Electronic Supplementary Information

Selective and Sensitive Colorimetric Sensor for CN- in Absence and Presence of Metal Ions (Cu2+/Ni2+): Mimicking Logic Gate Behaviour

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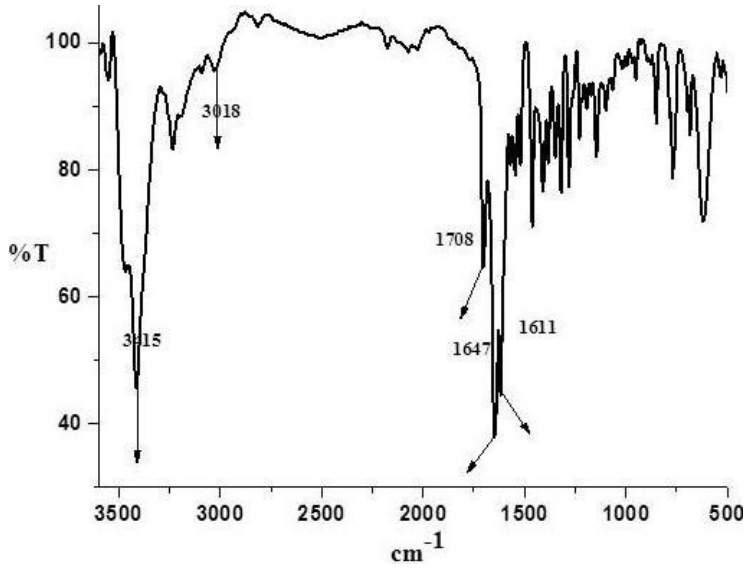
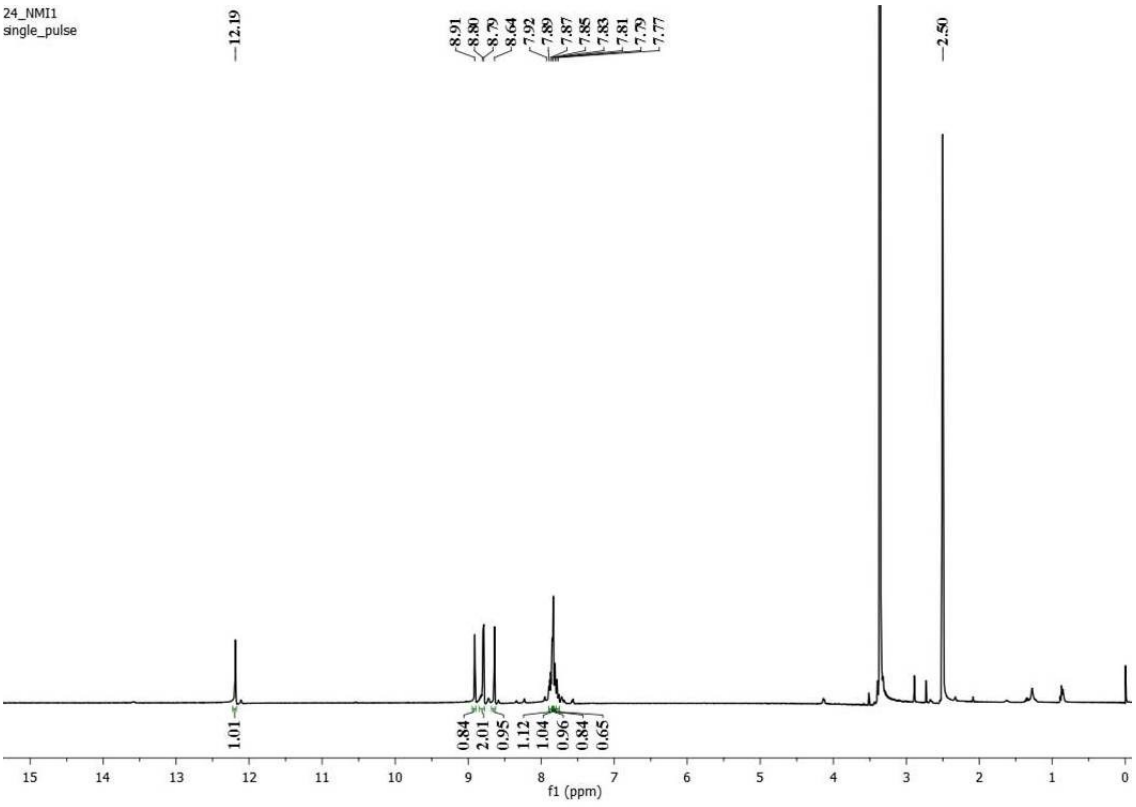
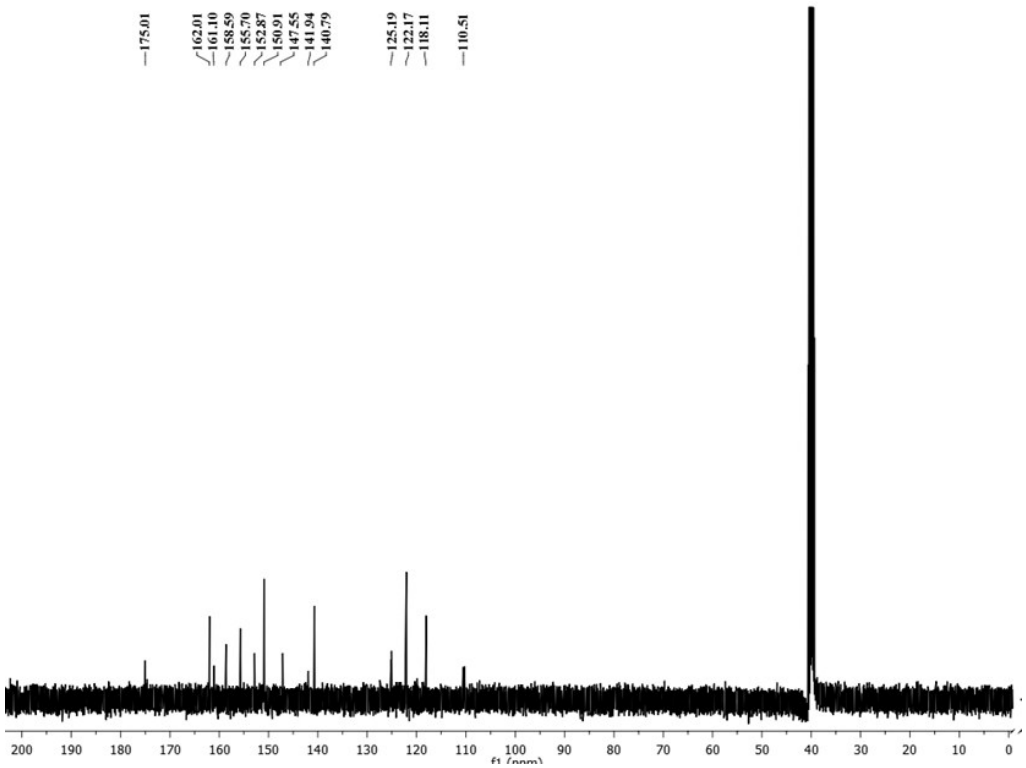


