

Supporting Information

A NBD-based two-in-one Cu²⁺/Ni²⁺ chemosensor with differential charge transfer processes

Richa Rani, Kamaldeep Paul and Vijay Luxami*
School of Chemistry and Biochemistry
Thapar University, Patiala-147004
vluxami@thapar.edu

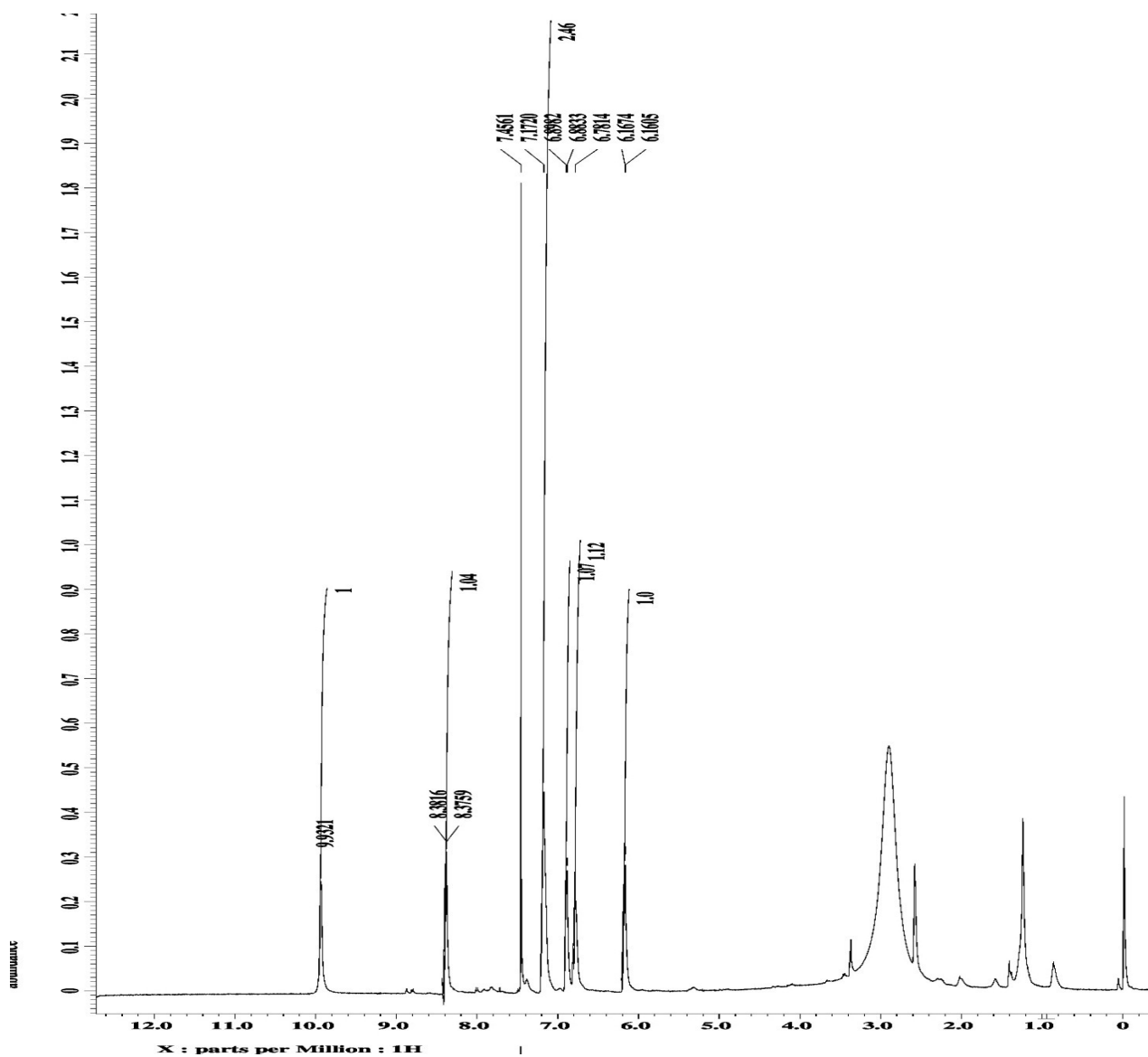


Figure SI 1: ¹H NMR spectrum of 2

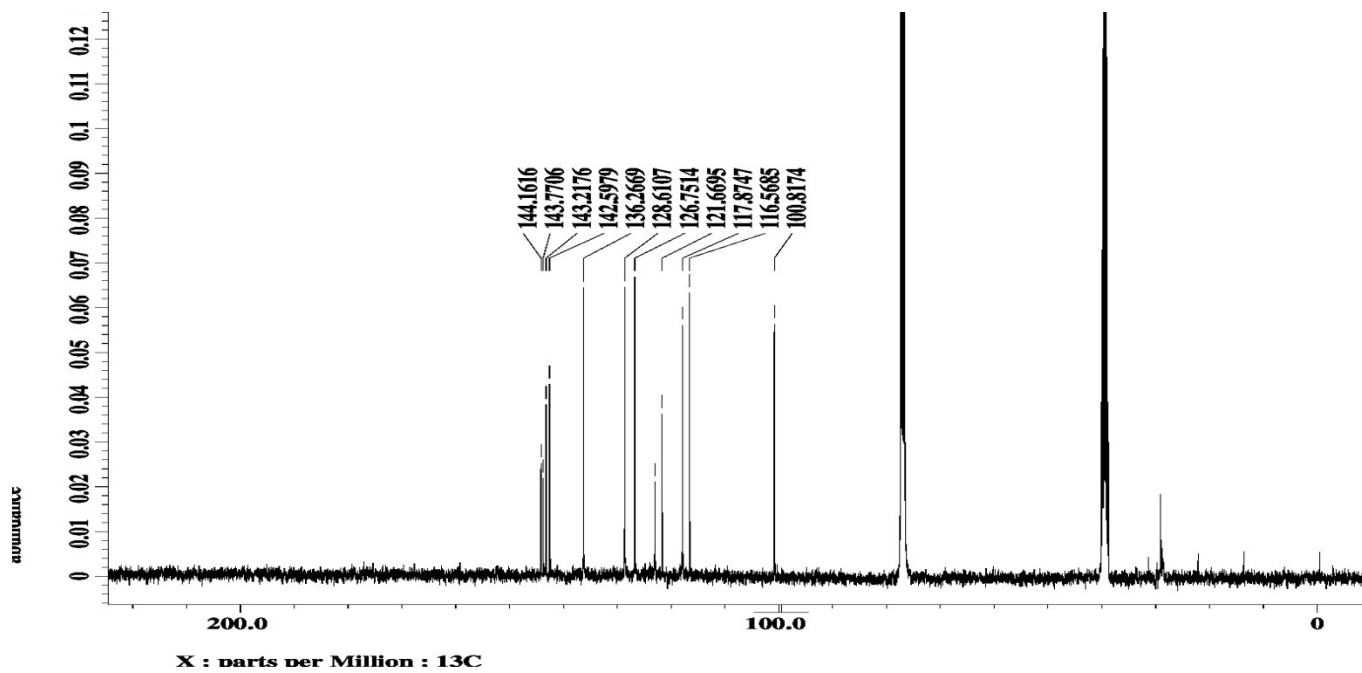


Figure SI 2: ^{13}C NMR spectrum of 2

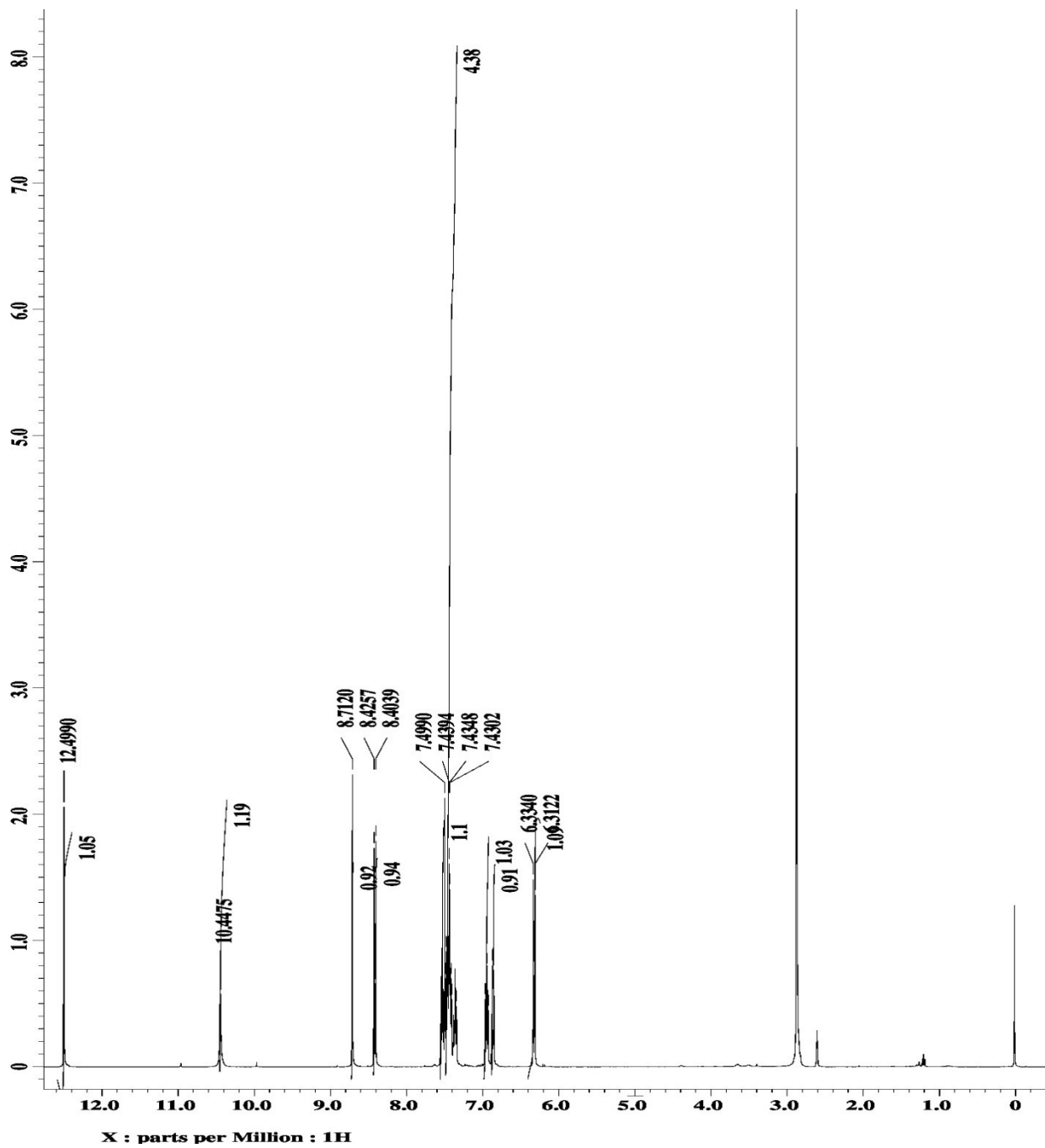


