## Supplementary Information

# Dihydro phenylquinazolinone based novel two-in-one colorimetric chemosensor for Nickel(II) and Copper(II) and its copper complex for fluorescent colorimetric nanomolar detection of cyanide anion

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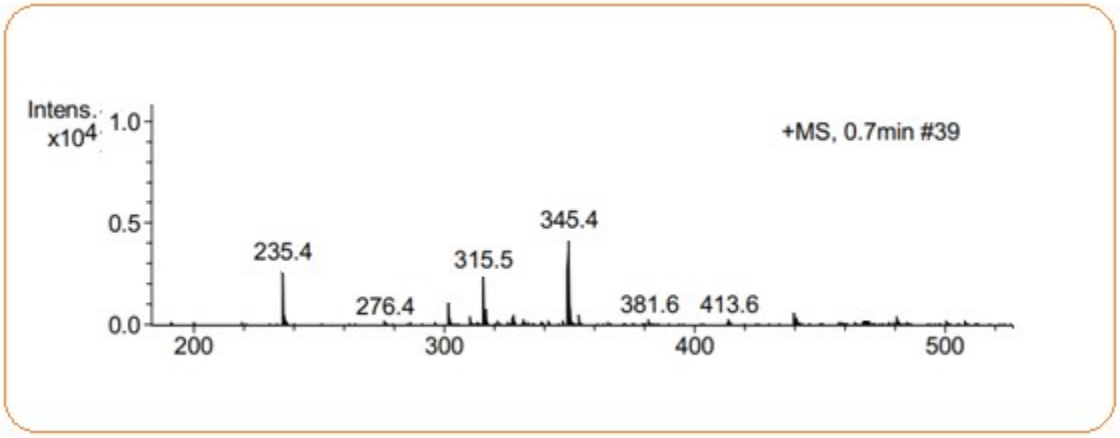



