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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Figure captions

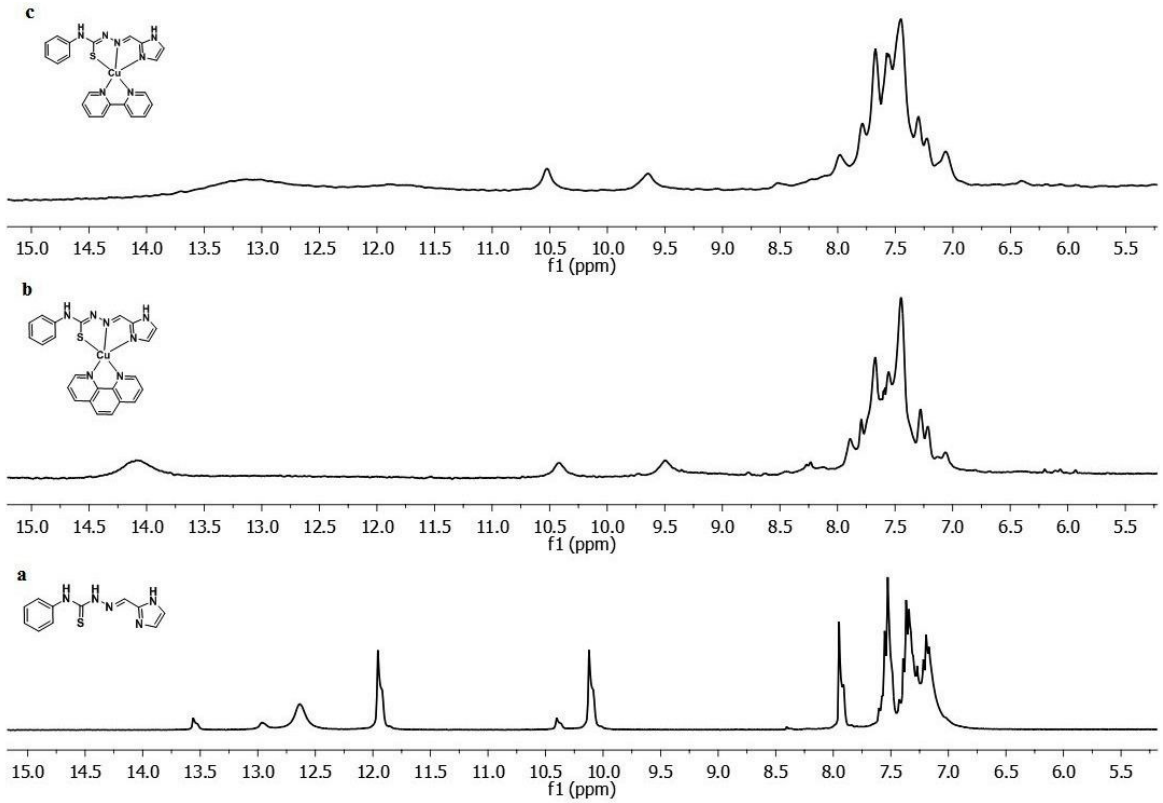

Fig. S1 ^{1}H NMR spectra of (a) ligand using DMSO-d_6 solvent (b) Cu(II) complexes of **1** and (c) **2** using in CD_3CN solvent.

