

Supporting Information

Aggregates of Triphenylene Based Chemosensing Ensemble for Sensitive Detection of Cyanide Ions in Aqueous Medium

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Effect of temperature on the absorption spectra of aggregates of copper ensemble of derivative 3

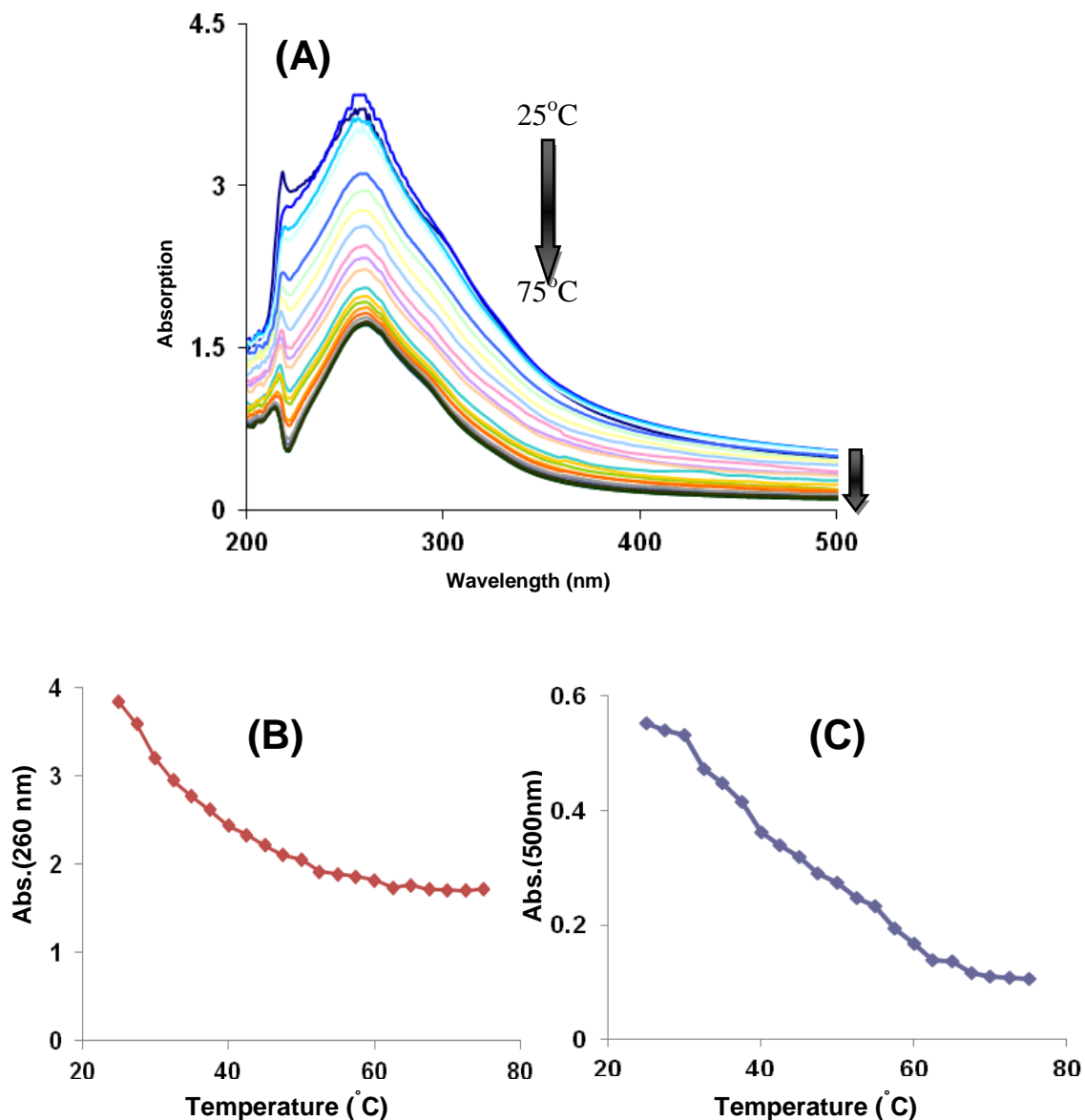


Figure S1: (A) Absorption spectra of aggregates of copper ensemble of derivative 3 upon increasing the temperature from 25 °C to 75 °C. (B-C) Change in the absorption intensity at 260 nm and 500 nm respectively upon increasing the temperature.