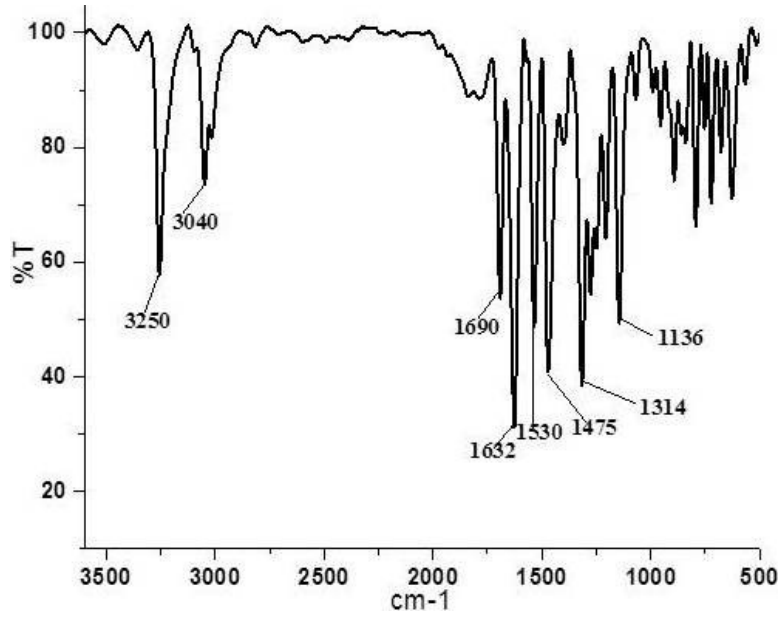
ESI Fig. S1: FTIR spectrum of L1.



