Kim, *Dalton Trans.*, 2016, **45**, 5700-5712.

3 A. K. Das, S. Goswami, G. Dutta, S. Maity, T. kanti Mandal, K. Khanra and N. Bhattacharyya, *Org. Biomol. Chem.*, 2016, **14**, 570-576.

4 R. Kaushik, A. Singh, A. Ghosh and D. A. Jose, *ChemistrySelect*, 2016, **1**, 1533-1540.

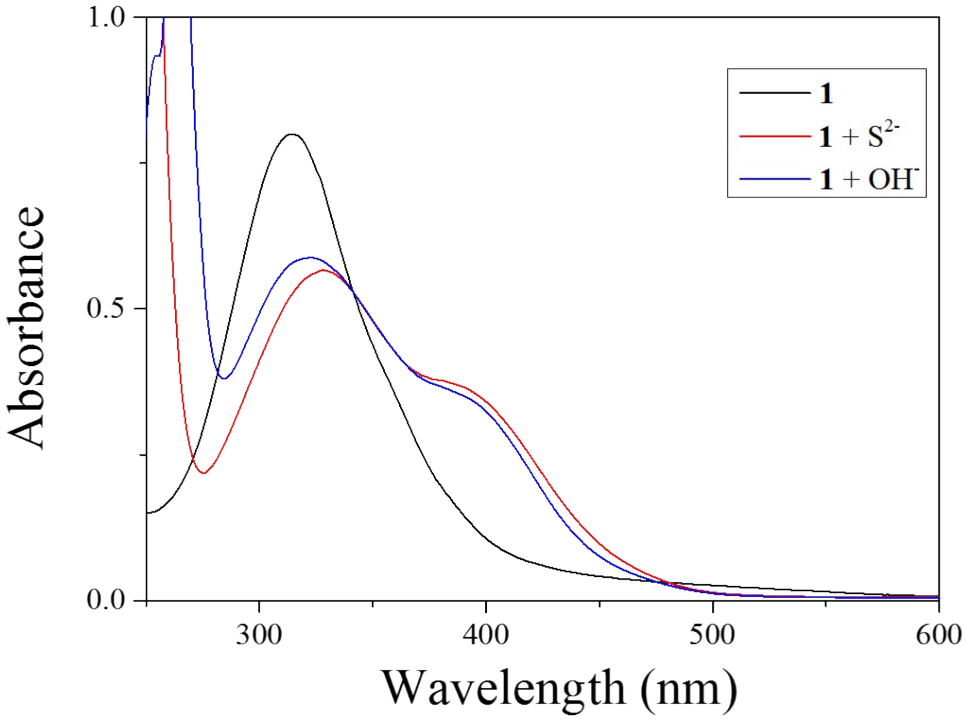


Fig. S1. Absorption changes of **1** (40 μM) in the presence of NaOH (160 equiv) and Na_2S (100 equiv), respectively, in bis-tris buffer.

