

Supporting Information

Synthesis and Characterization of Monometallic Rhenium(I) Complexes and their Application as Selective Sensor for Copper(II) ion

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Fig. S27 Relative emission intensity changes of Re(I) complex **1** with different metal ions.

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Fig. S32 Emission spectral changes observed with complex **3** (15 μM) with increasing concentration of Cu^{2+} ion in CH_3CN medium. $[\text{Cu}^{2+}] = (0\text{-}200 \mu\text{M})$.

Fig. S33 Emission spectral changes observed with complex **4** (15 μM) with increasing concentration of Cu^{2+} ion in CH_3CN medium. $[\text{Cu}^{2+}] = (0\text{-}200 \mu\text{M})$.

Fig. S34 Modified Benesi-Hildebrand plot for the emission enhancement of complex **1** in the presence of various concentrations of Cu^{2+} ions.

Fig. S35 Job's plot for the titration of complex **1** with Cu^{2+} ion.

Fig. S36 Calibration curve of complex **4** for Cu^{2+} . Insert: linear part of the calibration curve.

Fig. S37 Time resolved luminescence decay of complex **1** (15 μM) in the presence of Cu^{2+} ion (0 and 200 μM).

Fig. S38 Time resolved luminescence decay of complex **2** (15 μM) in the presence of Cu^{2+} ion (0 and 200 μM).

Fig. S39 Time resolved luminescence decay of complex **3** (15 μM) in the presence of Cu^{2+} ion (0 and 200 μM).

Fig. S40 Time resolved luminescence decay of complex **4** (15 μM) in the presence of Cu^{2+} ion (0 and 200 μM).

Table S1 The absorption spectral data of ligands **L1-L4** in CH₃CN–DMSO (99:1) medium.

Ligands	λ_{abs} , nm (λ_{max} , 10 ⁴ , dm ³ mol ⁻¹ cm ⁻¹)
L1	195 (11.3), 219 (3.2), 363 (1.6)
L2	195 (11.1), 222 (2.4), 376 (1.0)
L3	195 (11.0), 220 (2.9), 374 (1.2)
L4	195 (11.3), 224 (3.1), 369 (1.0)

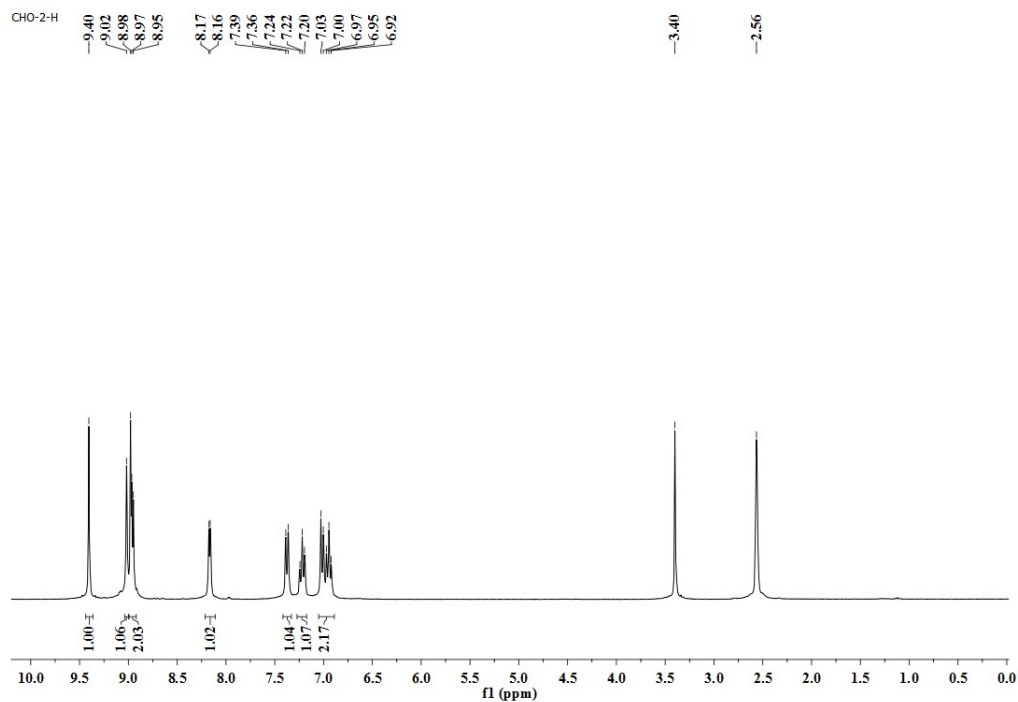


Fig. S1 ¹H NMR spectrum of ligand **L1**.

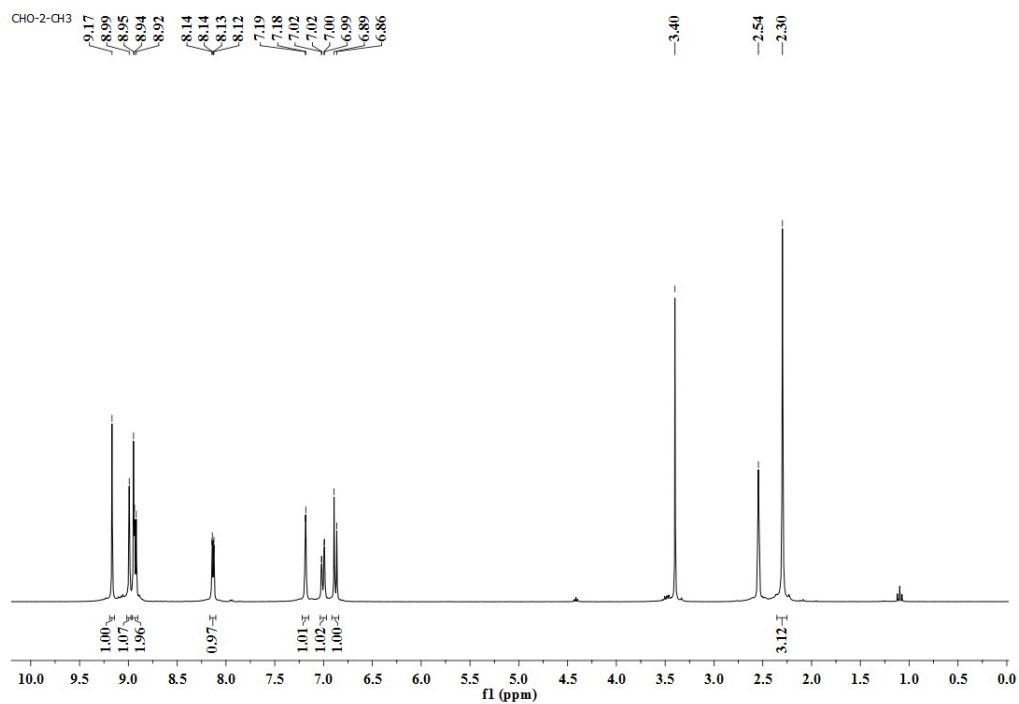


Fig. S2 ^1H NMR spectrum of ligand **L2**.

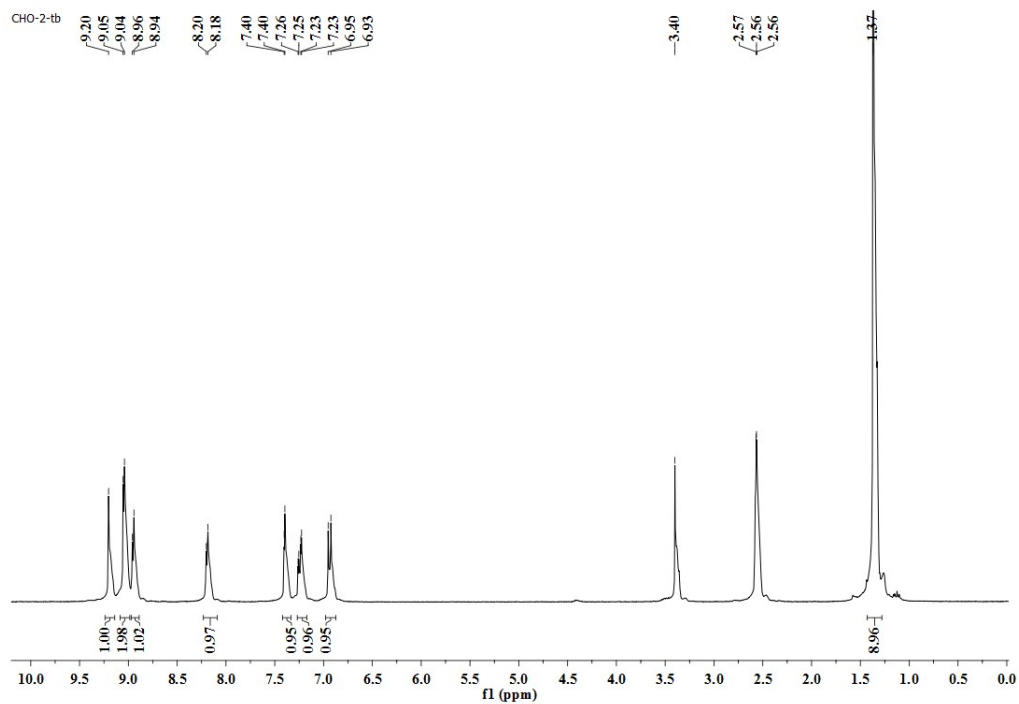


Fig. S3 ^1H NMR spectrum of ligand **L3**.