Effect of temperature on the fluorescence intensity of aggregates of copper ensemble of derivative 3

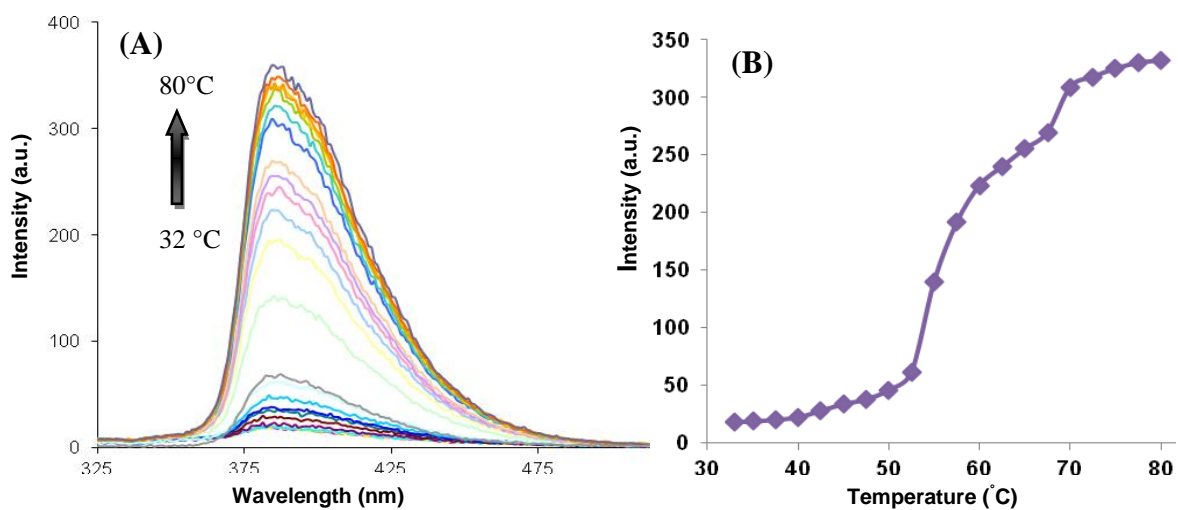


Figure: S2 (A) Fluorescence spectra of $3.Cu^{2+}$ upon increasing the temperature from 32 °C to 80 °C (B) Effect of increasing temperature on fluorescence intensity of aggregates of copper ensemble of **3**, $3.Cu^{2+}$ in EtOH:H₂O (8:2) λ_{ex} = 293 nm.

