

Supplementary Information

Mixed-ligand copper(II)-phenolate complexes: structure and studies on DNA/protein binding profile, DNA cleavage, molecular docking and cytotoxicity

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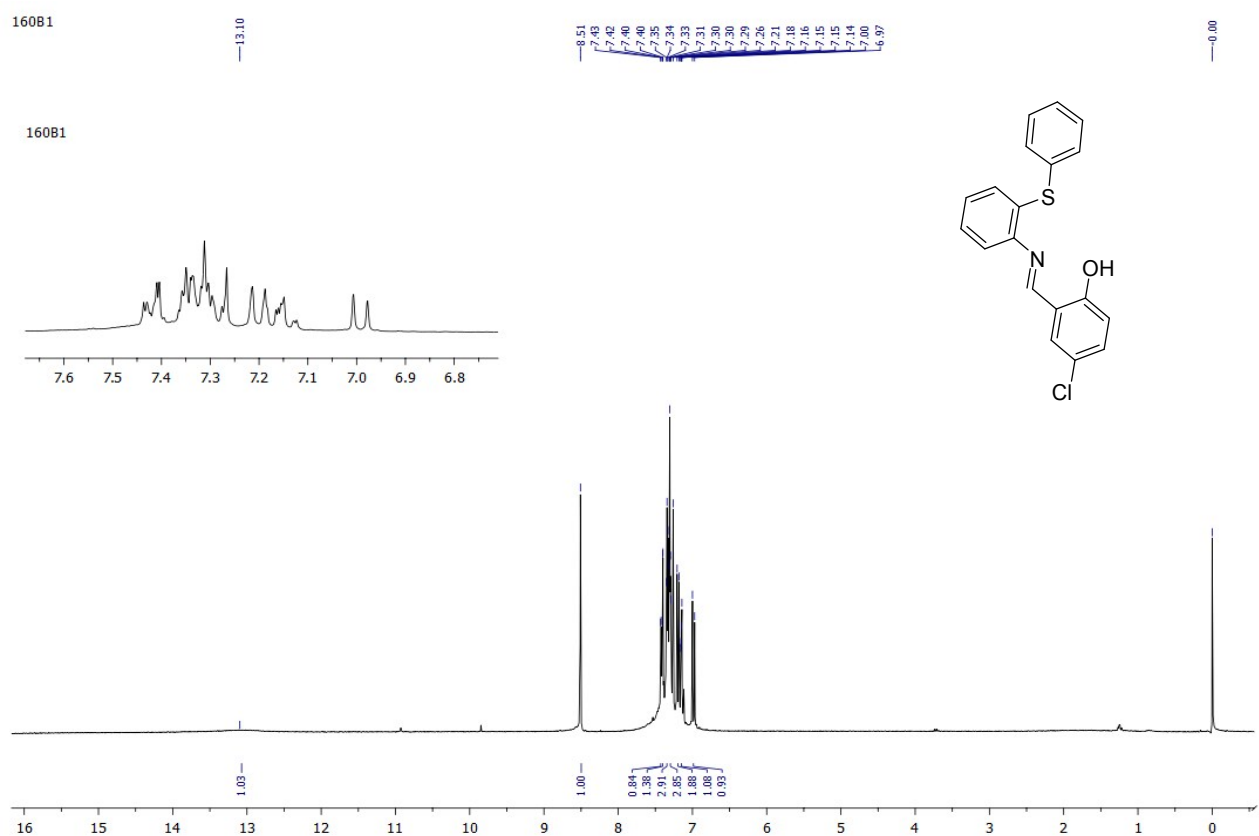


Fig. S1 ^1H -NMR spectra of 4-chloro-2-((2-phenylthio)phenylimino)methylphenol (L).

