Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Aggregation-induced emissive pyridoxal derived tetradentate Schiff base for the fluorescent turn-off sensing of copper(II) in aqueous medium

Vinita Bhardwaj[a], Lavani Hindocha[a], Ashok Kumar SK[b] and Suban K Sahoo[a,*]

[a] Department of Chemistry, Sardar Vallabhbhai National Institute Technology, Surat-395007, Gujarat, India.

[b] Materials Chemistry Division, School of Advanced Sciences, VIT University, Vellore-632014, India.

*E-mail: sks@chem.svnit.ac.in, subansahoo@gmail.com.

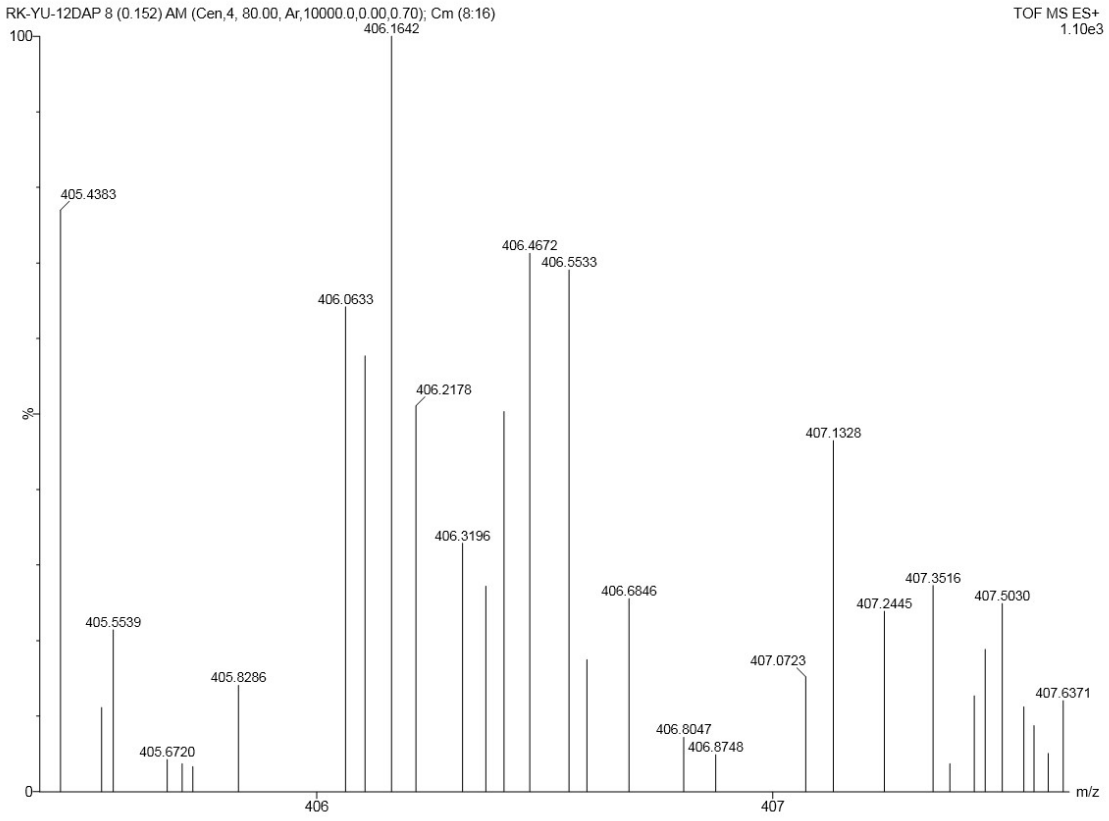


Fig. S1. HRMS of **L**.