**Fig. S1.** Mass spectra of **L**

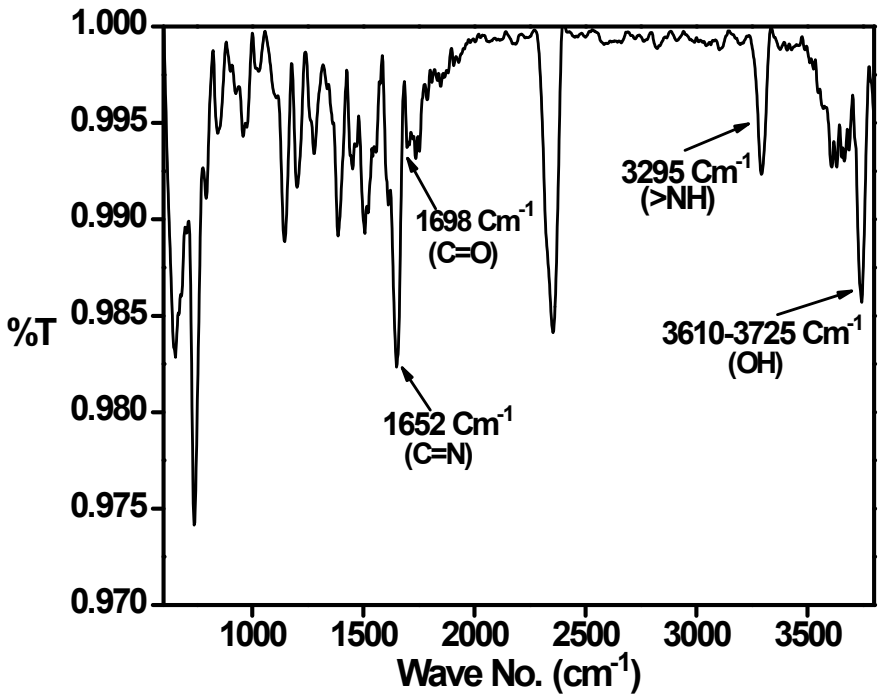



**Fig. S2.** IR spectra of **L**.

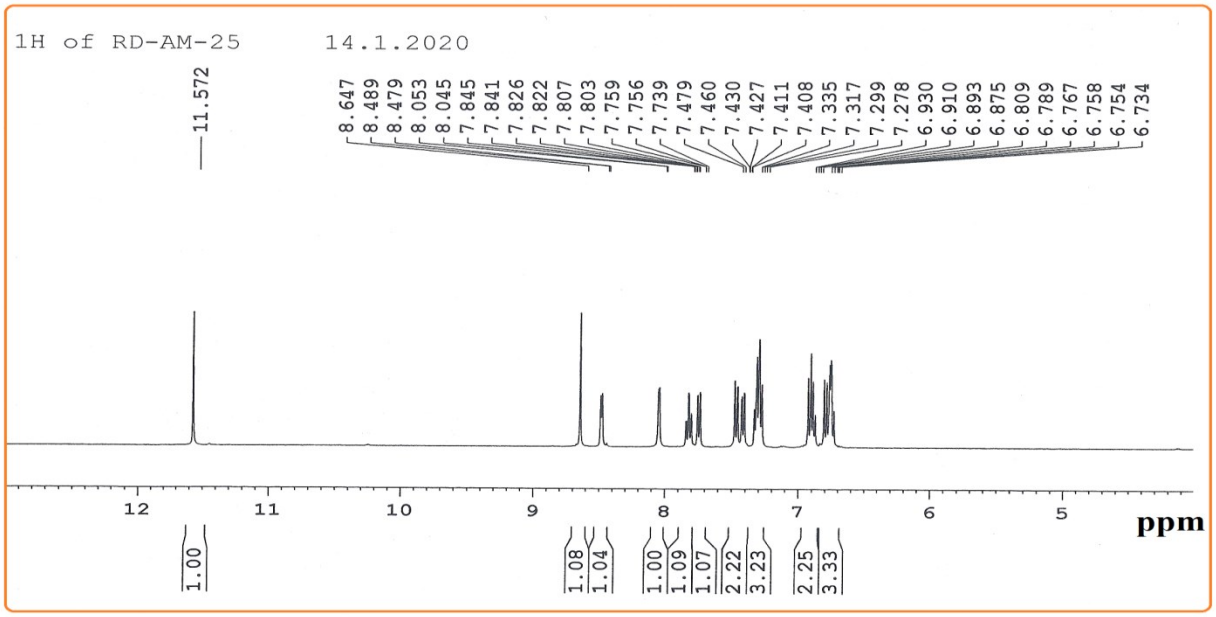



**Fig. S3.** Partial $^{1}$H-NMR spectra of **L** in DMSO-$d_6$.