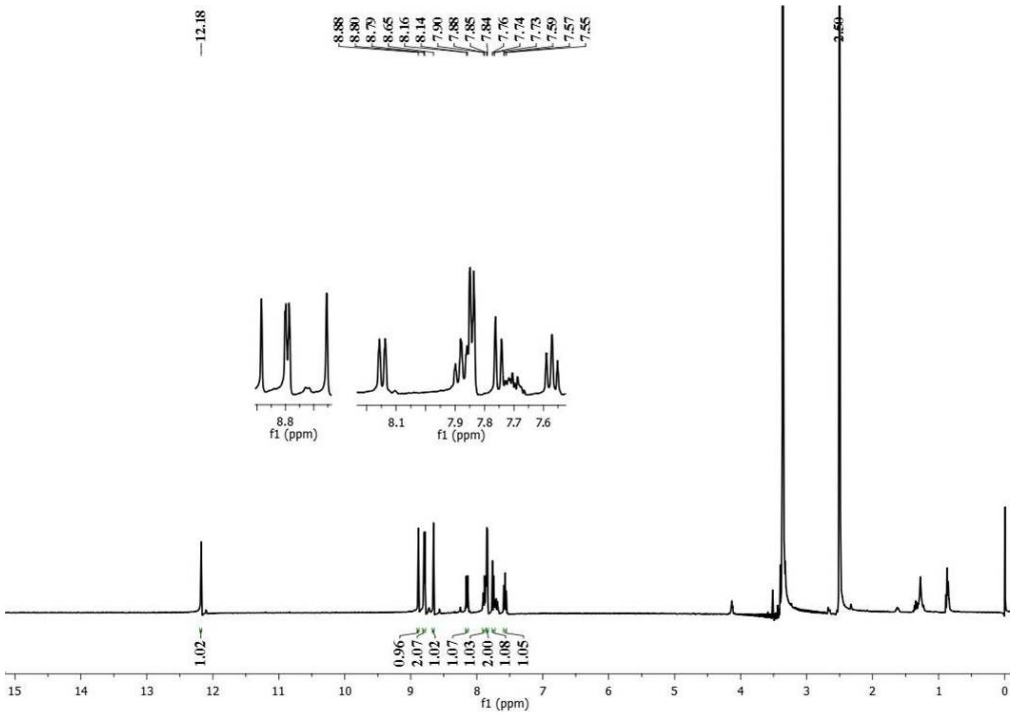
ESI Fig. S2: ^{1}H NMR spectrum of Probe in d_6 DMSO.