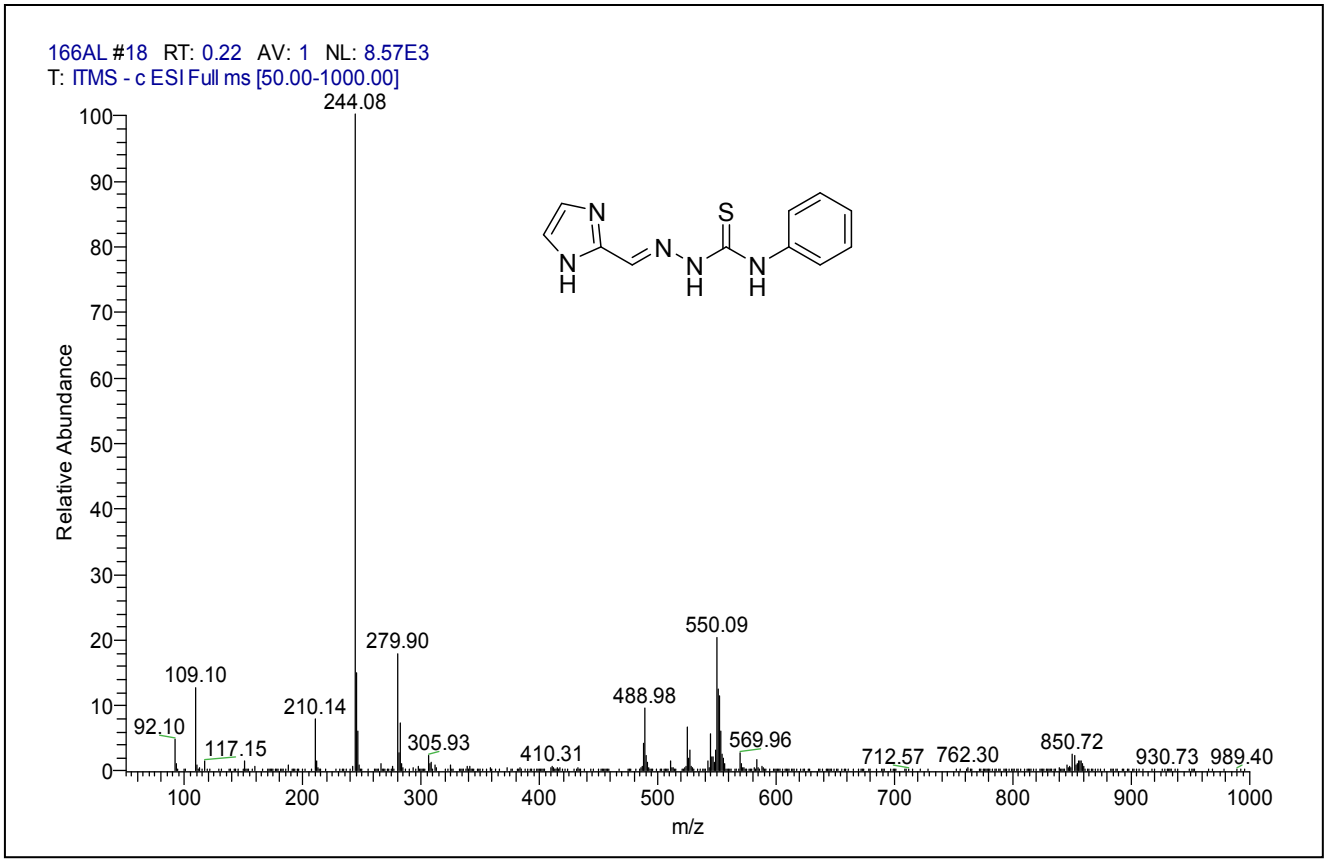

Fig. S2 ESI-MS spectrum of L.

