

Supporting information

Mixed-ligand copper(II) Schiff base complexes: the vital role of co-ligands in DNA/protein interactions and cytotoxicity

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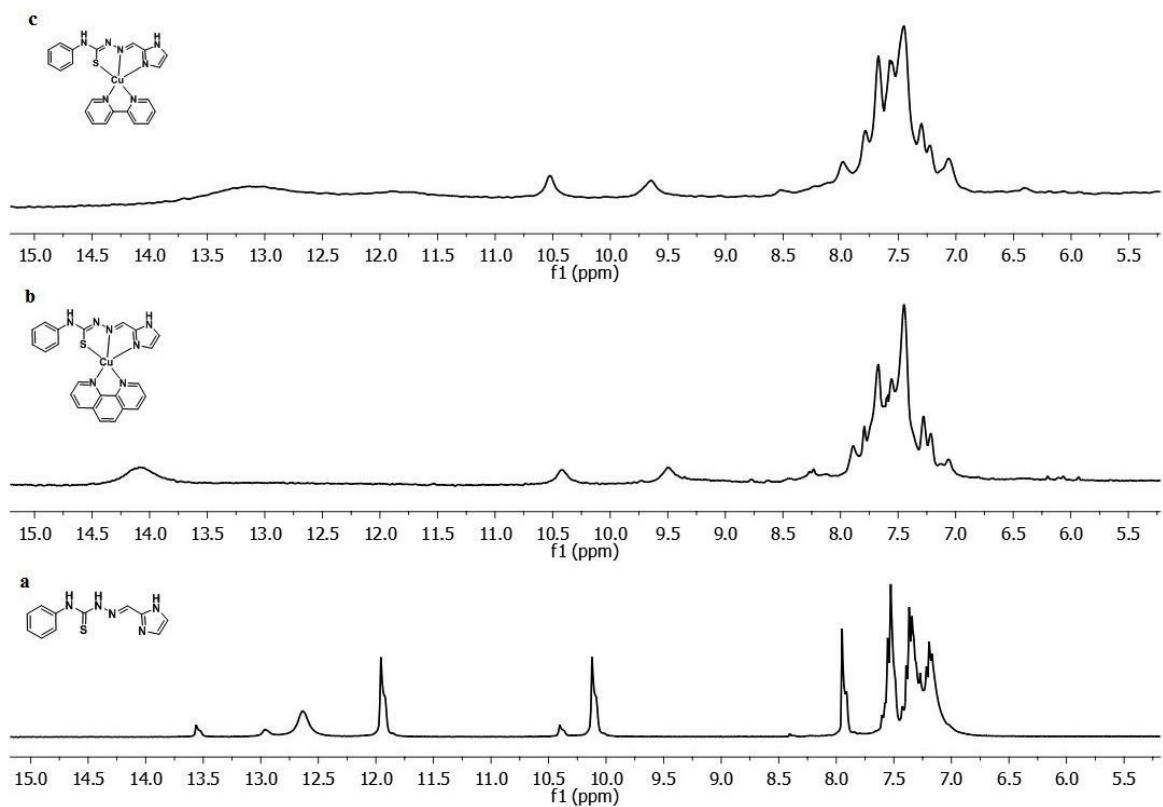


Fig. S1 ¹H NMR spectra of (a) ligand using DMSO-d₆ solvent (b) Cu(II) complexes of **1** and (c) **2** using in CD₃CN solvent.

166AL #18 RT: 0.22 AV: 1 NL: 8.57E3
T: ITMS - c ESI Full ms [50.00-1000.00]