160c2

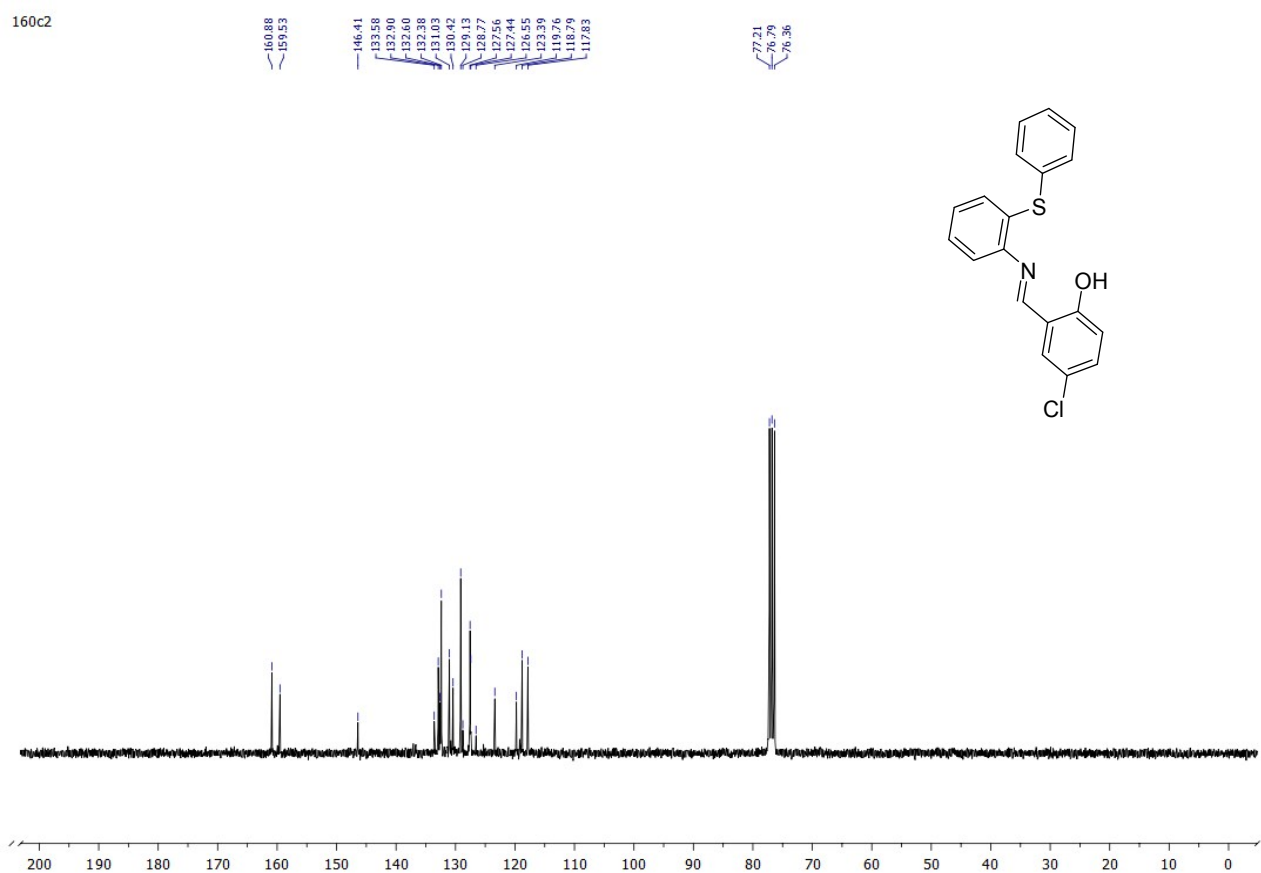


Fig. S2 ^{13}C -NMR spectra of 4-chloro-2-((2-(phenylthio)phenylimino)methyl)phenol (L).

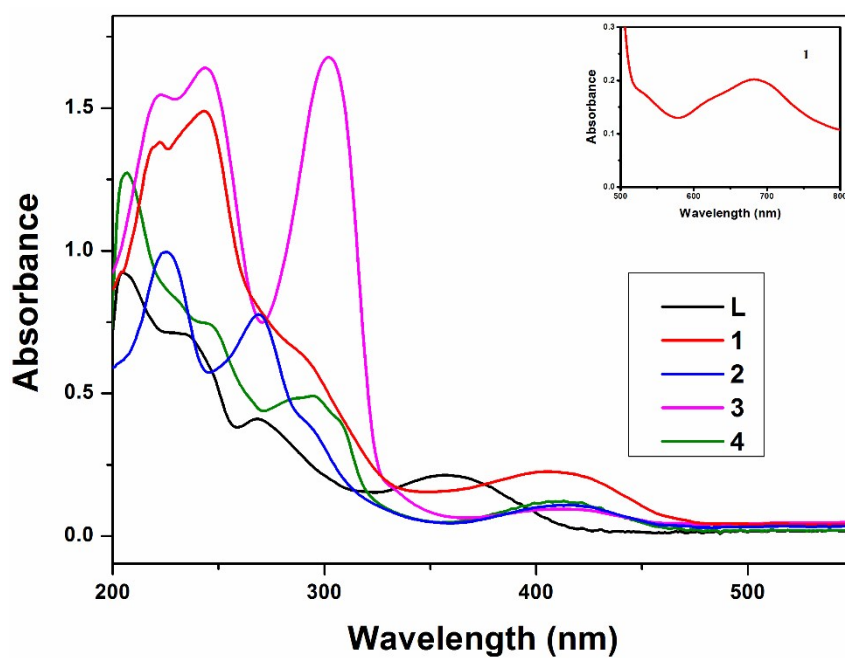


Fig. S3 UV-vis spectrum of L and complexes (1-4).