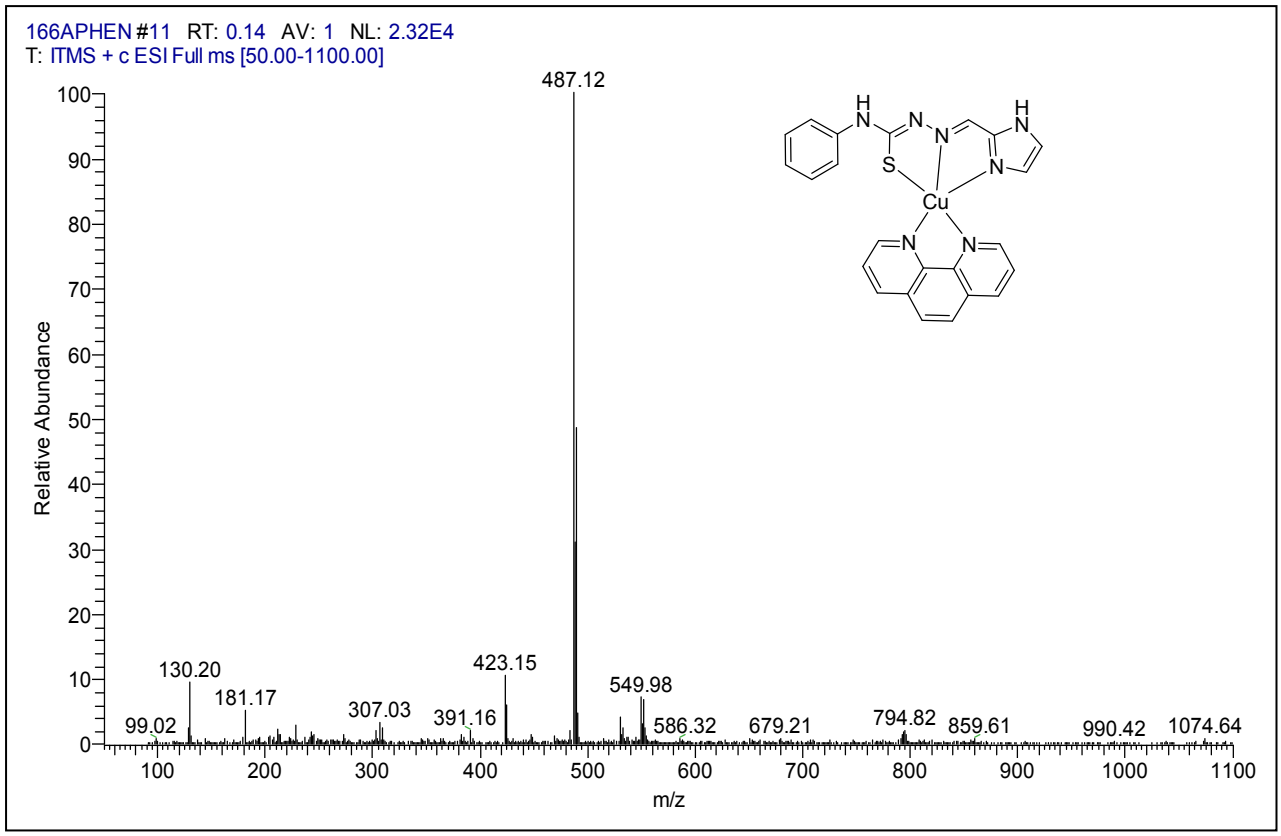

Fig. S3 ESI-MS spectrum of complex **1**.