Figure SI 3: ¹H NMR spectrum of probe 1

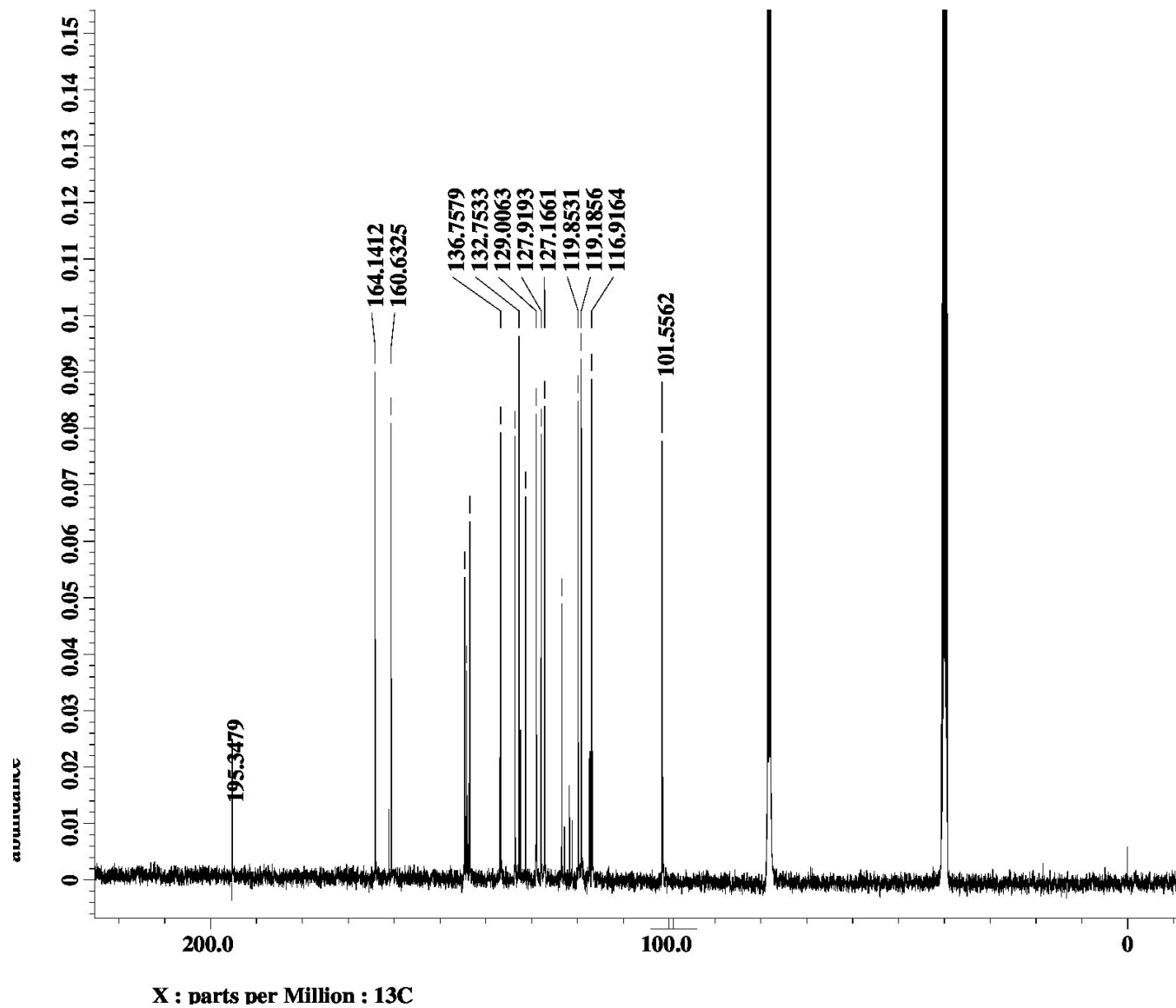


Figure S4: ¹³C NMR spectrum of probe 1

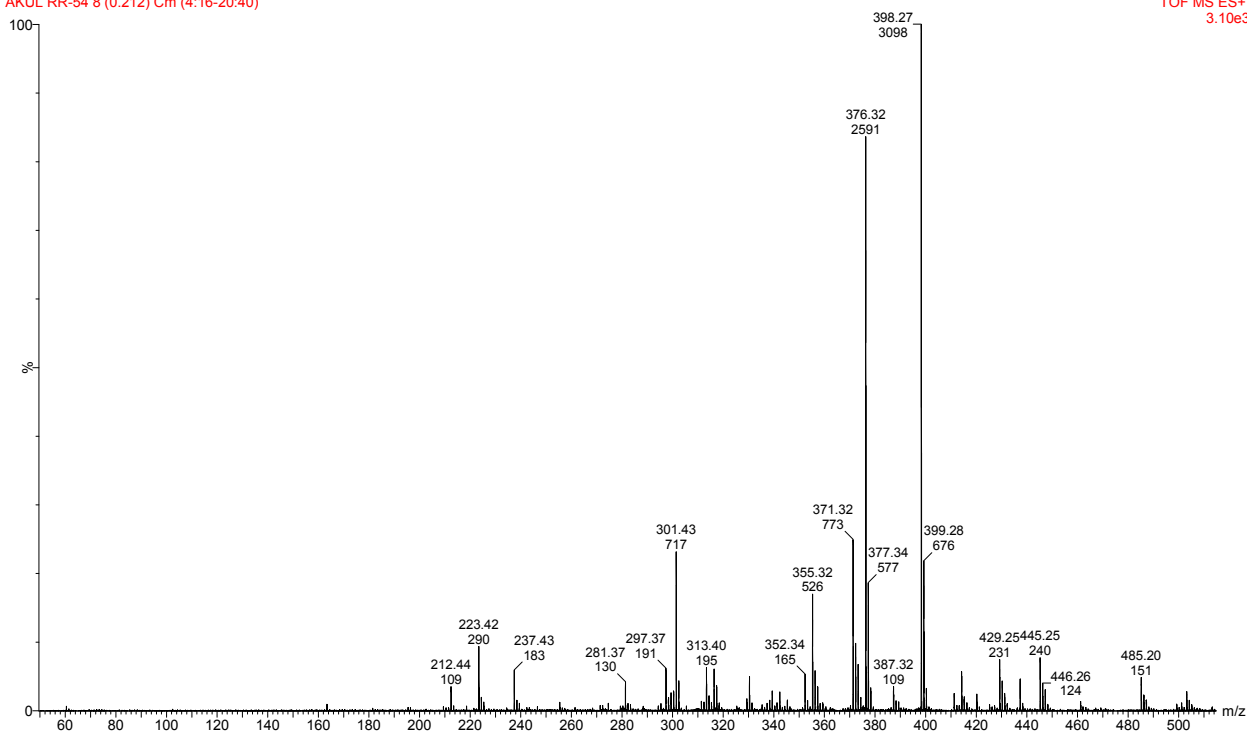


Figure S5: Mass spectrum of probe 1.

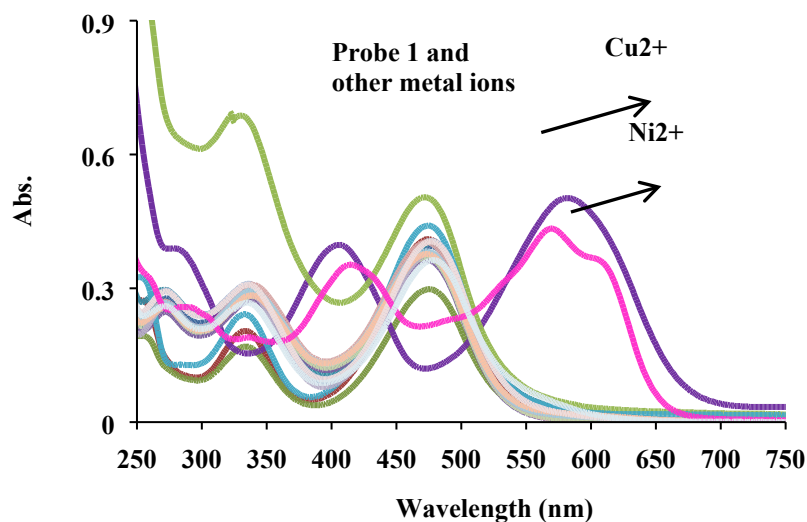