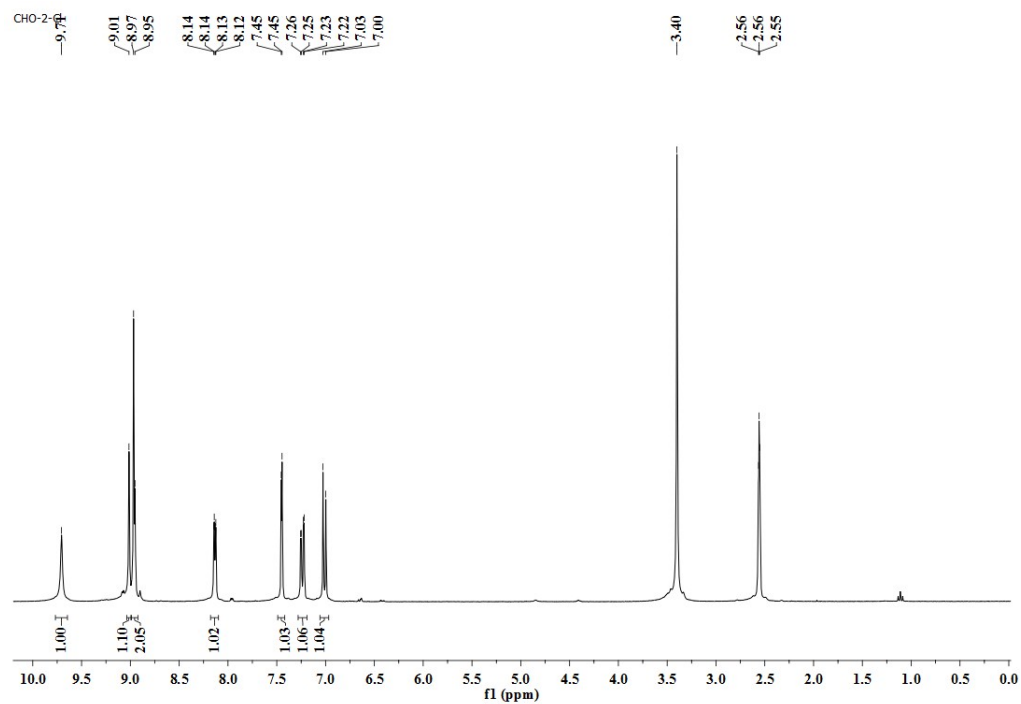


Fig. S4 ^1H NMR spectrum of ligand **L4**.

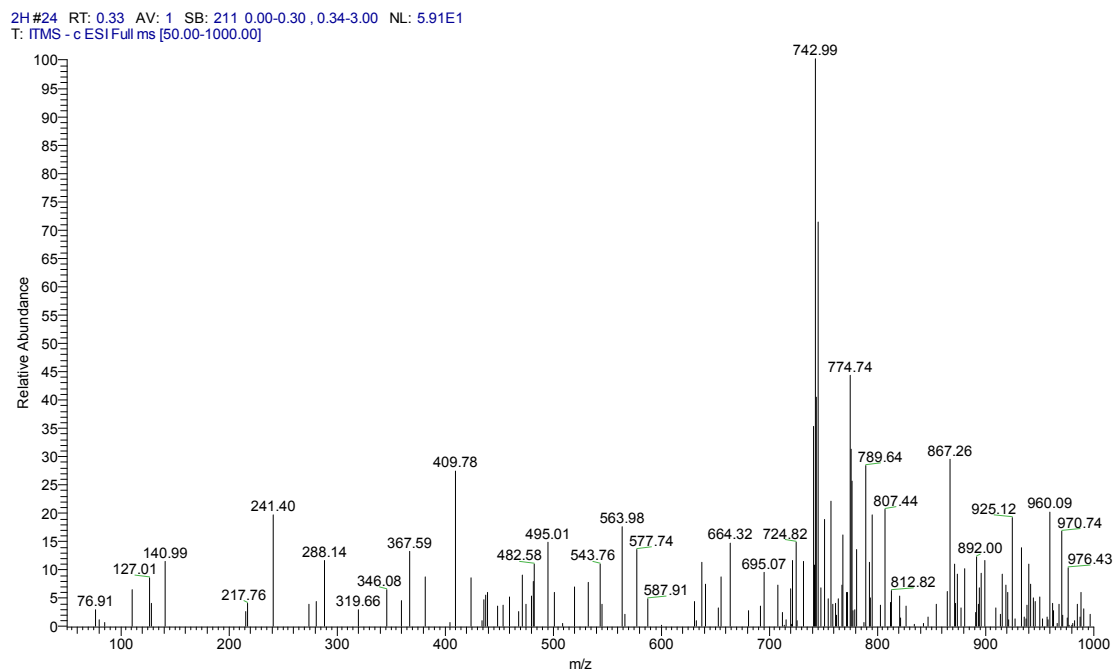


Fig. S5 ESI-MS spectrum of complex **1**.

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T: ITMS - c ESI Full ms [50.00-1000.00]

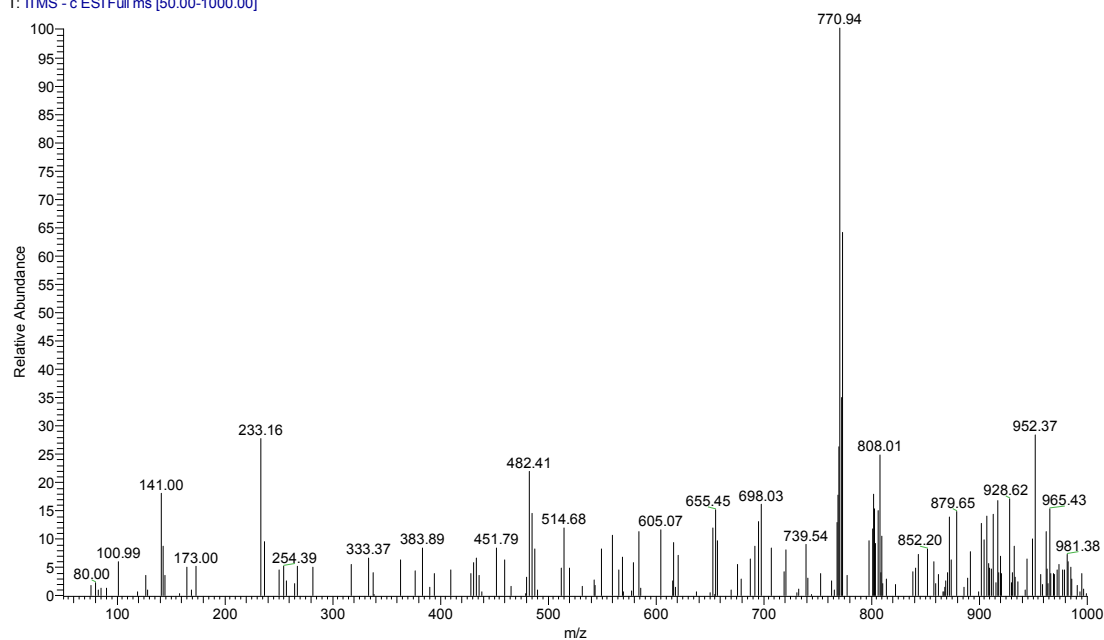


Fig. S6 ESI-MS spectrum of complex **2**.

2TB #58 RT: 0.81 AV: 1 SB: 206 0.02-0.59 , 0.65-2.94 NL: 8.47E1
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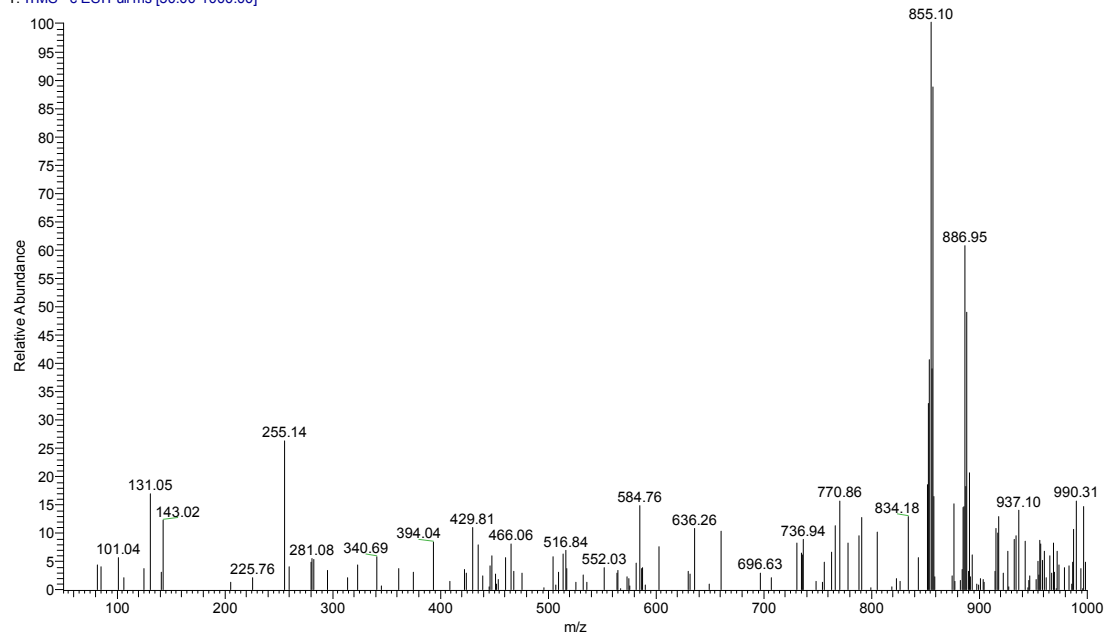


Fig. S7 ESI-MS spectrum of complex **3**.