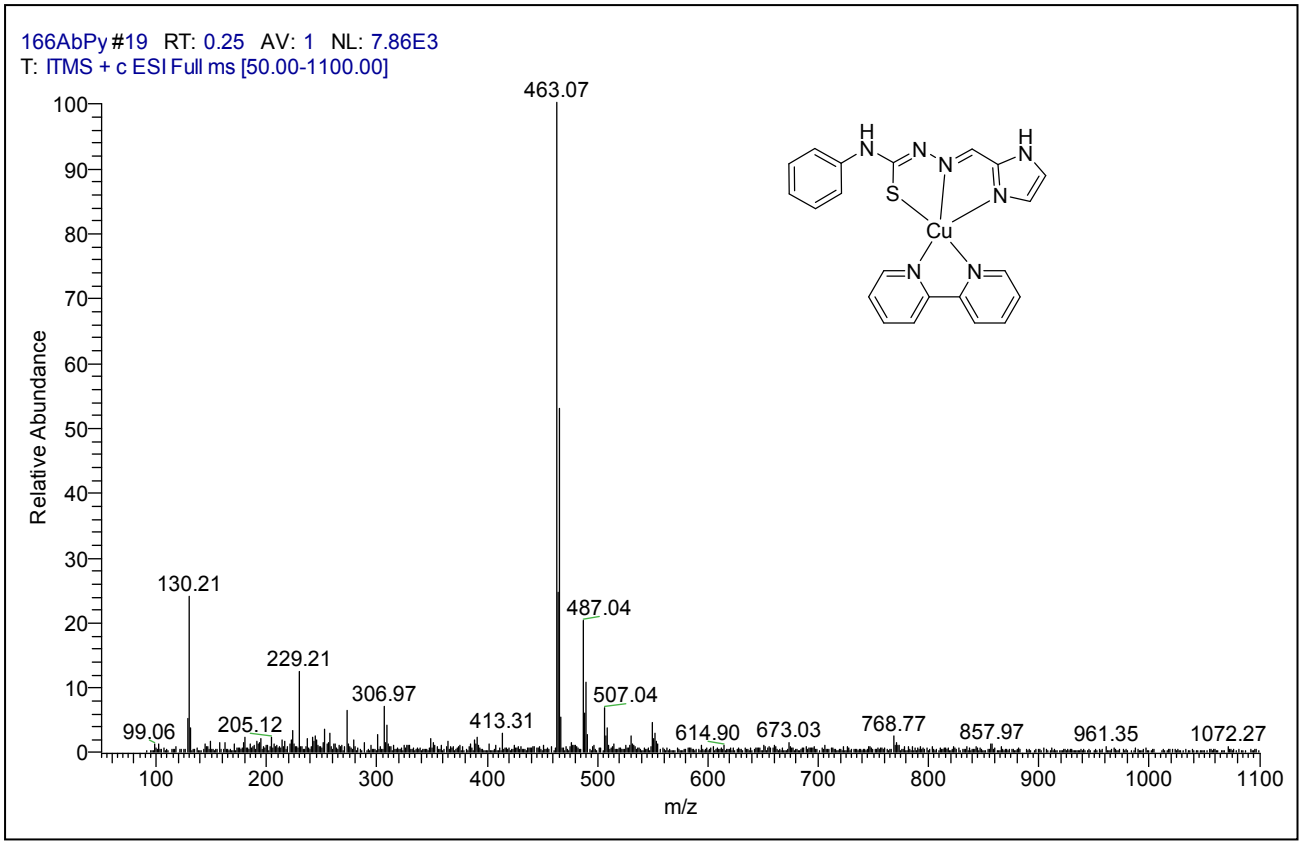

Fig. S4 ESI-MS spectrum of complex **2**.

