

Electronic Supplementary Information

Synthesis, Crystal structure and Bio-macromolecular interaction studies of pyridine-based thiosemicarbazone and its Ni(II) and Cu(II) complexes

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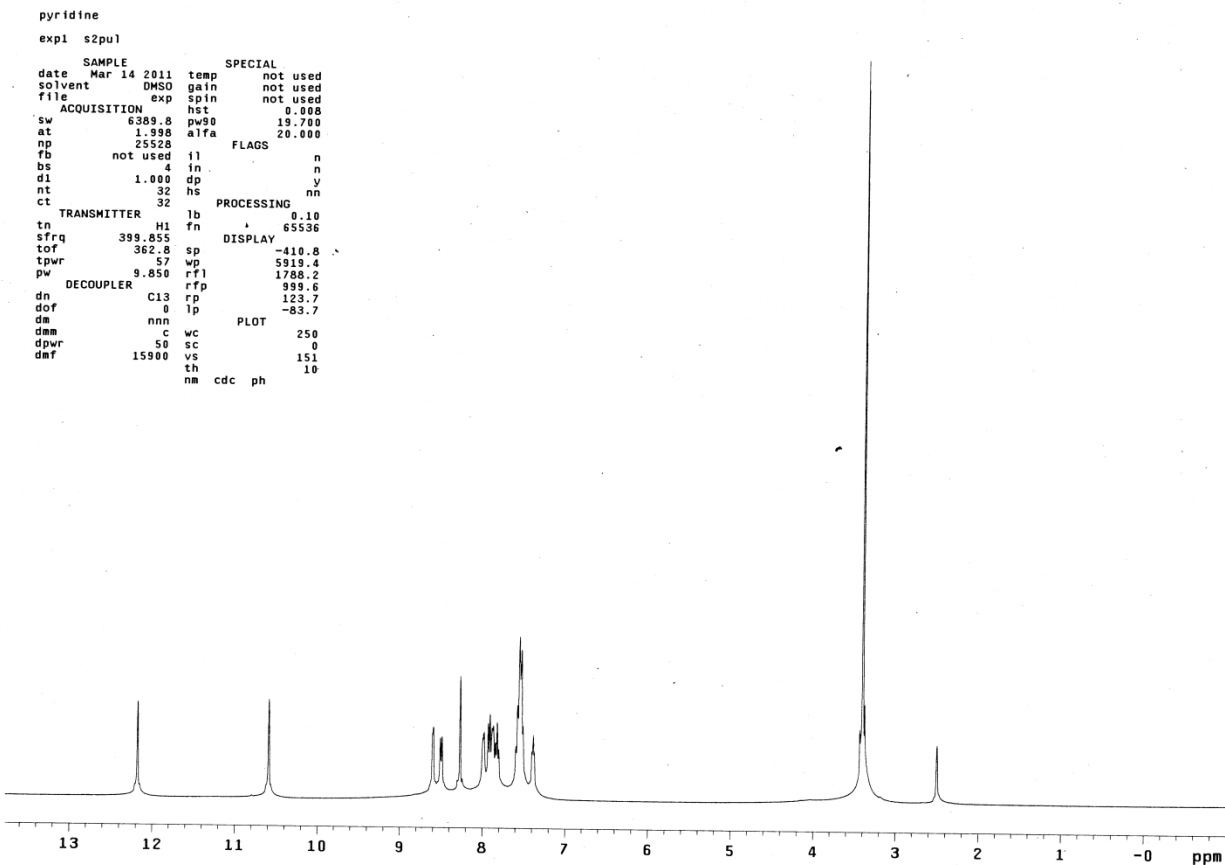


Fig.S1 ^1H NMR spectrum of LH.