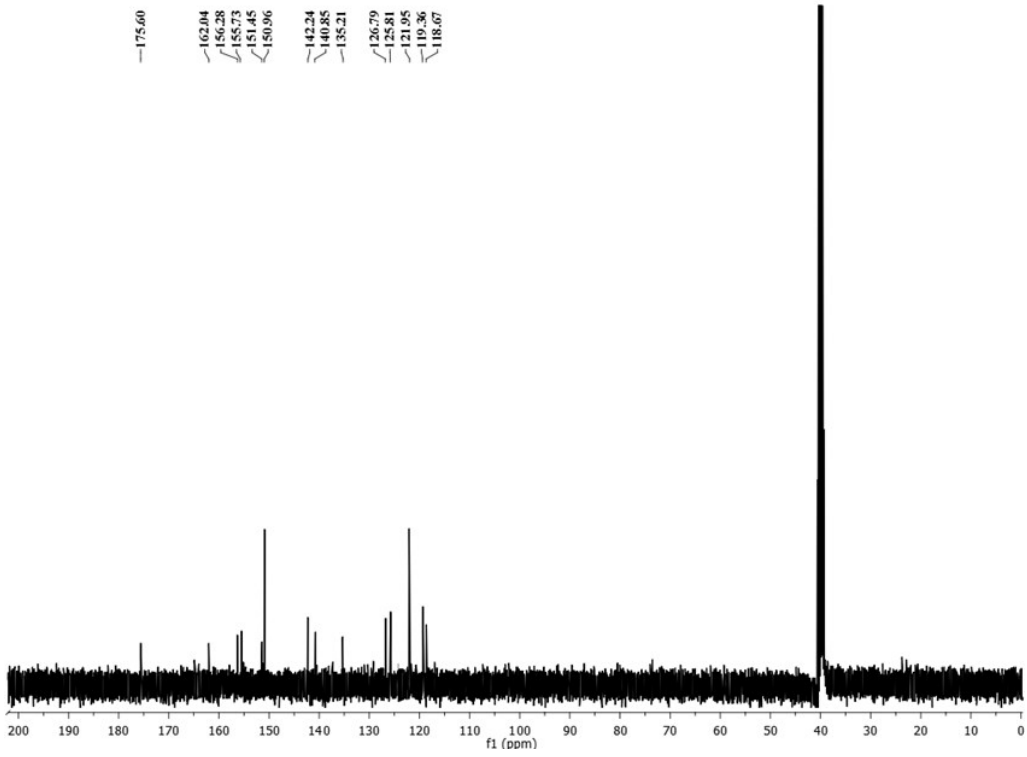
ESI Fig. S3: ^{13}C spectrum of L1 in d_6 DMSO.



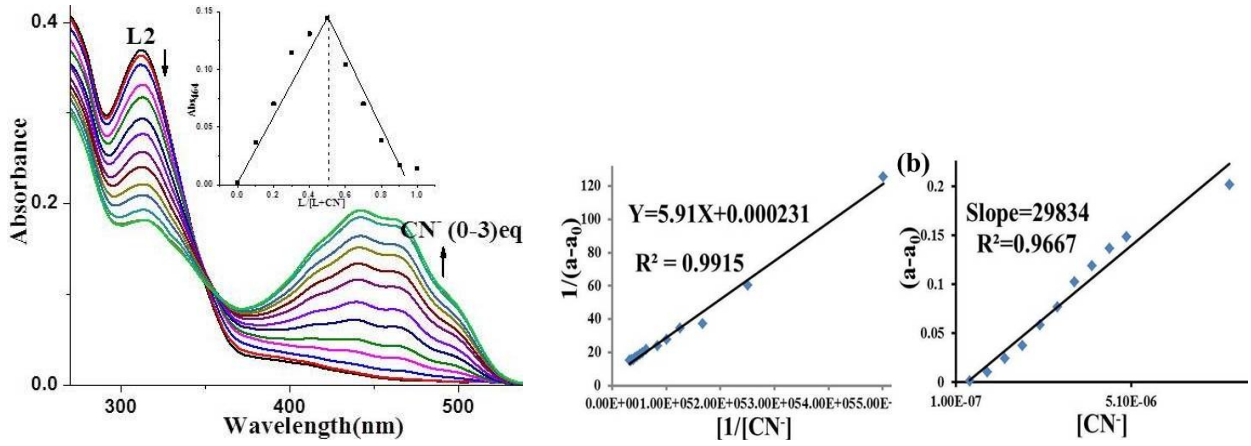
ESI Fig. S4: FTIR spectrum of L2.