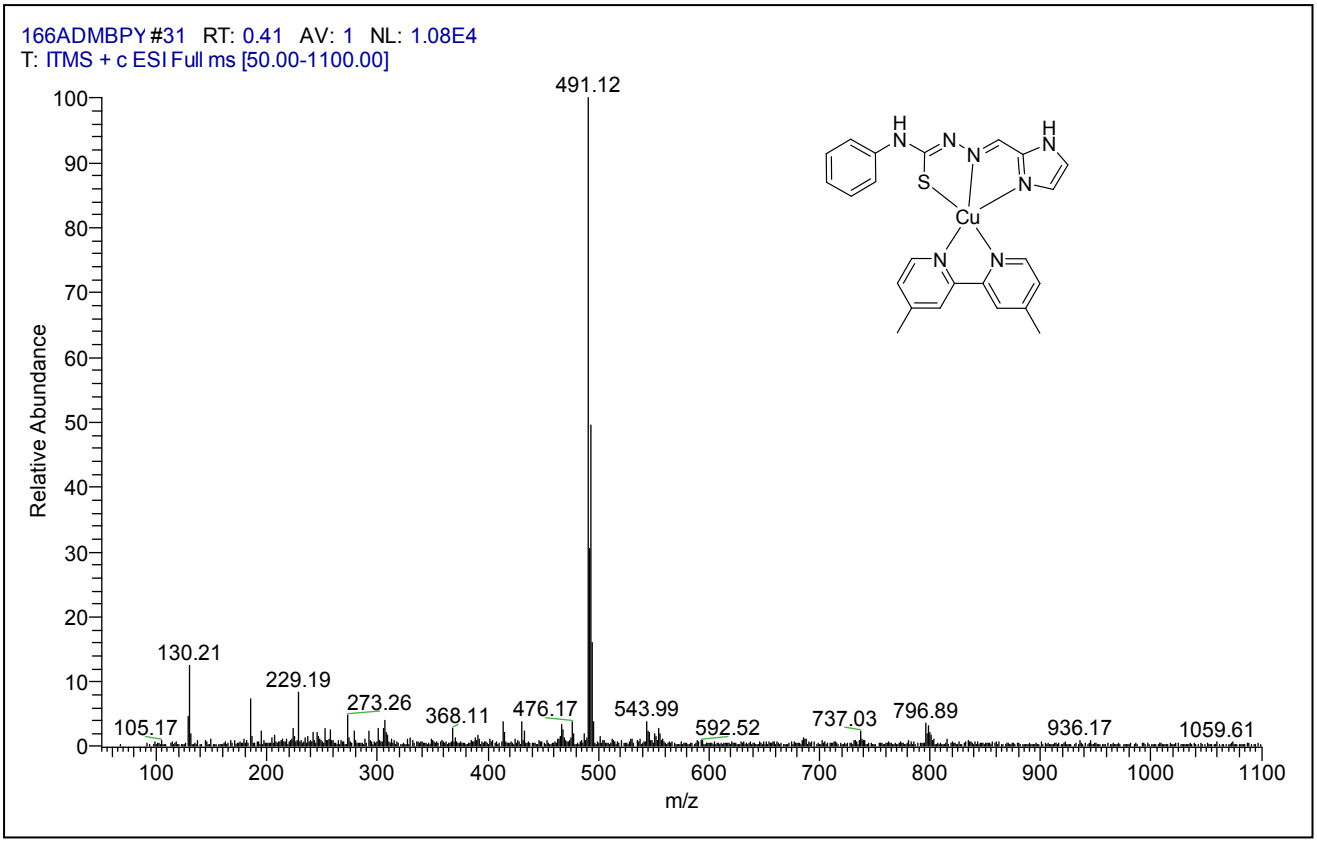

Fig. S5 ESI-MS spectrum of complex **3**.

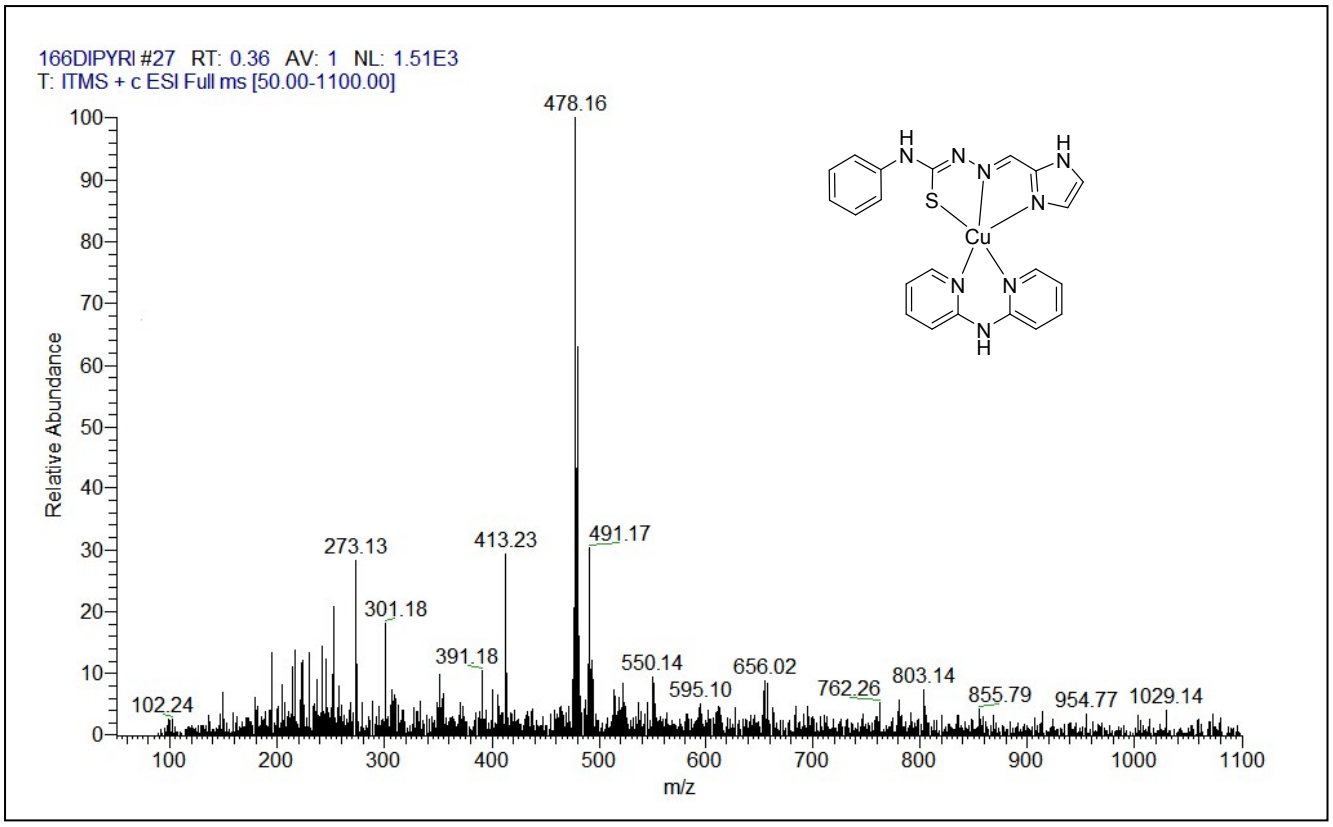

Fig. S6 ESI-MS spectrum of complex **4**.