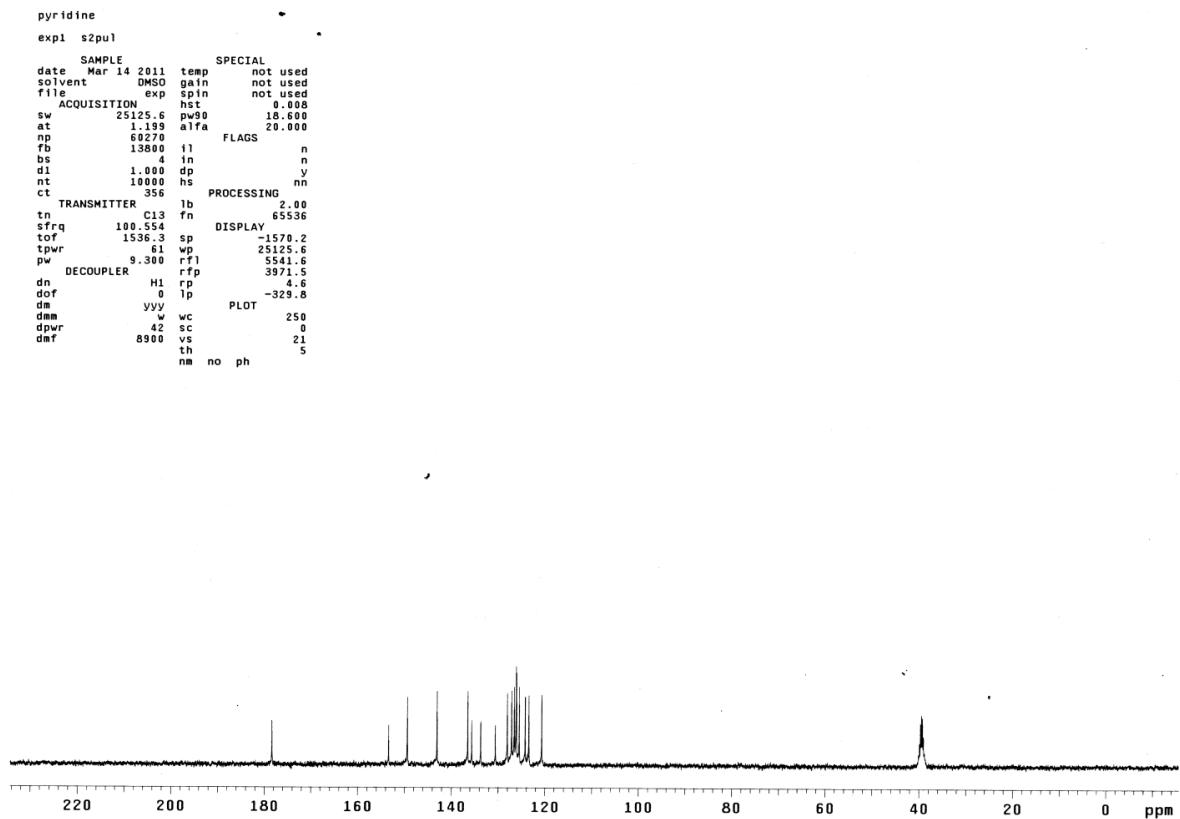


Fig.S2 ^{13}C -NMR spectrum of LH.

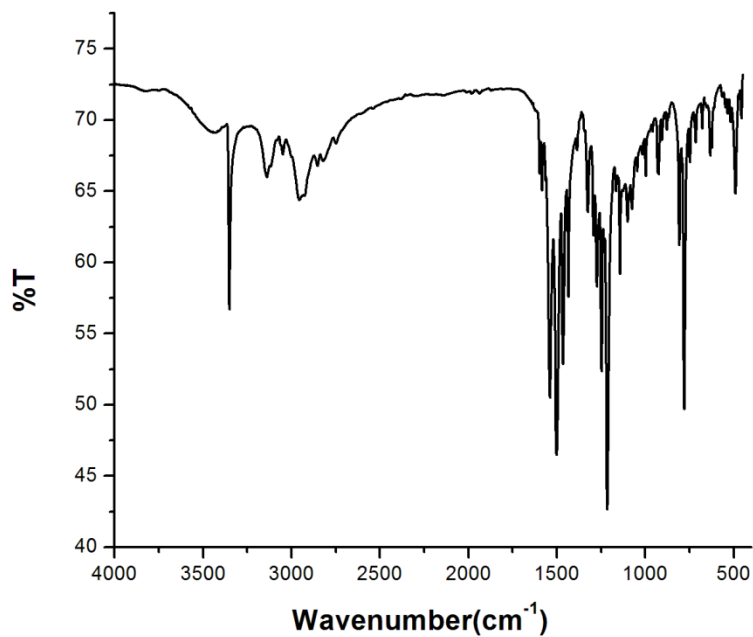


Fig.S3 IR-spectrum of LH.

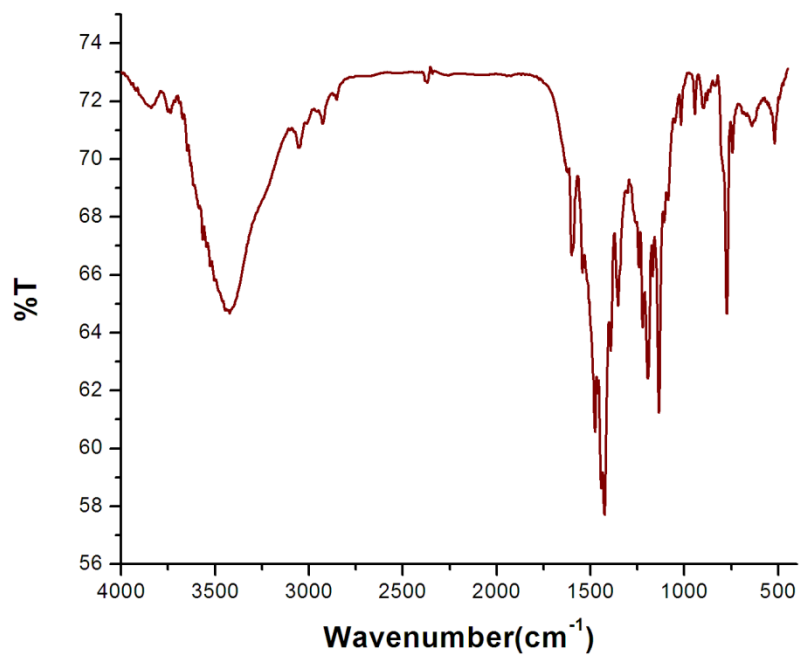


Fig.S4 IR-spectrum of Cu(L)Cl.