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T: ITMS -c ESI Full ms [50.00-1000.00]

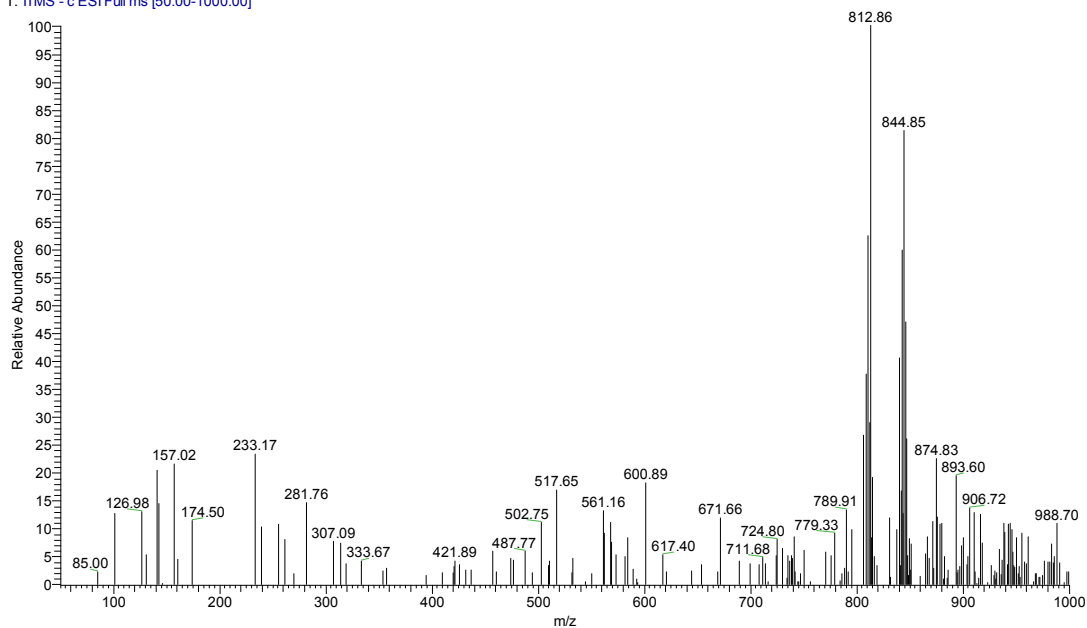


Fig. S8 ESI-MS spectrum of complex **4**.

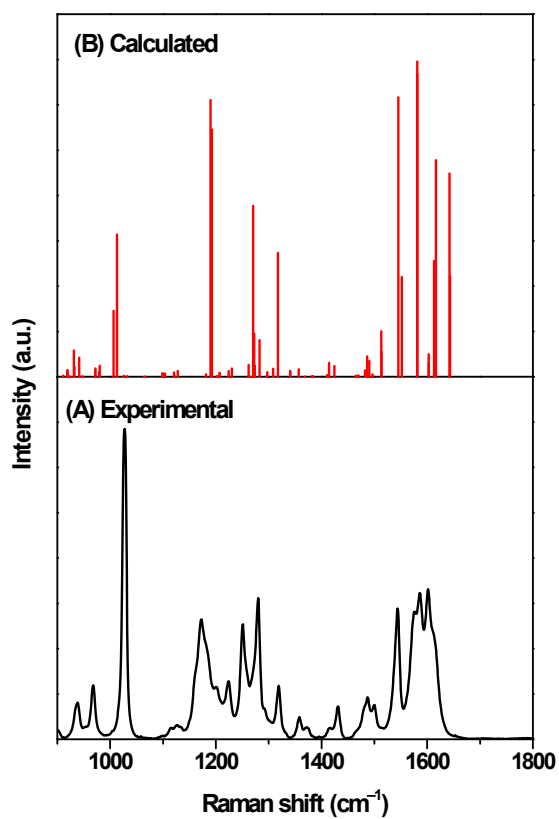


Fig. S9 (A) Experimental Raman spectrum of complex **3** in solid state and (B) calculated spectrum.

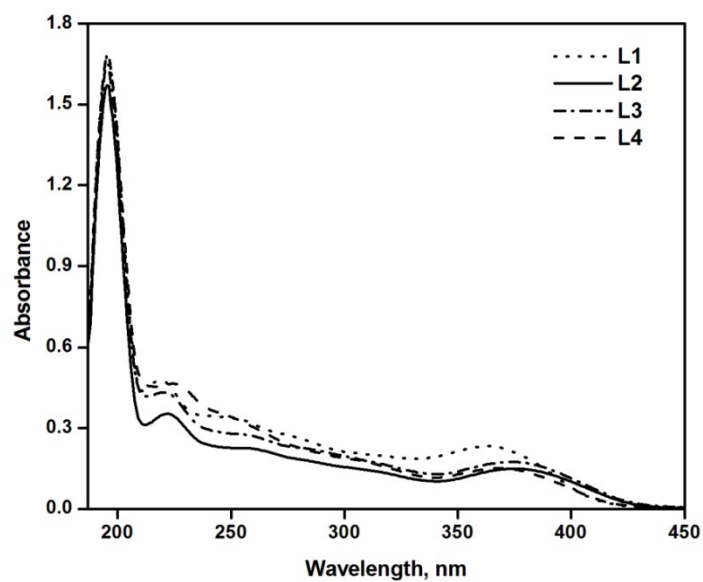


Fig. S10 Absorption spectra of ligands **L1-L4** (20 μ M) in CH_3CN -DMSO (99:1) medium.

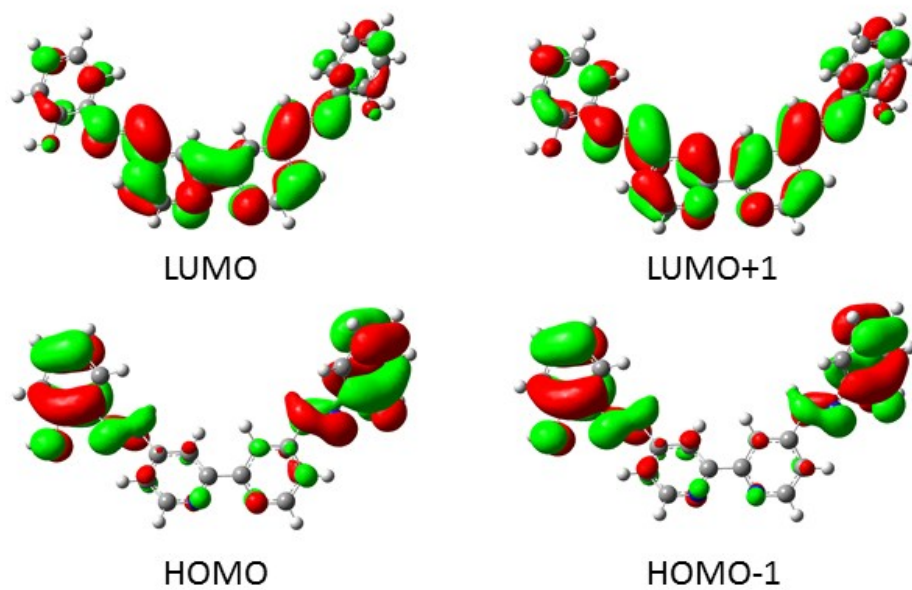


Fig. S11 MO pictures of HOMO-1, HOMO, LUMO and LUMO+1 of **L1**.