Figure S6: The UV-Visible spectra of probe 1 (20 μ M, CH₃OH: H₂O:: 1:1) in the presence of various metal ions (50 equiv.).

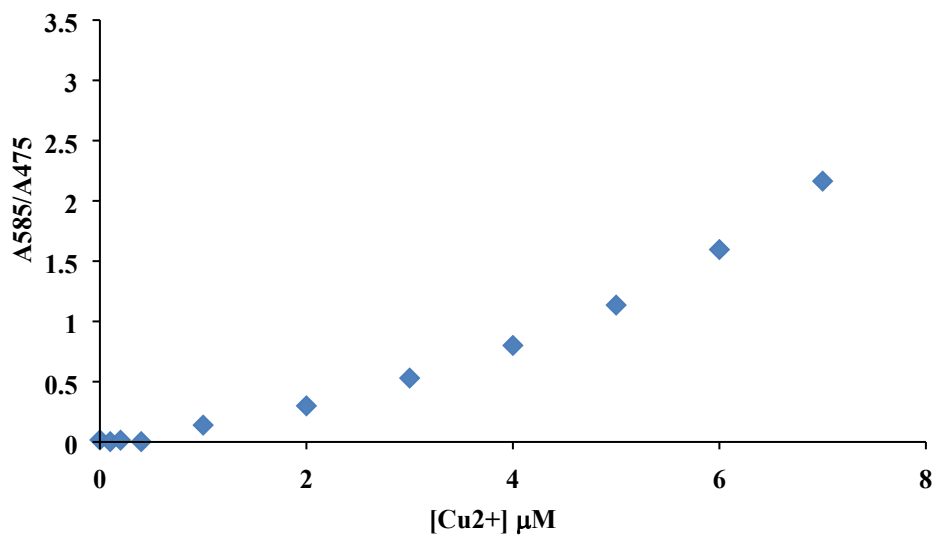


Figure S7: Ratiometric plot for the analysis of Cu²⁺ ions.