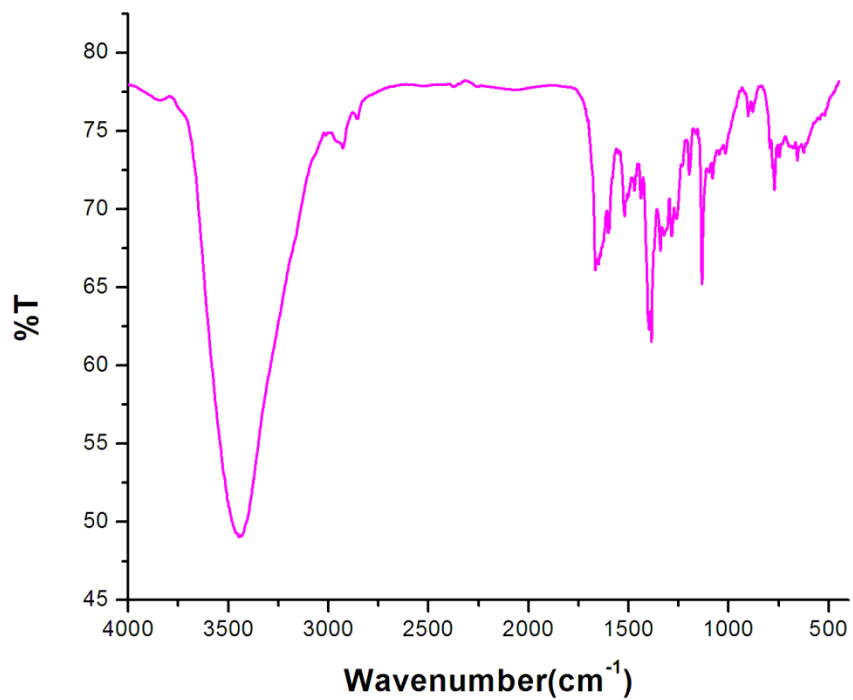


Fig.S5 IR-spectrum of Ni(L)₂.