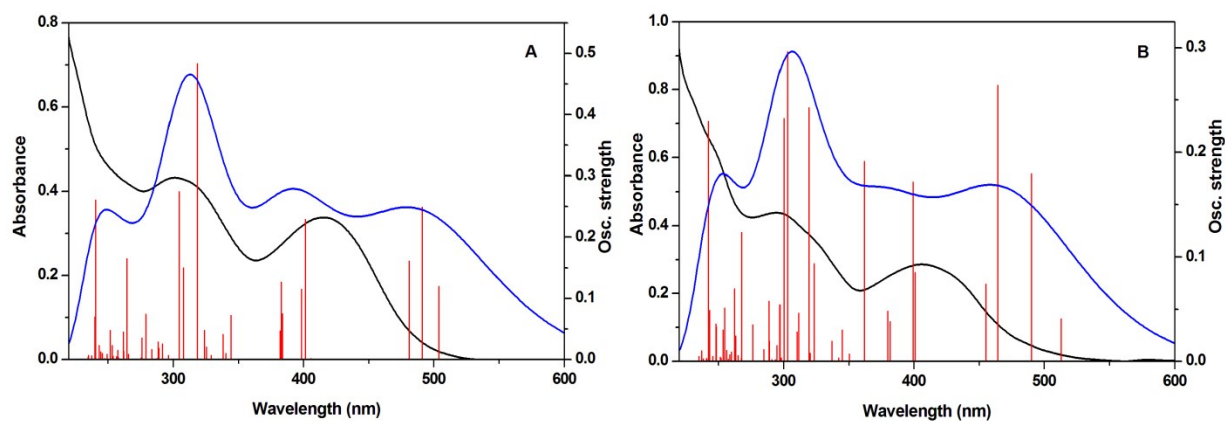


Fig. S12 Experimental (CH_3CN , black) and calculated (blue) UV-Vis absorption spectra of (A) complex **3** (15 μM) and (B) complex **4** (15 μM). The oscillator strength is represented by red lines.

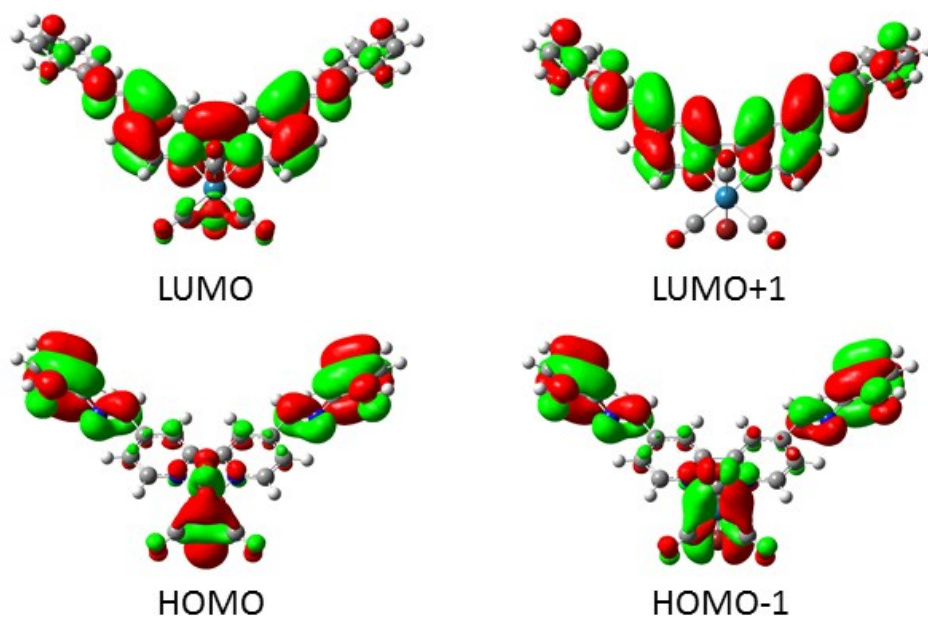


Fig. S13 MO pictures of HOMO-1, HOMO, LUMO and LUMO+1 of complex **1**.

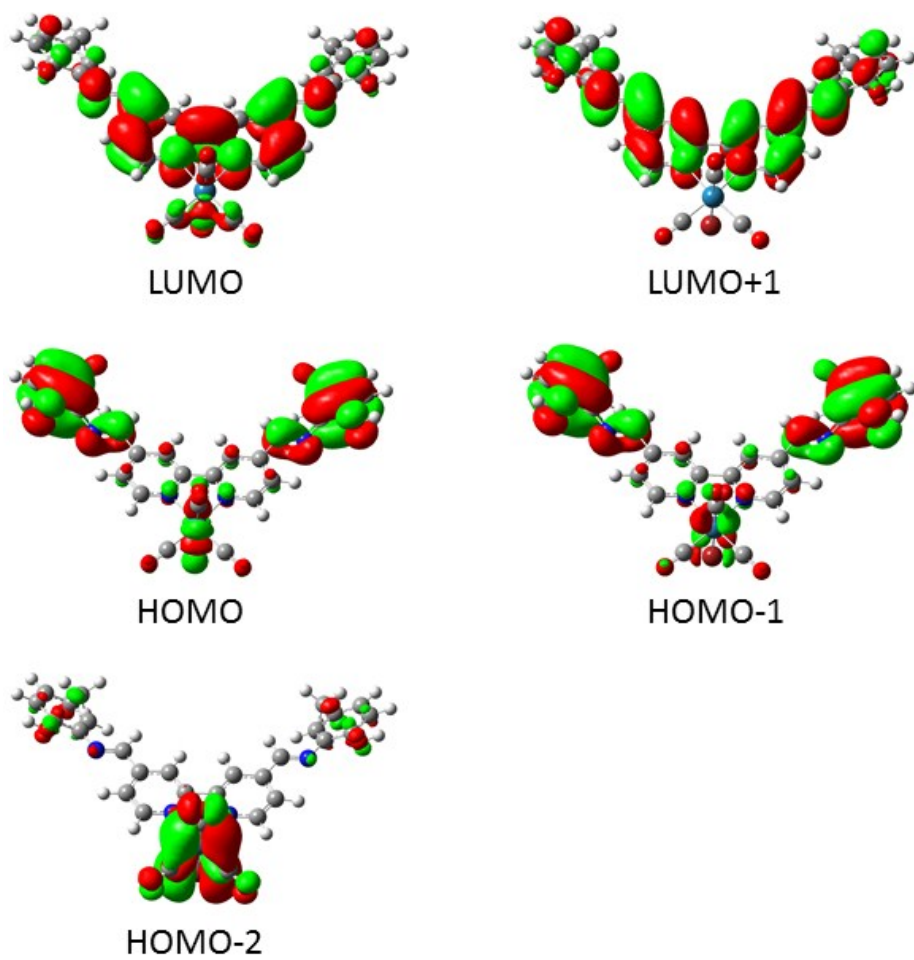


Fig. S14 MO pictures of HOMO-2, HOMO-1, HOMO, LUMO and LUMO+1 of complex **2**.

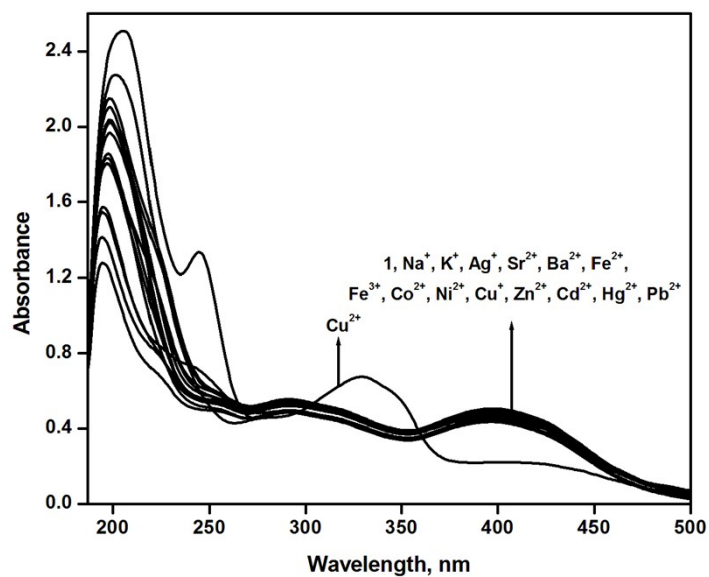


Fig. S15 Absorption spectral changes observed with complex 1 (15 μM) on the addition of different metal ions (50 μM) in CH_3CN medium.

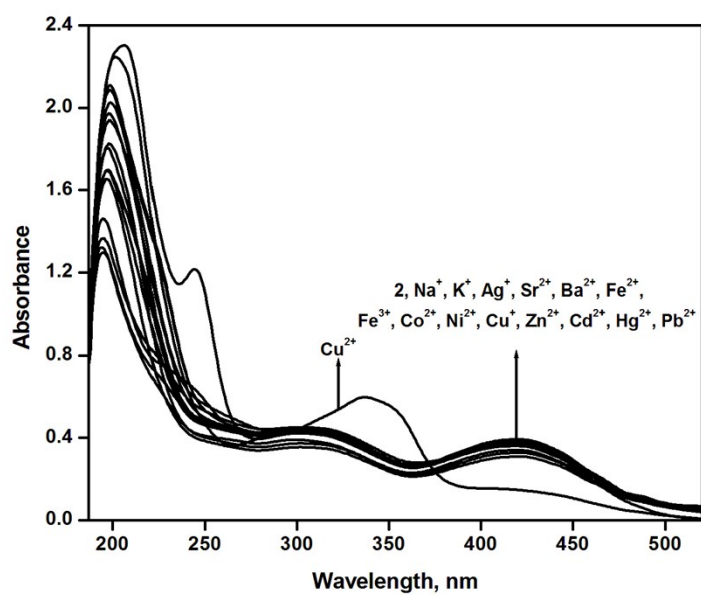


Fig. S16 Absorption spectral changes observed with complex 2 (15 μM) on the addition of different metal ions (50 μM) in CH_3CN medium.