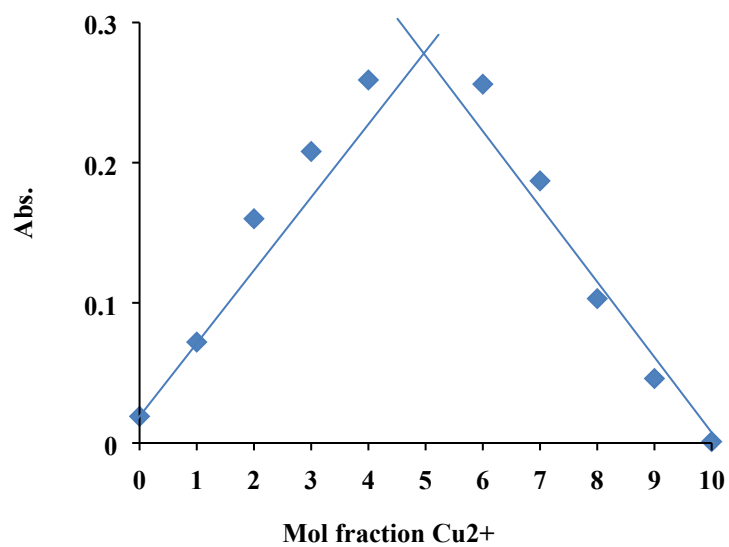


Figure S8: Job's plot showing the 1: 1 stoichiometry between probe 1 and Cu²⁺.

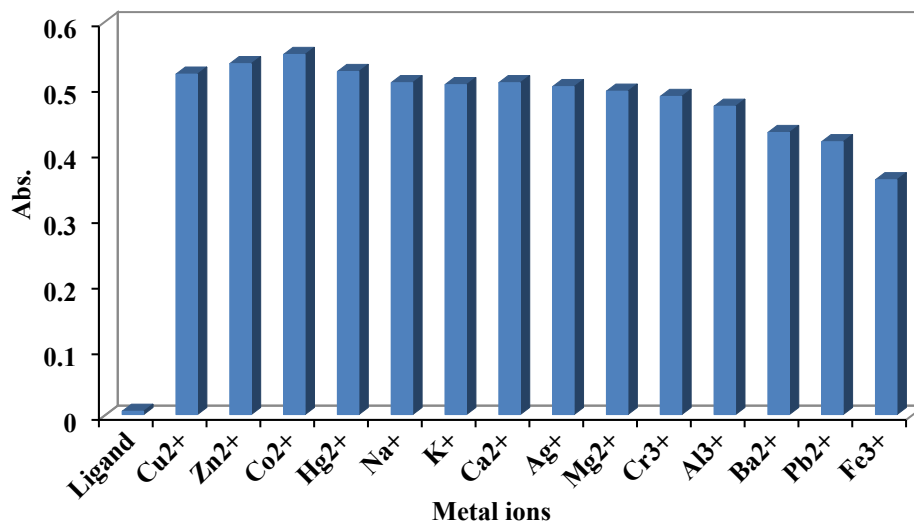


Figure S9: The absorption response of probe **1**. Cu²⁺ (20 μM, CH₃OH: H₂O:: 1:1) at 585 nm in the presence of various interfering metal ions (1 mM).

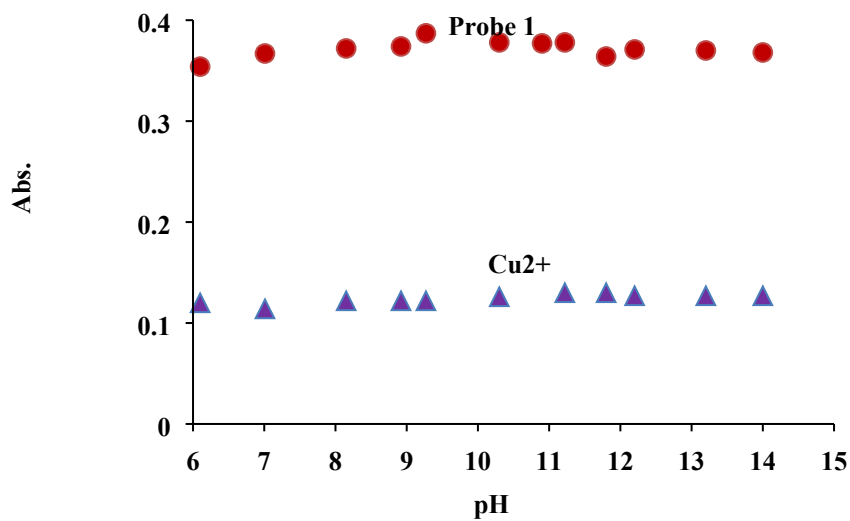


Figure S10: The effect of pH on absorption of probe **1** (475 nm) and probe **1**. Cu²⁺ (20 μM, CH₃OH: H₂O:: 1:1, 585 nm) .