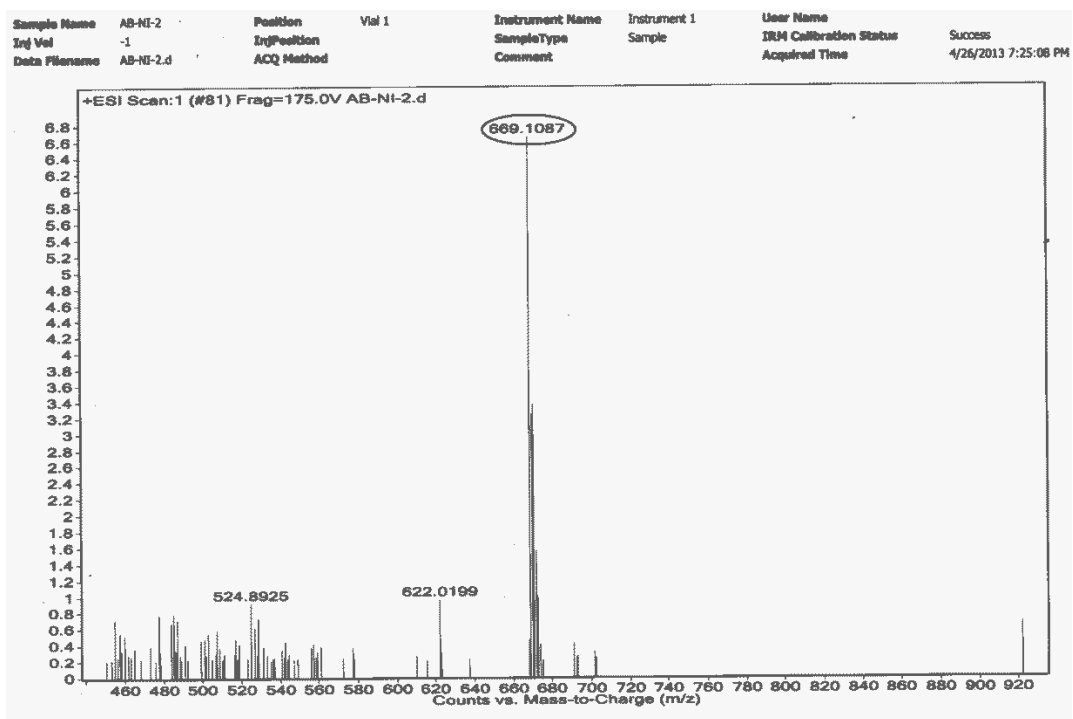


Fig. S6 Mass Spectrum of Ni(L)₂

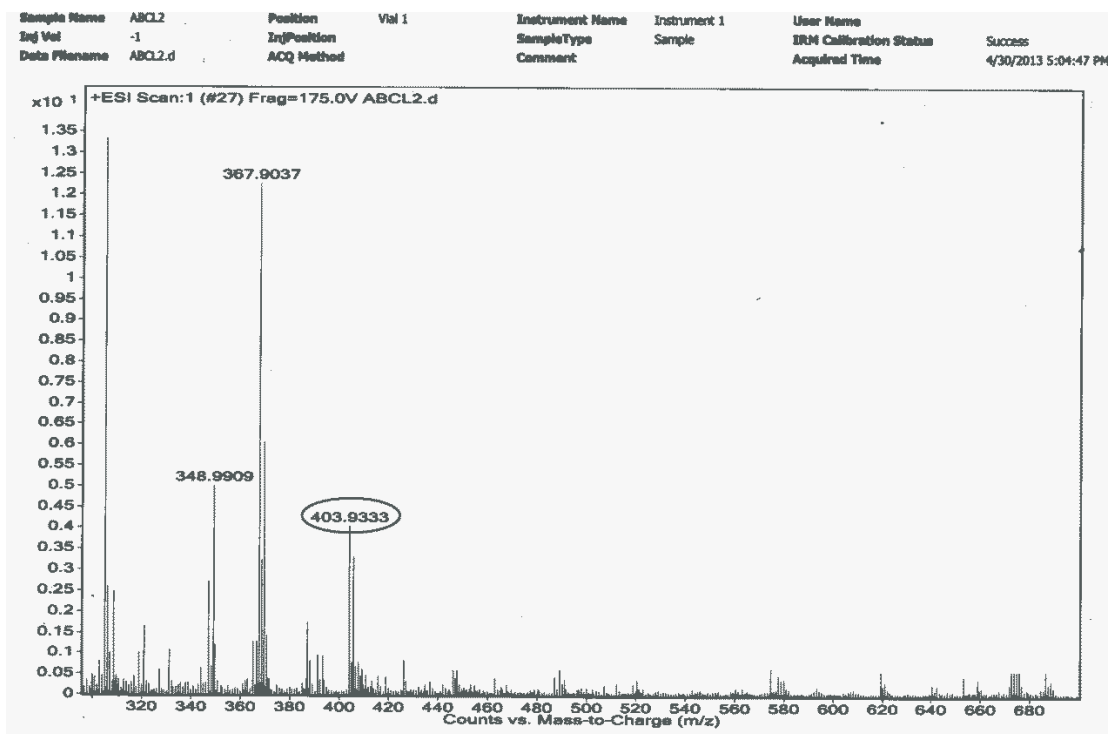


Fig. S7 Mass Spectrum of Cu(L)Cl

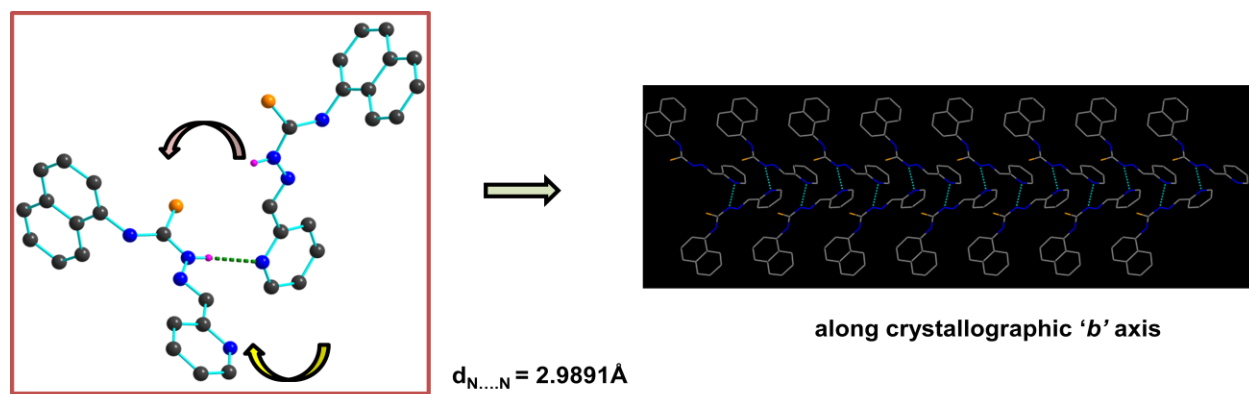


Fig. S8 Hydrogen bond directed packing diagram of ligand LH.

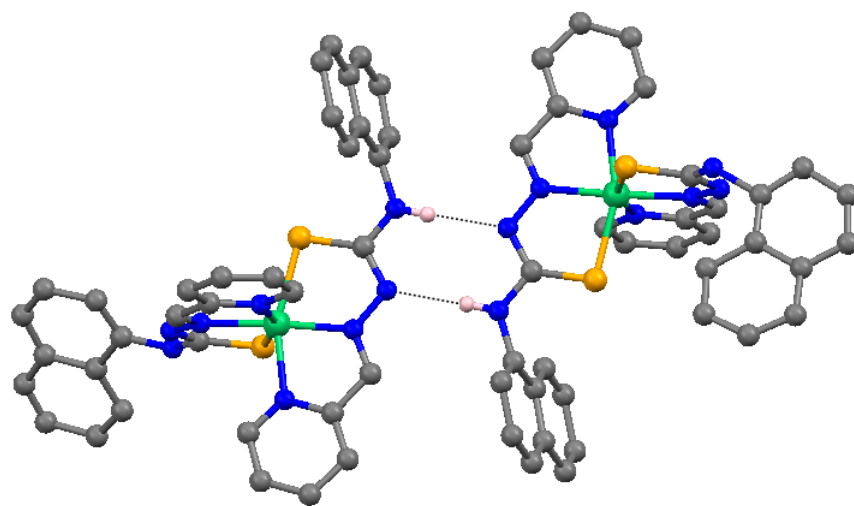


Fig. S9 Dimeric hydrogen bond integration between two Ni(II) complexes.