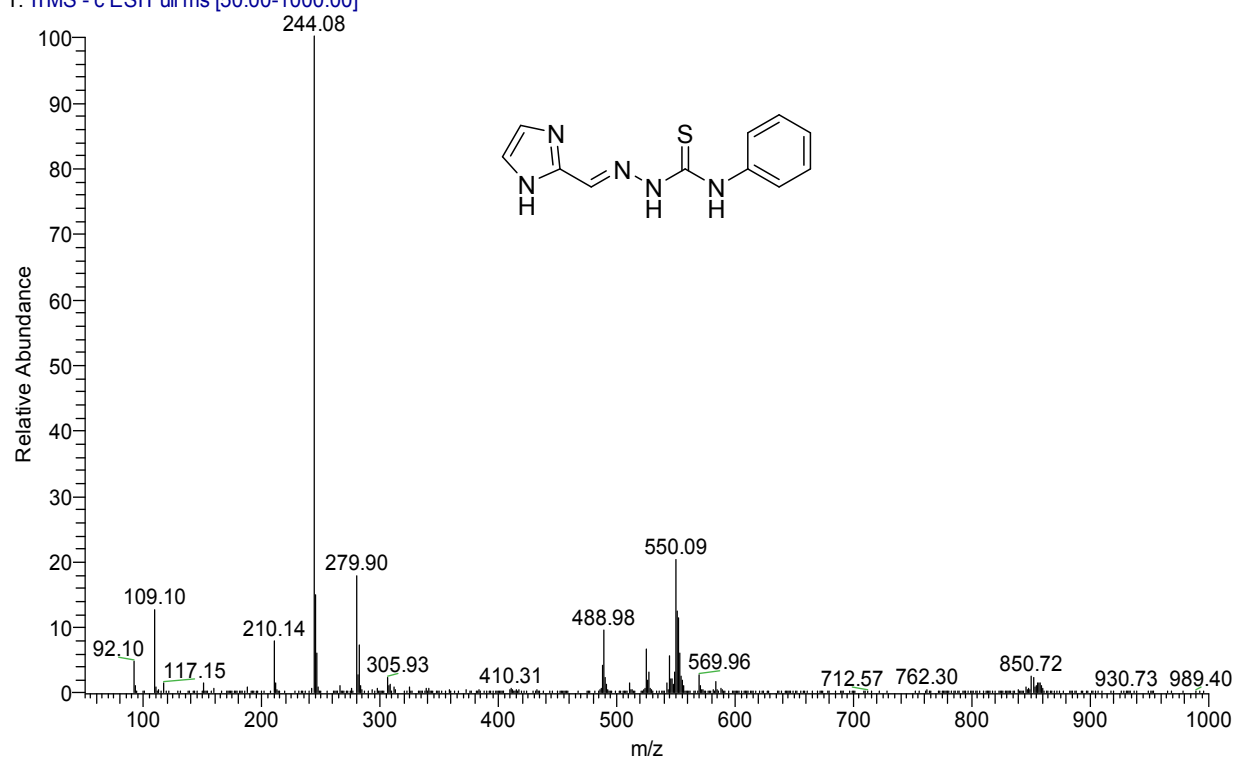


Fig. S2 ESI-MS spectrum of L.

166APHEN #11 RT: 0.14 AV: 1 NL: 2.32E4
T: ITMS + c ESI Full ms [50.00-1100.00]