XRD analysis of aggregates of copper ensemble of derivative 3

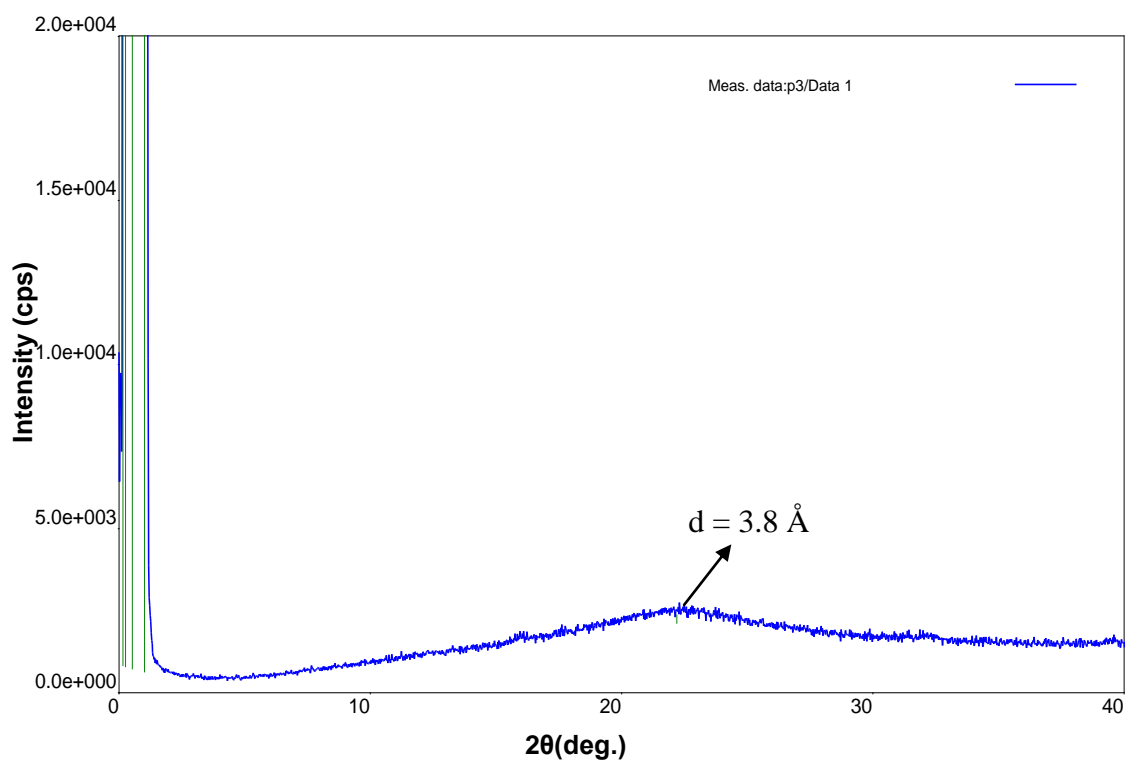