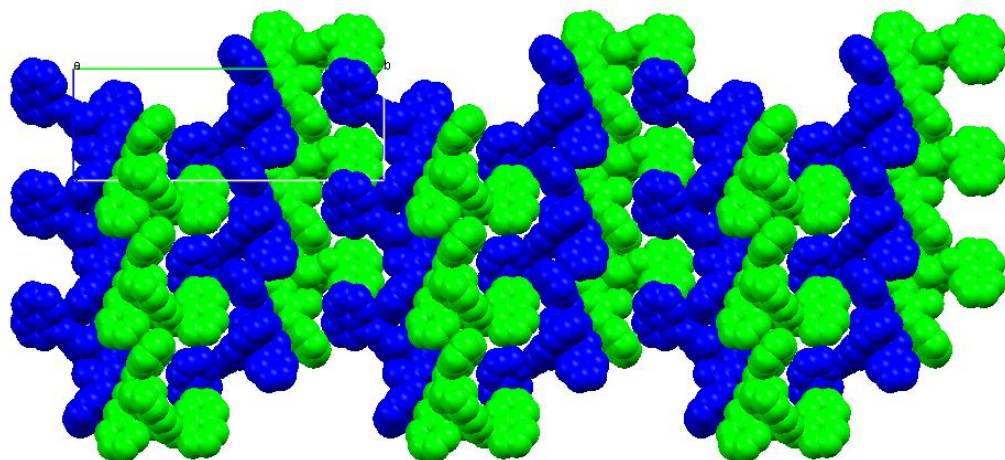


Fig. S10 Packing diagram of Ni(L)₂ along *a* axis. Solvent molecules are omitted for clarity.

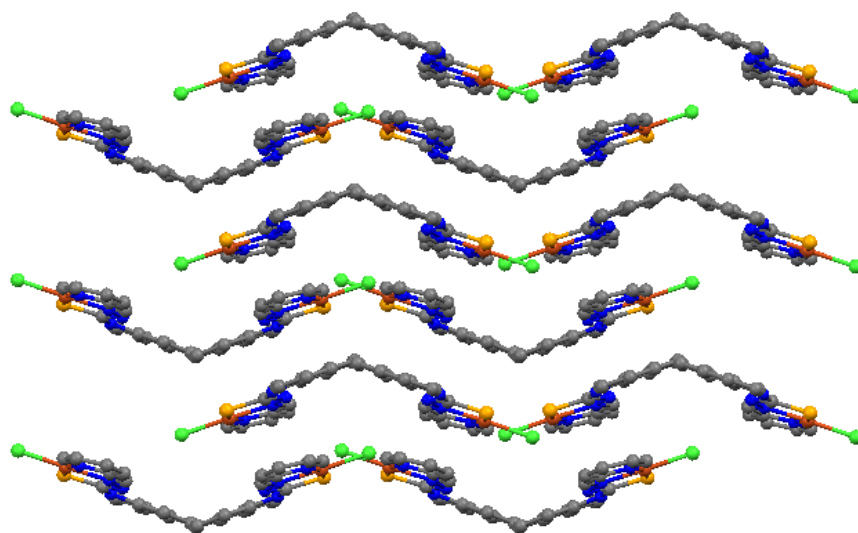


Fig. S11 Packing diagram of Cu(L)Cl along *c* axis.

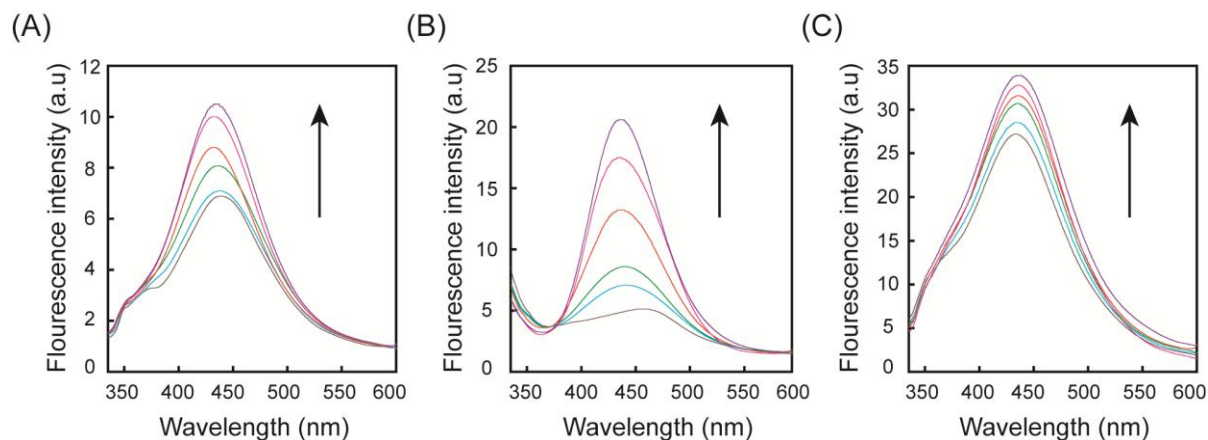


Fig. S12 Fluorescence titration spectra of (A) Compound 1, (B) Compound 2 and (C) Compound 3 with various concentration (6 μ M – 30 μ M) of CT DNA in PBS pH 7.4.