160BL #21 RT: 0.27 AV: 1 NL: 9.93E3
T: ITMS + c ESI Full ms [50.00-1000.00]

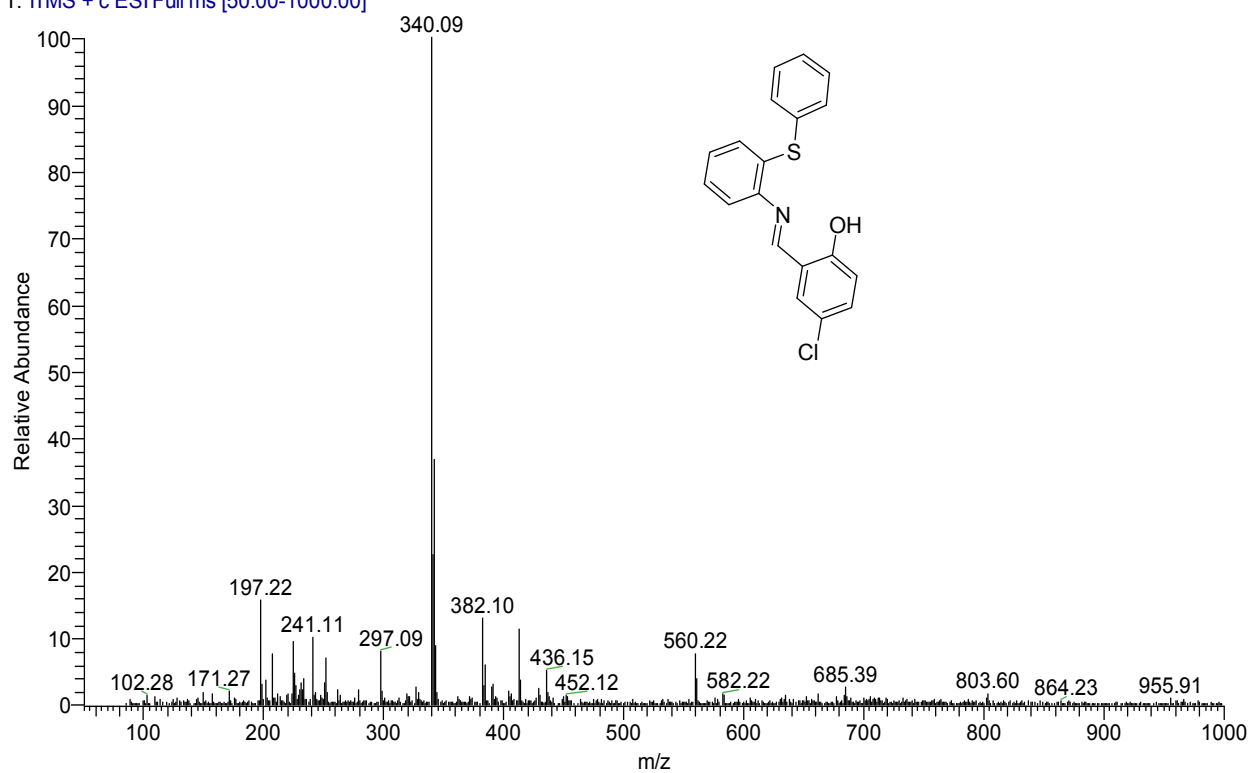


Fig. S4 ESI-MS spectra of Schiff base ligand (L).

16OBMC1_150123155420 #226 RT: 0.64 AV: 1 NL: 7.98E3
T: ITMS + c ESI Full ms [150.00-1000.00]