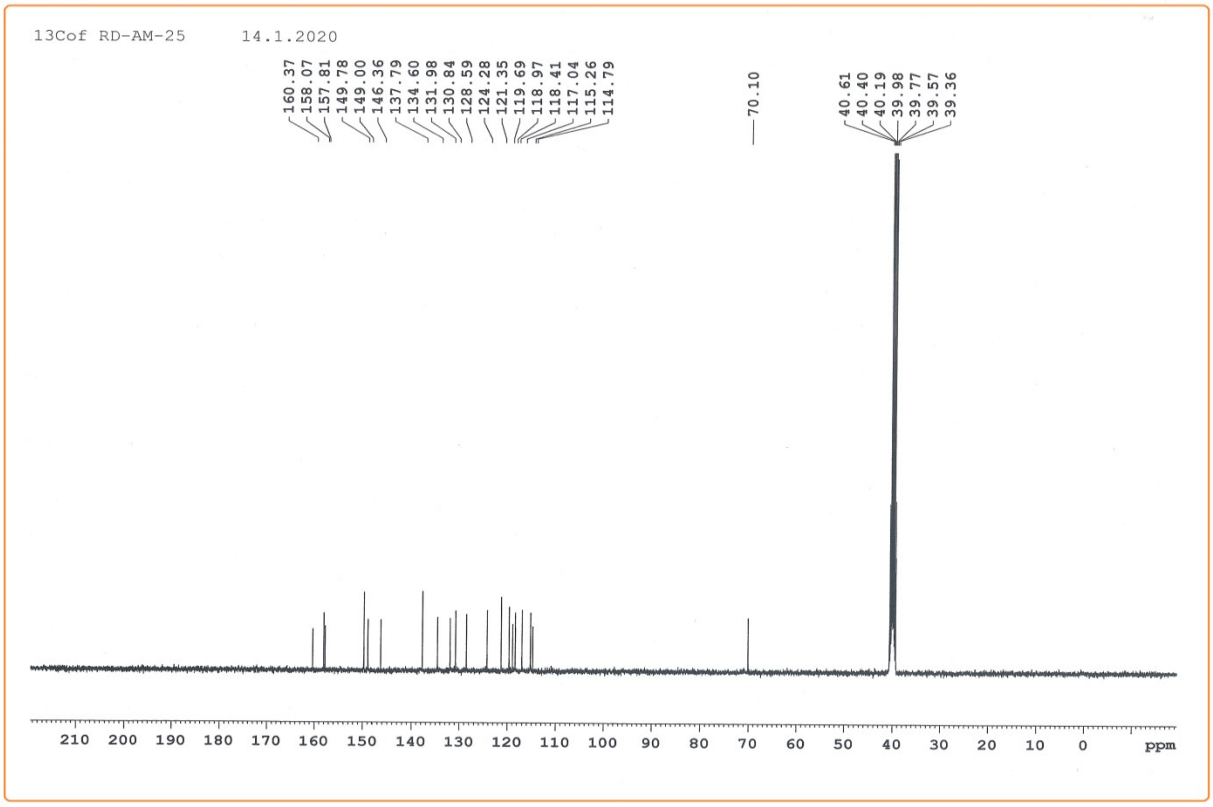



**Fig. S4.** $^{13}$C-NMR spectra of **L** in DMSO-$d_6$.

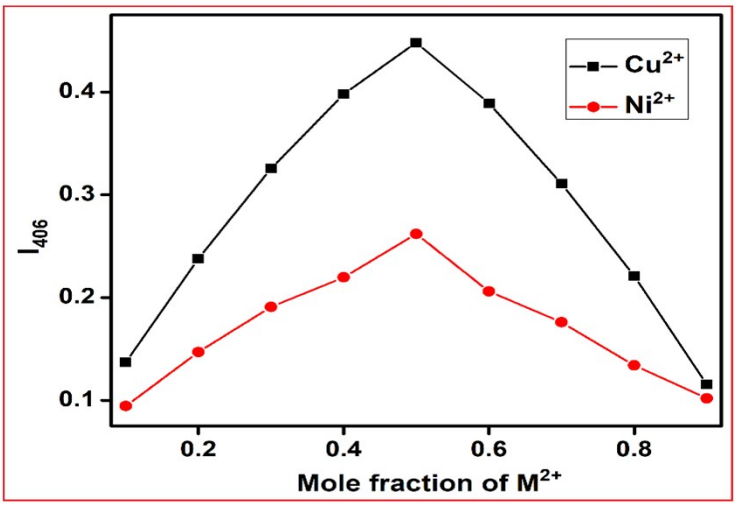



**Fig. S5:** Jobs Plot.

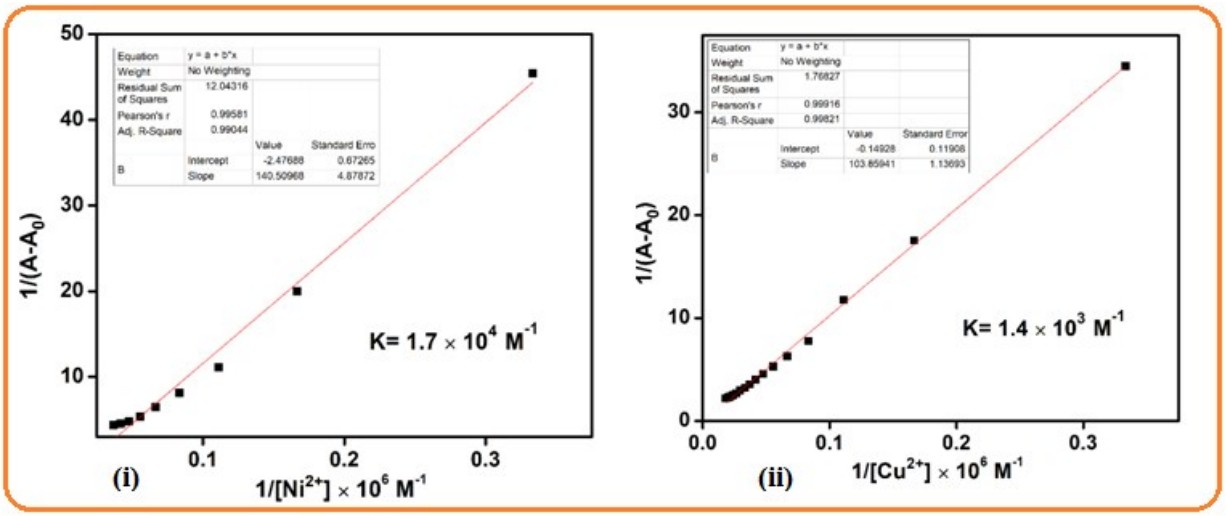