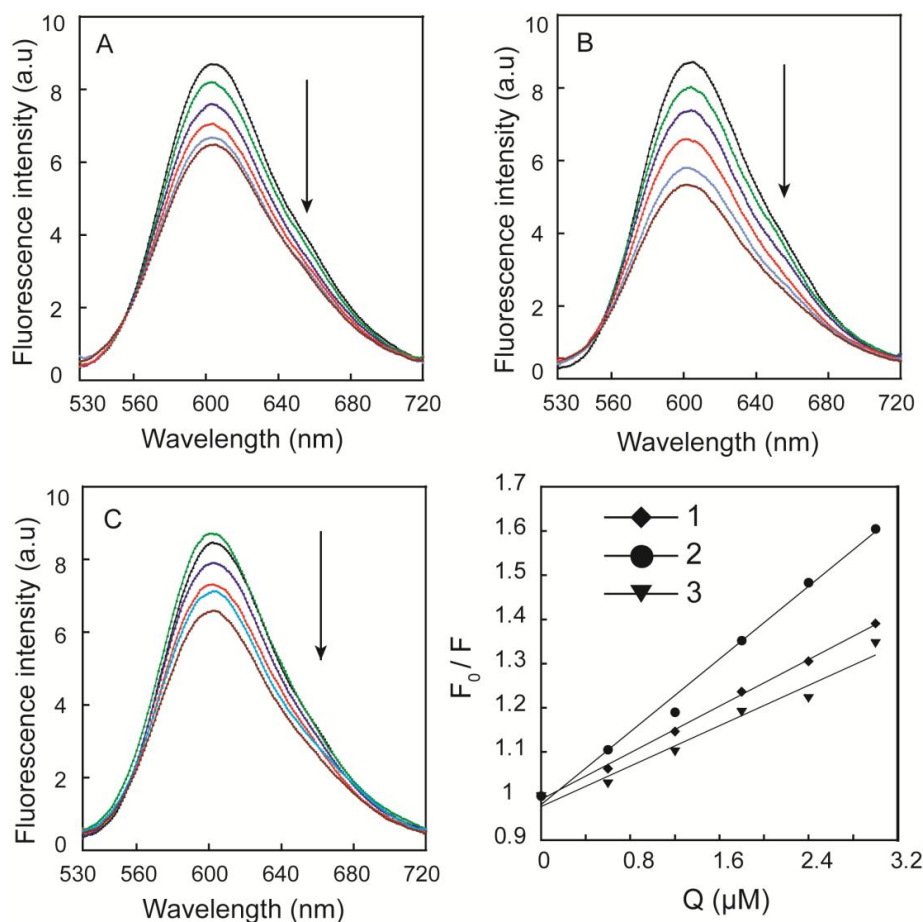


Fig. S13 Fluorescence quenching curves of ethidium bromide bound to CT-DNA by Compound 1(A), Compound 2(B) and Compound 3(C). [DNA] = 3 μ M, [EB] = 0.5 μ M and [Compound] = 0.6 μ M - 3.0 μ M. (D) Stern-Volmer plots of the fluorescence quenching by compounds.

