Electronic Supplementary Material (ESI) for RSC Advances.

Highly sensitive and selective "naked eye" sensing of Cu (II) by a novel amido-imine based receptor: a spectrophotometric and DFT study with practical application

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Table of contents:

1. Characterization of compound 1:

a) FTIR spectrum:

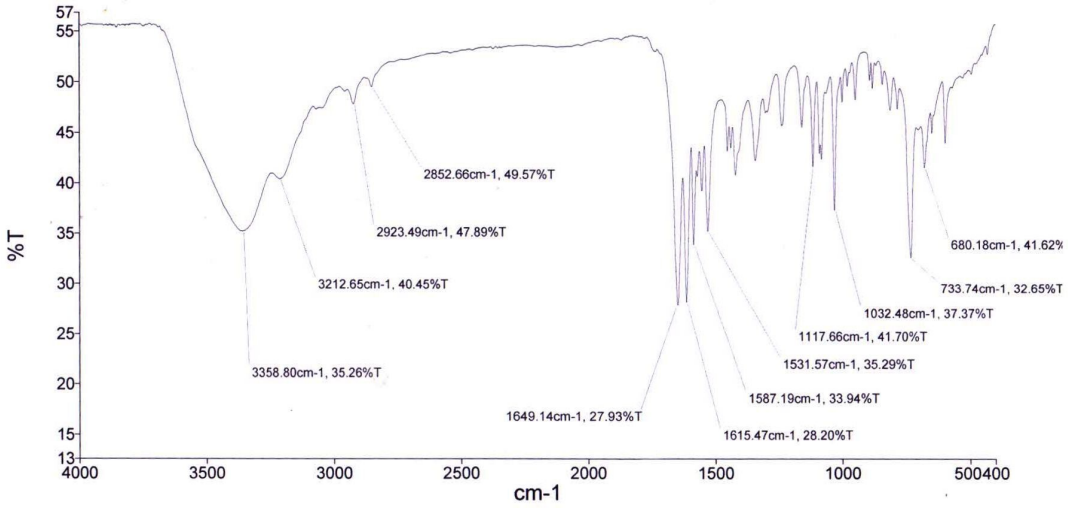

Fig S1: FTIR spectrum of 1

b) ^{1}H-NMR spectrum:

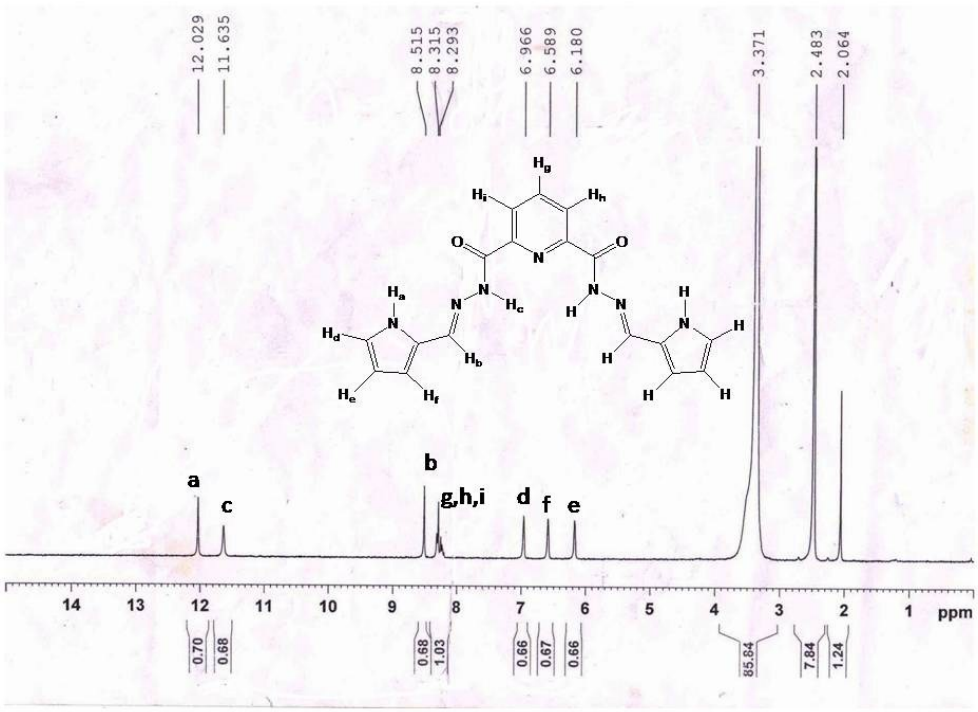

Fig S2: ^{1}H NMR of compound 1

c) ^{13}C NMR:

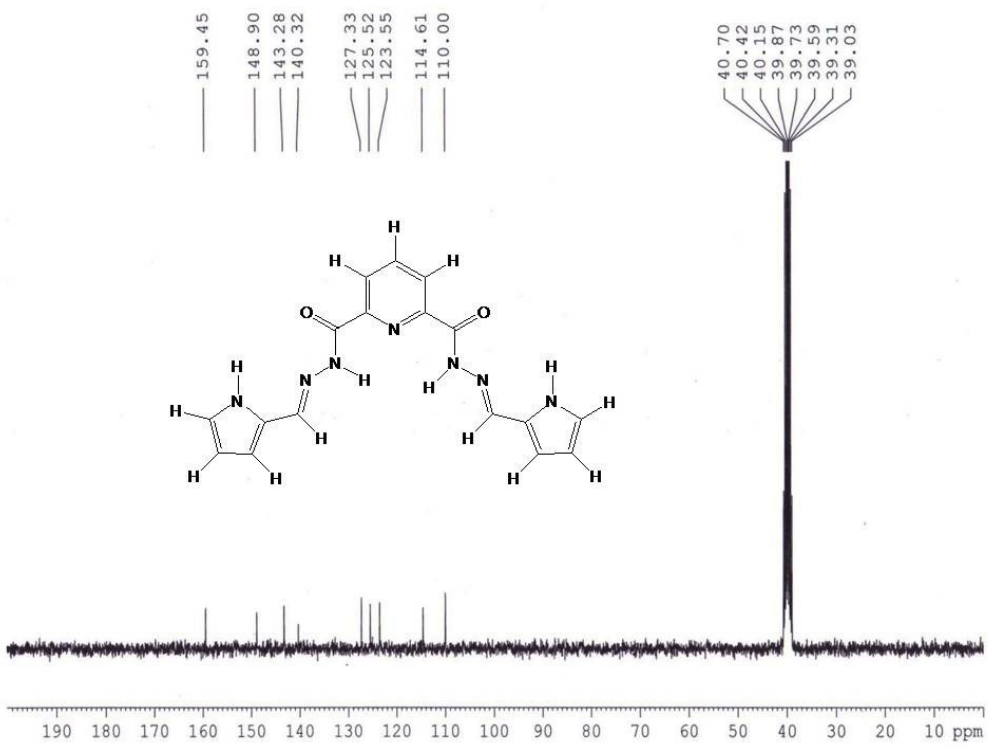

Fig S3: ^{13}C NMR of compound 1

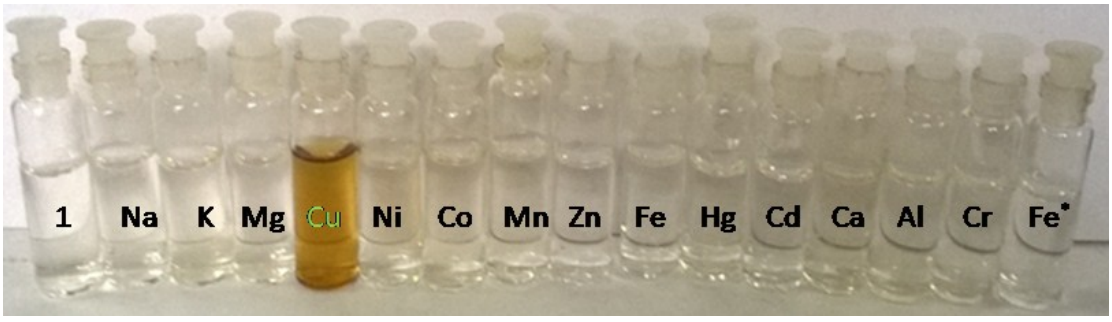

Fig S4: Change in color of receptor 1(far left) upon addition of 10 μM aqueous solution of various metals (Fe^{*} denotes Fe (III)).

2. UV-VIS Spectrum:

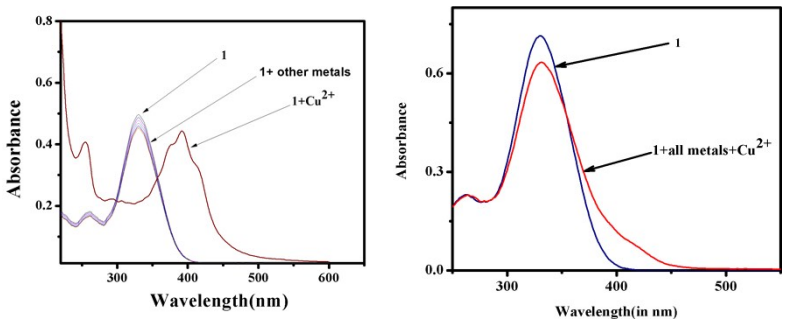

Fig S5a (left): Response of **1** to Cu^{2+} over other metals (Ni^{2+}, Co^{2+}, Mn^{2+}, Zn^{2+}, Fe^{2+}, Hg^{2+}, Cd^{2+} and Mg^{2+}). Fig S5b (right): Response of **1** to Cu^{2+}in a mixture of metals (Ni^{2+}, Co^{2+}, Mn^{2+}, Zn^{2+}, Fe^{2+}, Hg^{2+}, Cd^{2+} and Mg^{2+}) (2 equiv.).