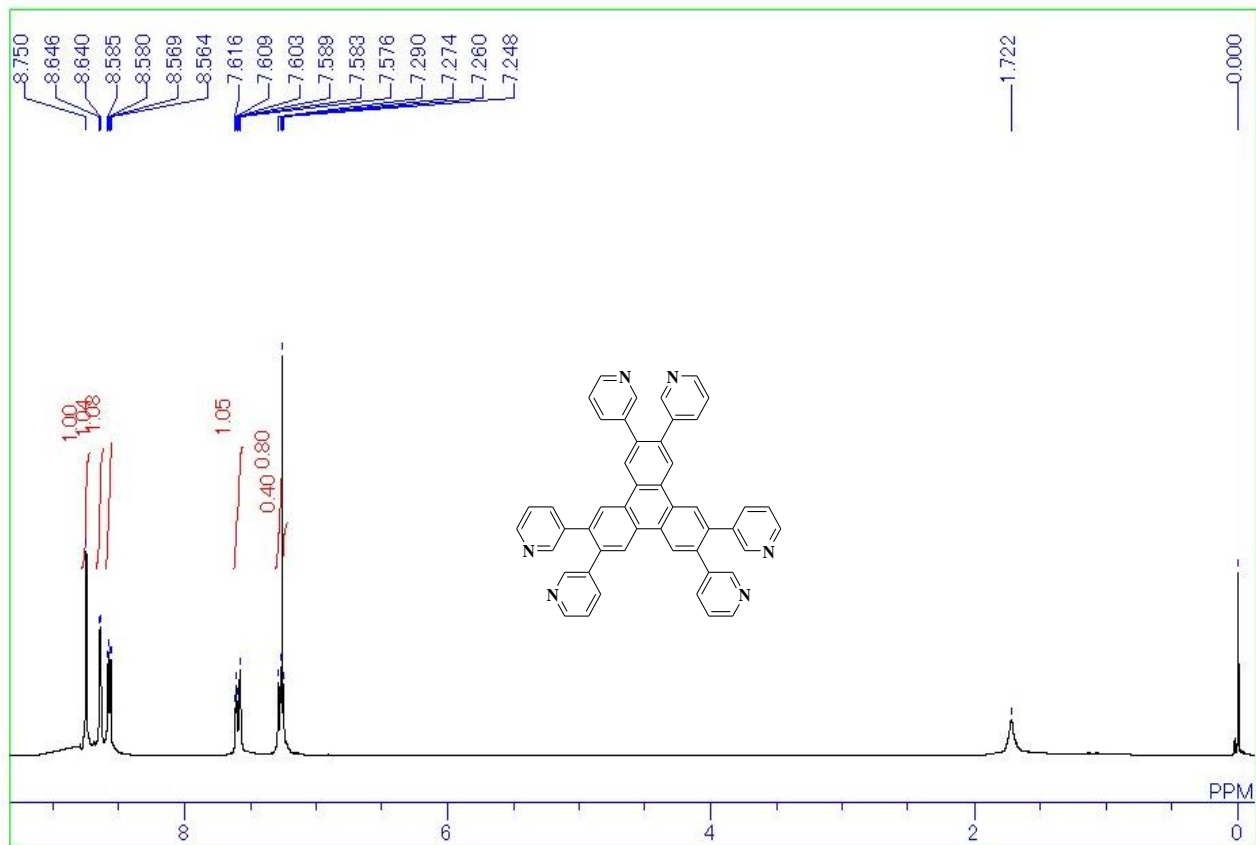
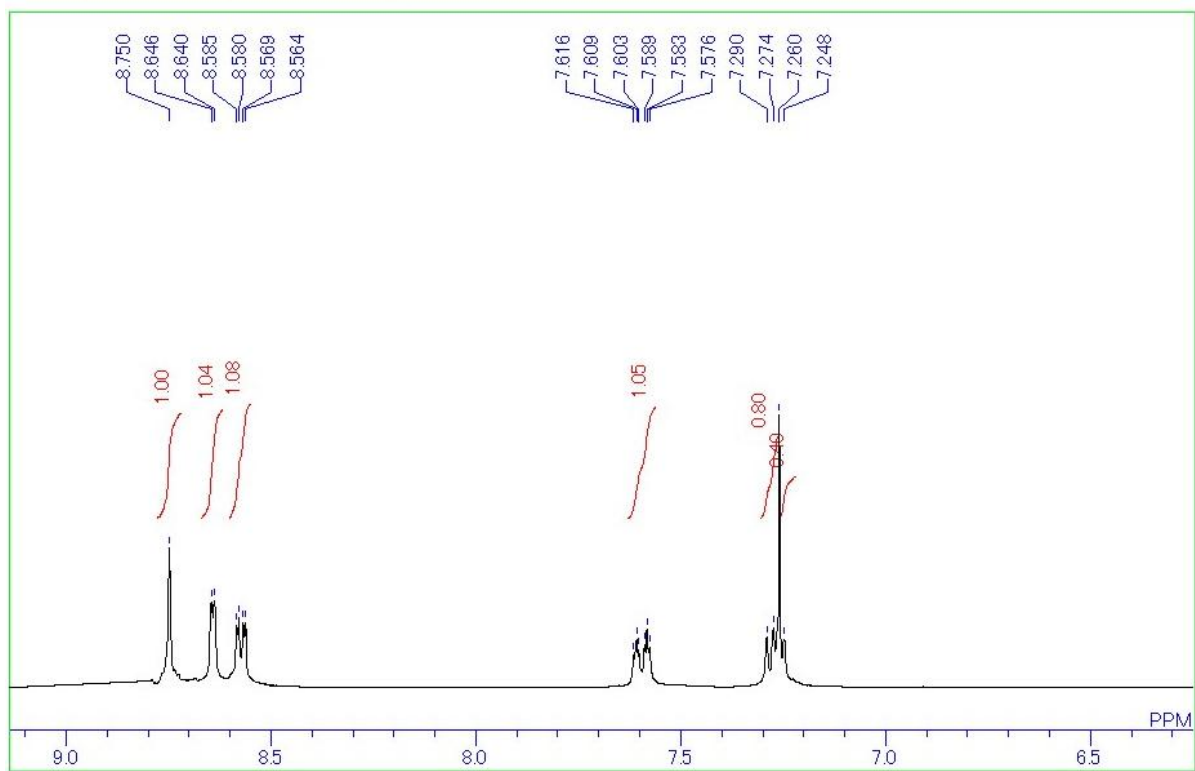