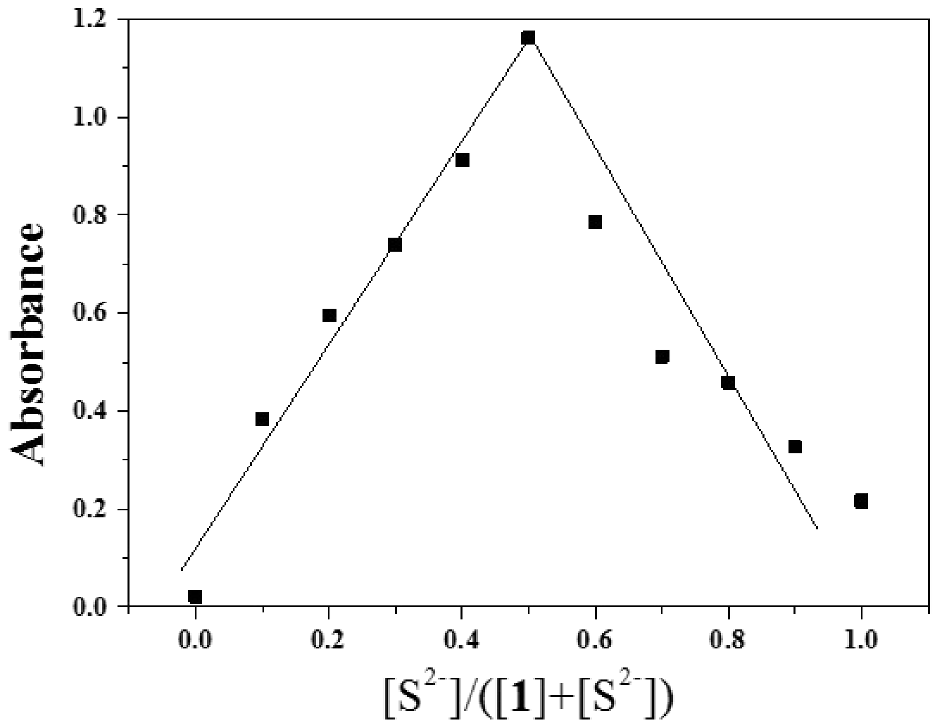


Fig. S2 Job plot of a 1:1 complex of receptor **1** and S^{2-} (absorbance at 400 nm). The total concentration of S^{2-} with receptor **1** was 100 μM.

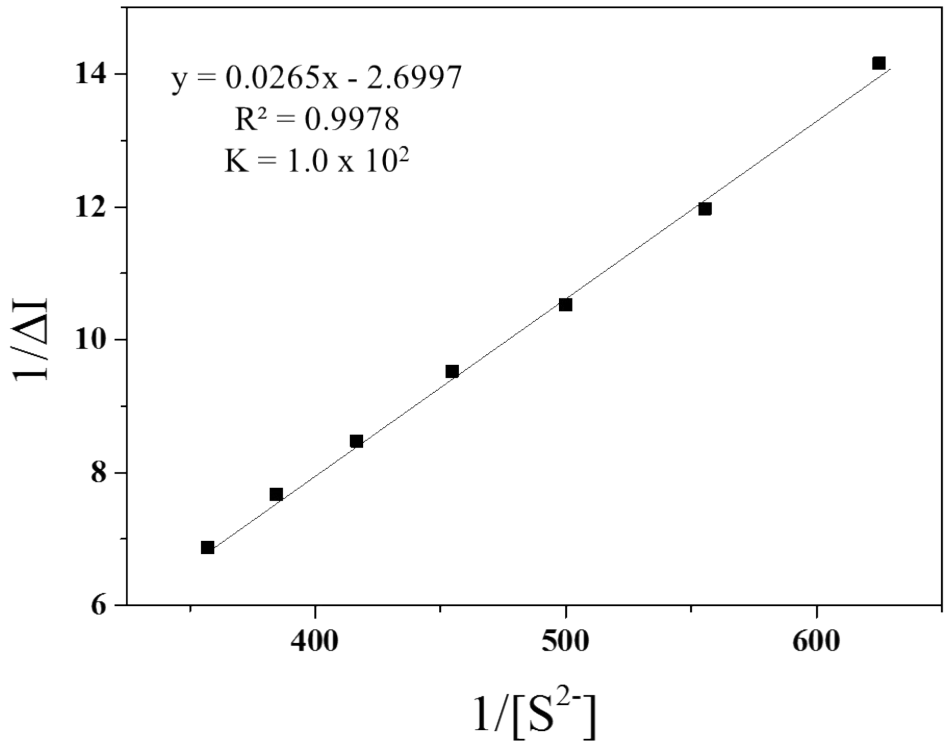


Fig. S3 Benesi-Hildebrand plot (at 400 nm) of **1** based on UV-vis titration, assuming 1:1 stoichiometry for association between **1** and S^{2-}.