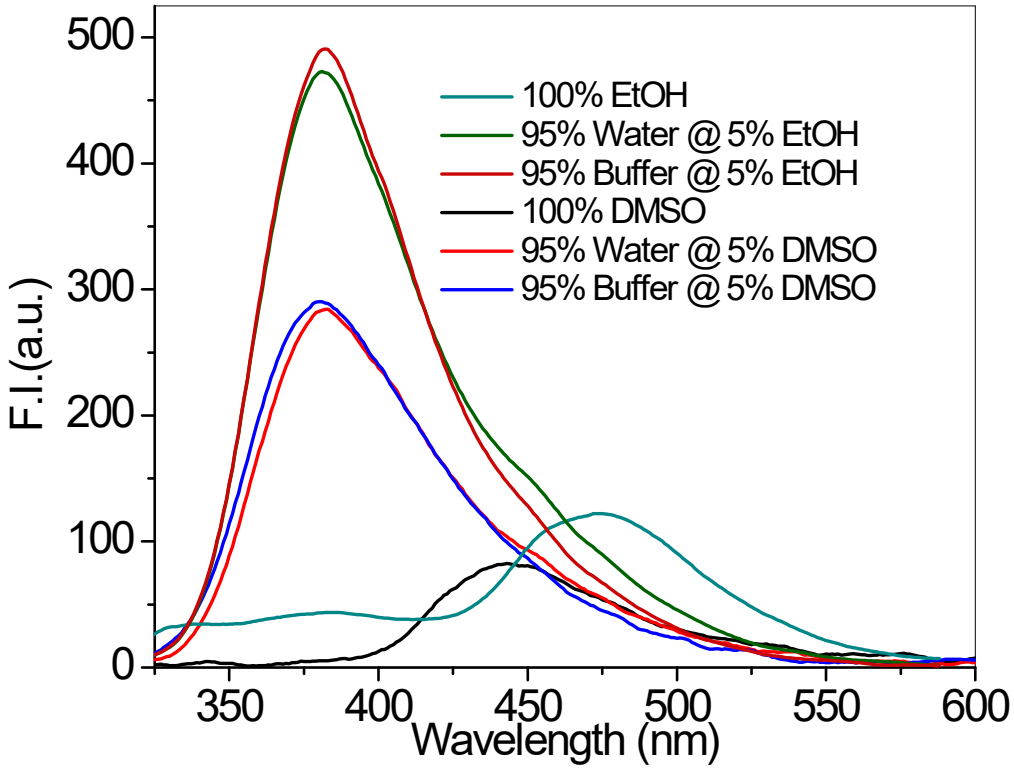


Fig. S2. The fluorescence spectral changes of **L** in pure EtOH/DMSO and EtOH/DMSO containing 95% water/HEPES buffer.

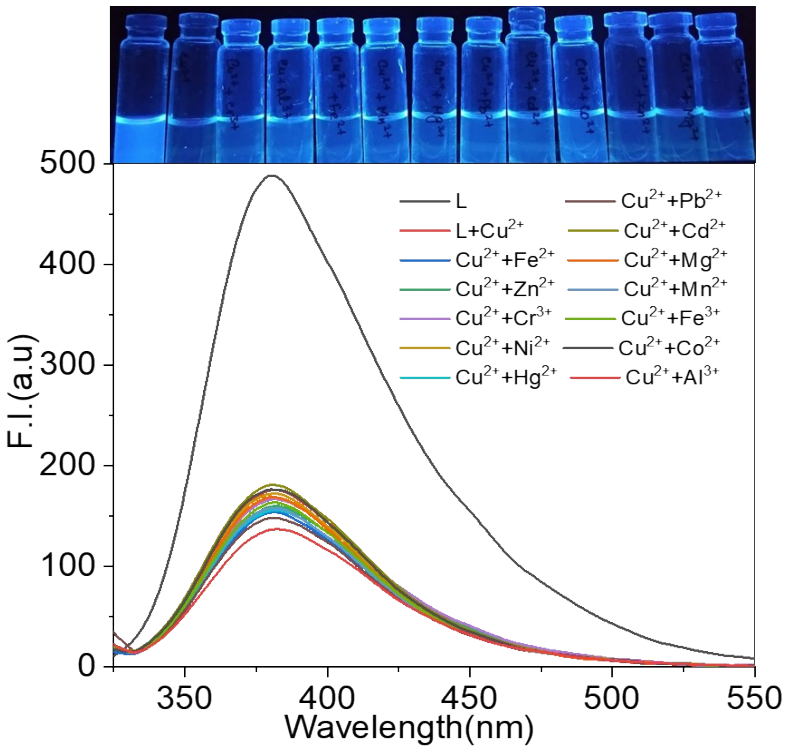


Fig. S3. The fluorescence spectral changes of **L** (5×10^{-5} M) with Cu^{2+} (5×10^{-5} M) in the presence of equimolar amount of other interfering metal ions (vials showed the corresponding fluorescent color changes irradiated with UV light at 365 nm).