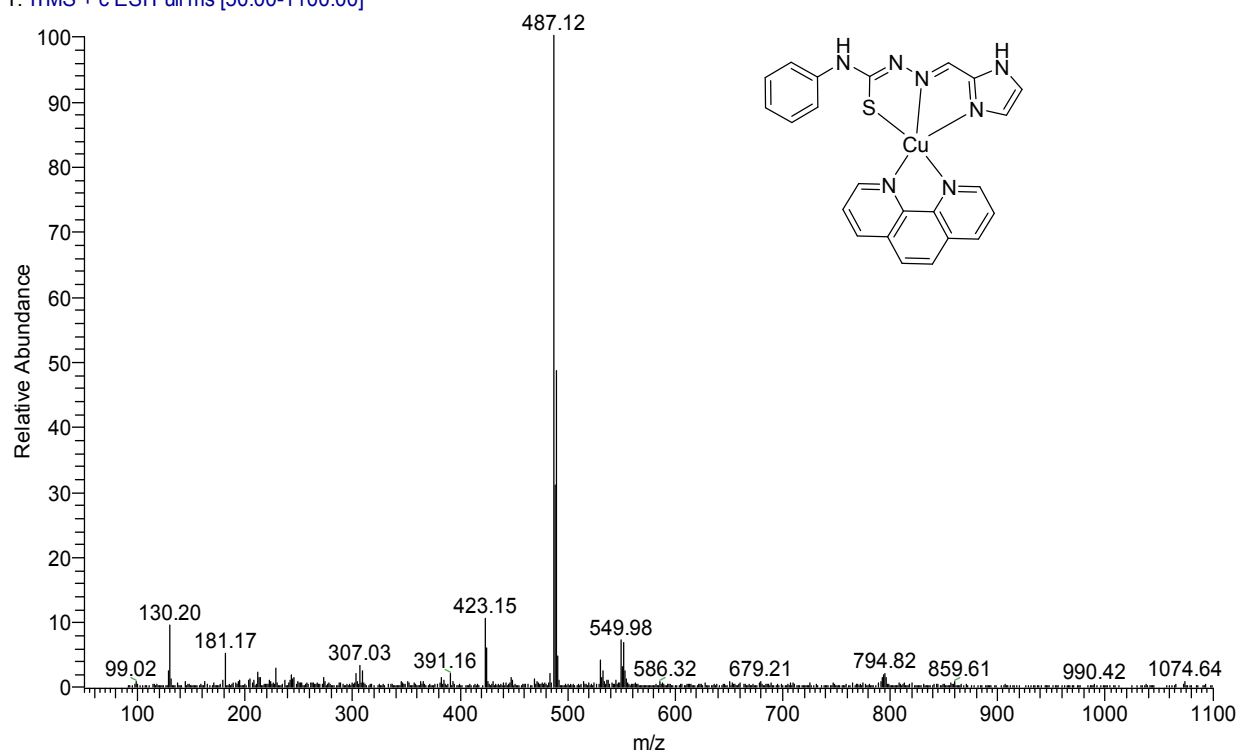


Fig. S3 ESI-MS spectrum of complex 1.

166AbPy#19 RT: 0.25 AV: 1 NL: 7.86E3
T: ITMS + c ESI Full ms [50.00-1100.00]

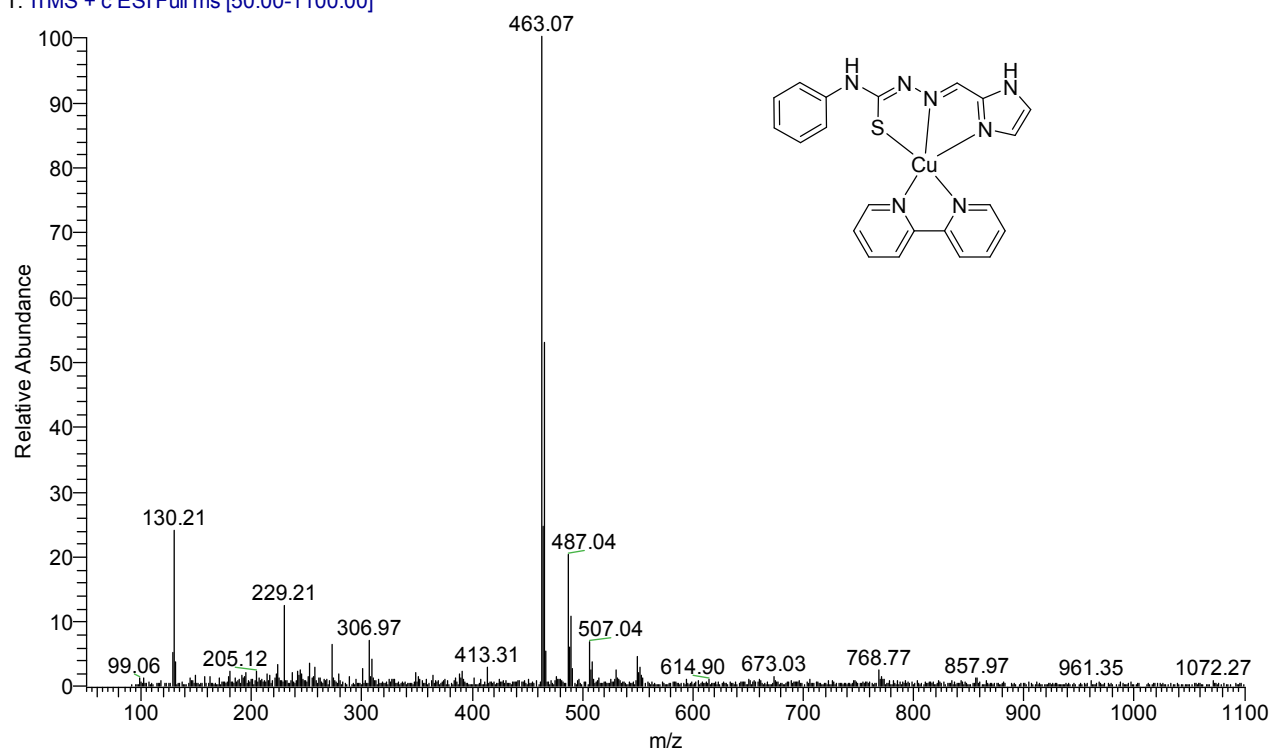


Fig. S4 ESI-MS spectrum of complex **2**.