Figure S4: Powder XRD pattern of aggregates of copper ensemble of triphenylene derivative 3

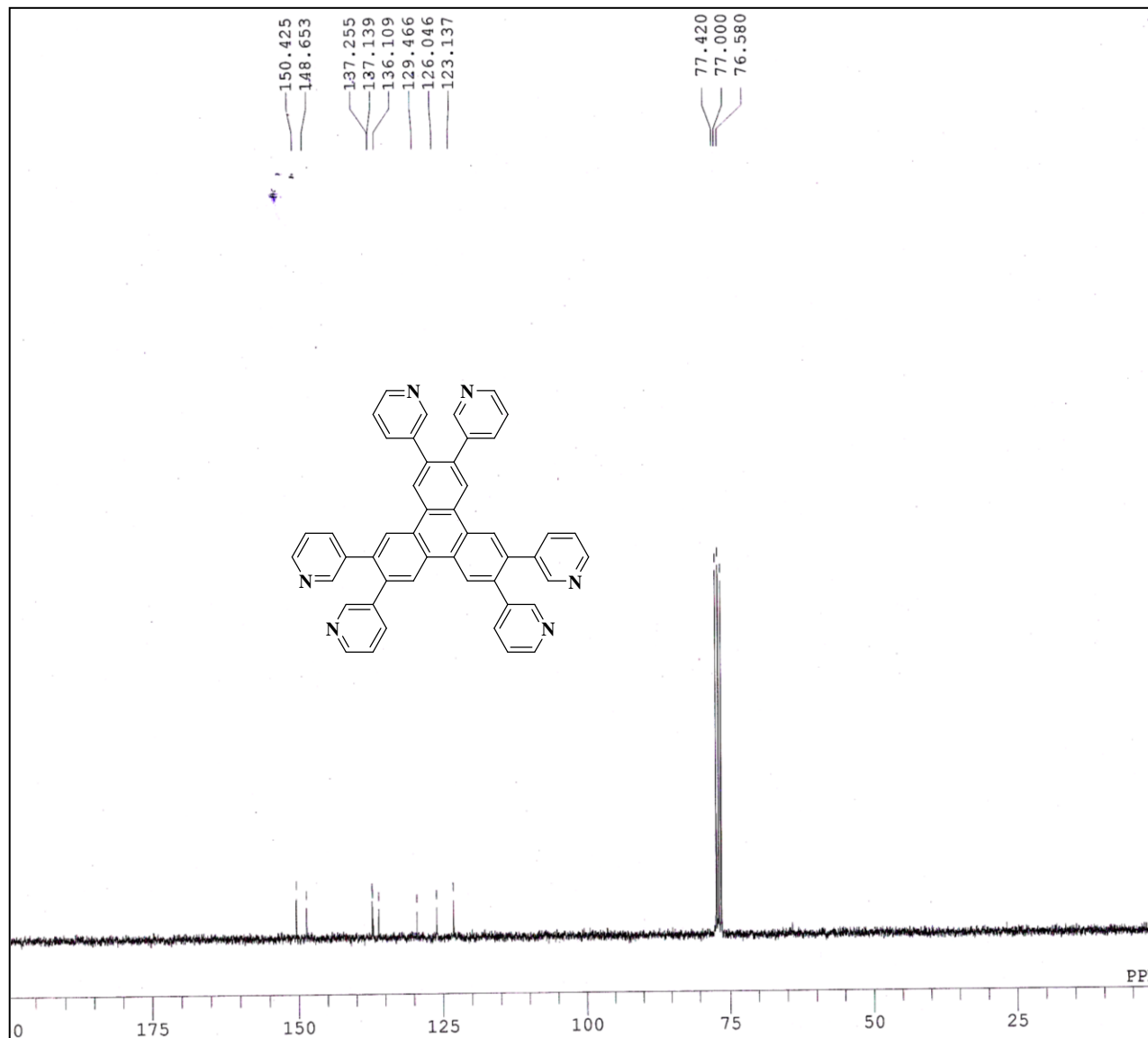