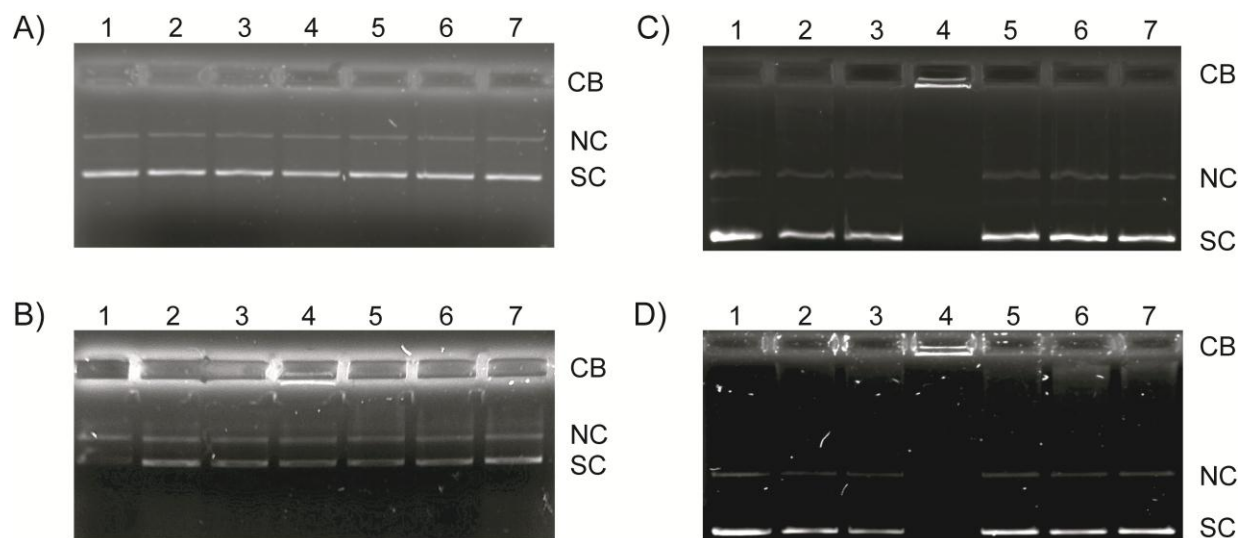


Fig. S14 Agarose gel electrophoresis to study pUC18 plasmid DNA cleavage activity of test compounds. Treatment of pUC18 plasmid DNA with 60 μM compound concentration was performed for (A) 1h and (B) 2h. Treatment of pUC18 plasmid DNA with 180 μM compound concentration was performed for (C) 1h and (D) 2h. Lanes: 1: untreated pUC18 plasmid DNA; 2: compound 1-treated, 3: compound 2-treated, 4: compound 3-treated, 5: Ni salt control; 6: Cu salt control; 7: DMSO control. CB: compound bound plasmid DNA; NC: nicked circular plasmid DNA, SC: super coiled plasmid DNA.

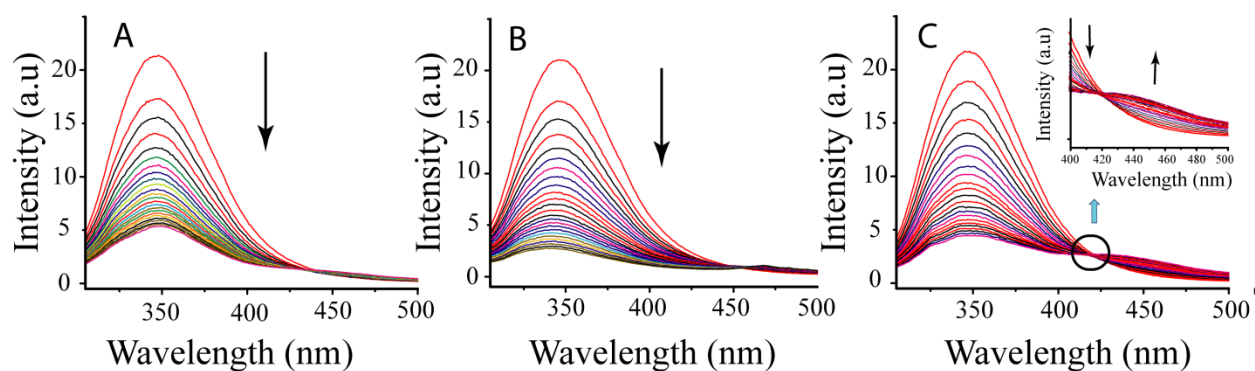


Fig. S15 Emission spectrum of BSA (1 μM ; $\lambda_{\text{exi}} = 295 \text{ nm}$; $\lambda_{\text{em}} = 345 \text{ nm}$) in the presence of increasing amounts of (A) compound 1, (B) compound 2 and (C) compound 3. The amount of the compounds was in the range of 0 μM - 40 μM .

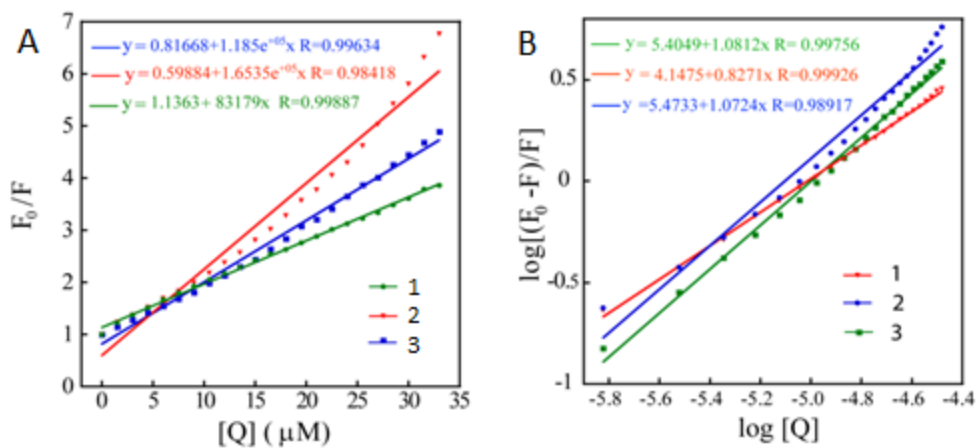


Fig. S16 (A) Stern–Volmer plot of BSA fluorescence titration for compound 1–3. (B) Scatchard plot of BSA fluorescence titration for compound 1–3.