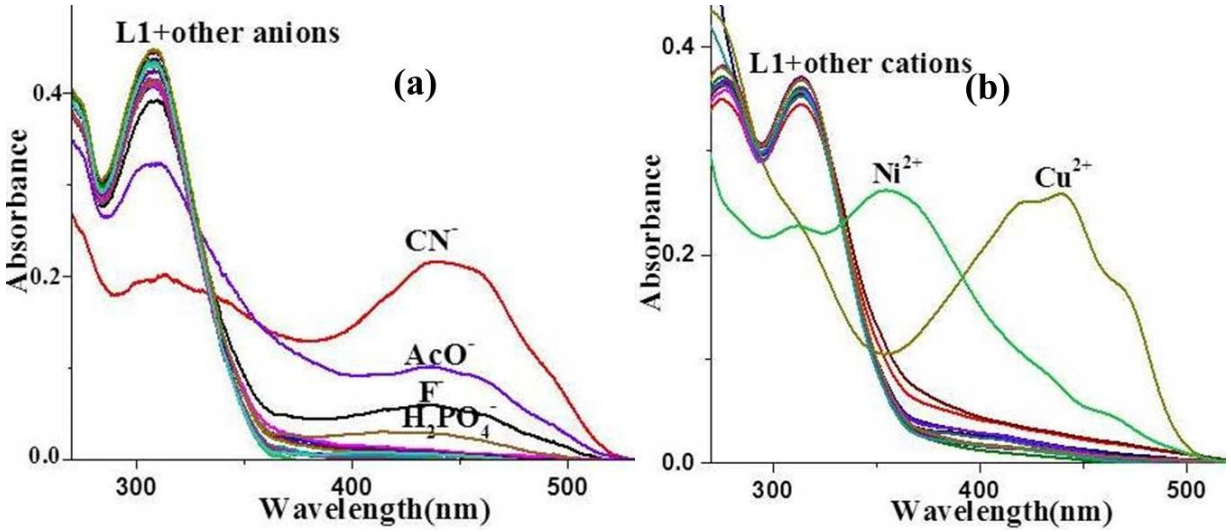
ESI Fig. S5: ^{1}H NMR spectrum of L2 in d_6 DMSO.



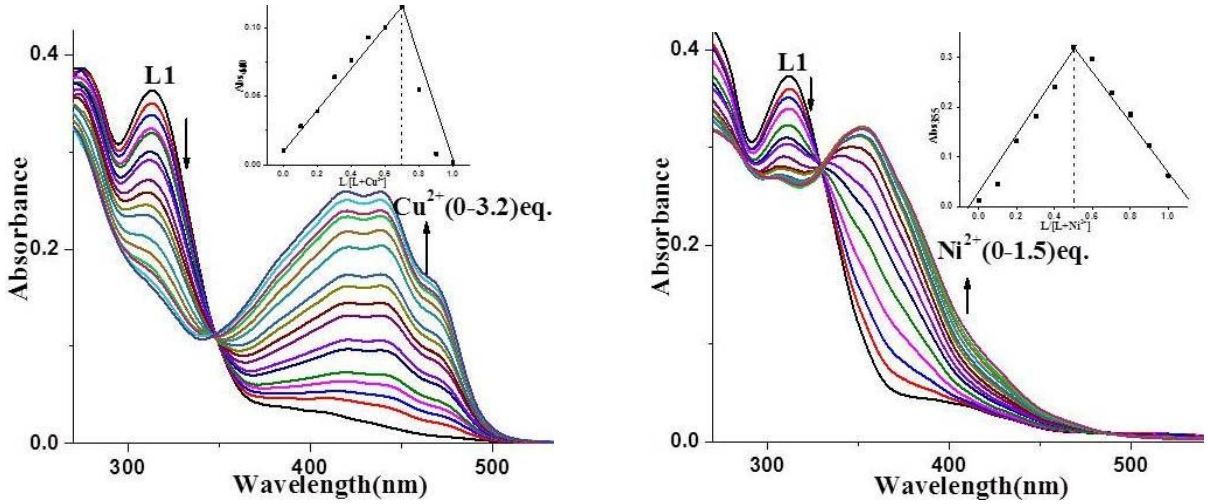
ESI Fig. S6: ^{13}C spectrum of L2 in d_6 DMSO.