^1H NMR spectrum of **3**



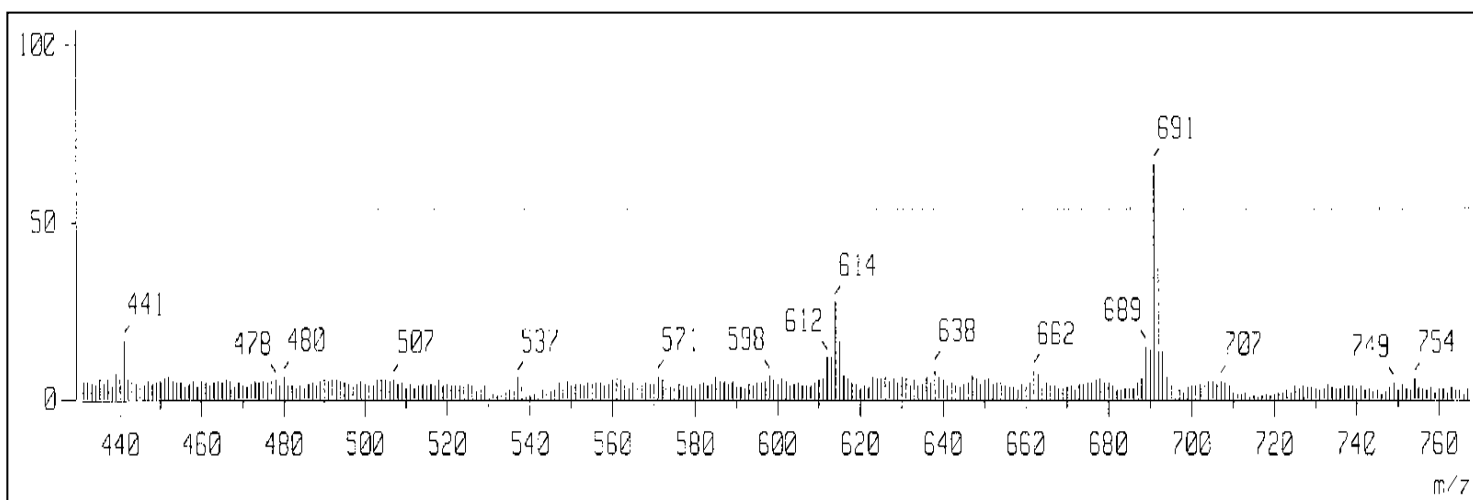
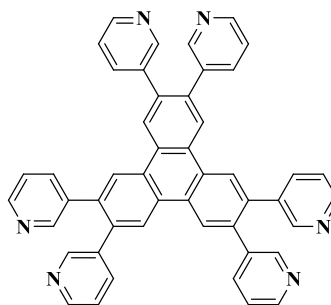
Expanded ^1H NMR spectrum of **3**