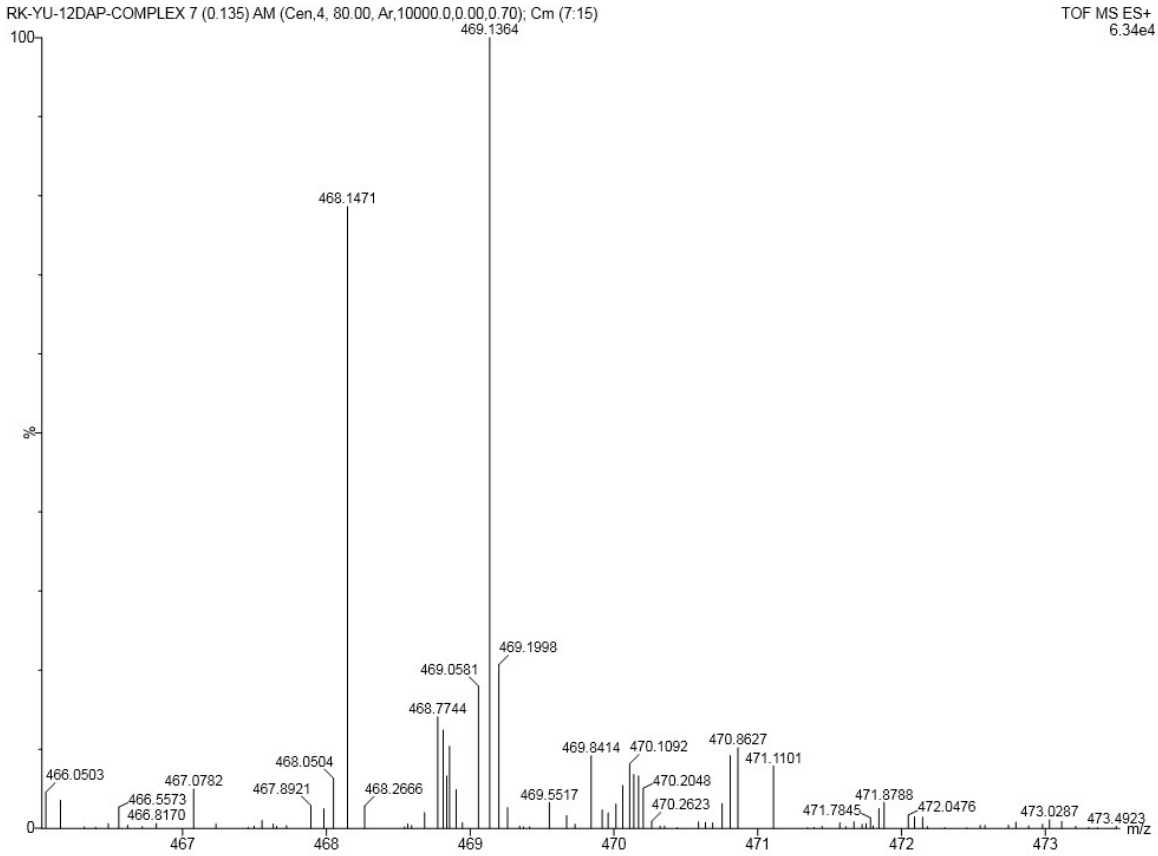


Fig. S4. HRMS of **L**-Cu^{2+}.