166ADMBPY#31 RT: 0.41 AV: 1 NL: 1.08E4
T: ITMS + c ESI Full ms [50.00-1100.00]

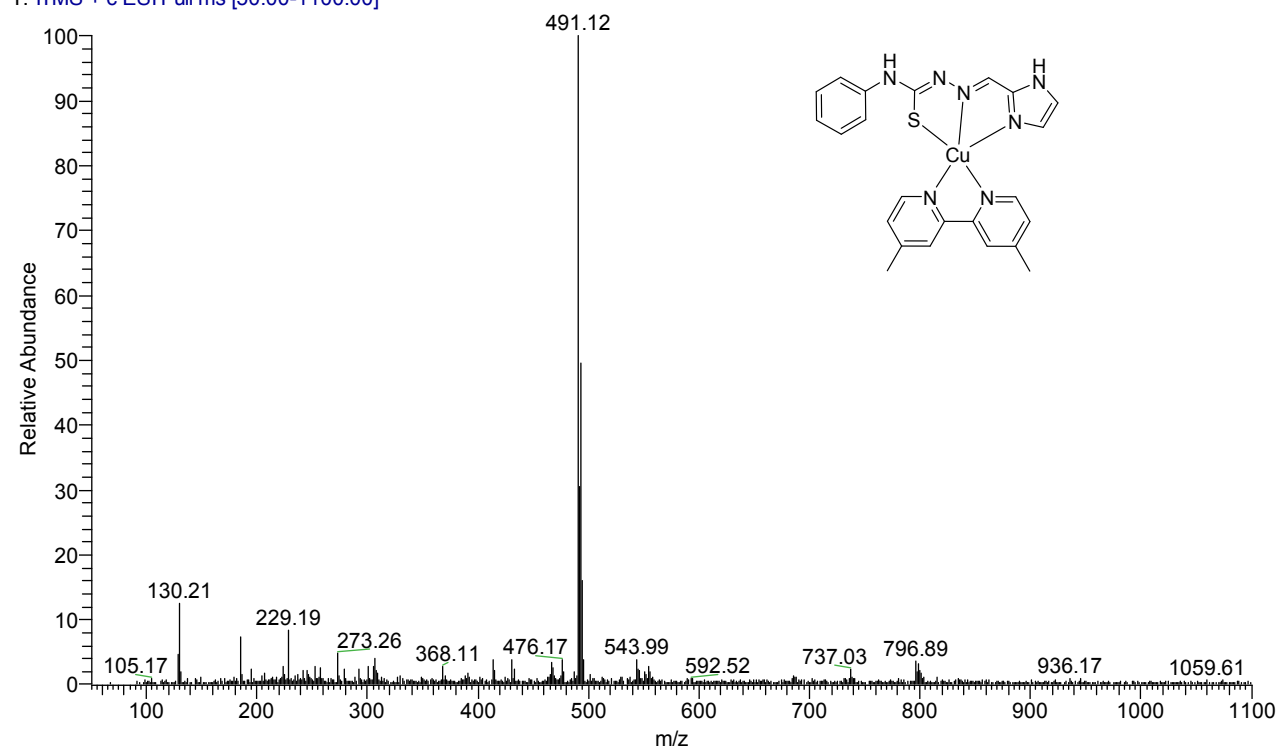


Fig. S5 ESI-MS spectrum of complex 3.

166DIPYRI#27 RT: 0.36 AV: 1 NL: 1.51E3
T: ITMS + c ESI Full ms [50.00-1100.00]