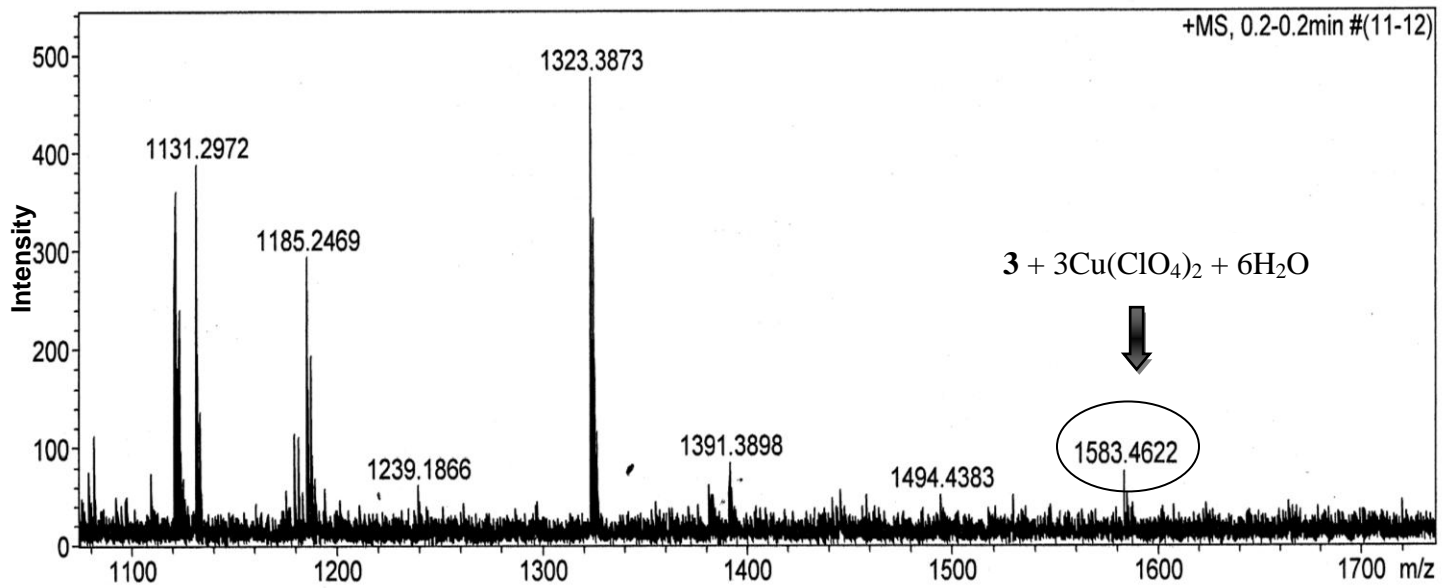
¹³C NMR spectrum of 3



FAB Mass spectrum of 3



ESI Mass spectrum of Cu complex of **3**



Fluorescence emission spectra of $3.Cu^{2+}$ upon the addition of NaCN in tap water