**Fig. S6.** Association constants of **L** towards (i) $Ni^{2+}$ and (ii) $Cu^{2+}$ ions.

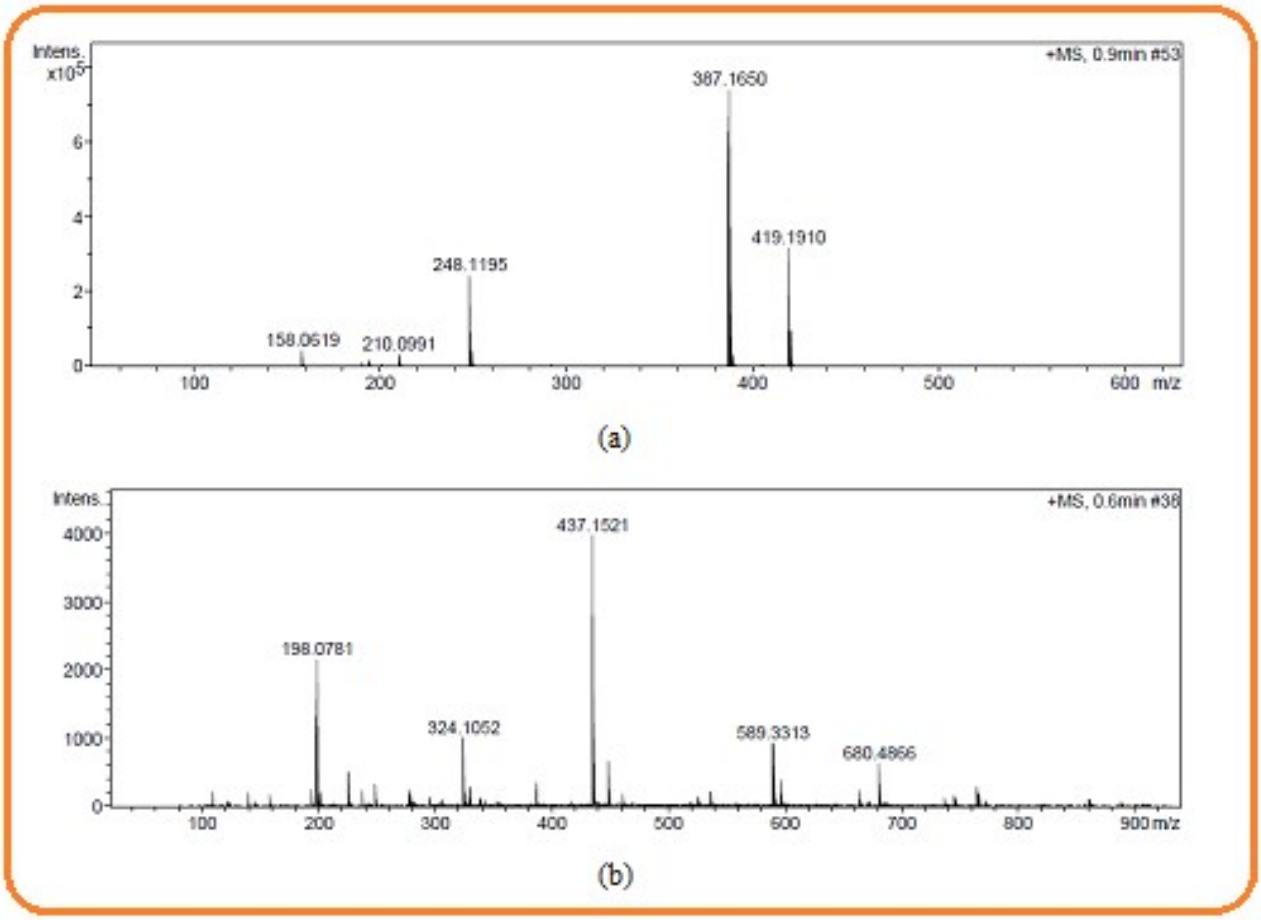



**Fig. S7.** ESI-Mass spectra of (a) **L**-$Ni^{2+}$ and (b) **L**-$Cu^{2+}$complexes.