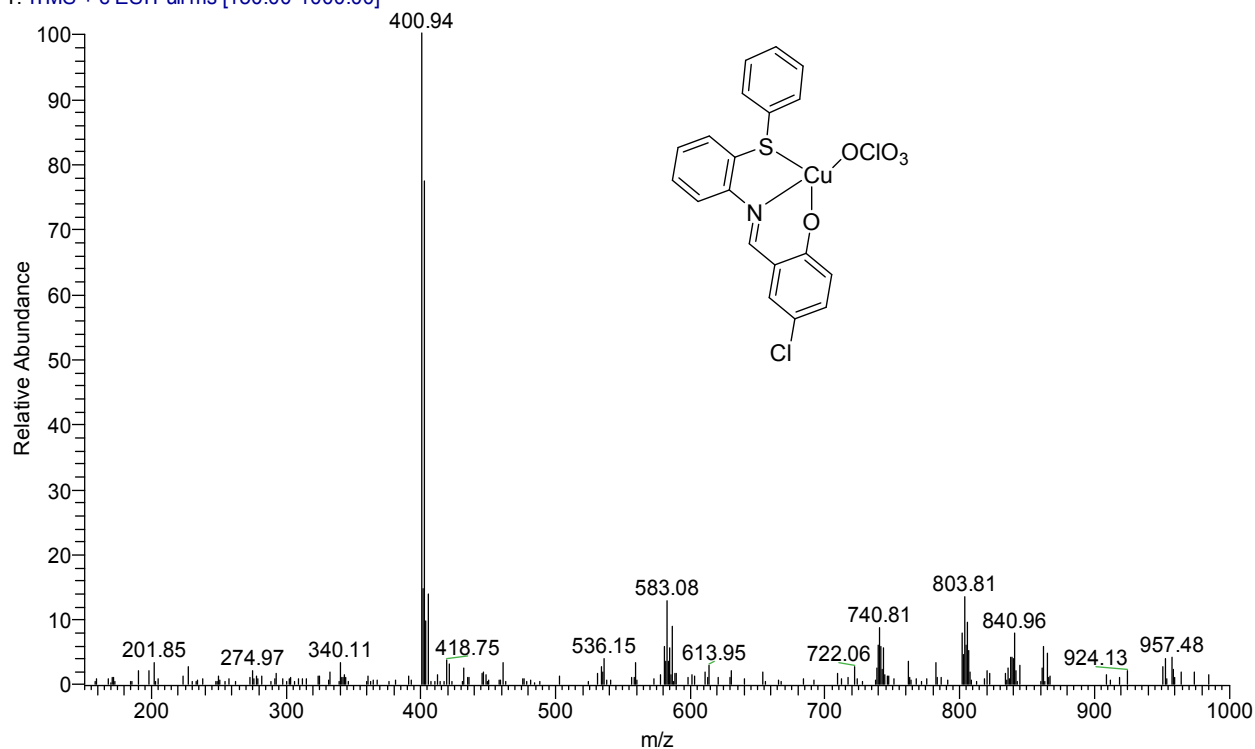


Fig. S5 ESI-MS spectra of Cu(II) complex 1.

160BCL1_150110183637 #171 RT: 0.49 AV: 1 NL: 1.30E4
T: ITMS + c ESI Full ms [150.00-1000.00]

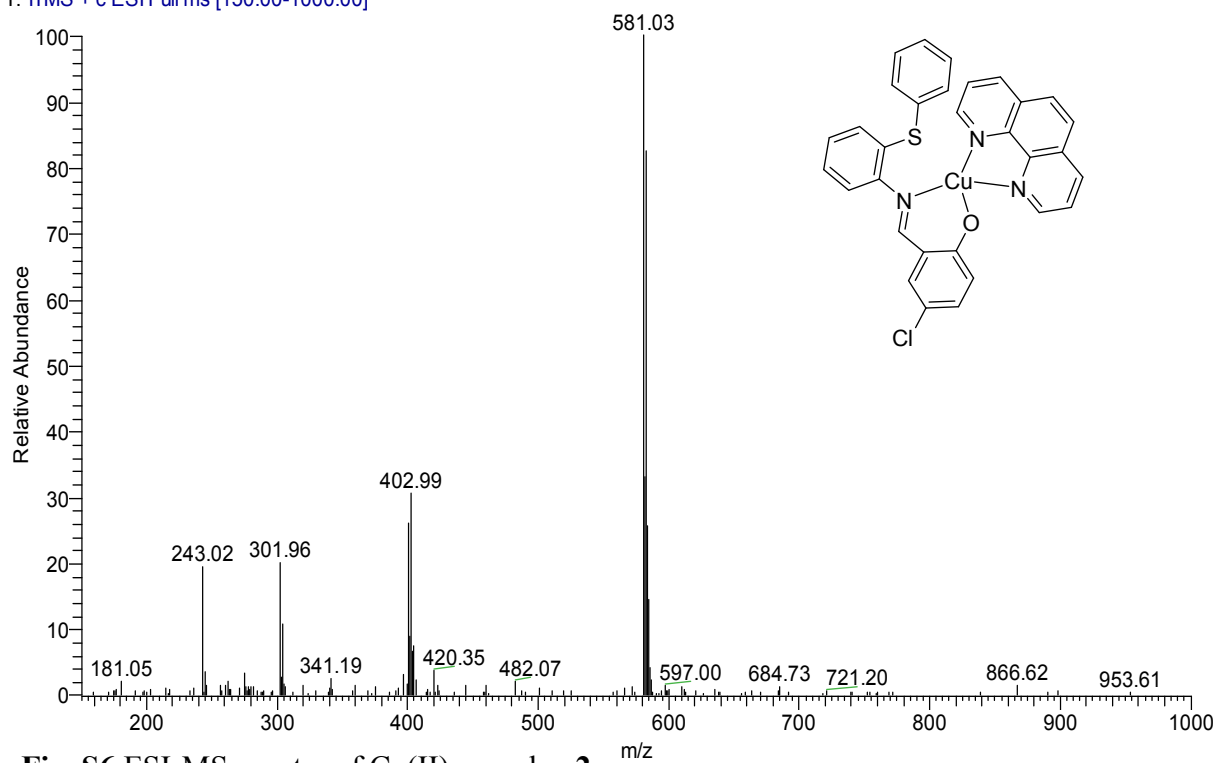


Fig. S6 ESI-MS spectra of Cu(II) complex 2.