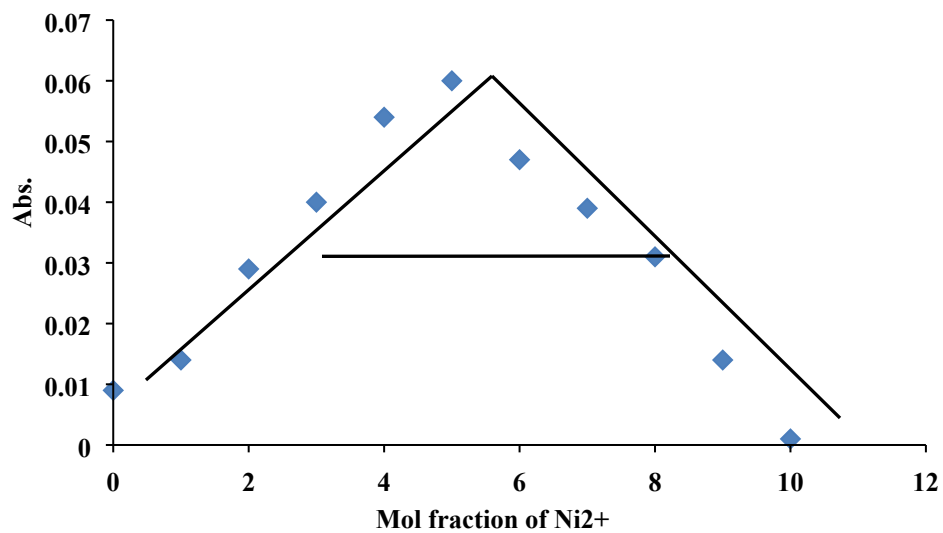


Figure S11: Job's plot showing the 1: 1 stoichiometry between probe **1** and Ni²⁺ at 575 nm.

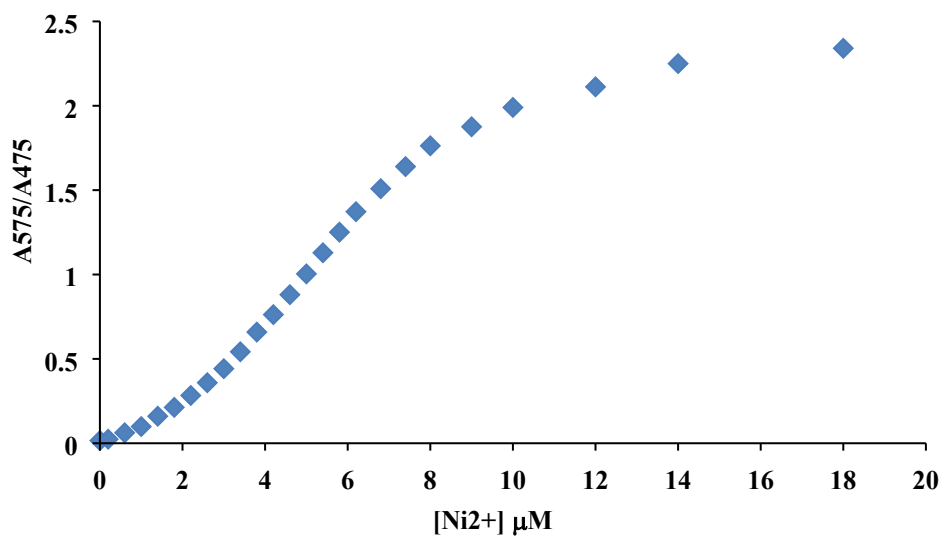


Figure S12: Ratiometric plot for the analysis of Ni²⁺ ions.

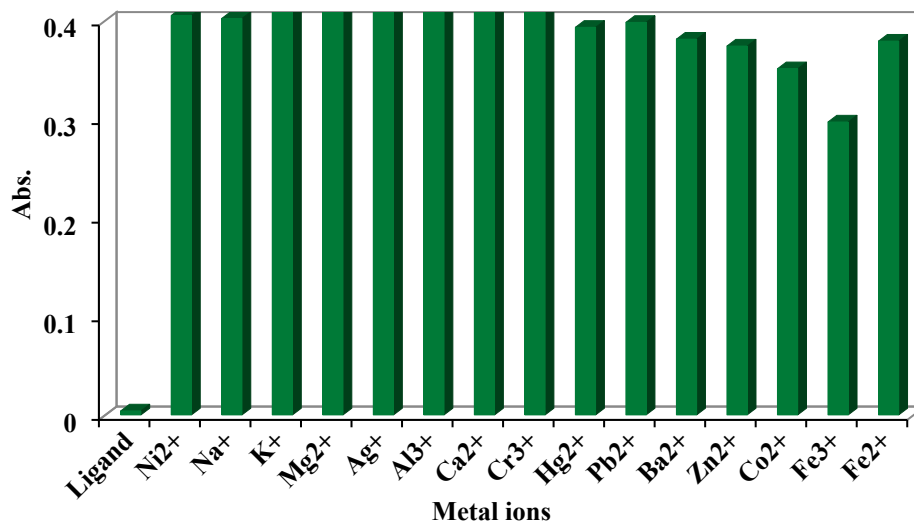


Figure S13: The absorption response of probe **1**. Ni²⁺ (20 μM, CH₃OH: H₂O:: 1:1) in the presence of various interfering metal ions (1mM) at 575 nm.