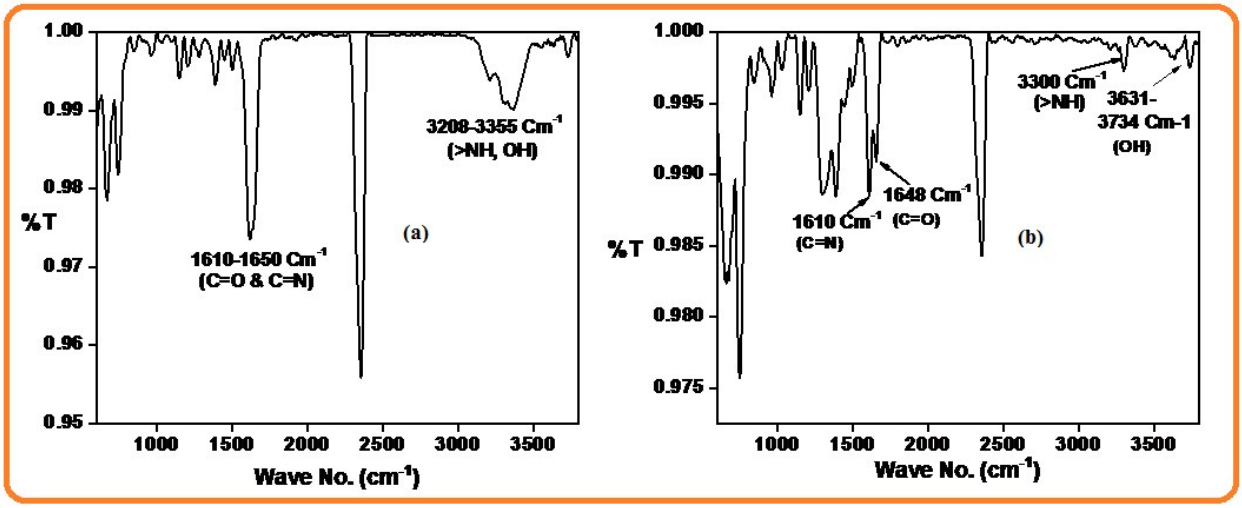



**Fig. S8.** FTIR spectra of [Ni**L**(OH)] (**1**) and [Cu**L**($OCH_3$)](**2**).

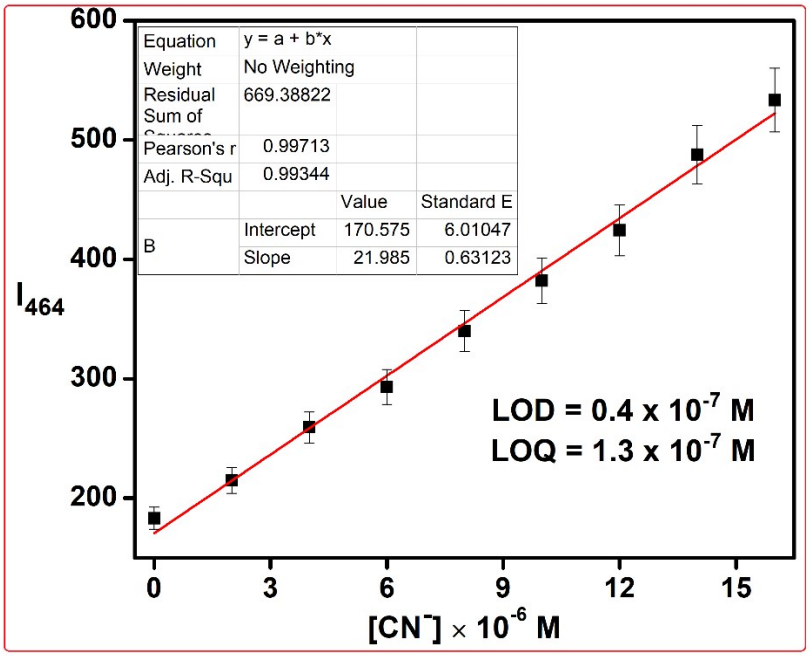



**Fig. S9.** Fluorometric detection limit of **L**+$Cu^{2+}$ towards $CN^-$ ion.