ESI Fig. S7: (a) Absorption titration spectra of L2 upon addition 0–3 eq. of CN^- , Inset: Jobs plot shows 1:1; (b) Benesi-Hilderbrand Plot and detection limit of L2 for the binding of CN^- in 10% aq.-DMSO solution (HEPES buffer 7.4).



ESI Fig. S8: (a) Interaction of L1 upon 5 eq. of anions in 100% DMSO solution; (b) Interaction of L1 upon 5 eq. of metal ions in 10% aq.-DMSO solution (HEPES buffer 7.4).

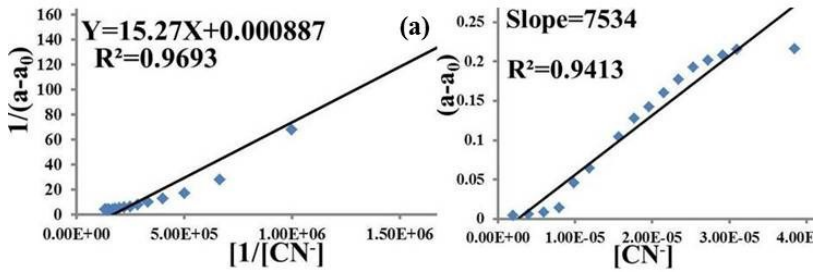


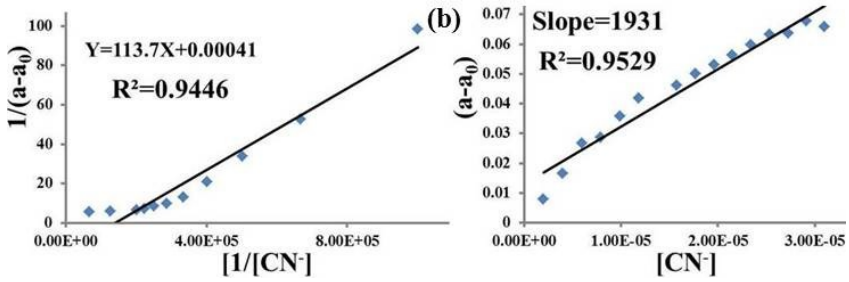
ESI Fig. S9: Absorption titration spectra of L1 upon addition of (0-3.2) eq.Cu^{2+} Inset: Jobs plot shows 1:2 and (0–1.5) eq. of Ni^{2+} Inset: Jobs plot shows 1:1 in 10% aq.-DMSO solution (HEPES buffer 7.4).