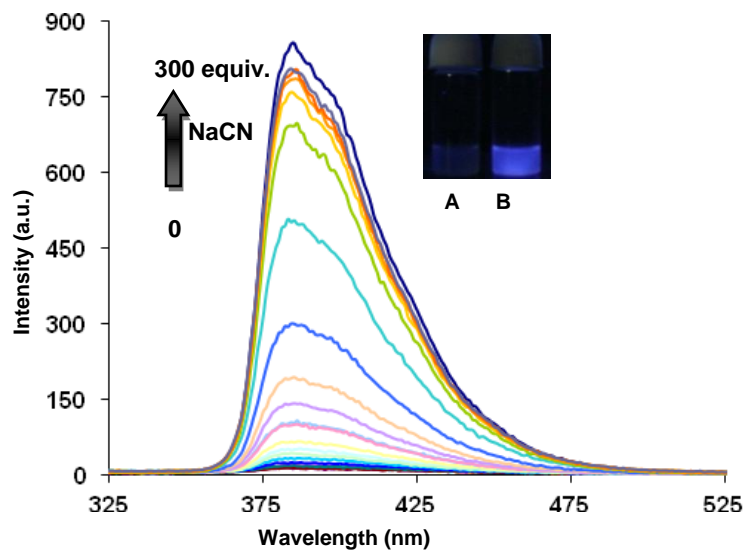


Figure S5: Fluorescence emission spectra of receptor $3.Cu^{2+}$ upon the addition of NaCN (0–300 equiv) in EtOH: H₂O (8:2) mixture. Inset shows fluorescence images of (A) copper ensemble, $3.Cu^{2+}$ (1×10^{-4} M) (B) $3.Cu^{2+}$ + NaCN in EtOH: H₂O (8:2) mixture.

Comparison of receptor 3 with other receptors reported in the literature

S.No.	References	Interference by other anions	Solvent system used for cyanide sensing	Detection limit of CN ⁻ ions	Ability to detect cyanide in tap water	Copper induced self-assembly
1	R. Yang, W. Wu, W.Wang, Z. Li, J. Qin <i>Macromol. Chem. Phys.</i> 2010, 211 , 18.	I ⁻ , OAc ⁻ , SO ₃ ²⁻	THF	0.47 ppm	NO	NO
2	Z. Li, X. Lou, H. Yu, Z. Li and J. Qin, <i>Macromolecules</i> , 2008, 41 , 7433.	I ⁻ , F ⁻ , SO ₄ ²⁻	THF	0.31 ppm	NO	NO
3.	Y. Liu, X. Lv, Y. Zhao, J. Liu, Y.-Q. Sun, P. Wang and W. Guo <i>J. Mater. Chem.</i> , 2012, 22 , 1747.	NO	CH ₃ CN/H ₂ O [9 : 1 (v/v)]	0.13 ppm	NO	NO
4	S. Dong, D. Ou, J. Qin, Z. Li <i>Journal of Polymer Science Part A: Polymer Chemistry</i> , 2011, 49 , 3314	I ⁻	THF	0.05 ppm	NO	NO
5	Q. Zeng, P. Cai, Z. Li, J. Qin and B. Z. Tang <i>Chem. Commun.</i> , 2008, 1094.	HPO ₄ ²⁻ , PO ₄ ³⁻	EtOH	1.82 ppm	NO	NO
6	X. Lou, Q. Zeng, Y. Zhang, Z. Wan, J. Qin and Z. Li <i>J. Mater. Chem.</i> , 2012, 22 , 5581	NO	EtOH	0.078	YES	NO

7	Y.-H.Tang, Y. Qu, Z. Song, X.-P. He, J. X., J. Hua and G.-R. Chen <i>Org. Biomol. Chem.</i> , 2012, 10 , 555	$\text{H}_2\text{PO}_4^{2-}$, HSO_4^-	MeOH	0.001 ppm (0.000962 ppm)	NO	NO
8	H.-C. Gee, C.-H. Lee, Y.-H. Jeong and W.-D. Jang <i>Chem. Commun.</i> , 2011, 47 , 11963	NO	CH_3CN	*	NO	NO
9	J. Wang and C.-S. Ha <i>Analyst</i> , 2011, 136, 1627	NO_3^- , H_2PO_4^-	$\text{H}_2\text{O}:\text{MeOH}$ (2:5; v/v)	*	NO	NO
10	V.Bhalla, H. Singh and M. Kumar <i>Dalton Trans.</i> , 2012, 41, 11413.	NO	DMSO	0.15 ppm	YES	NO
11	Receptor 3	NO	$\text{H}_2\text{O}:\text{EtOH}$ [2:8; (v/v)]	0.026 ppm	YES	YES

* No data available