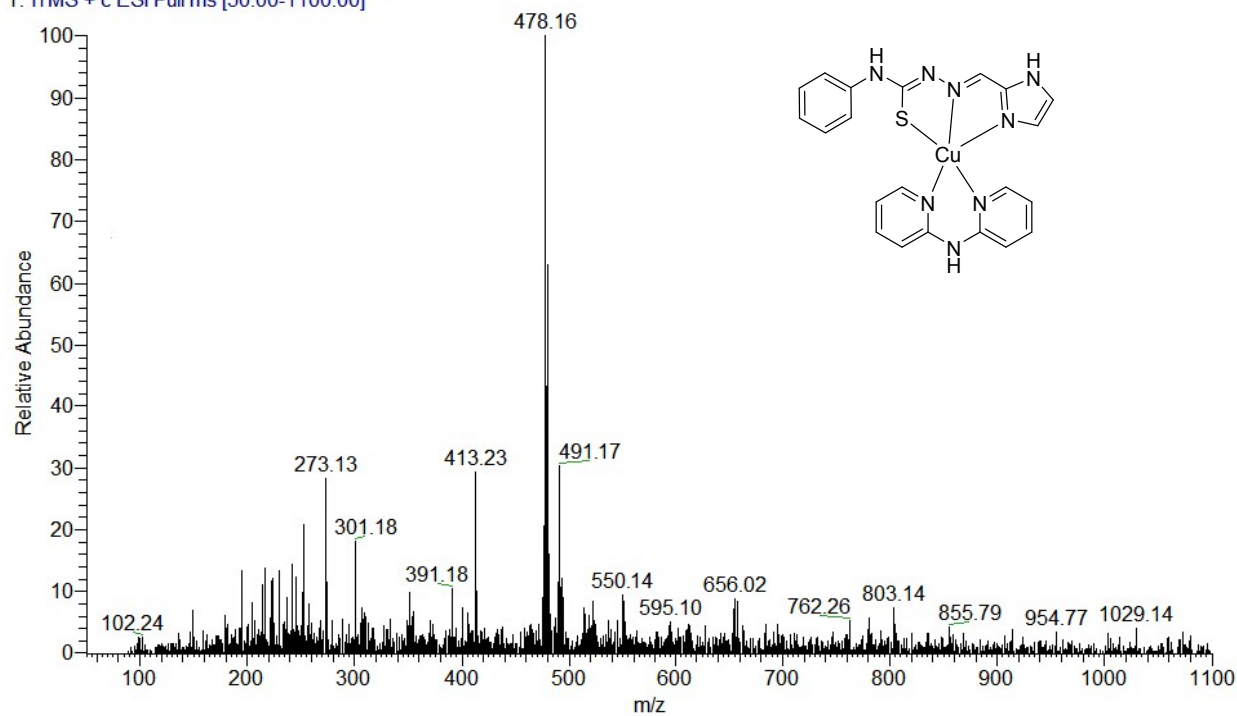


Fig. S6 ESI-MS spectrum of complex 4.