Determination of the detection limit

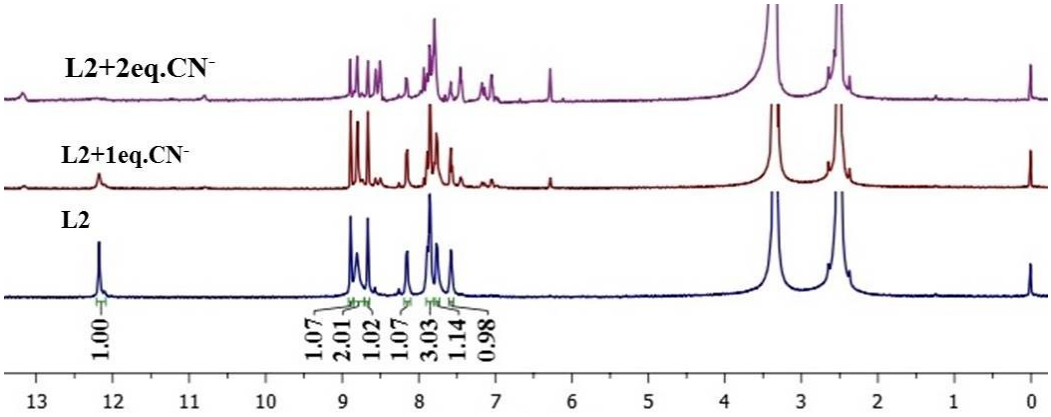
The detection limits of L1/L2 were determined from 3σ/slope, where σ is the standard deviation of the blank solution; S is the slope of the calibration curve.

CN^- complex	SD	Slope CN^-
L1	0.0097	38419
L2	0.00675	29834
L1+Cu^{2+}	0.009	7534
L1+Ni^{2+}	0.0041	1931.8

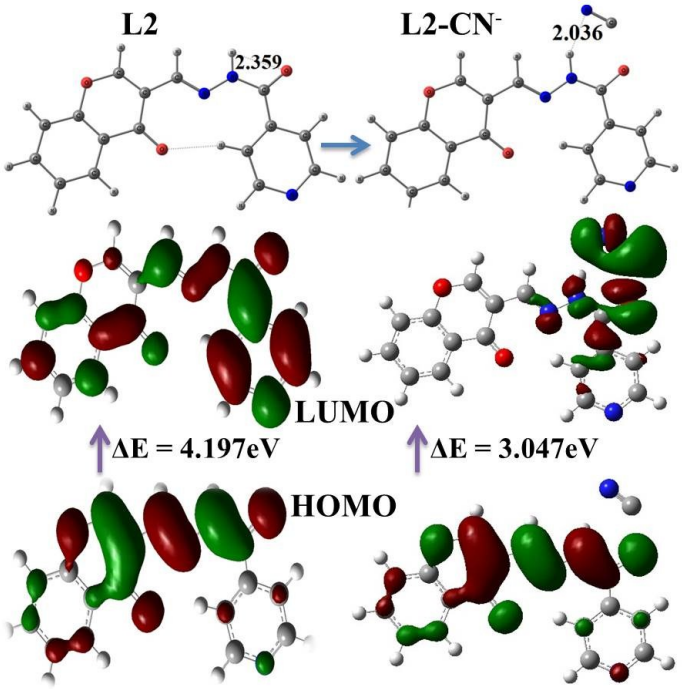




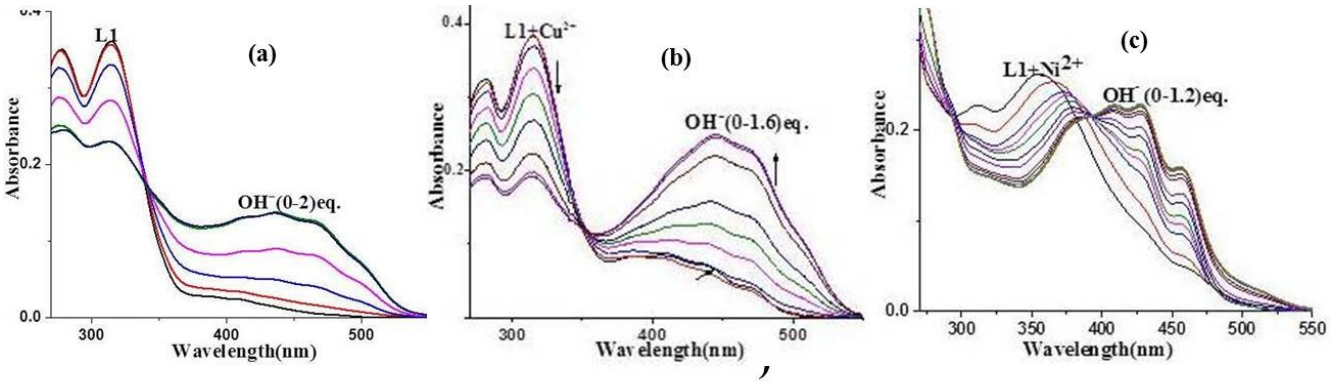
ESI Fig. S10: Benesi-Hilderbrand Plot and Limit of detection for the binding of CN^- (a) L1-Cu^{2+}



