Supporting Information

Cost-effective approach to detect Cu(II) and Hg(II) by integrating smartphone with the colorimetric response from NBD-benzimidazole based dyad

Thangaraj Anand and Suban K Sahoo*

Department of Applied Chemistry, SV National Institute of Technology (SVNIT), Surat-395007, India. (E-mail: suban_sahoo@rediffmail.com; Tel.: 91-261-2201855)

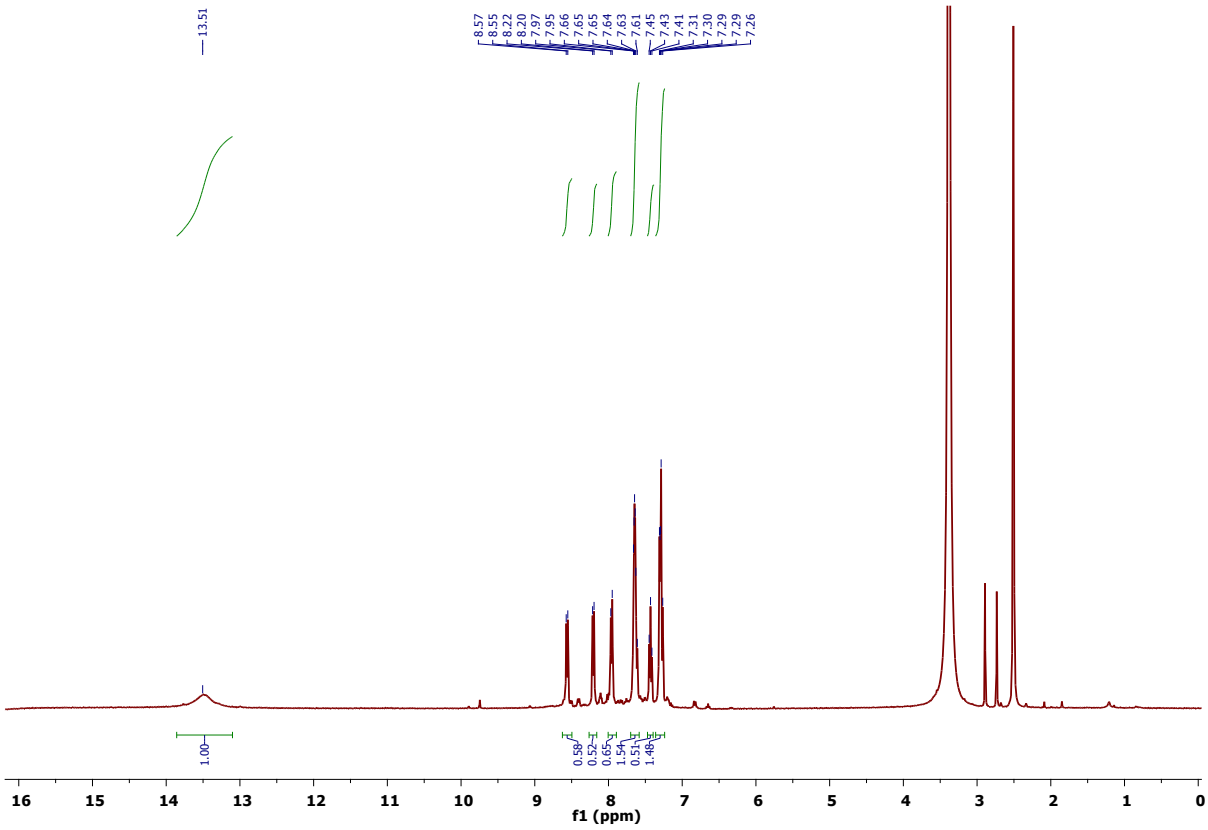

Fig. S1. ^{1}H NMR spectrum of the receptor **N1.**

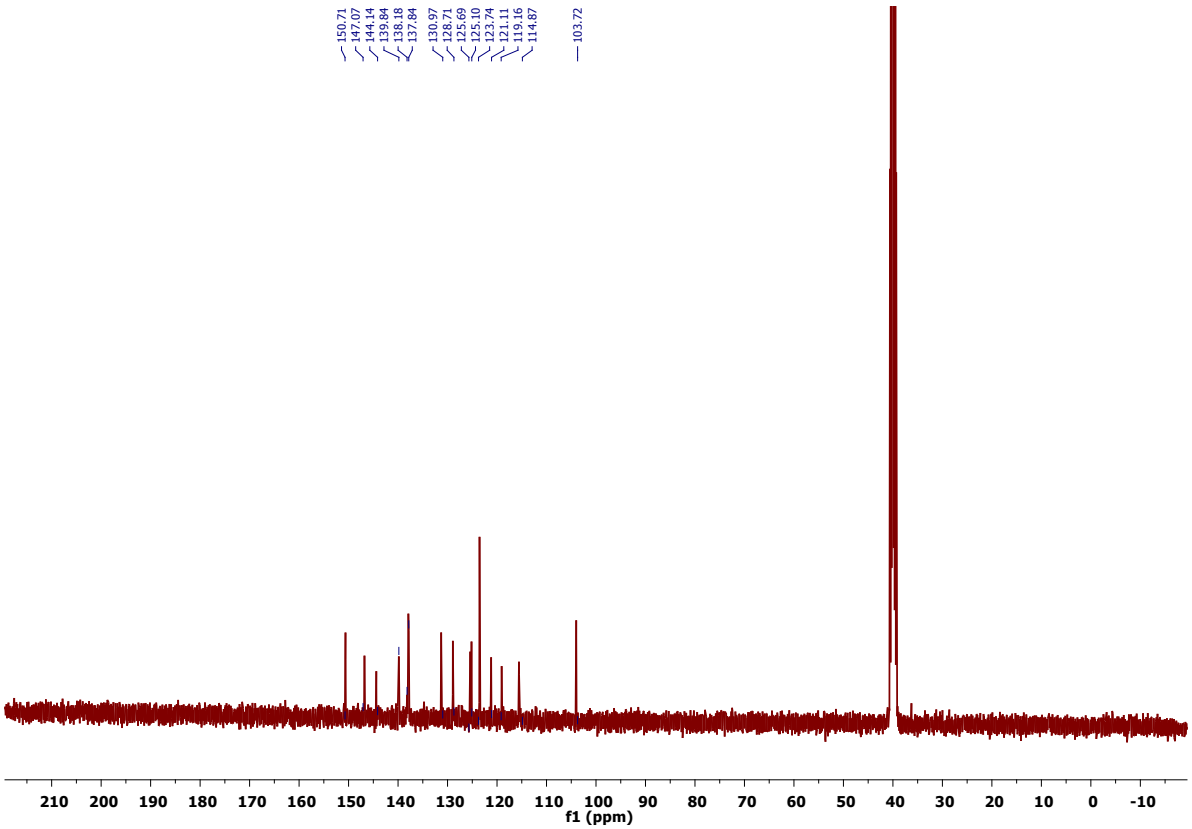

Fig. S2. ^{13}C NMR spectrum of the receptor **N1.**