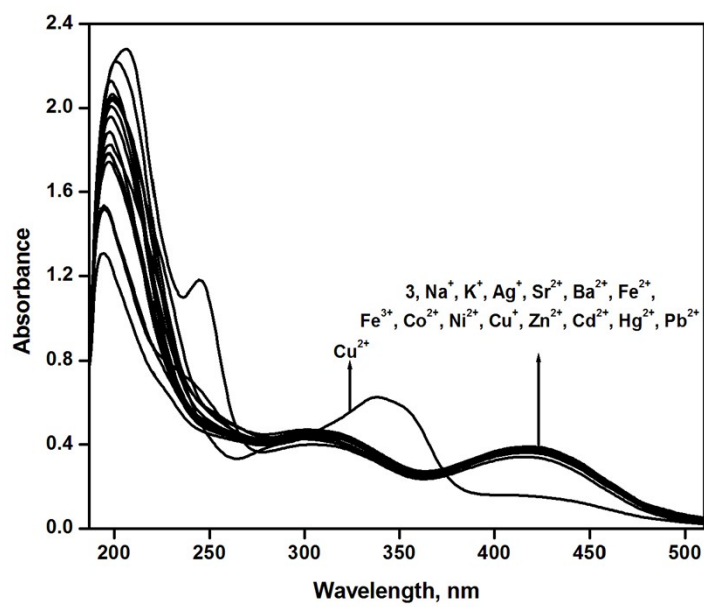


Fig. S17 Absorption spectral changes observed with complex **3** (15 μM) on the addition of different metal ions (50 μM) in CH_3CN medium.

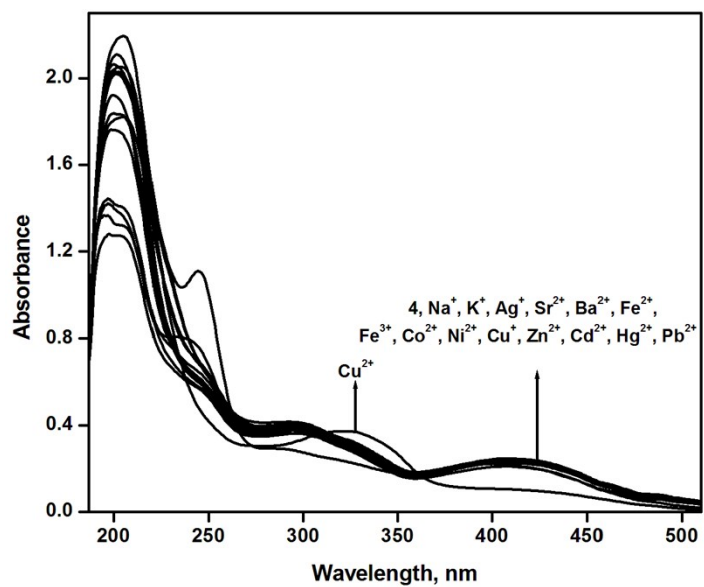


Fig. S18 Absorption spectral changes observed with complex **4** (15 μM) on the addition of different metal ions (50 μM) in CH_3CN medium.

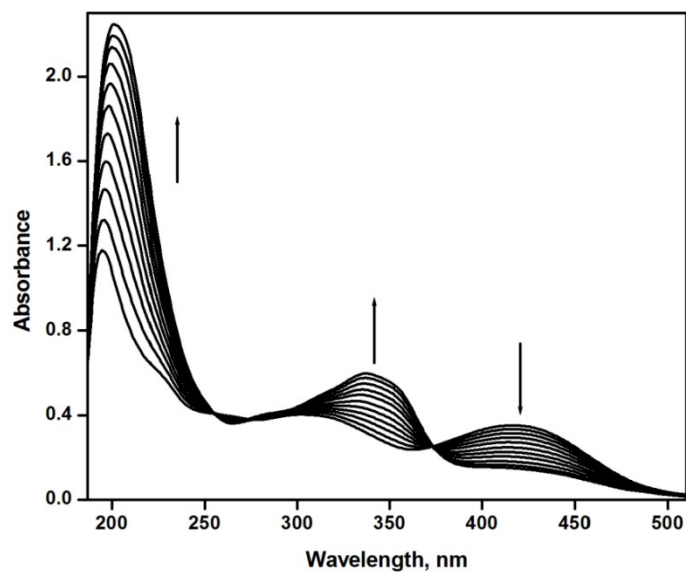


Fig. S19 Absorption spectral changes observed with complex **2** (15 μM) with increasing concentration of Cu²⁺ ion in CH₃CN medium. [Cu²⁺] = (0-50 μM).

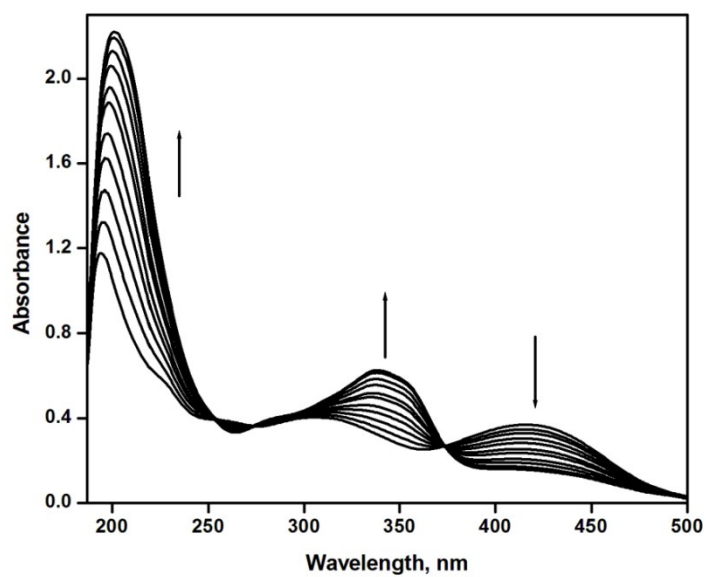


Fig. S20 Absorption spectral changes observed with complex **3** (15 μM) with increasing concentration of Cu²⁺ ion in CH₃CN medium. [Cu²⁺] = (0-50 μM).

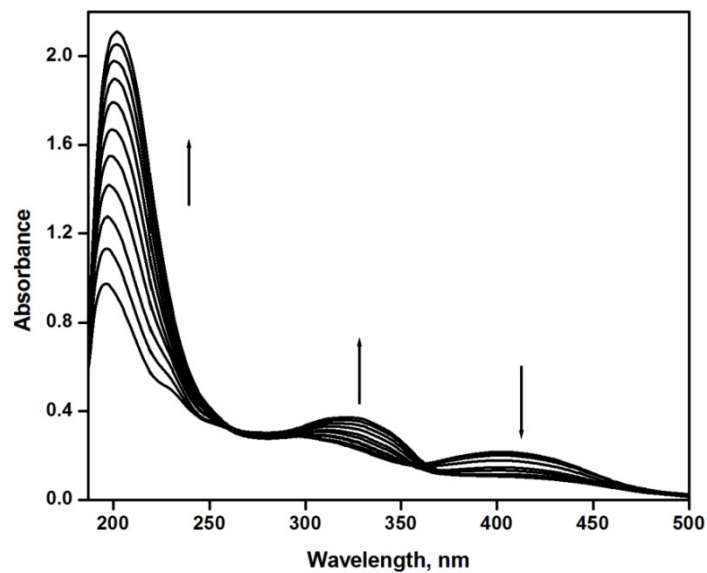


Fig. S21 Absorption spectral changes observed with complex **4** (15 μM) with increasing concentration of Cu²⁺ ion in CH₃CN medium. [Cu²⁺] = (0-50 μM).

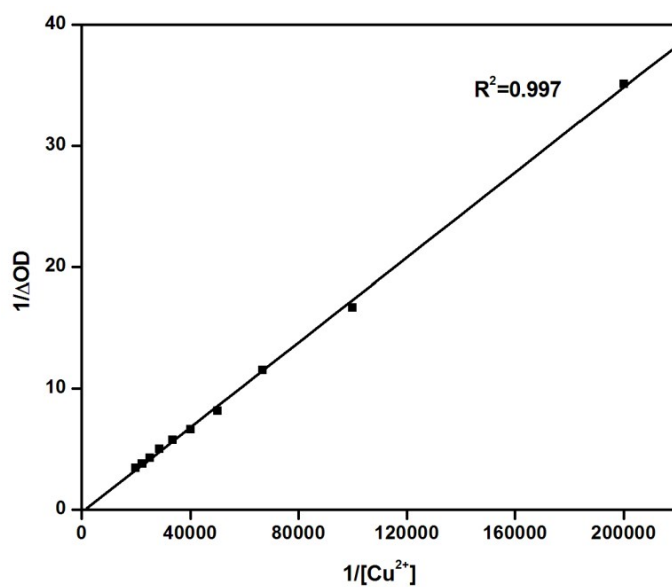


Fig. S22 Benesi-Hildebrand plot for the absorbance change of complex **1** in the presence of various concentration of Cu²⁺ ion.