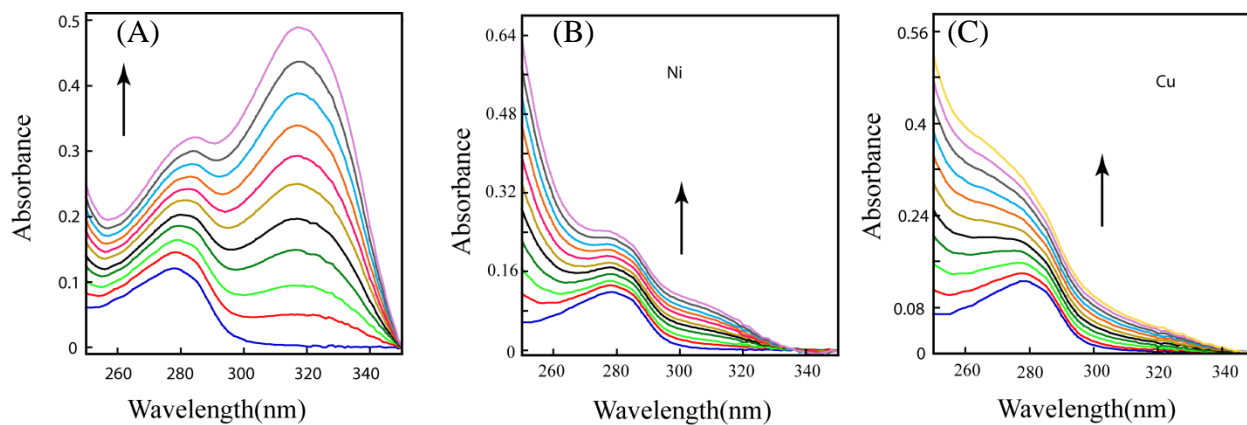


Fig. S17 UV-vis spectra of BSA in the presence of increasing amounts of (A) compound 1, (B) compound 2 and (C) compound 3.

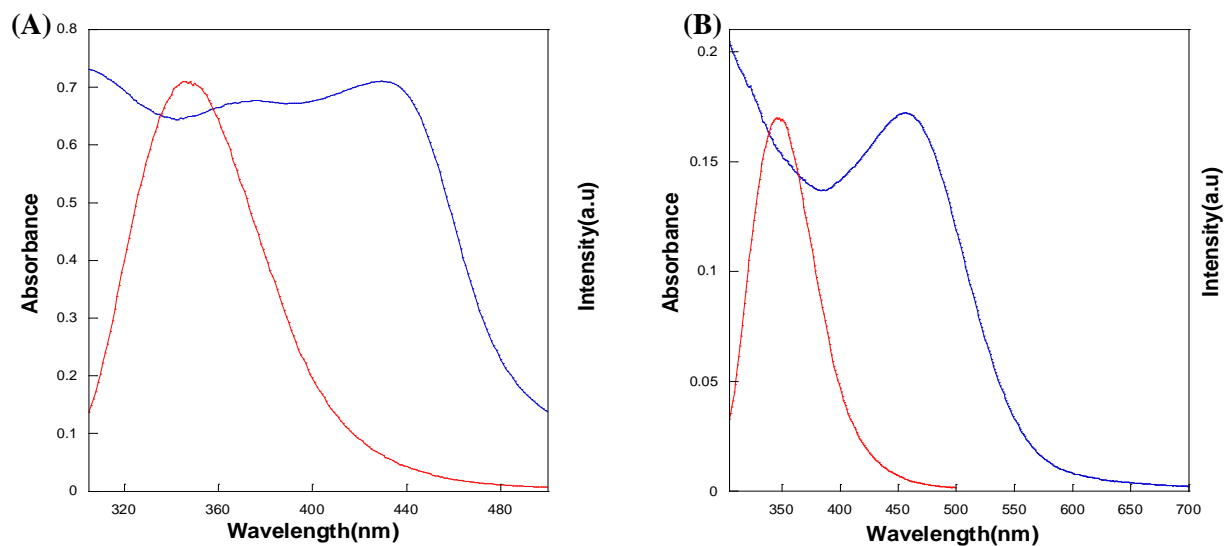


Fig. S18 The overlap of the fluorescence spectra of BSA (red line) and the absorption spectra (blue line) of (A) compound 2 and (B) compound 3.

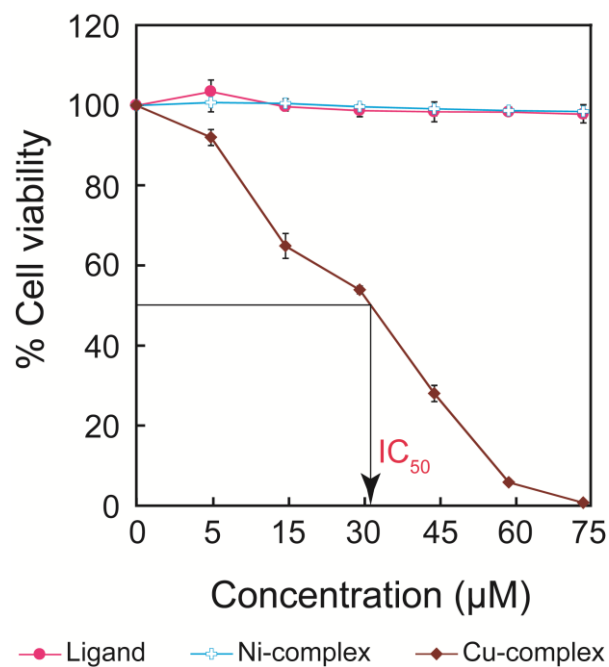


Fig. S19 Determination of IC_{50} value for complex 3.