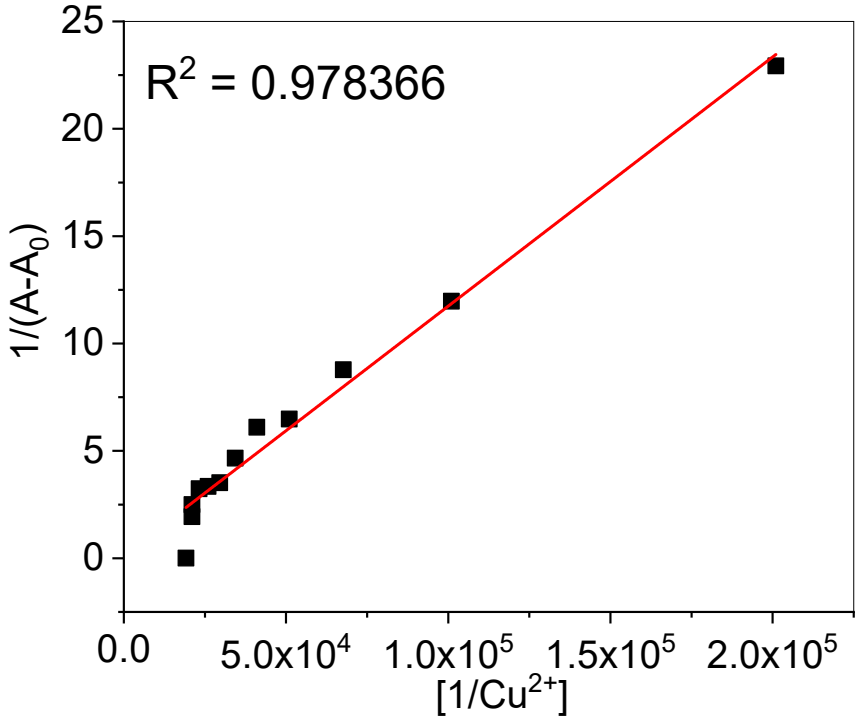


Fig. S5. B-H plot for the estimation of **L**-Cu^{2+} binding constant by using UV-Vis titration data.