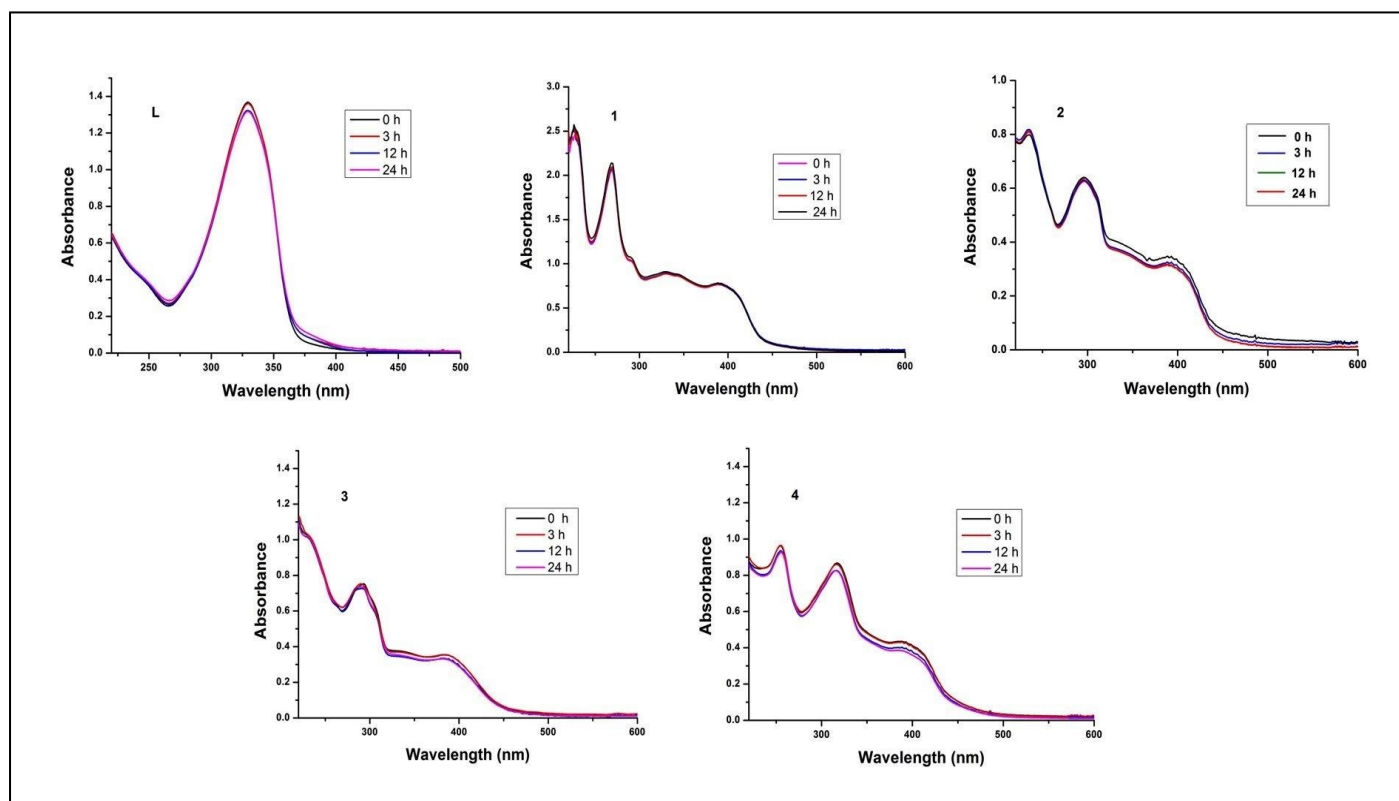


Fig. S7 Stability of L and complexes 1-4 were monitored for 0-24 h in MeOH/Tris-HCl buffer solution at room temperature.

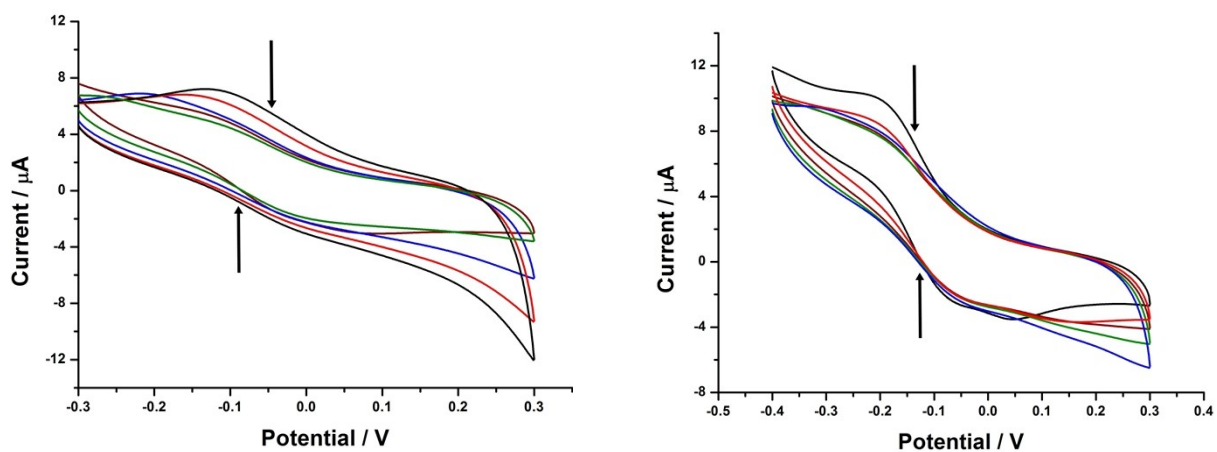


Fig. S8 CV of complexes **2** and **3** in the absence and presence of HS-DNA at scan rate of 100 mV/s.

