Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications
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Supplementary Material

Design, synthesis and crystal structure determination of dinuclear copper- based potential chemotherapeutic drug entity; *in vitro* DNA binding, cleavage studies and an evaluation of genotoxicity by micronucleus test and comet assay

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Figure Captions

Fig. S1. EPR spectra of complex **1b** and **2b** at variables temperature in solid state.

Fig. S2. EPR spectra of complex **1b** and **2b** at variables temperature in liquid state (MeOH).

Fig. S3. H–bonding network of complex **1b**.

Fig. S4. Packing of complex **1b** along three crystallographic axes.

Fig. S5. Absorption spectral traces of **2a** and **2b** (a,b) in Tris HCl buffer upon addition of CT DNA at 25 °C. Inset: Plots of [DNA]/ ε_b vs [DNA] for the titration of CT DNA with complexes ■, experimental data points; full lines, linear fitting of the data. [complex] 6.67 x 10^{-6} M, [DNA] 0-33.3 x 10^{-6} M.

Fig. S6. Emission spectra of **2a** and **2b** (a, b) in Tris HCl buffer DNA in the presence of DNA at 25 °C. [DNA] 0-33.3 x 10^{-6} M. Arrow shows the intensity changes upon increasing concentration of the complexes.

Fig. S7. Fluorescence emission spectra of the EB-CT DNA system in the absence and presence of complexes. **2a** and **2b** (a,b) at 25 °C. [complex], [EB], [DNA] = 1 X 10^{-5} M.

Fig. S8. CD spectra of CT DNA alone and in presence of **2a** and **2b** (a,b)in Tris HCl buffer at 25 ^{o}C. [Complex] = 1 x10^{-7} M, [DNA] =1 x10^{-7} M. Sky blue line represent DNA alone, dark blue line represent S-enantiomer interacting with DNA and red line represent R-enantiomer interacting with DNA.

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Fig. S9. The cleavage patterns of the agarose gel electrophoresis for pBR322 plasmid DNA (300 ng) by **1**–**2** (**a** and **b**) at 25 °C after 45 minutes of incubation in buffer (5mM Tris HCl/ 50 mM NaCl, pH= 7.2). Lane 1, DNA; Lane 2, 0.05 mmol metal complex+ DNA**;** Lane 3, 0.10 mmol metal complex + DNA; Lane 4, 0.15 mmol metal complex + DNA; Lane 5, 0. 20 mmol metal complex + DNA; Lane 6, 0.25 mmol metal complex + DNA.

Fig. S10. (a) Mean comet tail length (TL), (b) Mean Olive tail moment (OTM) for peripheral blood lymphocytes (PBL) in control and groups treated with CDDP, **1b**, and Extra Virgin Olive oil (EVOO) and their combination in healthy *Rattus norvegicus* (Wistar rats). Values are expressed as mean ± SD (n=5). Values that do not share a common superscript letter differ significantly at $p<0.05$(One-way ANOVA followed by Tukey test).

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Figures

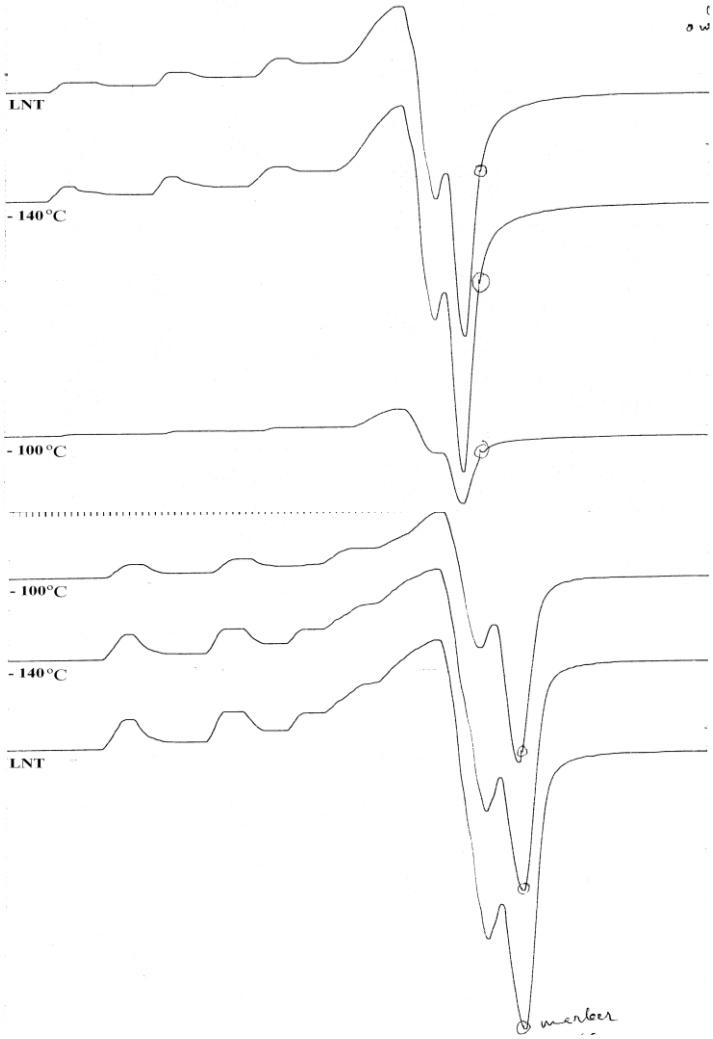
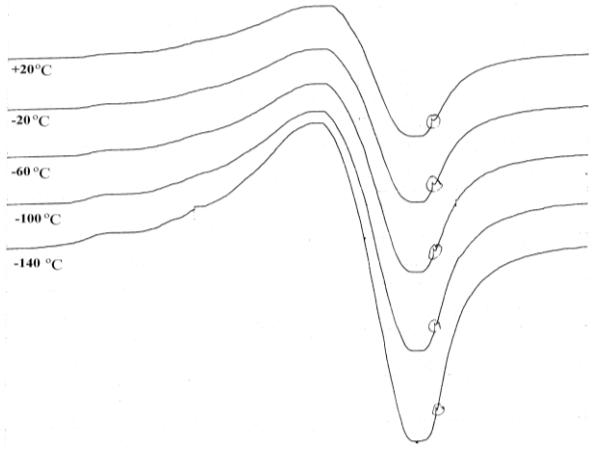