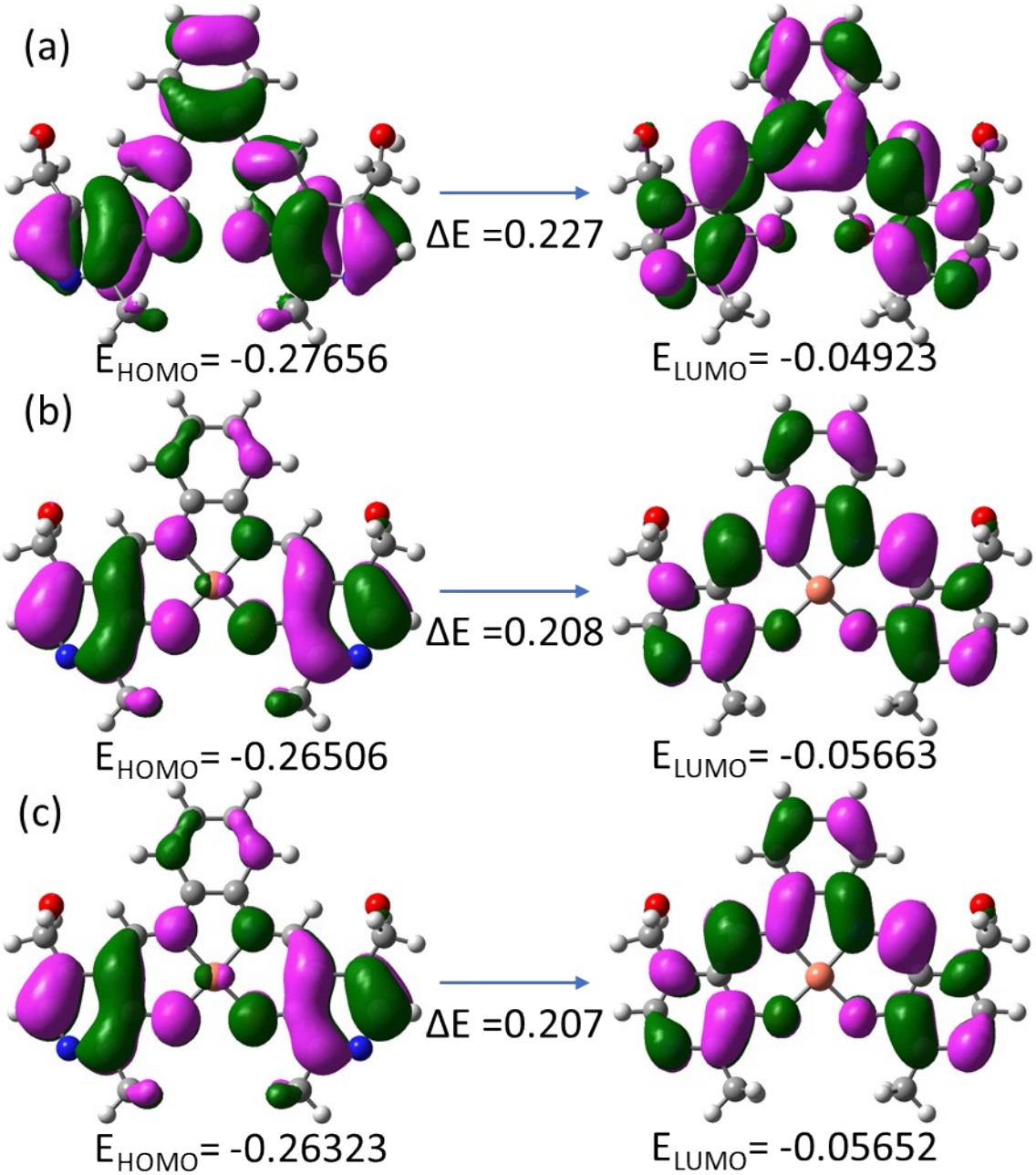


Fig. S6. DFT computed HOMO and LUMO diagrams of (a) **L**, (b) **L**-Cu^{2+} (alpha MO's) and (c) **L**-Cu^{2+} (beta MO's).

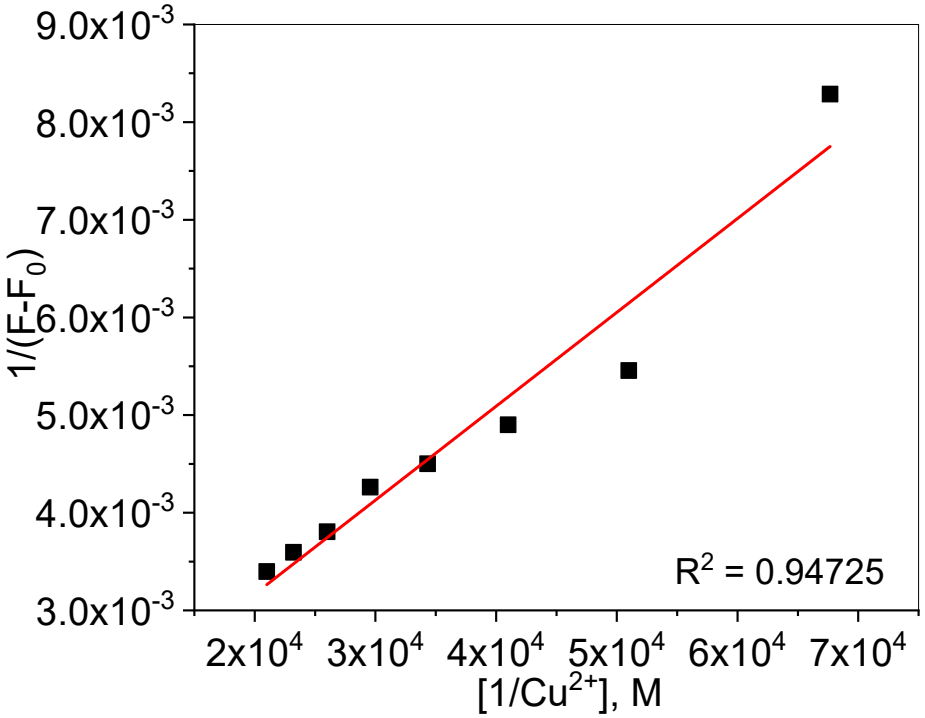


Fig. S7. B-H plot for the estimation of **L**-Cu^{2+} binding constant by using fluorescence titration data.