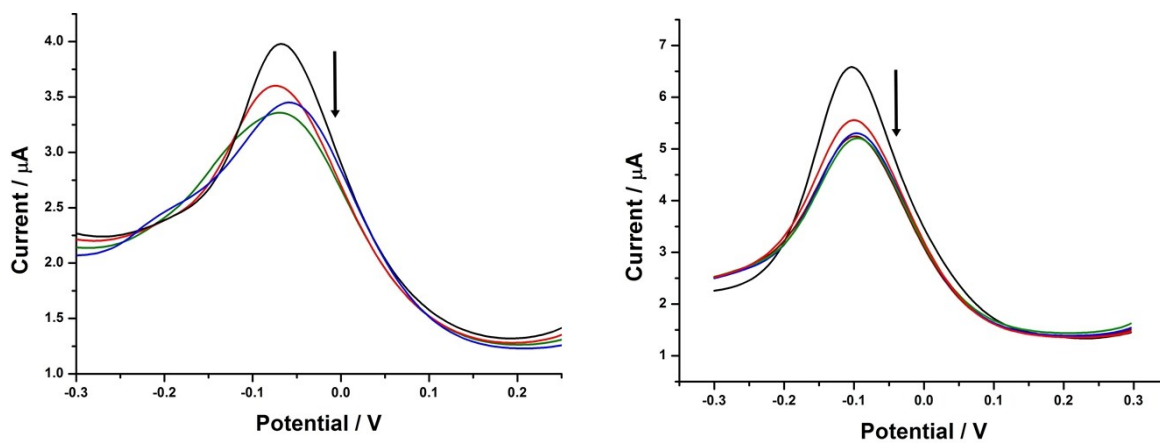
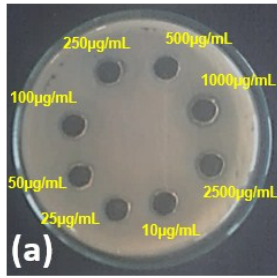


Fig. S9 DPV of complexes **2** and **3** in the absence and presence of HS-DNA in buffer/CH₃CN solution.

P. aeruginosa



S. aureus

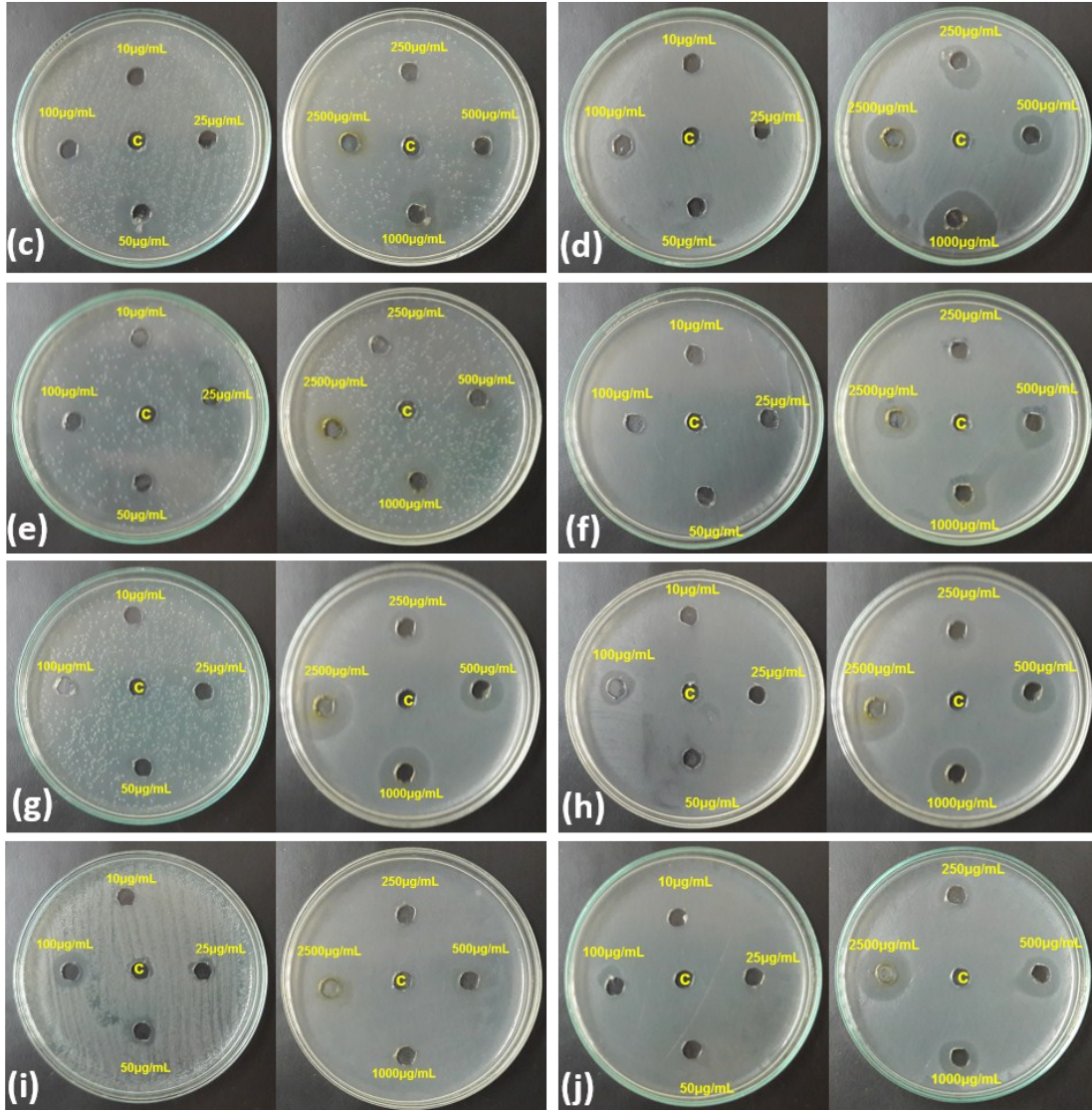
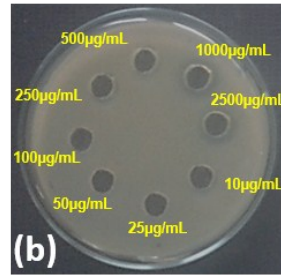