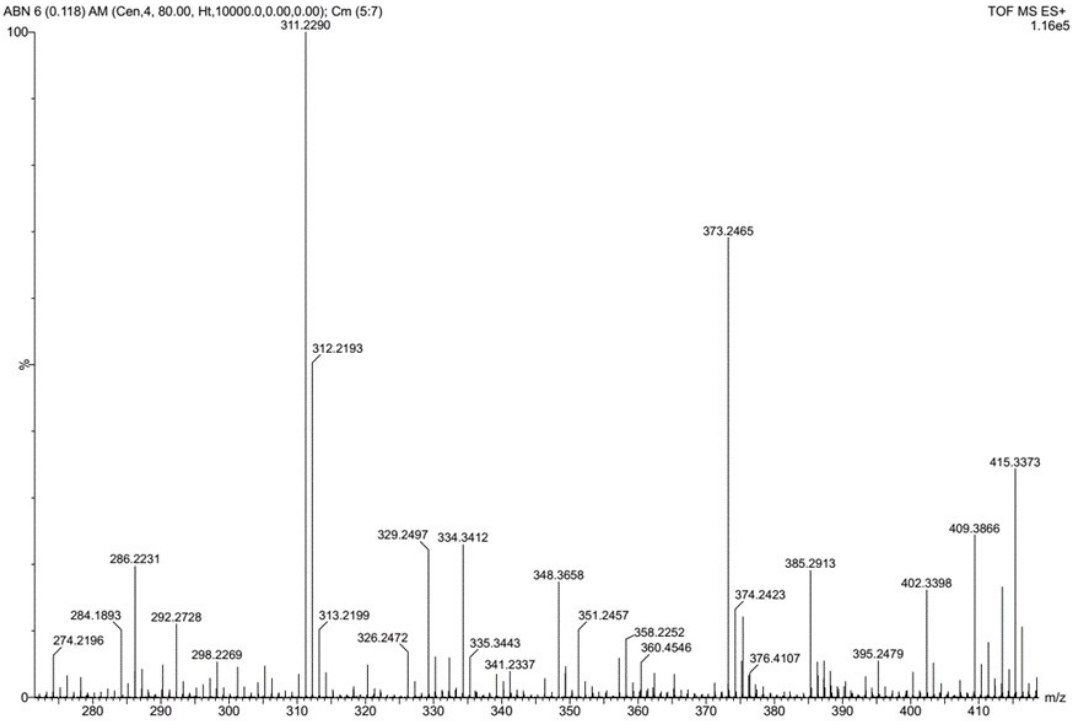

Fig. S3. HRMS spectrum of the receptor **N1.**

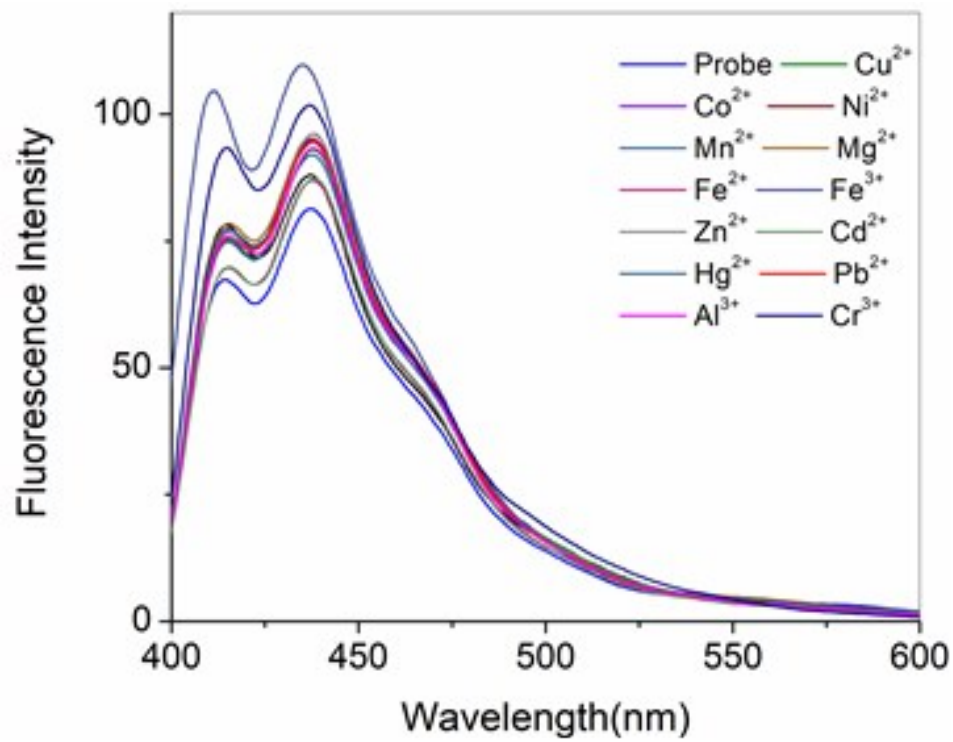

Fig. S4. Fluorescence spectral changes of **N1** (50 μL, 2.5×10^{-5} M) in CH_3OH:H_2O (1:1, v/v) upon addition of different metal ions (50 μL, 1×10^{-3} M, H_2O).