16OBCL2_150110183637 #190 RT: 0.54 AV: 1 NL: 5.22E3
T: ITMS + c ESI Full ms [150.00-1000.00]

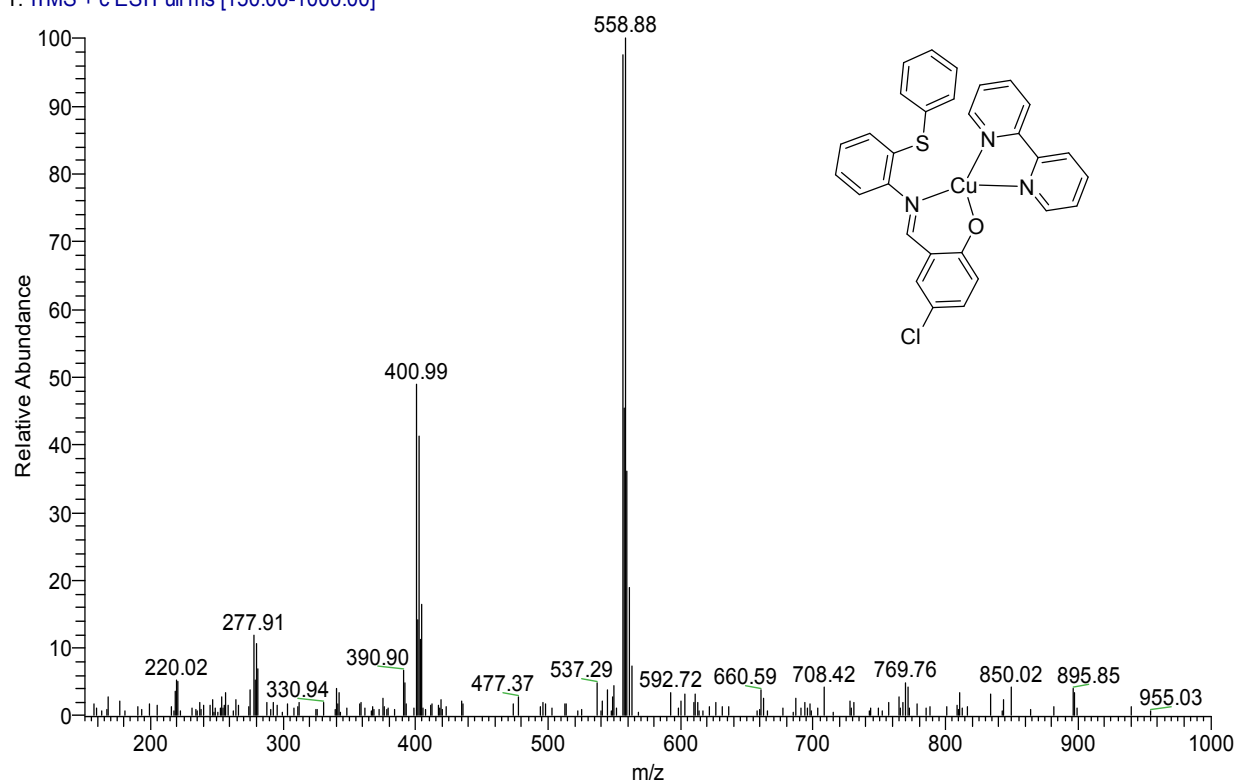


Fig. S7 ESI-MS spectra of Cu(II) complex **3**.

16OBCL3_150123155420 #124 RT: 0.35 AV: 1 NL: 7.91E3
T: ITMS + c ESI Full ms [150.00-1000.00]