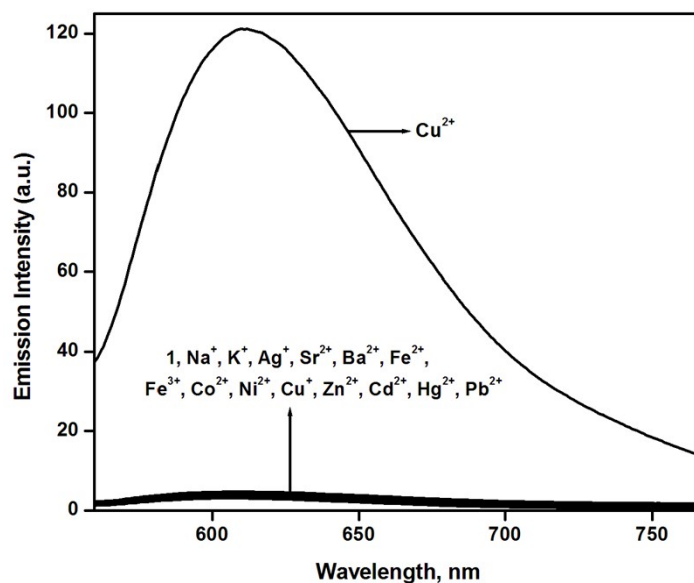


Fig. S23 Emission spectral changes observed with complex **1** (15 μM) on the addition of different metal ions (200 μM) in CH_3CN medium.

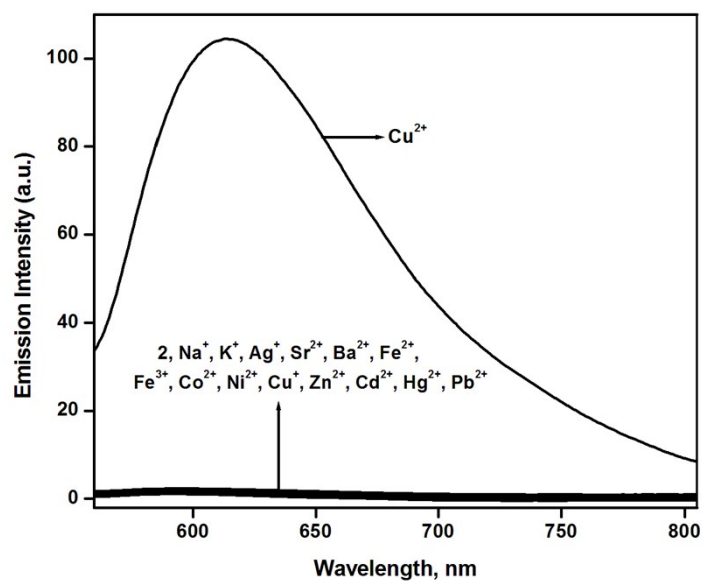


Fig. S24 Emission spectral changes observed with complex **2** (15 μM) on the addition of different metal ions (200 μM) in CH_3CN medium.

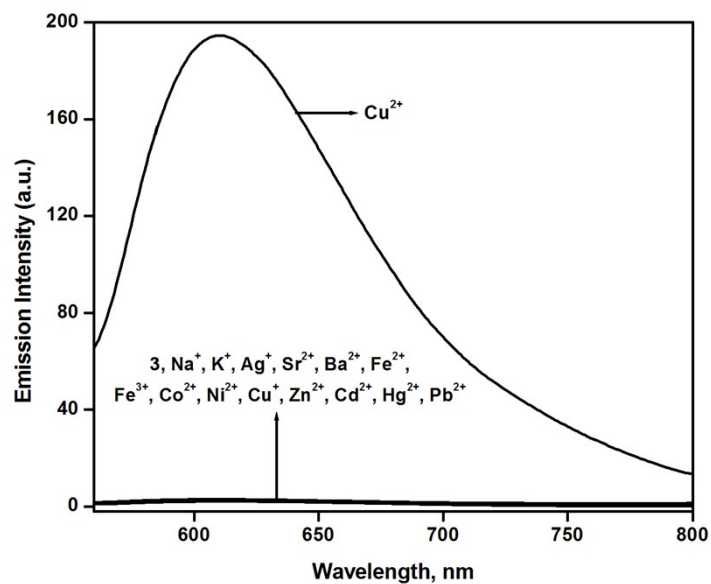


Fig. S25 Emission spectral changes observed with complex **3** (15 μM) on the addition of different metal ions (200 μM) in CH_3CN medium.

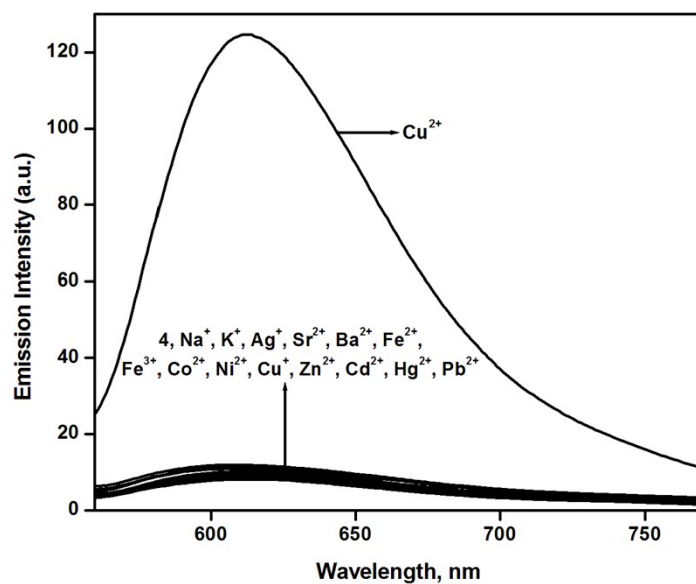


Fig. S26 Emission spectral changes observed with complex **4** (15 μM) on the addition of different metal ions (200 μM) in CH_3CN medium.

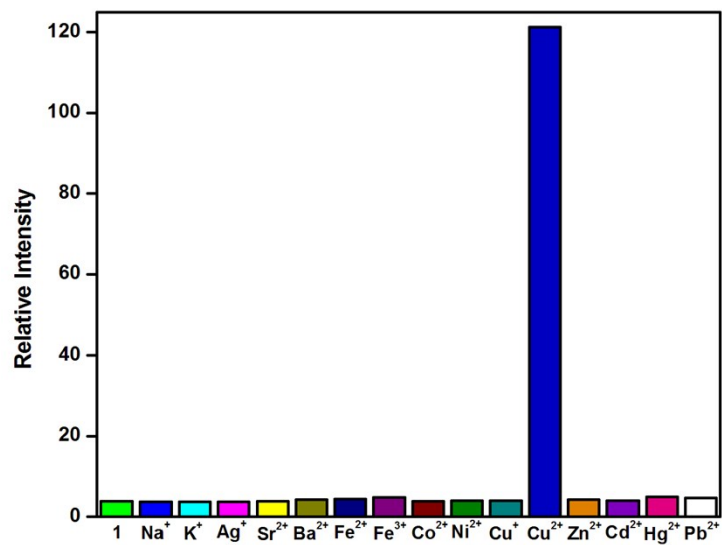


Fig. S27 Relative emission intensity changes of Re(I) complex **1** with different metal ions.

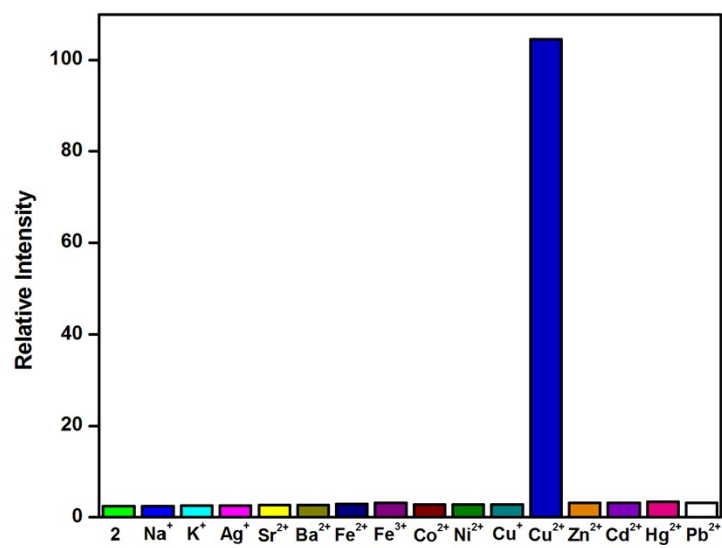


Fig. S28 Relative emission intensity changes of Re(I) complex **2** with different metal ions.