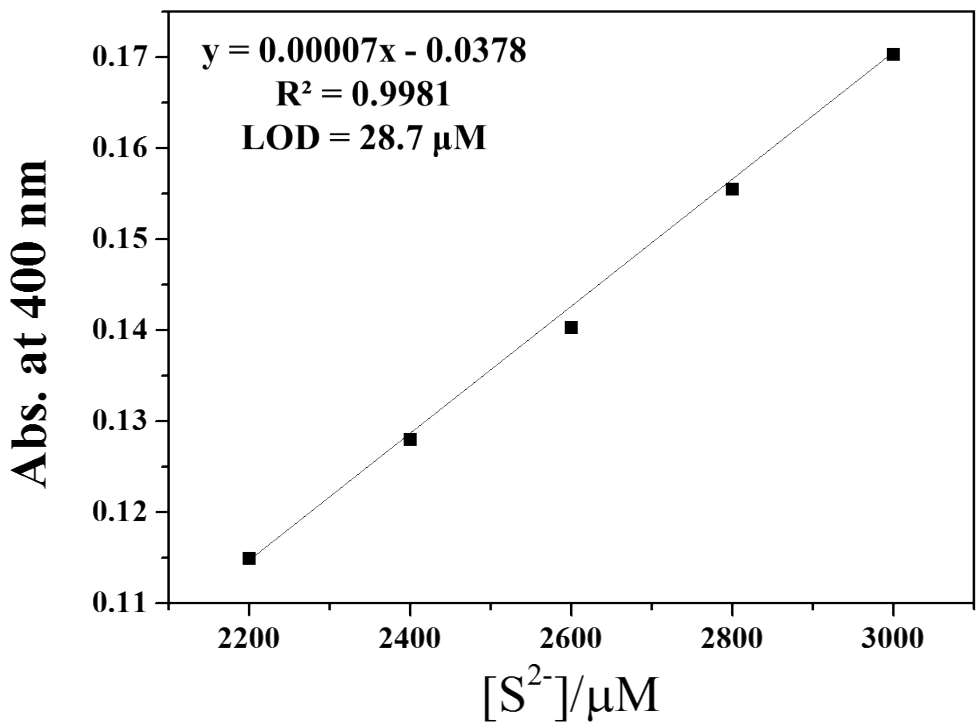


Fig. S4 Determination of the detection limit based on UV-vis titration in the ratio (absorbance intensity at 400 nm) of **1** (40 μM) with S^{2-}.

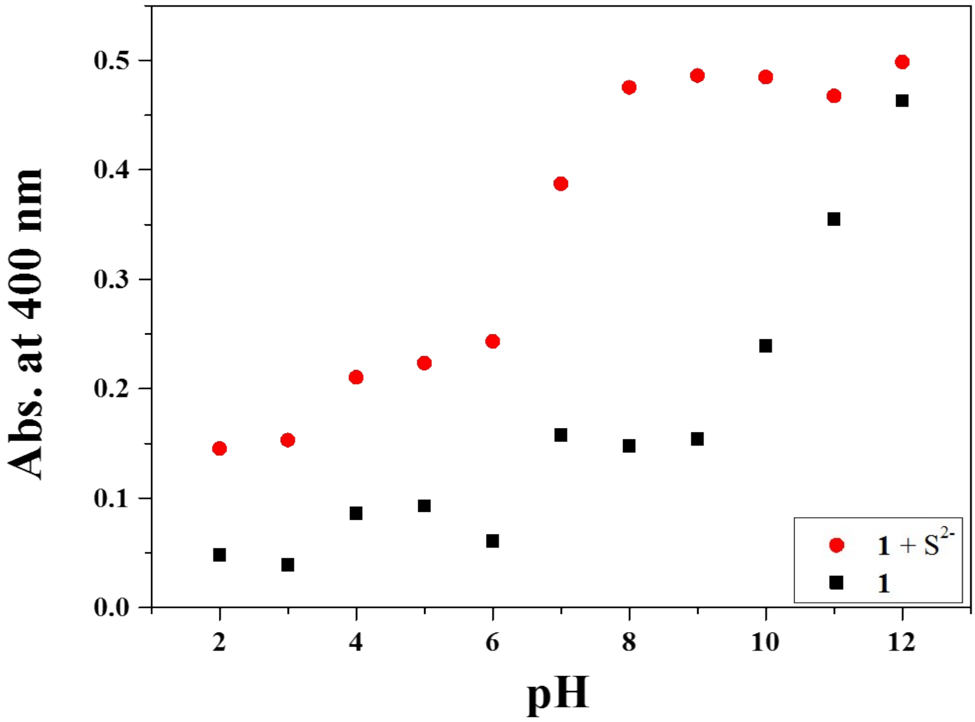
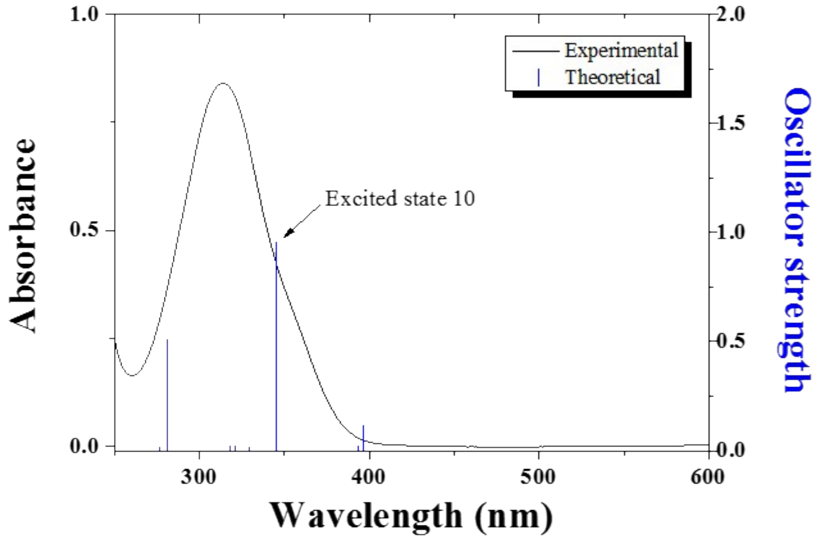