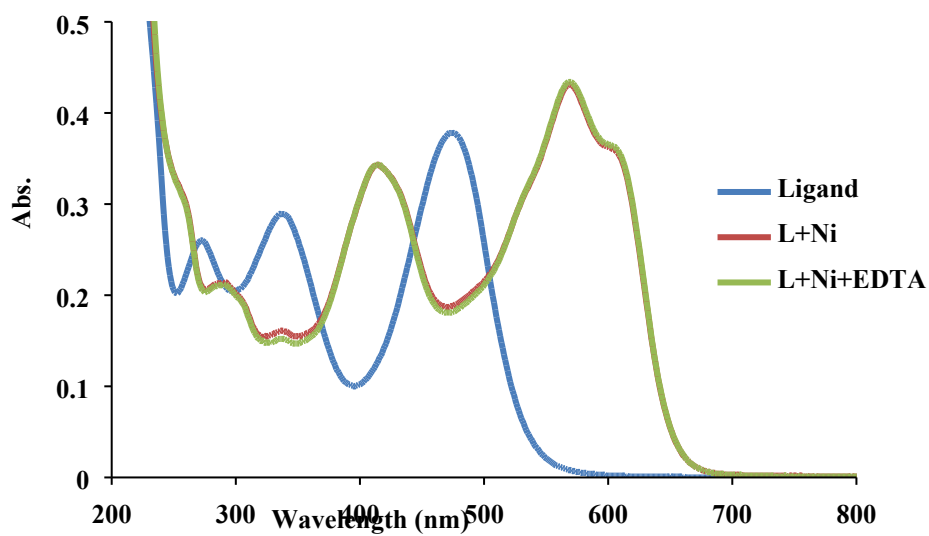


Figure S14: Effect of addition of EDTA on absorption spectra of probe **1**.Ni²⁺ complex.

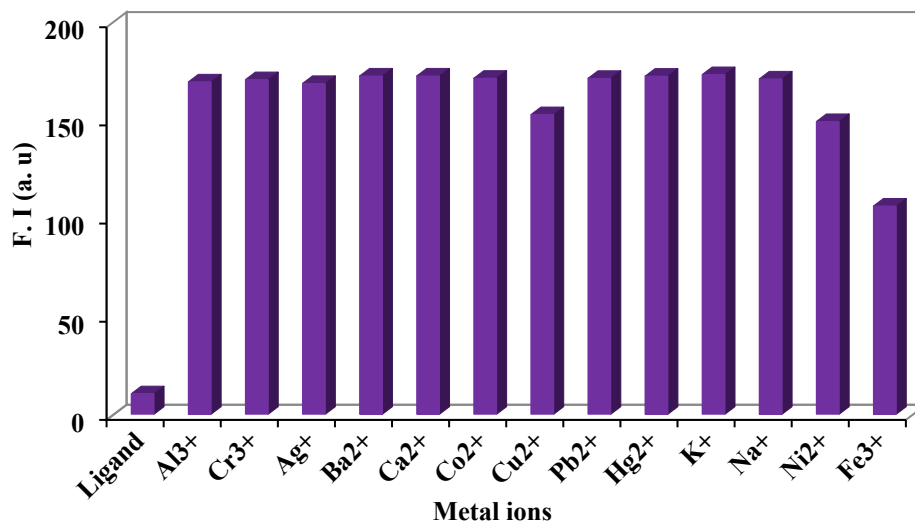


Figure S15: The absorption response of probe **1**. Al³⁺ (10 μM, CH₃OH: H₂O:: 1:1) in the presence of various interfering metal ions (1mM).

Table S1: Comparison of bond distances of probe **1** with Cu²⁺ and Ni²⁺

Bond Distance (Å)	M = Cu ²⁺	M = Ni ²⁺
Salicyl H-O...M	1.9587	1.8793
NBD =N...M	1.9908	1.8920
H-N...M	2.0672	1.9692
Schiff =N...M	1.9057	1.8457

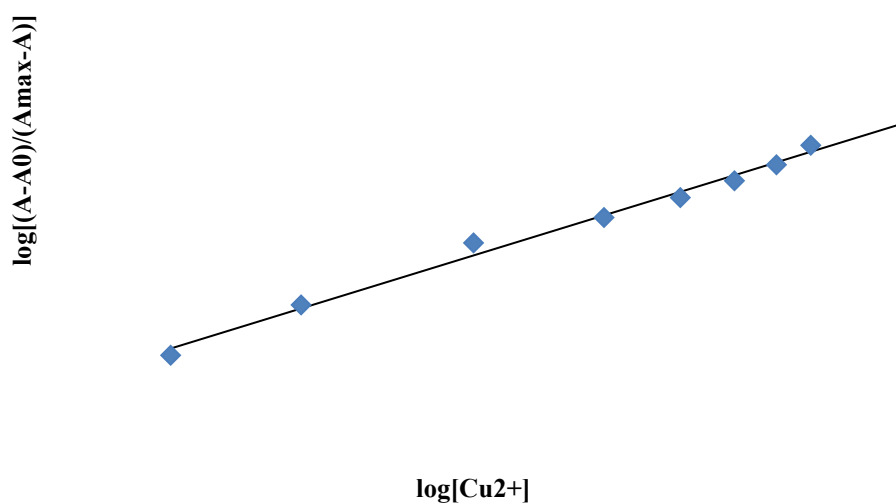


Figure S16: Spectral linear curve fit data for incremental addition of Cu^{2+} to probe **1** ($20 \mu\text{M}$, $\text{CH}_3\text{OH}:\text{H}_2\text{O}::1:1$, HEPES buffer, $\text{pH} = 7.0$).