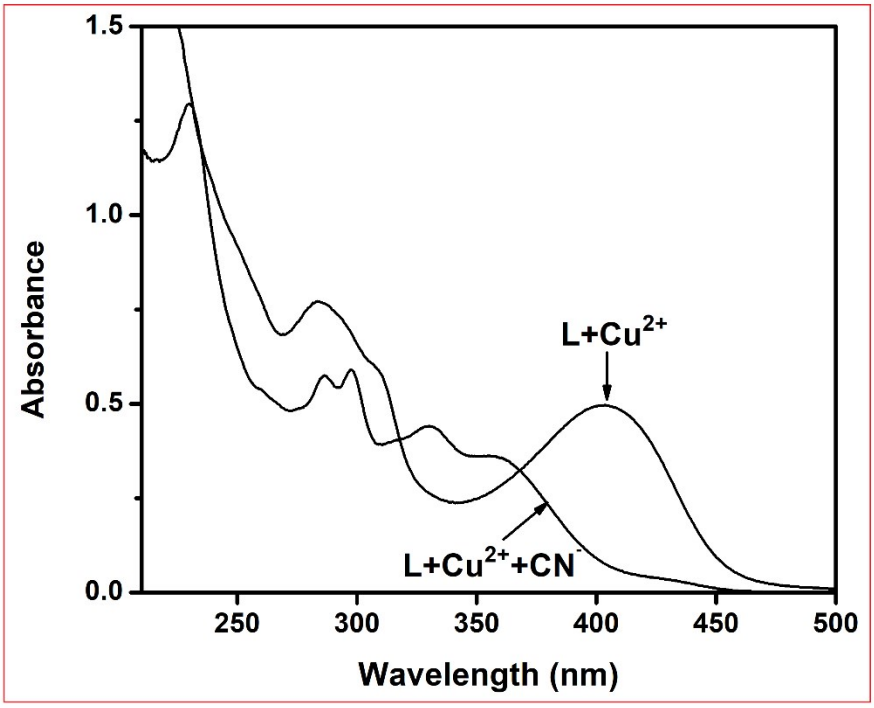



**Fig. S10.** UV-Vis absorption response of probe **L**+$Cu^{2+}$ (10 μM) in methanol-*tris*-HCl buffer (1:1 v/v) upon addition of $CN^-$ anions (5 equiv.).