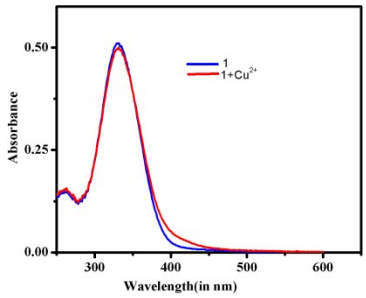

Fig S6: Response of 1 towards 2 µL of 10 µM aqueous solution of Cu^{2+}

3. Limit of detection (LOD):

Table of concentration and absorbance values:

Table-S1:

$[Cu^{2+}](4.0\times10^{-8}$ (M))	Absorbance at 392 nm
2	0.093
4	0.135
6	0.185
8	0.245
10	0.285
12	0.337
14	0.389
16	0.434
18	0.464
20	0.496
22	0.521

We have,

Standard deviation (S.D) of the blank solution = 5.471×10^{-4}

Slope of the calibration curve= 4.355×10^{5} M^{-1}

Thus, LOD= (3×S.D)/Slope = 3.989×10^{-9} M≈ 4.0×10^{-9} M

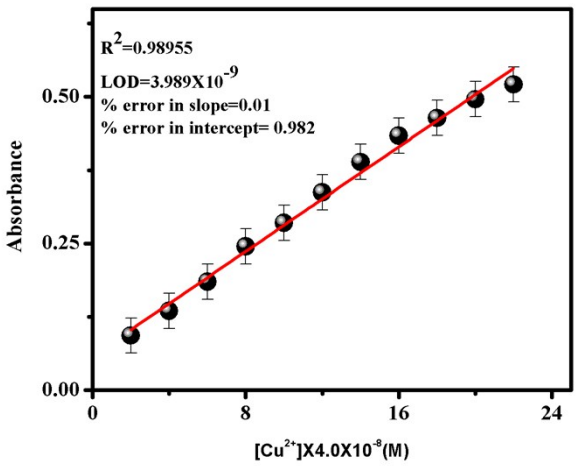

Fig S7: Plot of Absorbance vs. concentration of Cu (II) for calculating LOD

4. IR spectrum of Complex:

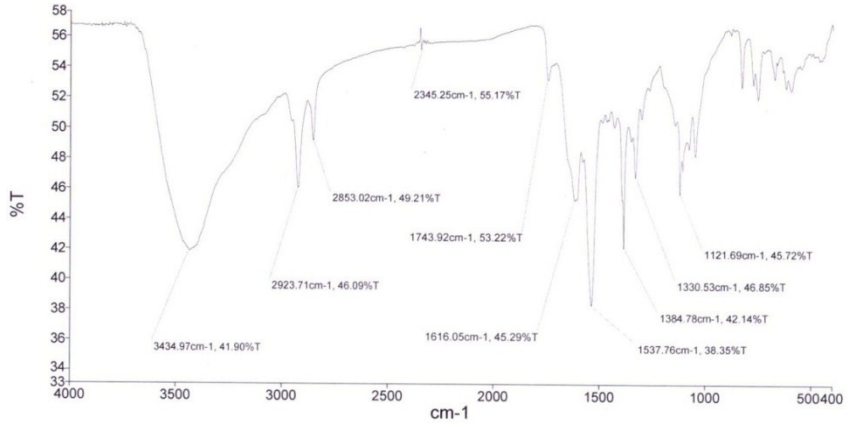

Fig S8: IR spectrum of complex of 1 with Cu^{2+}

5. Table for optimized structure parameters:

Following are tabulated the bond lengths (in Å) of the functional groups of 1 as well as its complex for showing the effect of complexation on bond length as obtained from DFT (B3LYP/6-311++g**) optimized structures of 1 and its Cu(II) complex.

Table-S2:

Species	**C=O(in Å)**	**C-N(in Å)**	**N-H(in Å) (amide)**	**N-N(in Å)**	**C=N (in Å) (imine)**	**N-H(in Å) (pyrrole)**
1	1.21451	1.37049	1.01614	1.35739	1.28503	1.00865
1+Cu^{2+}	1.25407	1.36583	––	1.36429	1.31169	––