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**Electronic Supplementary Information (ESI) for New Journal of Chemistry** 

## Unpredicted formation of copper(II) complexes containing 2-thiophen-2-yl-1-thiophen-2-ylmethyl-1h-benzoimidazole and most promising *in vitro* cytotoxicity in MCF-7 and HeLa cell lines over *cisplatin*

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Fig. S1. Stability of the ligand and complexes in 0.1 % DMSO in aqueous and PBS buffer medium



Fig. S2. NMR spectra of Ligand in DMSO solvent







Fig. S4. EPR spectrum of Complex 1b in Room Temperature at X-band.



Fig. S5. The circular dichroism spectra of free CT-DNA (10  $\mu$ m) and after the addition of the ligand and complexes 1a and 1b (10  $\mu$ m).



Fig. S6. Absorption titration spectra of ligand and complexes 1a and1b with BSA



Fig. S7. Synchronous spectra of BSA (10  $\mu$ M) in the presence of increasing concentration of Ligand and complexes 1a and 1b for a wavelength difference of  $\Delta\lambda = 60$  nm.





Fig. S8. DPPH scavenging activity of the ligand and new Cu(II) complexes.



**Fig. S9.** The ligand and newly synthesized copper complexes (**1a** and **1b**) inhibit MCF-7 cell proliferation in a dose dependent manner. MCF-7 cells were treated with different concentrations of complexes for 48 h, the cell viability was determined and the results were expressed as percentage cell viability with control. Results shown are mean, which are three separate experiments performed in triplicate,



**Fig. S10.** The ligand and newly synthesized copper complexes (**1a** and **1b**) inhibit HeLa cell proliferation in a dose dependent manner. HeLa cells were treated with different concentrations of complexes for 48 h, the cell viability was determined and the results were expressed as percentage cell viability with control. Results shown are mean, which are three separate experiments performed in triplicate.



**Fig. S11**. The ligand and newly synthesized copper complexes (**1a** and **1b**) inhibit human normal Embryonic Kidney cells proliferation in a dose dependent manner. Cells were treated with different concentrations of complexes for 48 h, the cell viability was determined and the results were expressed as percentage cell viability with control. Results shown are mean, which are three separate experiments performed in triplicate.



Table S1: Selected bond lengths (Å) and bond angles (°) of Cu(II) complexes

	Bond lengths		Bond angles	
Complex 1a	Cu(1)-Cl(1)	2.205(2)	N(1)-Cu(1)- Cl(1)	96.66(18)
	Cu(1)-N(1)	1.975(6)	N(1)-Cu(1)-N(3)	168.2(3)
	Cu(1)-N(3)	1.980(6)	N(3)-Cu(1)-Cl (1)	94.2(2)
	Cu(1)-N(3)	1.975(7)	N(3)-Cu(1)-Cl(1)	168.4(2)
			N(3)-Cu(1)-N(1)	92.8(2)
			N(3)-Cu(1)-N(3)	77.0(3)
Complex 1b	Cu(1)-Cl(13)	2.2632(2)	Cl(1)-Cu(1)-Cl(1)	180.0
	Cu(1)-N(1)	1.990(6)	N(1)-Cu(1)-Cl(1)	88.35(11)
			N(1)-Cu(1)-Cl (1)	91.65(11)
			N(1)-Cu(1)-Cl(1)	180.0
			N(1)-Cu(1)-N (1)	180.0

Bond lengths	Experimental	DFT
Cu(1)-Cl(1)	2.205	2.312
Cu(1)-N(1)	1.975	1.995
Cu(1)-N(3)	1.980	2.080
Cu(1)-N(3)	1.975	2.000
Bond Angles	Experimental	DFT
N(1)-Cu(1)-Cl(1)	96.66	96.35
N(1)-Cu(1)-N(3)	168.2	169.19
N(3)-Cu(1)-Cl(1)	94.2	94.40
N(3)-Cu(1)-Cl(1)	168.4	168.29
N(3)-Cu(1)-N(1)	92.8	94.74
N(3)-Cu(1)-N(3)	77.0	74.62

Table. S2. Experimental and theoretical calculations of complex 1a

Table S3: The  $K_b$ ,  $K_{sv}$  and  $K_{app}$  values for the interactions of ligand and complexes with CT-DNA

Compound	$K_b/\mathrm{M}^{-1}$	$K_{sv}/M^{-1}$	$K_{app}/\mathrm{M}^{-1}$
Ligand	1.89±0.33×10 <sup>4</sup>	1.98±0.08×10 <sup>3</sup>	$1.60 \times 10^{6}$
Complex 1a	6.75±0.25×10 <sup>5</sup>	2.59±0.03 ×10 <sup>3</sup>	1.58×10 <sup>6</sup>
Complex 1b	2.52±0.25×10 <sup>5</sup>	$2.21\pm0.06 \times 10^{3}$	1.61×10 <sup>6</sup>

**Table S4:** Quenching constant ( $K_{sv}$ ), binding constant ( $K_{bin}$ ) and number of binding sites (n) for the interactions of ligand and complexes (**1a** and**1b**) with BSA

Compound	$K_{SV}/M^{-1}$	K <sub>bin</sub> /M <sup>-1</sup>	'n'
Ligand	1.029±0.03 x 10 <sup>4</sup>	2.011±0.10×10 <sup>3</sup>	$0.8163 \pm 0.01$
Complex 1a	$2.805.\pm0.08\times10^4$	$8.600 \pm 0.18 \times 10^4$	$1.1169 \pm 0.03$
Complex 1b	$2.076 \pm 0.06 \times 10^4$	$8.074 \pm 0.19 \times 10^{3}$	$0.9006 \pm 0.03$

Table S5: The radical scavenging activity of the ligand and the new Cu(II) complexes

Compound	IC <sub>50</sub> values ( $\mu$ g /ml)
	DPPH <sup>.</sup>
Standard	57.62±0.99

Ligand	27.61±0.35
Complex 1a	12.27±0.18
Complex 1b	15.18±0.16