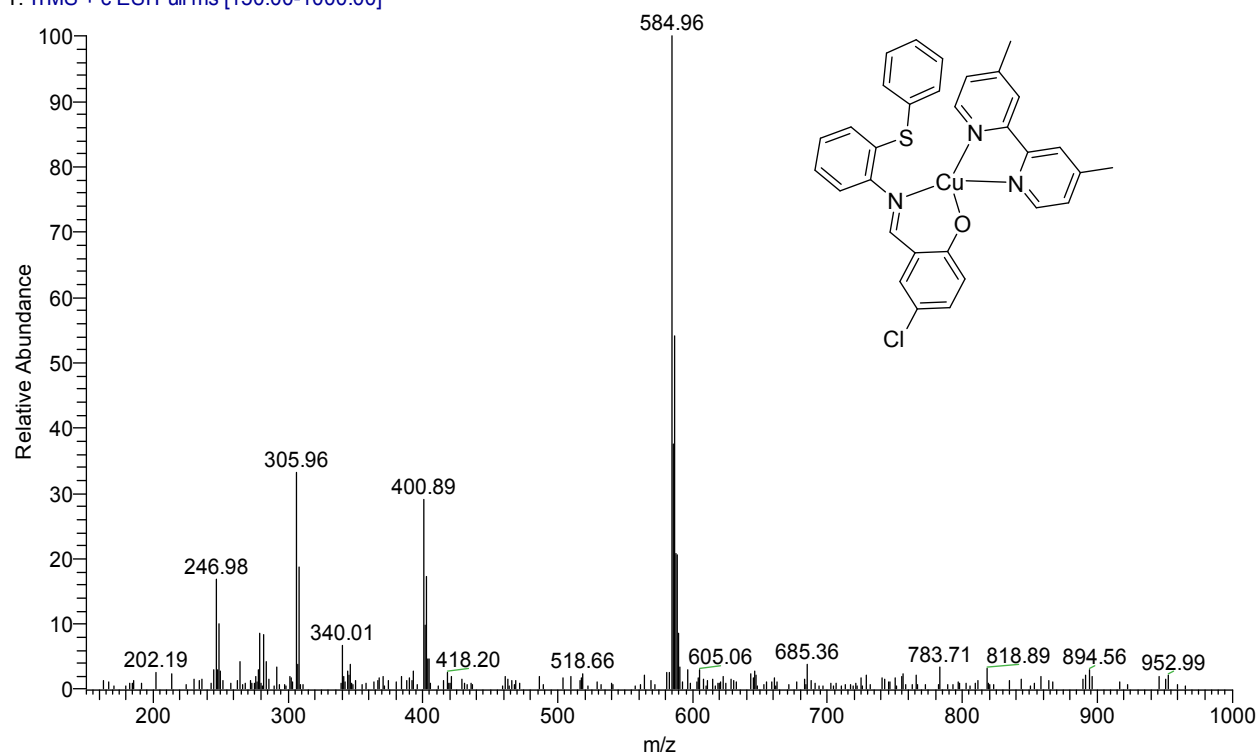


Fig. S8 ESI-MS spectra of Cu(II) complex **4**.

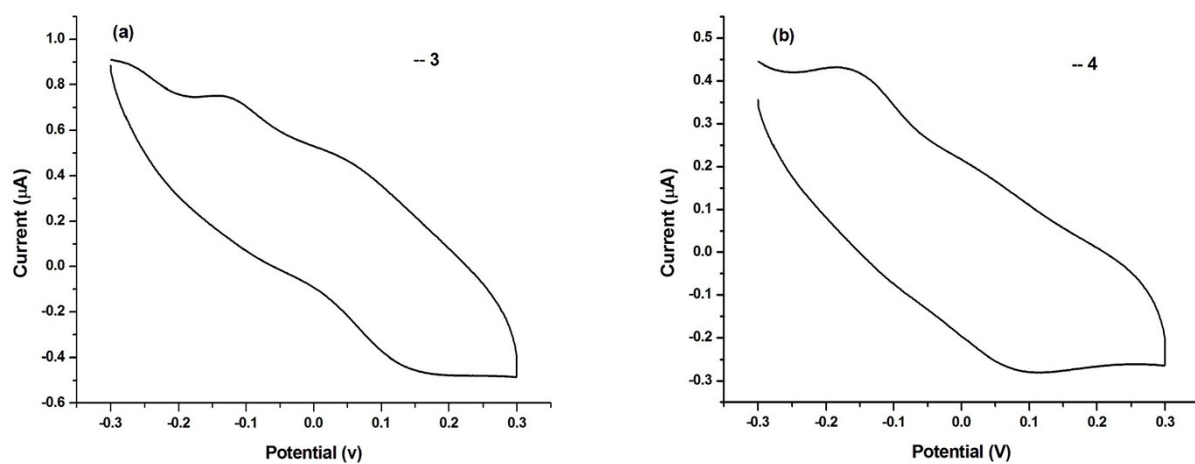


Fig. S9 Cyclic voltammograms of the complexes **3** (a) and **4** (b) in CH_3CN (0.1 TBAP) on a GC working electrode. Scan rate 100 mV s^{-1}