Fig. S5 UV-vis absorbance (400 nm) of **1** and **1**-S^{2-} at pH 2-12 in bis-tris buffer at room temperature.

(a)

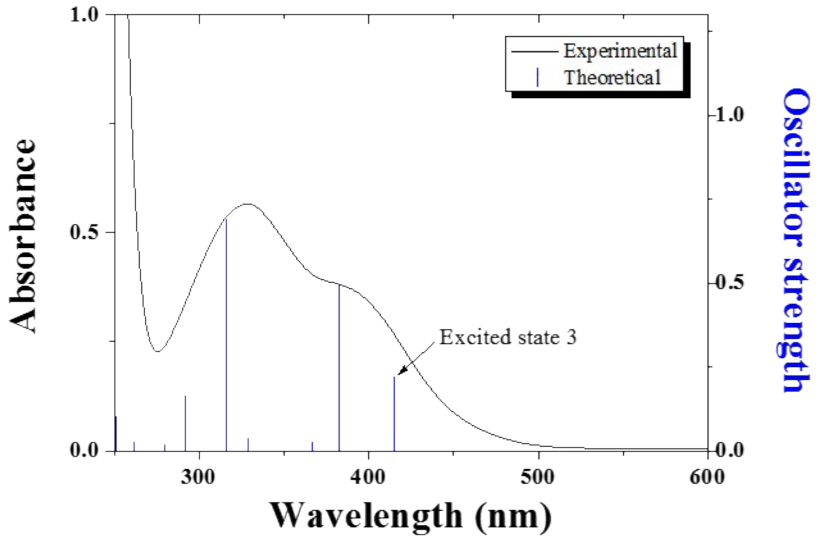


(b)

Excited state 10	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H → L	345.6	98	$\pi \rightarrow \pi^*$	0.9581

Fig. S6 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**. (b) The major electronic transition energy and molecular orbital contributions for **1** (H = HOMO and L = LUMO).

(a)



(b)

Excited state 3	Wavelength (nm)	Percent (%)	Main character	Oscillator strength
H → L + 1	414.88	98	ICT	0.2214

Fig. S7 (a) The theoretical excitation energies and the experimental UV-vis spectrum of **1**$^-$. (b) The major electronic transition energy and molecular orbital contributions for **1**$^-$ (H = HOMO and L = LUMO).