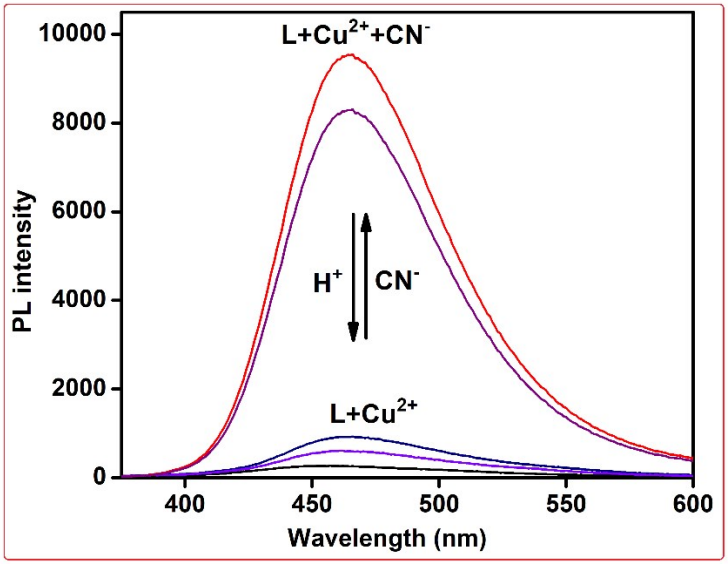



**Fig. S11**. Reversibility of **L**+$Cu^{2+}$ towards $CN^-$.

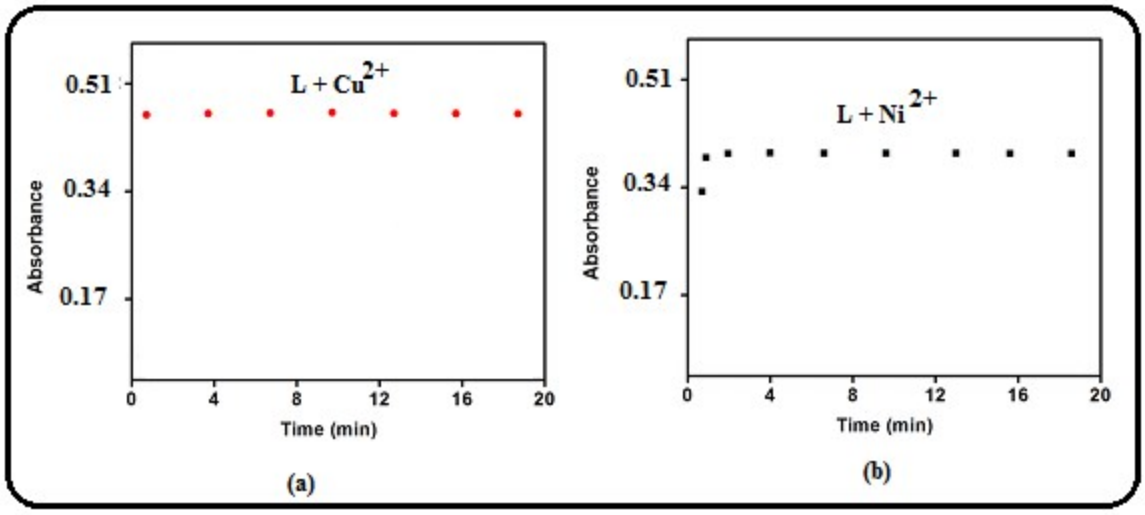



**Fig. S12.** Time responses of **L** towards $Cu^{2+}$ and $Ni^{2+}$.

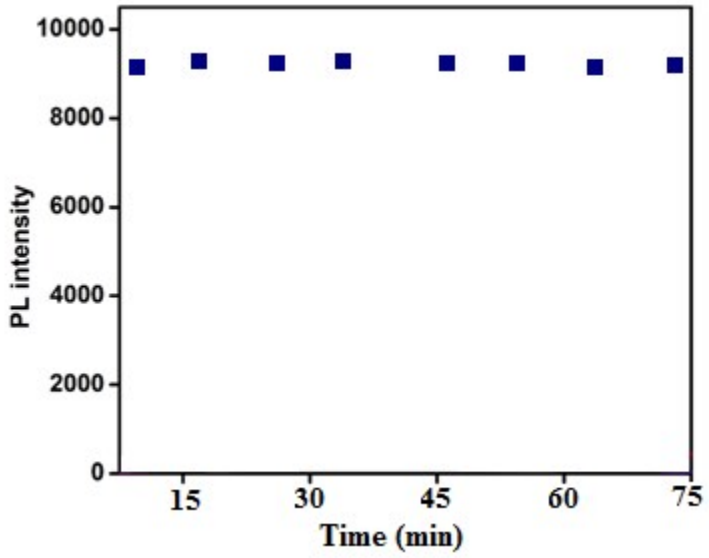
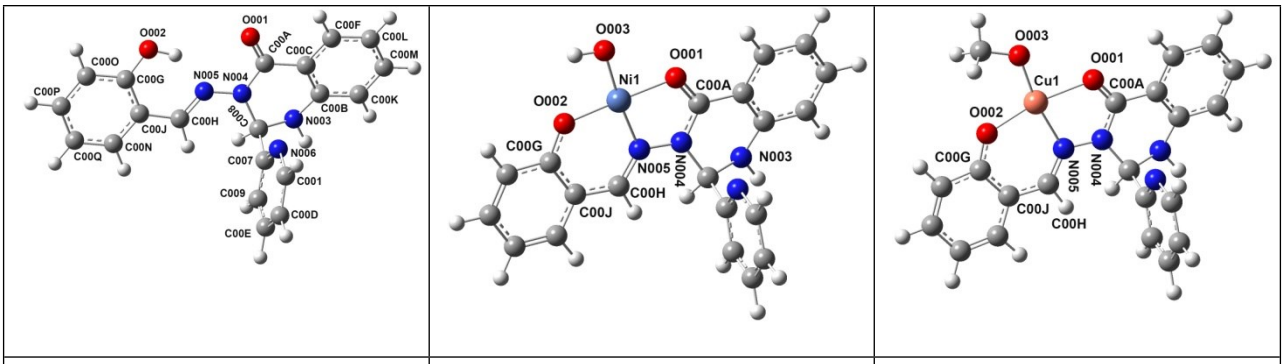