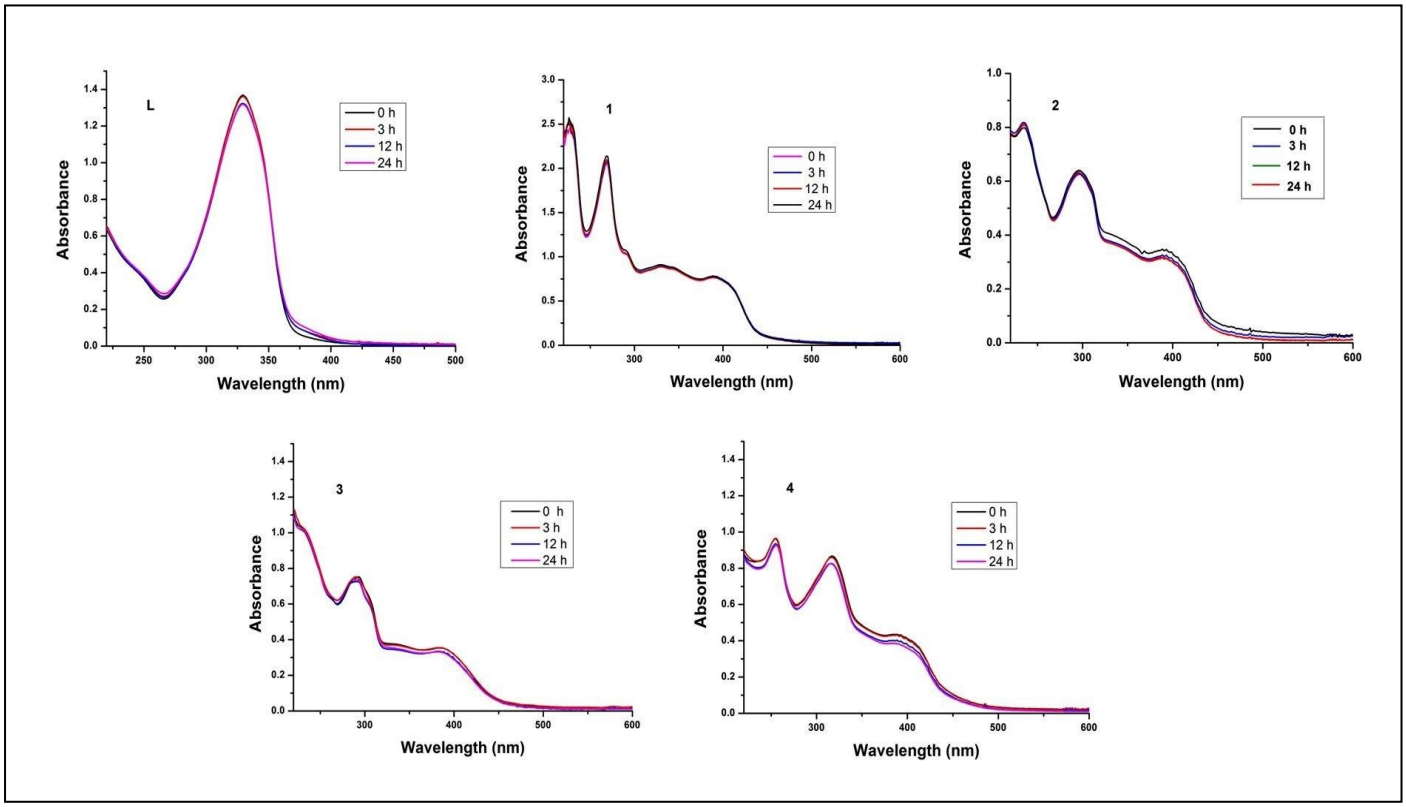

Fig. S7 Stability of L and complexes **1-4** were monitored for 0-24 h in MeOH/Tris-HCl buffer solution at room temperature.