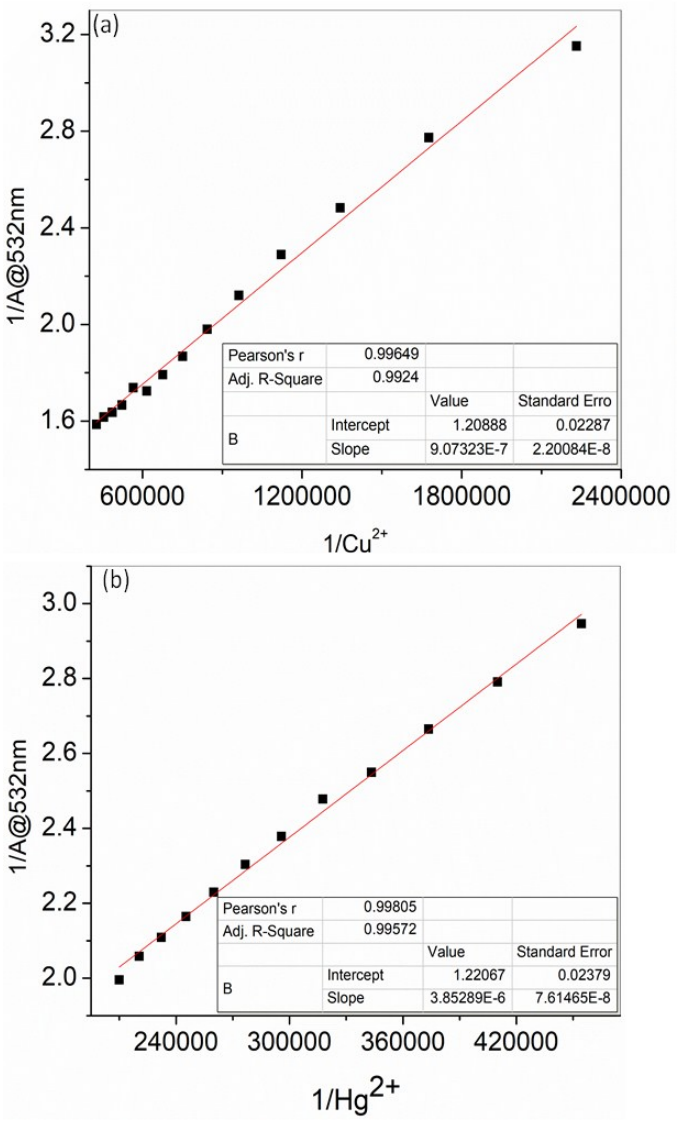

Fig. S5. (a) The B-H plot of fluorescence curve of **N1** in the presence of Cu^{2+} ion. (b) B-H plot of fluorescence data of **N1** in the presence of Hg^{2+} ion.