Fig. S10 Antibacterial activity of compound with *Pseudomonas aeruginosa* [(a) L (c) 1 (e) 2 (g) 3 and (i) 4] and *S. aureus* [(b) L (d) 1 (f) 2 (h) 3 and (j) 4].

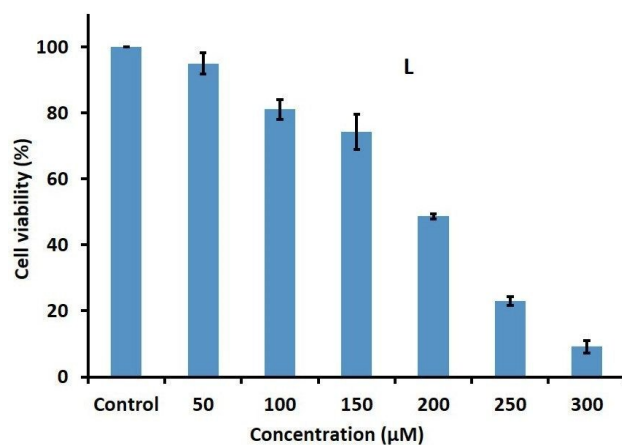


Fig. S11 Cell viability of AGS gastric cancer cells after exposure with L for 24 h.

Table S1 The calculated free energy, inhibitory constant and binding region of the Cu(II) complexes with B-DNA (1BNA)

Complexes	Free energy of binding (FEB) (kcal/mol)	Inhibitory constant (µM)	Binding region
1	-4.66	383.0	Guanine, Cytosine, Adenine
2	-4.19	845.4	Guanine, Cytosine
3	-4.34	658.3	Guanine, Cytosine, Adenine
4	-3.99	1190.0	Guanine, Cytosine, Adenine, Thymine

Table S2 Means of inhibition zones diameter obtained by agar well diffusion method against *Staphylococcus aureus* and *Pseudomonas aeruginosa*.

Complex	Means of zones of bacterial growth inhibition (mm)	
	<i>S. aureus</i>	<i>P. aeruginosa</i>
1	14	17
2	12	14
3	13	15
4	12	11

Table S3: Means of inhibition zones diameter obtained by agar well diffusion method against *Staphylococcus aureus*.

Compound	Zones of growth inhibition (mm)							
	10 (µg/mL)	25 (µg/mL)	50 (µg/mL)	100 (µg/mL)	250 (µg/mL)	500 (µg/mL)	1000 (µg/mL)	2500 (µg/mL)
L	7	7	7	8	9	9	10	10
1	10	10	11	13	15	16	18	22
2	10	10	10	11	13	14	16	17
3	10	10	10	12	14	16	19	17
4	10	10	10	10	12	14	15	20

Table S4: Means of inhibition zones diameter obtained by agar well diffusion method against *Pseudomonas aeruginosa*.

Compound	<i>Zones of growth inhibition (mm)</i>							
	10 ($\mu\text{g/mL}$)	25 ($\mu\text{g/mL}$)	50 ($\mu\text{g/mL}$)	100 ($\mu\text{g/mL}$)	250 ($\mu\text{g/mL}$)	500 ($\mu\text{g/mL}$)	1000 ($\mu\text{g/mL}$)	2500 ($\mu\text{g/mL}$)
L	6	6	6	6	8	8	11	11
1	11	11	16	18	19	20	21	23
2	10	10	14	15	14	17	18	20
3	10	11	12	16	17	18	20	22
4	10	10	10	10	12	13	14	15