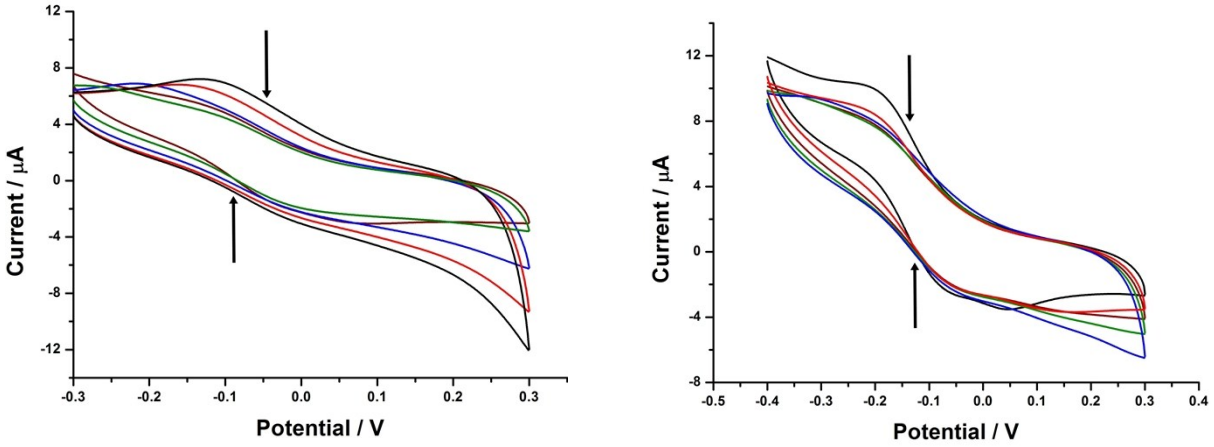

Fig. S8 CV of complexes **2** and **3** in the absence and presence of HS-DNA at scan rate of 100 mV/s.

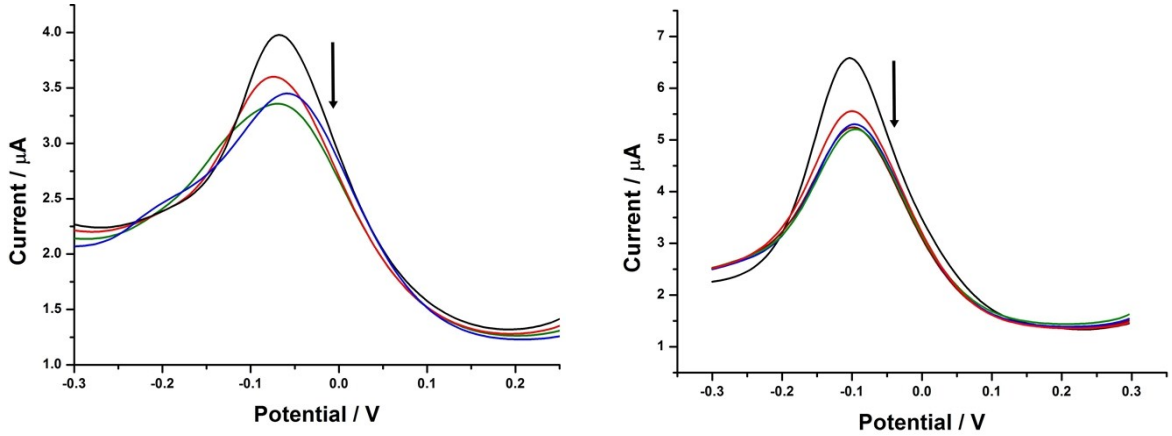

Fig. S9 DPV of complexes **2** and **3** in the absence and presence of HS-DNA in buffer/CH_3CN solution.