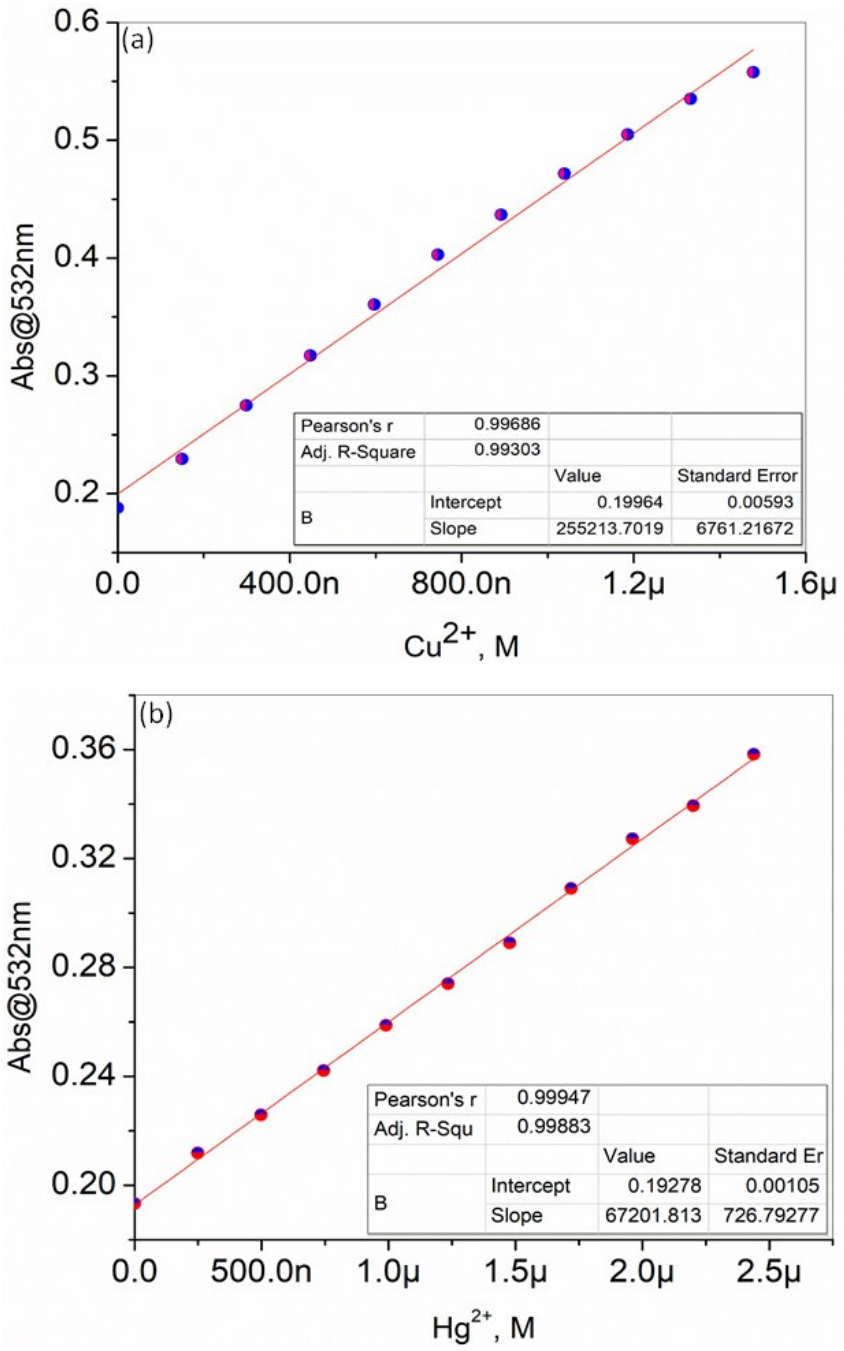

Fig. S6. (a) Calibration curve to estimate the LOD of **N1** for Cu^{2+} and Hg^{2+} (b) in aqueous methanol medium.

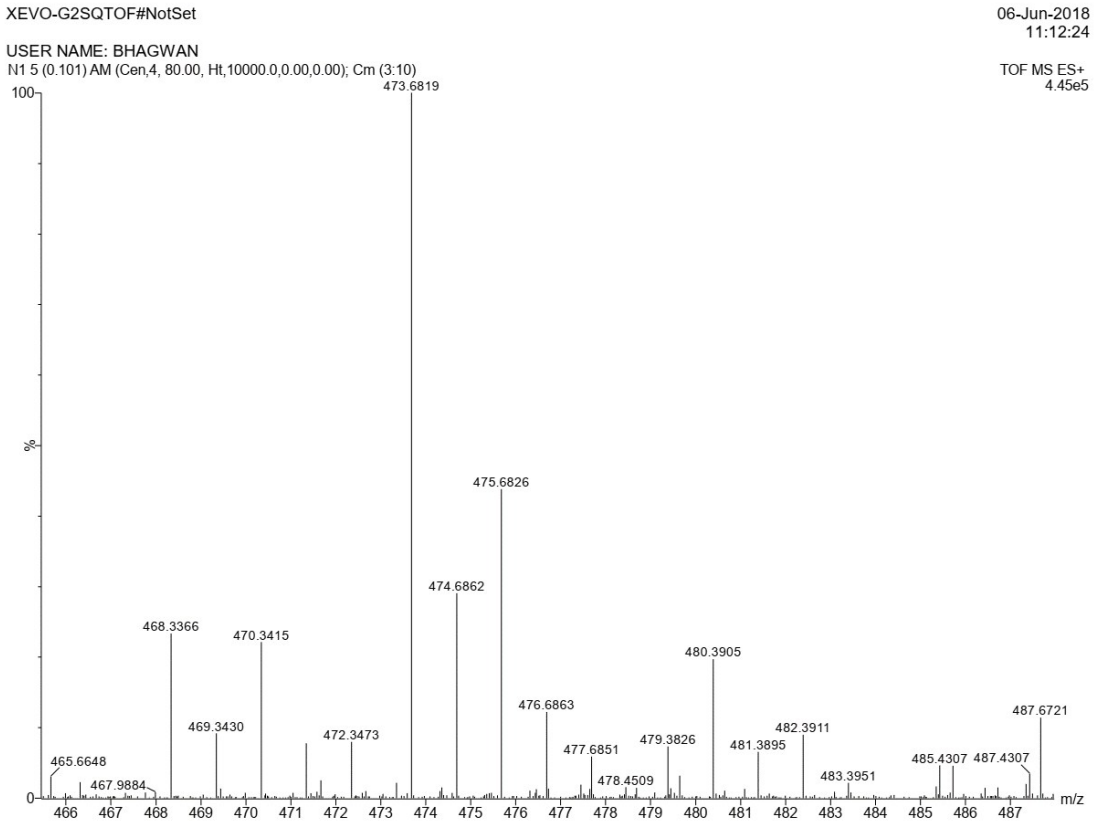

Fig. S7. HRMS spectrum of receptor **N1** with Cu^{2+} ion.