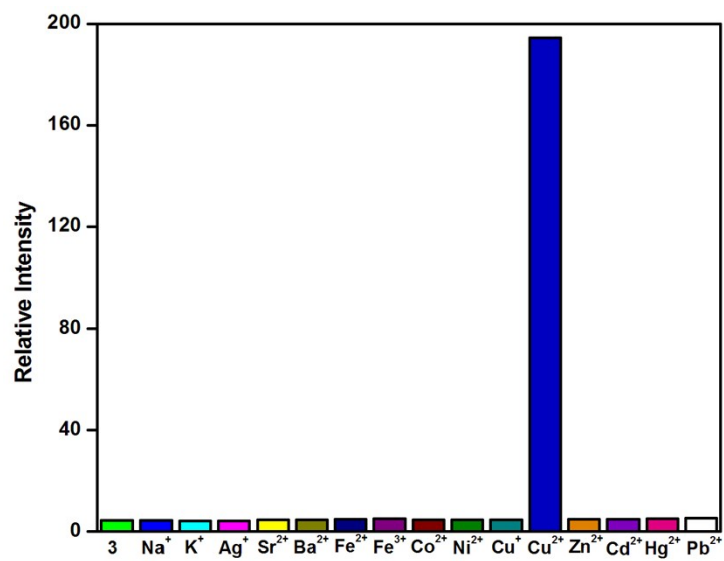


Fig. S29 Relative emission intensity changes of Re(I) complex **3** with different metal ions.

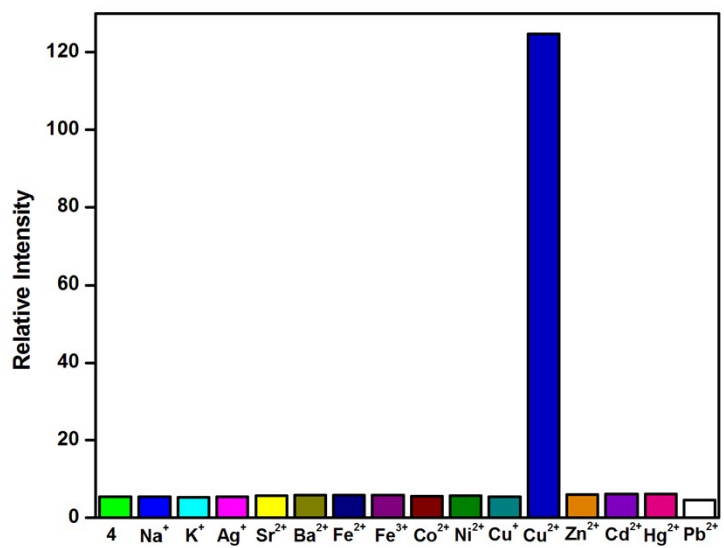


Fig. S30 Relative emission intensity changes of Re(I) complex **4** with different metal ions.

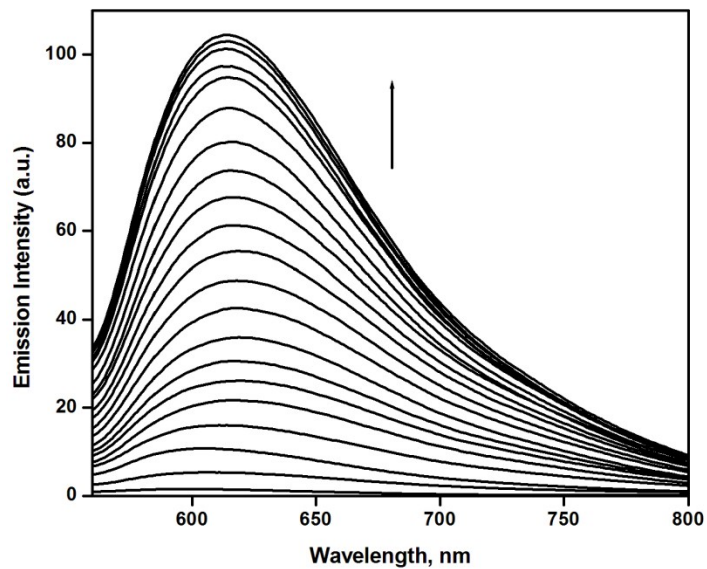


Fig. S31 Emission spectral changes observed with complex **2** (15 μM) with increasing concentration of Cu²⁺ ion in CH₃CN medium. [Cu²⁺] = (0-200 μM).

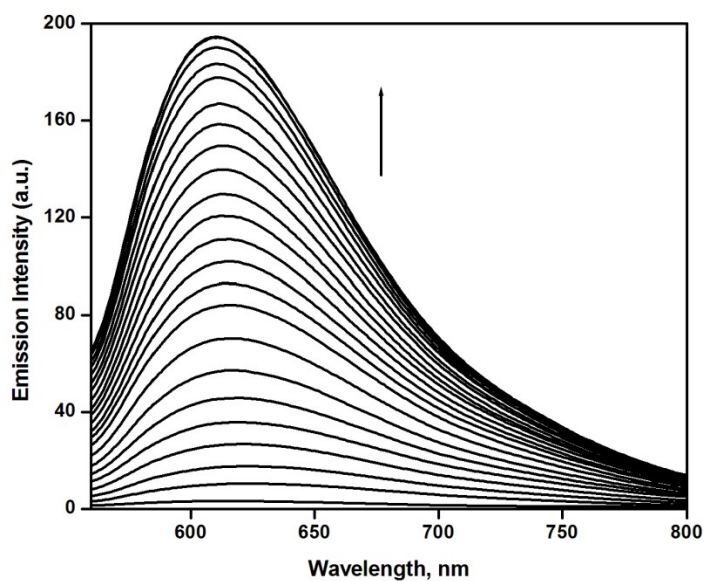


Fig. S32 Emission spectral changes observed with complex **3** (15 μM) with increasing concentration of Cu²⁺ ion in CH₃CN medium. [Cu²⁺] = (0-200 μM).

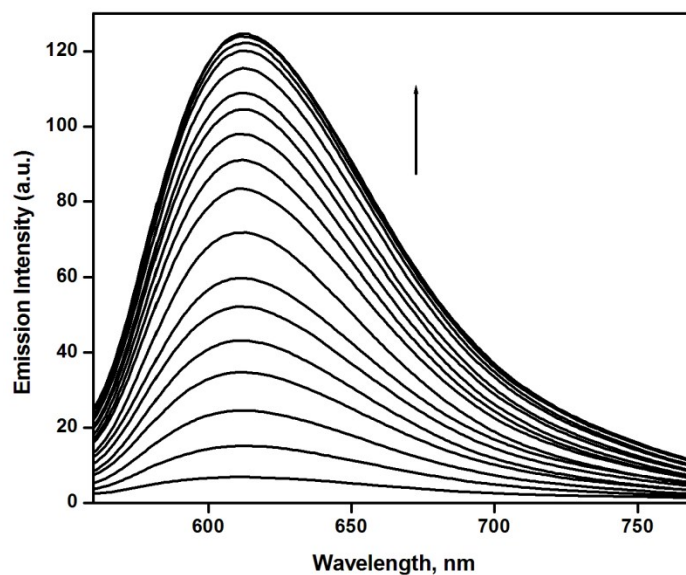


Fig. S33 Emission spectral changes observed with complex **4** (15 μM) with increasing concentration of Cu^{2+} ion in CH_3CN medium. $[\text{Cu}^{2+}] = (0\text{-}200 \mu\text{M})$.

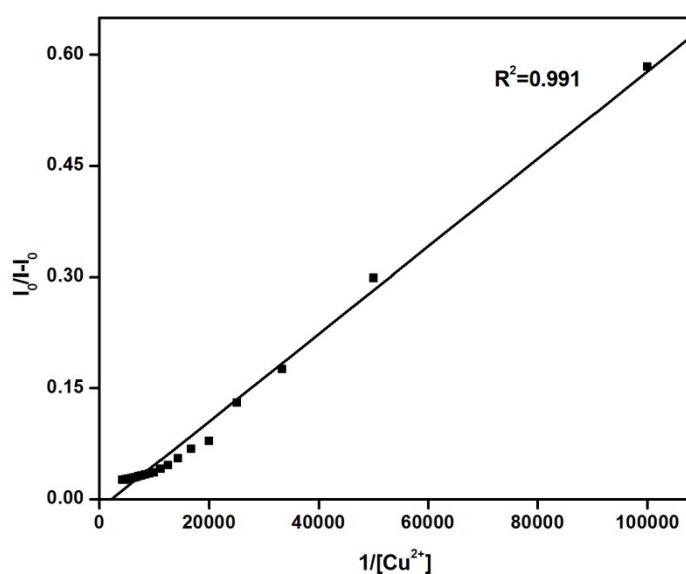


Fig. S34 Modified Benesi-Hildebrand plot for the emission enhancement of complex **1** in the presence of various concentrations of Cu^{2+} ions.