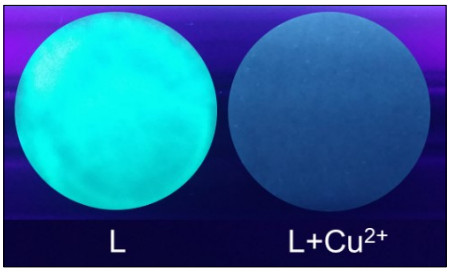


Fig. S8. Fluorometric test strips coated with **L** for the detection of Cu^{2+} ions under UV lamp at 365 nm.

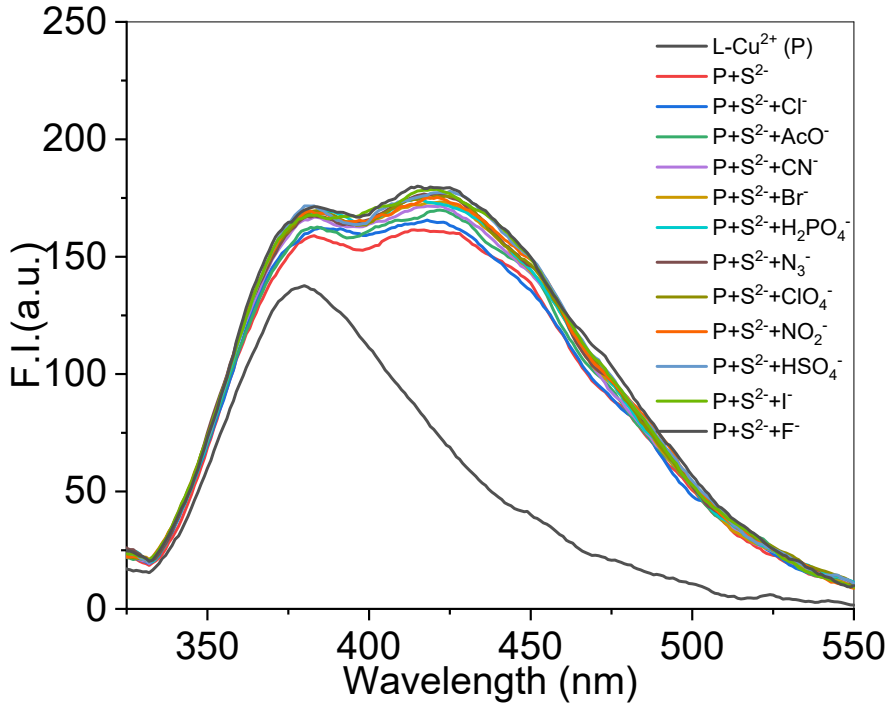


Fig. S9. The fluorescence spectral changes of **L**-Cu^{2+} (5×10^{-5} M) with S^{2-} (5×10^{-5} M) in the presence of equimolar amount of other interfering anions.