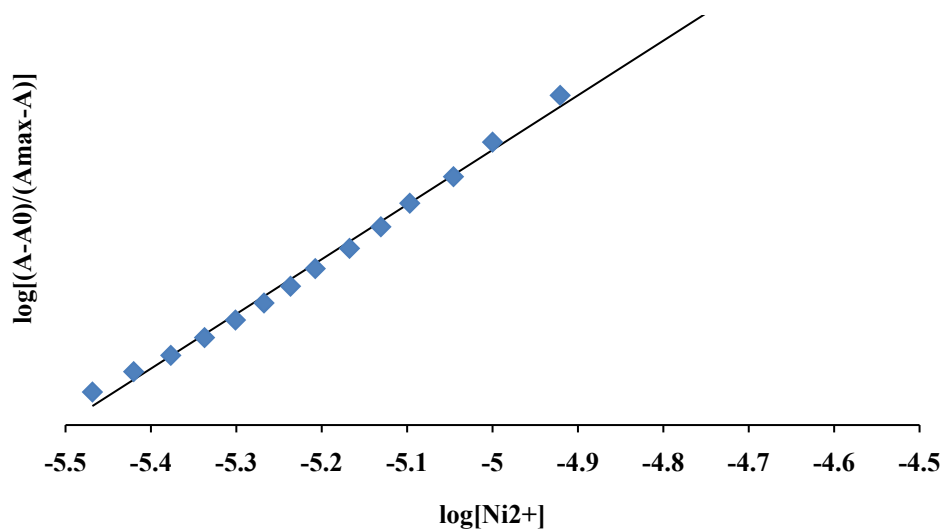


Figure S17: Spectral linear curve fit data for incremental addition of Ni^{2+} to probe **1** ($20 \mu\text{M}$, $\text{CH}_3\text{OH}:\text{H}_2\text{O}::1:1$, HEPES buffer, $\text{pH} = 7.0$).

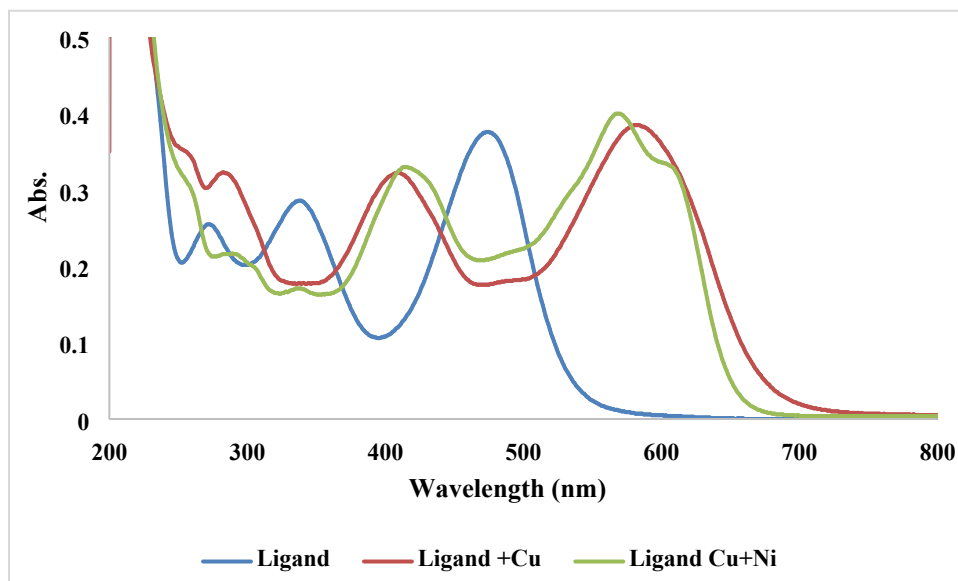


Figure S18: Effect of addition Ni^{2+} on absorption spectrum (1:1) probe **1**. Cu^{2+} ($20 \mu\text{M}$, $\text{CH}_3\text{OH}:\text{H}_2\text{O}::1:1$, HEPES buffer, $\text{pH} = 7.0$).

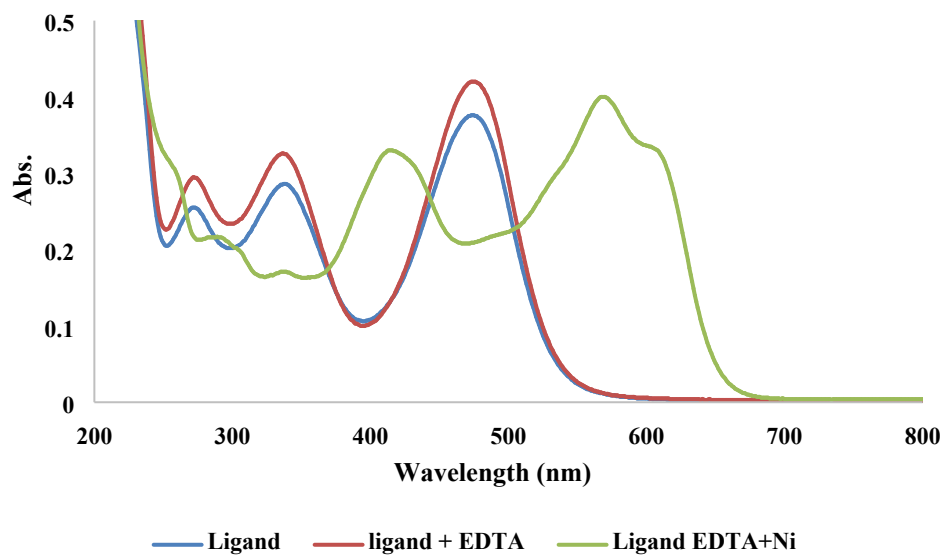


Figure S19: Effect of addition Ni^{2+} on absorption spectrum probe 1 having EDTA (1 equiv.) (20 μM , $\text{CH}_3\text{OH}:\text{H}_2\text{O}::1:1$, HEPES buffer, $\text{pH} = 7.0$).