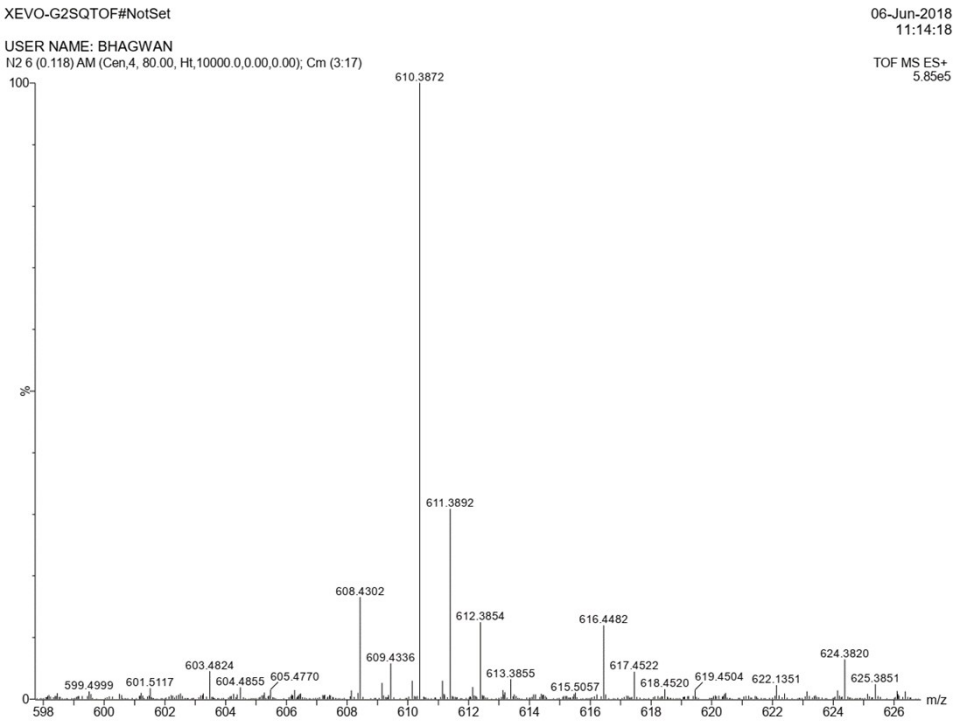

Fig. S8. HRMS Spectrum of receptor **N1** with Hg^{2+} ion.