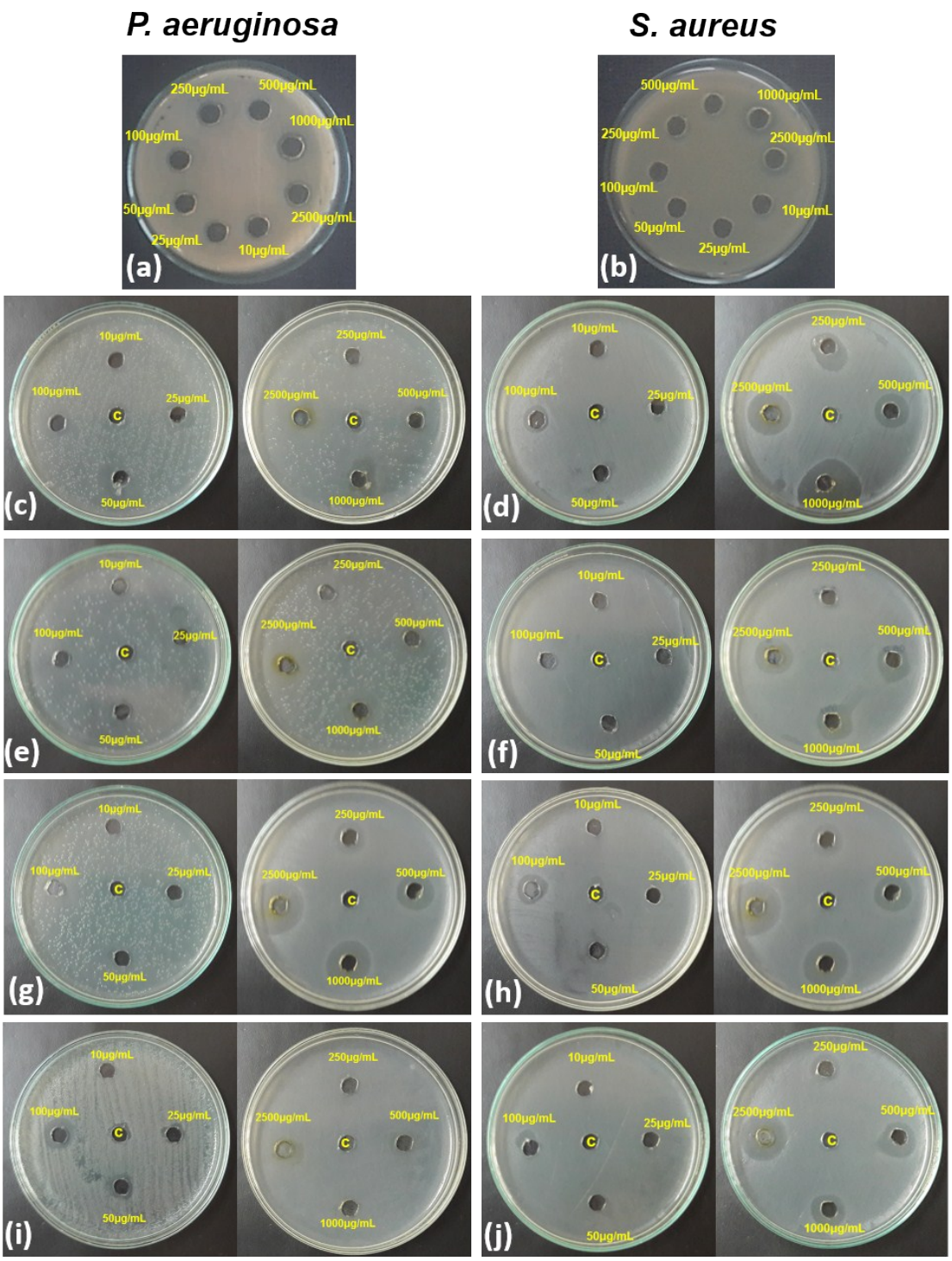

Fig. S10 Antibacterial activity of compound with *Pseudomonas aeruginosa* [(a) L (c) **1** (e) **2** (g) **3** and (i) **4**] and *S. aureus* [(b) L (d) **1** (f) **2** (h) **3** and (j) **4**].

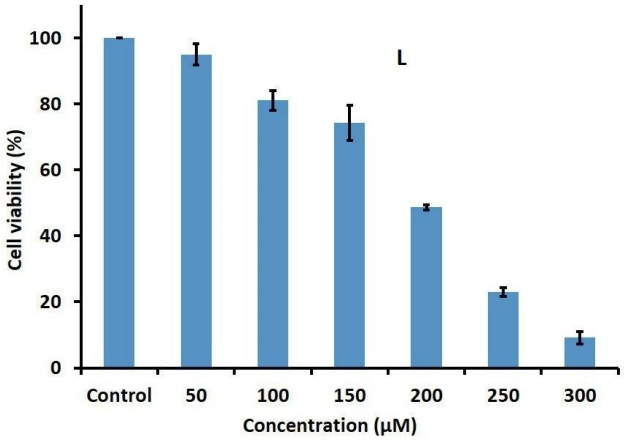

Fig. S11 Cell viability of AGS gastric cancer cells after exposure with L for 24 h.

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)	
	S. aureus	***P. aeruginosa***
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	***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	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