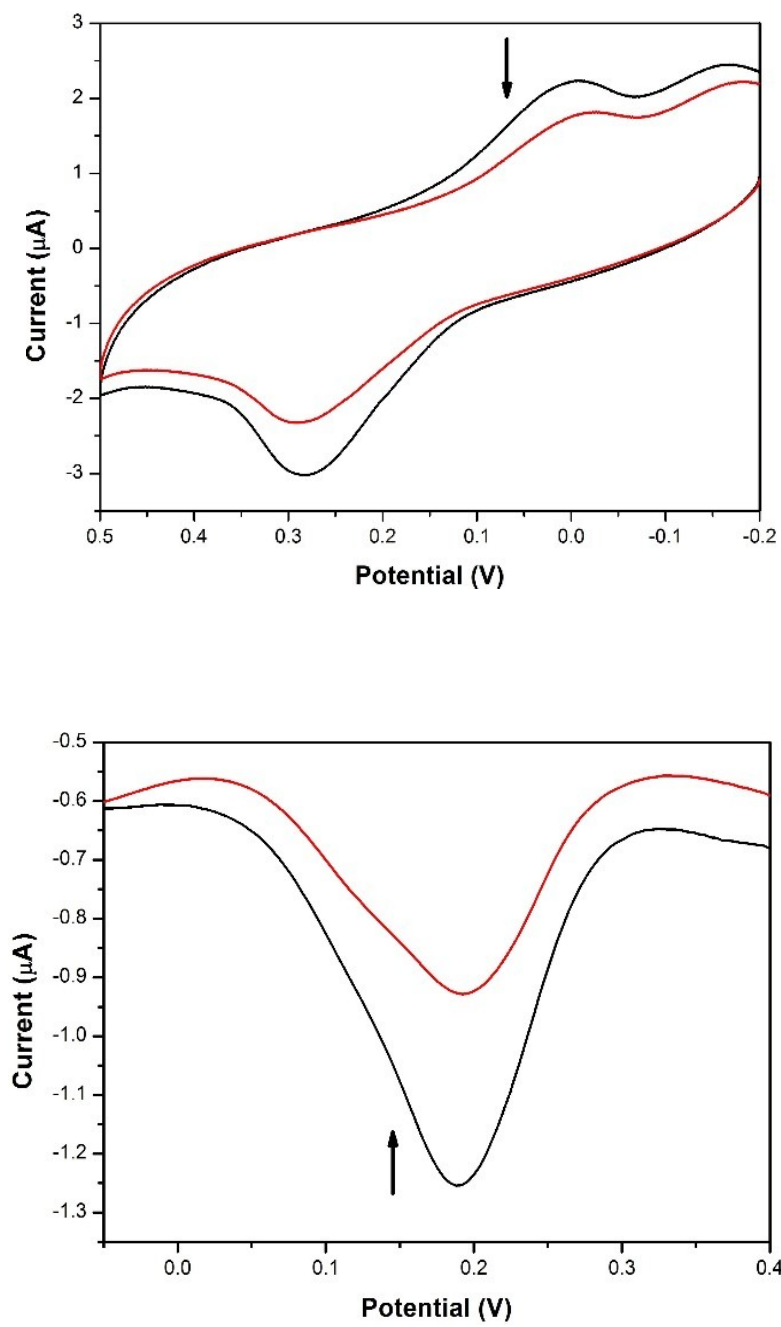


Fig. S10 CV and DPV of **1** in the absence and presence of HS-DNA at scan rate of 100 mV s^{-1} .

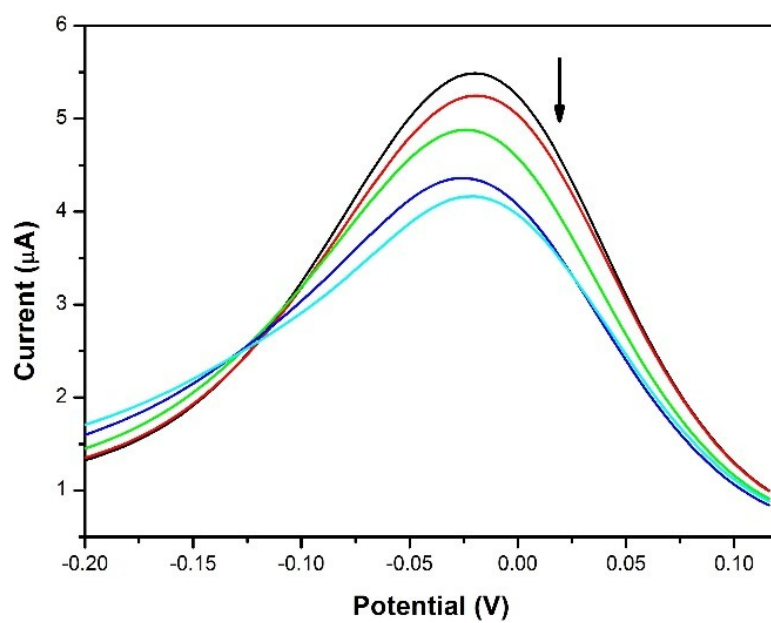
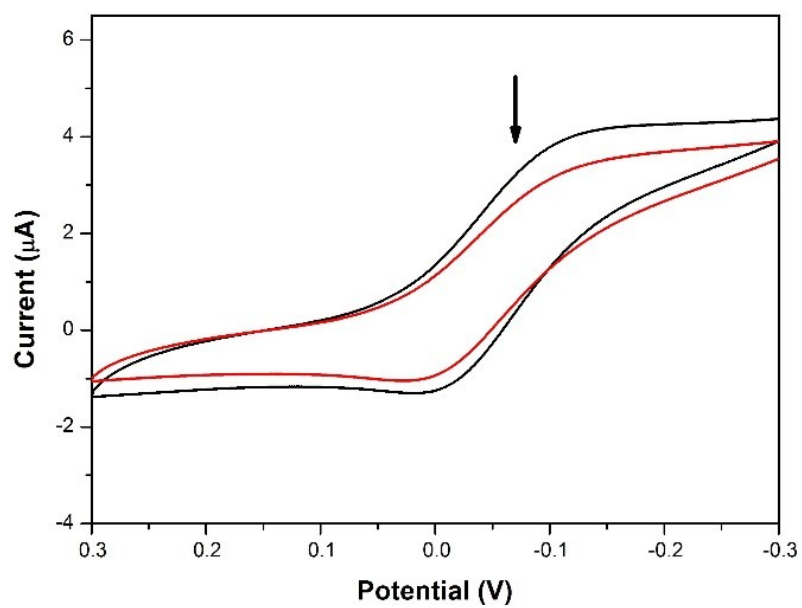


Fig. S11 CV and DPV of **2** in the absence and presence of HS-DNA at scan rate of 100 mV s^{-1} .