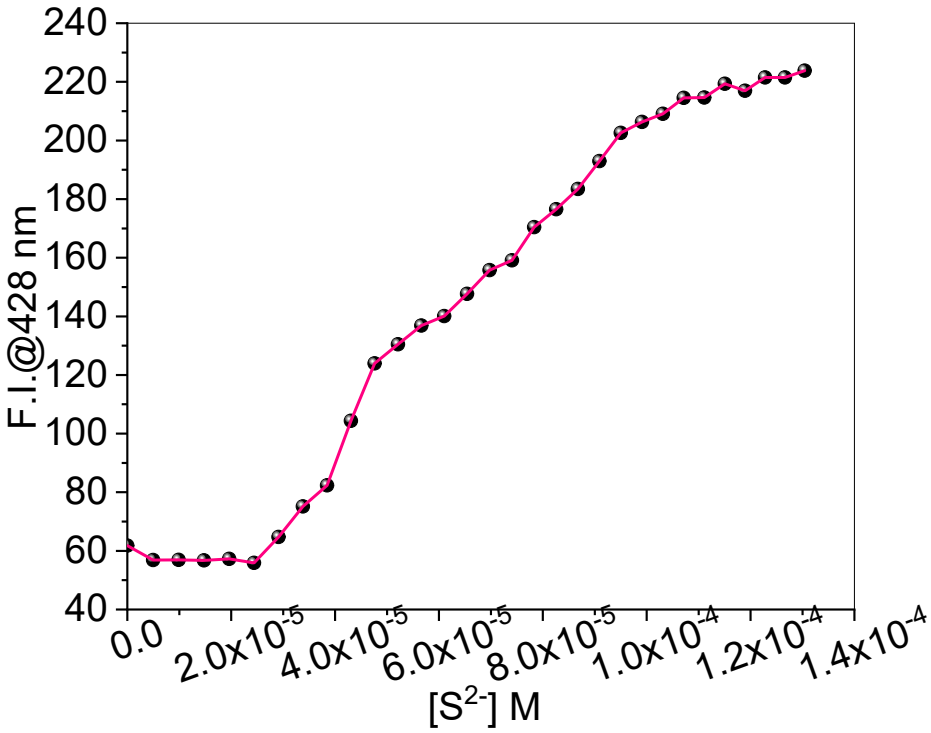


Fig. S10. The change in fluorescence intensity of **L**-Cu^{2+} (5×10^{-5} M, λ_{exc} = 300 nm) at 428 nm with increasing amounts of S^{2-} in EtOH:HEPES buffer (5% EtOH, pH = 7.4).

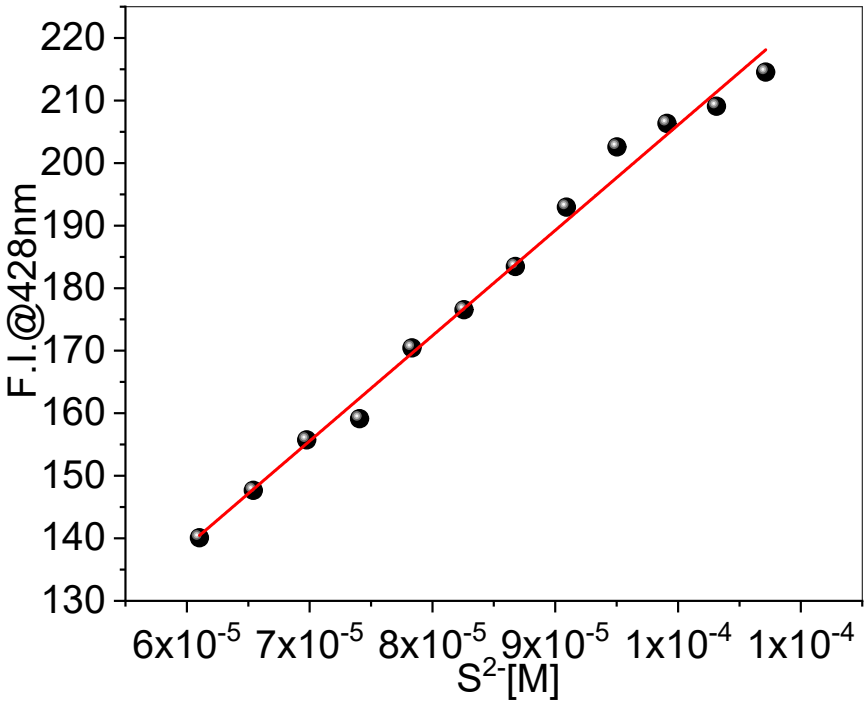
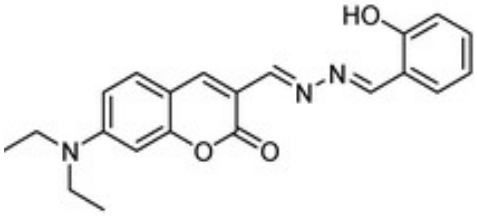
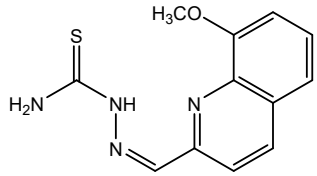
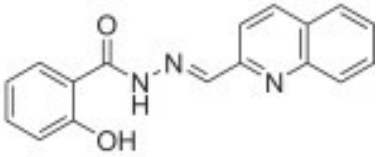
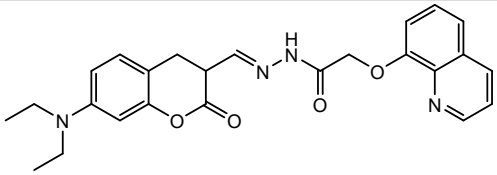
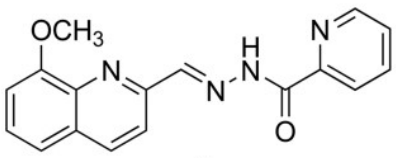
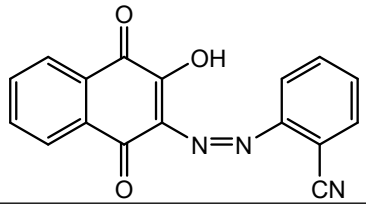
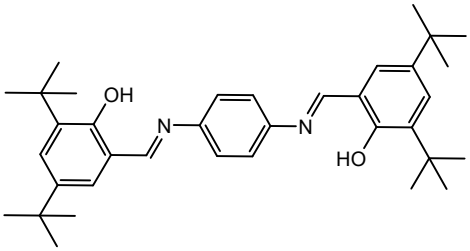
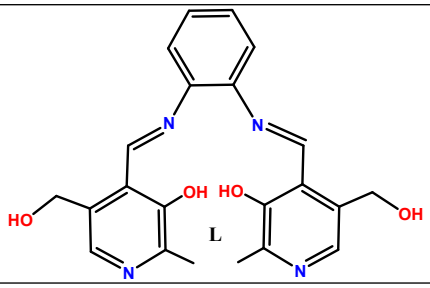