ESI Fig. S11: Stacked ^1H NMR titration of L2 in d_6 DMSO.



ESI Fig.S12: DFT Optimized structure and HOMO/LUMO energy band gap of L2 and L2-CN^-.



ESI Fig. S13: Absorption titration spectra of (a) L1; (b) L1-Cu^{2+}; (c) L1-Ni^{2+} with TBAOH solution.

Table S1: Solvatochromic studies of L1 with CN^- in different polar solvents.

Solvent	λ_{abs} of L1	λ_{abs} of L1-CN^-
DCM	306	310
ACN	306	427
DMSO	308	455
MeOH	310	465

Table S2: Comparison of proposed probe with previously reported (containing –NH group) literatures by colorimetric method.

Previously literatures	**Selective Anions**	**Solvent System**	**Binding Constant (M^{-1})**
Tetrahedron Letters 2013, 54, 5612–5615 (28a)	F^-, AcO^-	ACN	1.22×10^4, 2.59×10^4
Anal. Methods, 2013, 5, 6401–6410 (28b)	F^-, AcO^-	DMSO	4.30×10^3, 3.80×10^3 (S1) 2.26×10^4, 2.13×10^4 (S2)
RSC Adv., 2016, 6, 16586-16597 (28c)	CN^-, S^{2-}	buffer/DMSO (1 : 9, v/v).	4.20×10^3, 1.20×10^3

Analytica Chimica Acta, 2010, 663,77–84 (28d)	F^-, CN^-	DMSO	-------
Sensors and Actuators B, 2016, 231, 768–778 (28e)	F^-, CN^-	50% aq. DMF	5.53×10^5, 8.27×10^4 (R-Cu complex) 7.58×10^5, 9.87×10^4 (R-Co complex) 2.60×10^6, 9.04×10^4 (R-Ni complex) ---------- 7.13×10^4 (R-Zn complex)
Sensors and Actuators B, 2014, 204, 125–135 (22a)	CN^-, AcO^-	DMSO	7.52, 7.07 (N1) 8.52, 7.86 (N2)
Dalton Trans., 2016, 45, 1166-1175 (16d)	F^-, CN^-	ACN (2.5% DMSO)	1.17×10^4, 4.9×10^4 (R) 1.37×10^5, 1.19×10^4 (R-Cu complex)
This work	CN-	H_2O -DMSO- (10%)	3.83×10^4 (R) 1.72×10^5 (Cu complex) 2.80×10^5 (Ni complex)

R= synthesized ligand

Table S3: Analytical results of CN^- detection in water samples.

Sample	Added [CN-](μM) added	By Absorption spectra[CN-][a] (μM)	Determined [CN-](μM) AAS	Recovery%
Roorkee Tap water	20	19.8 ± 0.5	19.86	99%
Haridwar water	20	19.7 ± 0.2	19.82	98.5%
Roorkee water	20	19.96 ± 0.7	20.1	100.5%

[a]Mean value ± standard deviation (triplicate measurement)