**Fig. S13.** Time responses of **L** + $Cu^{2+}$ towards $CN^{-}$.




| **L** | [Ni**L**(OH)] (**1**) | [Cu**L**($OCH_3$)](**2**) |
|---|---|---|

**Fig. S14.** Geometry optimized structure of **L**, [Ni**L**(OH)](**1**) and [Cu**L**($OCH_3$)] (**2**).

**Table S1** Recent chemosensor / materials for detection of $CN^-$ .

| **Chemosensor/Material** | **Method used** | **LOD** | **Reference** |
|---|---|---|---|
| Biometal organic Framework | Fluorescent turn on | $1.9x10^{-8}$ | 1 |
| Zn-coordination Polymer | Fluorescent turn off | $9.0x10^{-6}$ | 2 |
| Gold nanocluster | Fluorescent turn off | $2.0x10^{-7}$ | 3 |
| Phenothiazine derivative | Fluorescent turn off | $3.2x10^{-9}$ | 4 |
| Naphthoquinone-indole ensembles | Fluorescent turn on | $2.1x10^{-9}$ | 5 |
| Dihydro phenylquinazolinone | Fluorescent turn on | $4.0x10^{-8}$ | Present study |

**Table S2** Selected bond parameters for geometry optimized structures of [Ni**L**(OH)] (**1**) and [CuL($OCH_3$)] (**2**).

| Bond Parameter | Optimized [Ni**L**(OH)] (**1**) | Bond Parameter | Optimized [Cu**L**($OCH_3$)] (**2**) |
|---|---|---|---|
| Bond length (Å) | | | |
| Ni1-O001 | 1.85077 | Cu1-O001 | 1.94818 |
| Ni1-O002 | 1.91286 | Cu1-O002 | 2.09329 |
| Ni1-O003 | 1.83519 | Cu1-O003 | 1.85210 |
| Ni1-N005 | 1.89700 | Cu1-N005 | 2.06074 |
| C00A-O001 | 1.31071 | C00A-O001 | 1.29399 |
| O002-C00G | 1.26594 | O002-C00G | 1.24454 |
| N005-C00H | 1.47200 | N005-C00H | 1.46496 |
| N004-N005 | 1.39162 | N004-N005 | 1.38971 |
| Bond angle ($^0$) | | | |
| O001-Ni1-O003 | 90.02333 | O001-Cu1-O003 | 99.24156 |
| O001- Ni1-N005 | 95.50909 | O001-Cu1-N005 | 91.02902 |
| O002- Ni1-N005 | 83.09986 | O002-Cu1-N005 | 76.91589 |
| O002- Ni1-O003 | 91.36677 | O002-Cu1-O003 | 92.83055 |

| | | | |
|---|---|---|---|
| O001- Ni1-O002 | 178.58167 | O001-Cu1-O002 | 167.88140 |
| O003- Ni1-N005 | 174.46376 | O003-Cu1-N005 | 169.70270 |

**References**


1. A. Karmakar, B. Joarder, A. Mallick, P. Samanta, A. V. Desai, S. Basu and S. K. Ghosh, Aqueous phase sensing of cyanide ions using a hydrolytically stable metalorganic framework, *Chem. Commun*., 2017, **53**, 1253–1256.
2. L. D. Rosales-Vázquez,J. Valdes-García, I.J. Bazany-Rodríguez, J. M. Germán-Acacio, D. Martínez-Otero, A. R. Vilchis-Néstor, R. Morales-Luckie, V. Sánchez-Mendieta and A. Dorazco-González, A sensitive photoluminescent chemosensor for cyanide in water based on a zinc coordination polymer bearing ditert-butyl-bipyridine, *Dalton Trans*., 2019,**48**, 12407-12420
3. Y. Liu, K. Ai, X. Cheng, L. Huo and L. Lu, Gold-nanoclusterbased fluorescent sensors for highly sensitive and selective detection of cyanide in water, *Adv. Funct. Mater*., 2010, **20**, 951–956
4. F.A. M. Al‑Zahrani, R.M. El‑Shishtawy, A.M. Asiri, A.M. Al‑Soliemy,K.A. Mellah, N.S. E. Ahmed and A. Jedid, A new phenothiazine‑based selective visual and fuorescent sensor for cyanide, *BMC Chemistry*, 2020, **14**, 2.
5. P. Jayasudha, R. Manivannan, S. Ciattini, L. Chelazzi and K. P. Elango, Selective sensing of cyanide in aqueous solution by quinone-indole ensembles – quantitative effect of substituents on the HBD property of the receptor moiety, *Sens. Actuators B*, 2017, **242**, 736–745.