Fig. S11. The calibration plot for the estimation of LOD for S^{2-}.

Table S1. Comparison of **L** with reported fluorescent turn-off sensors.

Sensors	Medium	λ_{exc} / λ_{em}	LOD	Ref.
	MeOH-water (v/v = 1 : 1, 10 mM HEPES, pH 7.0)	467 nm/537 nm	0.27 μM	1
	HEPES buffer (1‰ DMSO, pH = 7.4)	340 nm/512 nm	0.44 μ M	2
	DMSO/HEPE S (20 mM, pH 7.22, 9:1, v/v)	410 nm/468 nm	8.68 μ M	3
	H_2O (containing 5% DMSO)	467 nm/517 n m	10.8 μ M	4

	HEPES buffered (1‰ DMSO, pH = 7.4)	340 nm/523 nm	0.3 μM	5
	DMSO/H_2O	300 nm/383 nm	0.27 μ M	6
	DMF/H_2O	386 nm/ 554 nm	0.35 μM	7
	EtOH:HEPES buffer (5% EtOH, pH = 7.4)	300 nm/380 nm	0.53 μM	**This work**

References

1. J.-T. Yeh, W.-C. Chen, S.-R. Liu and S.-P. Wu, *New J. Chem.*, 2014, **38**, 4434.
2. L. Tang, P. Zhou, Q. Zhang, Z. Huang, J. Zhao and M. Cai, *Inorg. Chem. Commun.*, 2013, **36**, 100-104.
3. C. Gao, X. Liu, X. Jin, J. Wu, Y. Xie, W. Liu, X. Yao and Y. Tang, *Sens. Actuators, B*, 2013, **185**, 125.
4. F. Chen, F. Hou, L. Huang, J. Cheng, H. Liu, P. Xi, D. Bai and Z. Zeng, *Dyes Pigm.*, 2013, **98**, 146
5. L. Tang, P. Zhou, Z. Qi, Z. Huang, J. Zhao and M. Cai, *Bull. Korean Chem. Soc.*, 2013, **34**, 2256.
6. M. Sonawane, S.K. Sahoo, J. Singh, N. Singh, C.P. Sawant and A. Kuwar, *Inorg. Chim. Acta*, 2015, **438**, 37-41.
7. P. Torawane, S. K. Sahoo, A. Borse and A. Kuwar, *Luminescence*. 2017, **0**, 1–5.

****