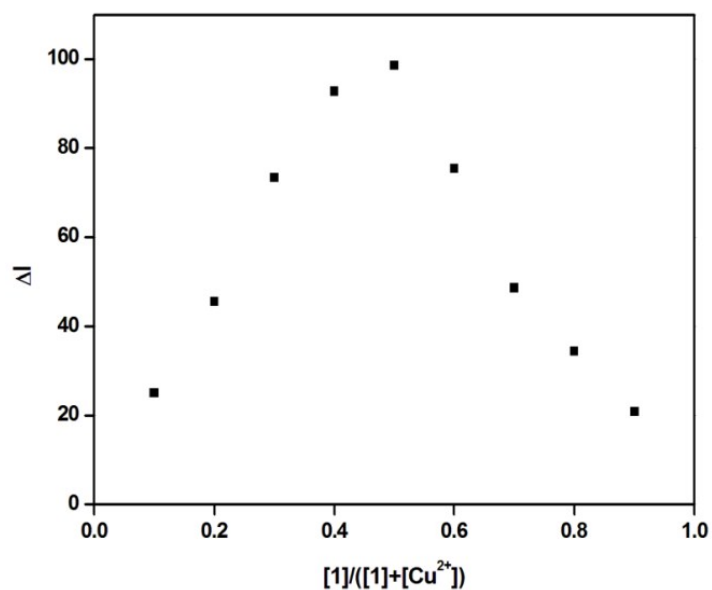


Fig. S35 Job's plot for the titration of complex **1** with Cu^{2+} ion.

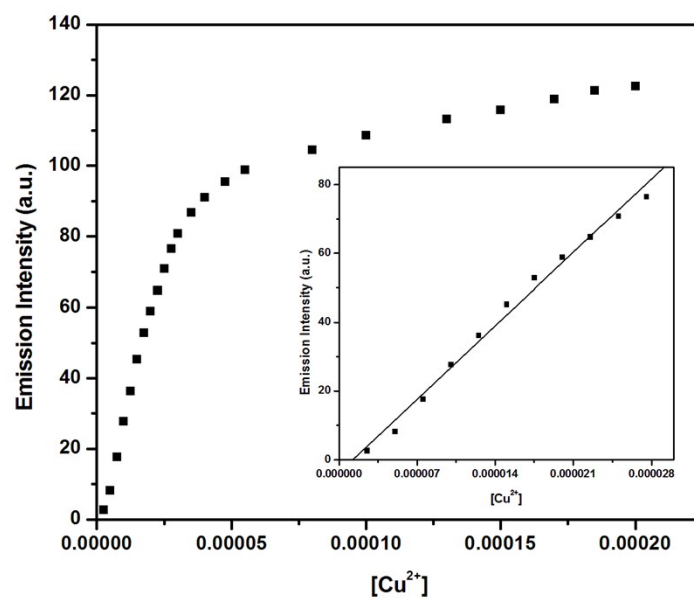


Fig. S36 Calibration curve of complex **4** for Cu^{2+} . Insert: linear part of the calibration curve.

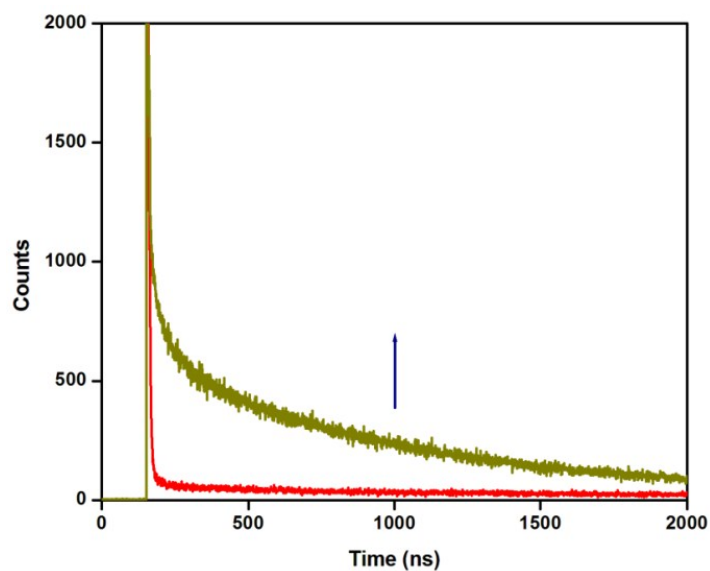


Fig. S37 Time resolved luminescence decay of complex **1** (15 μM) in the absence and in the presence of Cu²⁺ ion (200 μM).

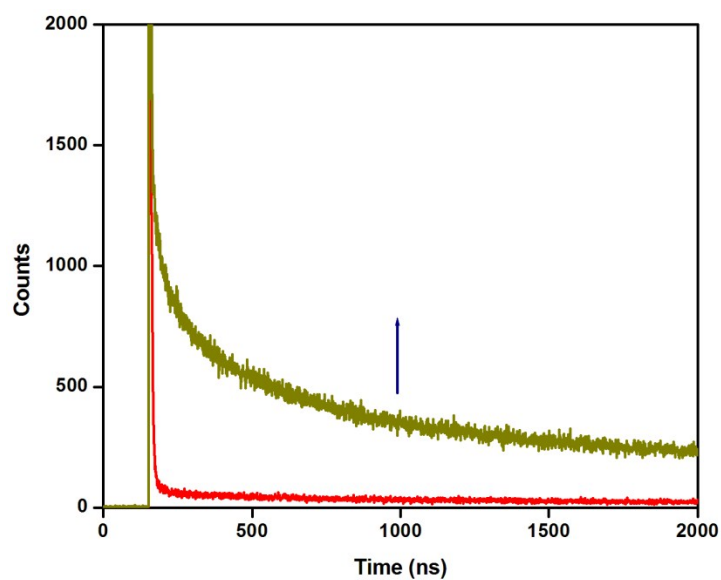


Fig. S38 Time resolved luminescence decay of complex **2** (15 μM) in the absence and in the presence of Cu²⁺ ion (200 μM).

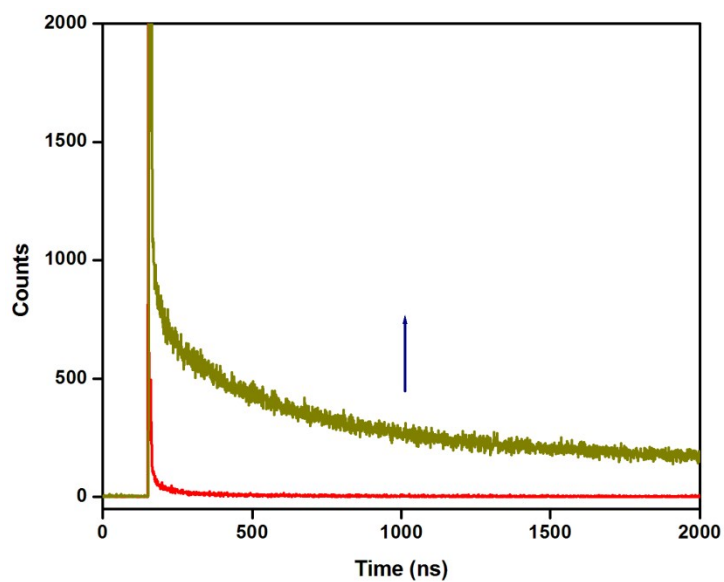


Fig. S39 Time resolved luminescence decay of complex **3** (15 μM) in the absence and in the presence of Cu²⁺ ion (200 μM).

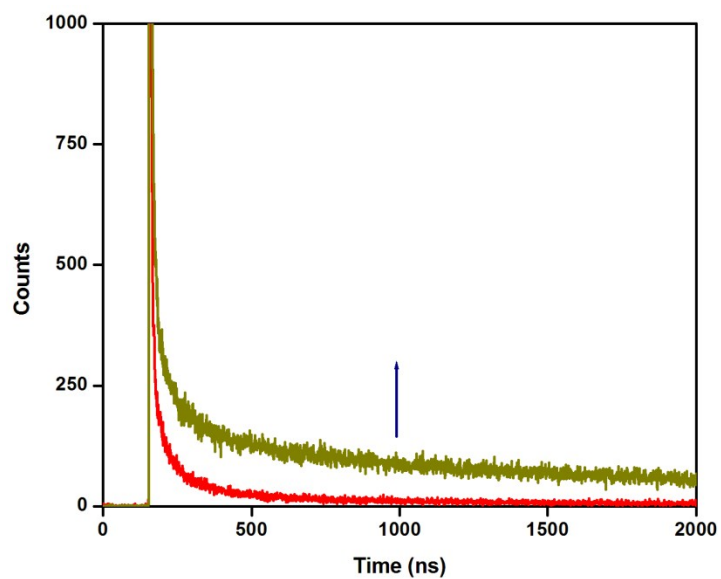


Fig. S40 Time resolved luminescence decay of complex **4** (15 μM) in the absence and in the presence of Cu²⁺ ion (200 μM).