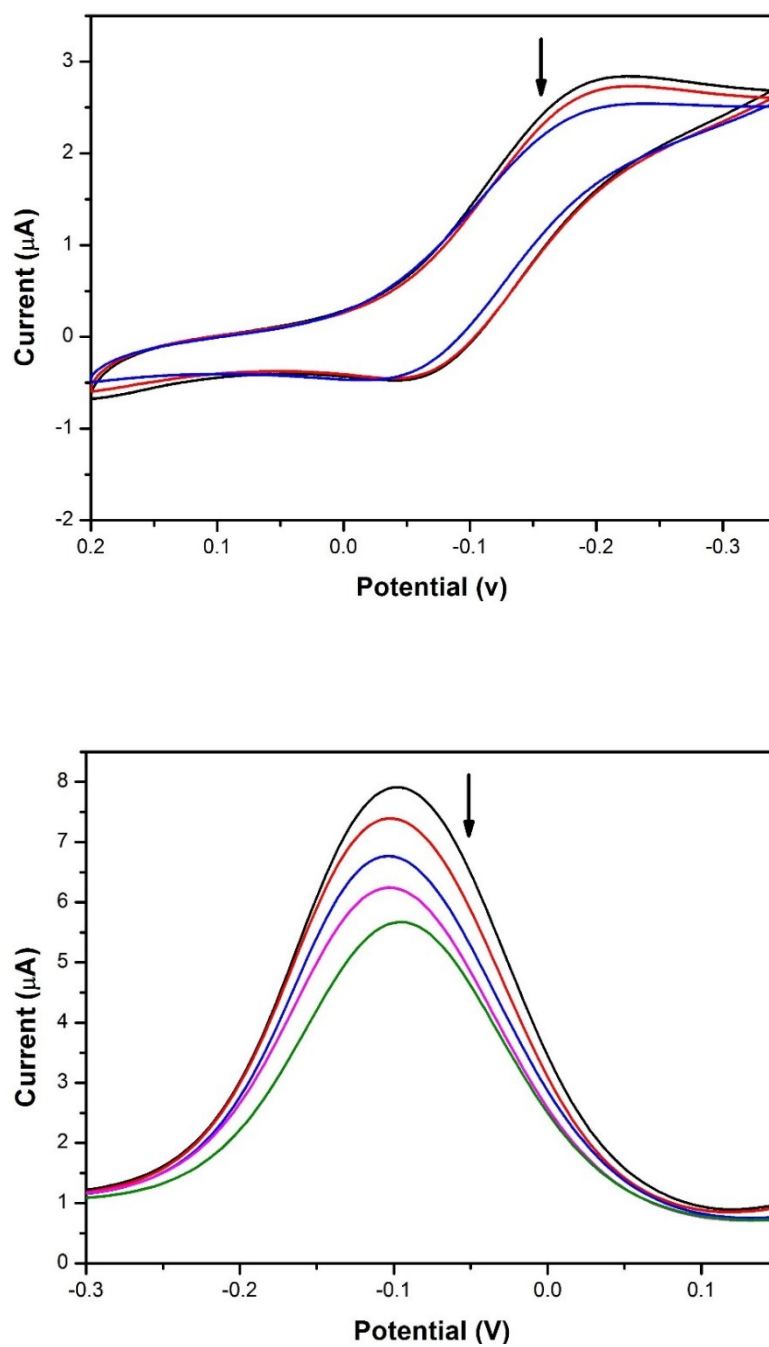


Fig. S12 CV and DPV of **4** in the absence and presence of HS-DNA at scan rate of 100 mV s^{-1} .

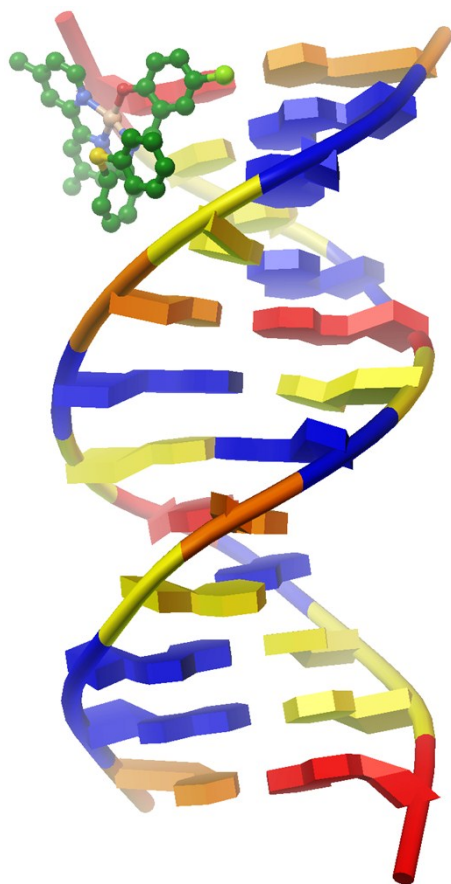


Fig. S13 Docked image of 423D bound ligand with remove of ClO₄ coordinate.

Table S1:

The calculated E-total value of docking protocol was validated with the removal of ClO₄ from complex **4** with DNA (423D)

Complex	E-Total Value (kcal mol ⁻¹)	Inhibitory constant (μM)	Binding region
423D bound ligand	-4.31	692.14	AT-GC