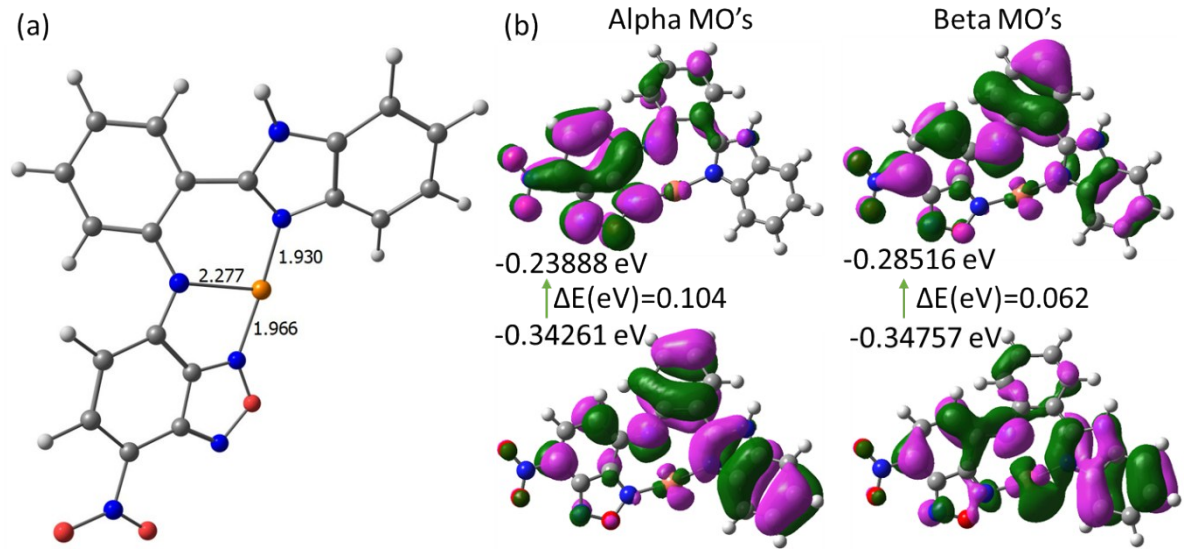

Fig. S9. DFT computed 3D structure of the **N1**-Cu^{2+} complex and it's HOMO's and LUMO's diagrams along with the two band gaps for alpha and beta MO's. In open-shell system with unpaired electron, the band gap is also calculated from the highest singly occupied MO (SOMO) to the next LUMO, which is estimated as 0.05746 eV (ΔE = -0.28516 + 0.34262) for **N1**-Cu^{2+}.

Table S1. Comparison table of some reported works on Cu^{2+} and Hg^{2+} sensors with **N1.**

S.No	Compound	Selectivity	Response	Sensitivity (M)	Mechanism	Reference
1	Naphthalic anhydride-Morpholine conjugate	Hg^{2+} Cu^{2+}	Turn-on Turn-off	6.11×10^{-8}	PET Paramagnetic effect	1
2	Bodipy derivative	Hg^{2+} Cu^{2+} Pb^{2+}	Colorimetric fluorescence	0.07×10^{-6} 0.27×10^{-6} 0.14×10^{-6}	ICT	2
3	Rhodamine 6g hydrazone	Hg^{2+} Cu^{2+}	Colorimetric fluorescence	2.96×10^{-6} 6.88×10^{-6}	CHEF Hydrolysis	3
4	Phenothiazine conjugate	Hg^{2+} Cu^{2+}	Colorimetric And turn off	80×10^{-9} 97×10^{-9}	Chemodosimeter Paramagnetic effect	4
5	Benzothiazole system	Hg^{2+} Cu^{2+}	Fluorescence	7.6×10^{-9} 2.4×10^{-9}	Chemodosimeter ESIPT and Paramagntic effect	5
6	Ferrocenyl derivative	Hg^{2+} Cu^{2+}	Colorimetric Fluorescence	7.19×10^{-7} 6.77×10^{-7}	PET	6
8	Pyrimidin-4yl-phenothiazine derivative	Hg^{2+} Cu^{2+}	Colorimetric Fluorescence	9.06×10^{-7} 3.78×10^{-7}	Chemodosimeter	7
10	Triphenylamine derivative	Hg^{2+} Cu^{2+}	Colorimetric Fluorescence	2.3×10^{-6} ---	Energy transfer Cyclisation	8
11	**NBD-aminophenyl benzimidazole**	**Hg^{2+} Cu^{2+}**	**Colorimetric**	**1.23×10^{-7} 4.70×10^{-7}**	**ICT**	**Our work**

References:

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Table S2. UV-Vis spectrophotometric determination of spiked Cu^{2+} and Hg^{2+} ions concentration by using the receptor **N1**.

Water	**[Cu^{2+}], M added**	**[Cu^{2+}], M found**	**Recovery %**
Tap Water	1.48×10^{-6}	1.43×10^{-6}	96.88
	1.91×10^{-6}	1.95×10^{-6}	102
	2.34×10^{-6}	2.37×10^{-6}	101
River Water	1.48×10^{-6}	1.33×10^{-6}	90.16
	1.91×10^{-6}	1.78×10^{-6}	93.16
	2.34×10^{-6}	2.31×10^{-6}	98.63
Water	**[Hg^{2+}], M added**	**[Hg^{2+}], M found**	**Recovery %**
Tap Water	1.48×10^{-6}	1.60×10^{-6}	108
	1.96×10^{-6}	2.22×10^{-6}	113
	2.44×10^{-6}	2.61×10^{-6}	107
River Water	1.48×10^{-6}	1.34×10^{-6}	90.70
	1.96×10^{-6}	1.85×10^{-6}	94.70
	2.44×10^{-6}	2.38×10^{-6}	97.60

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