Fig. S1



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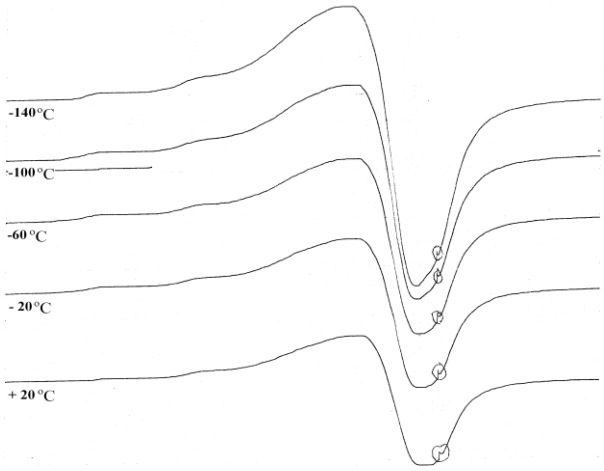


Fig. S2

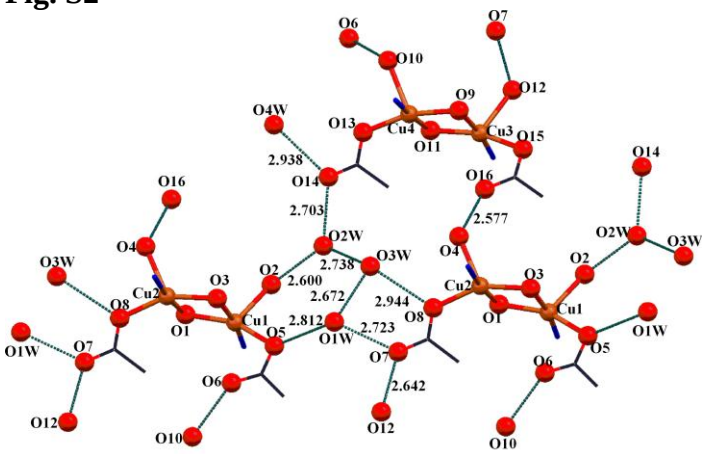
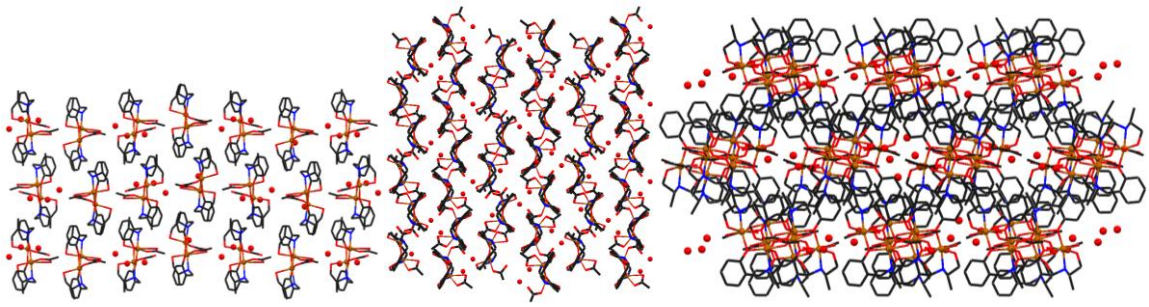


Fig. S3



a–axis ***b–axis*** ***c–axis***

Fig. S4

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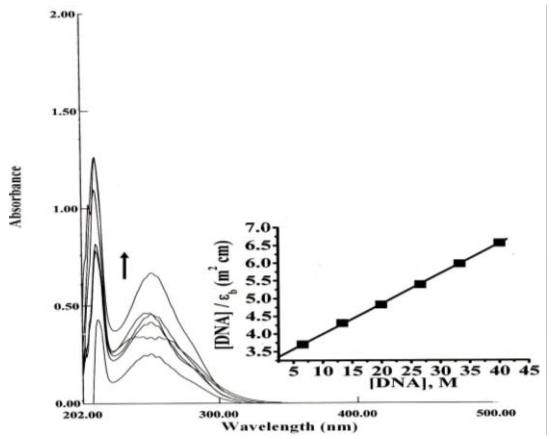
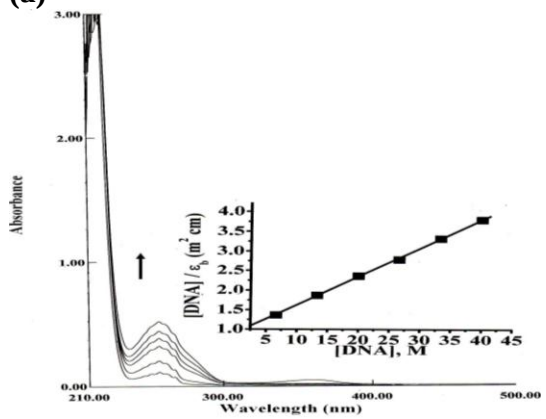
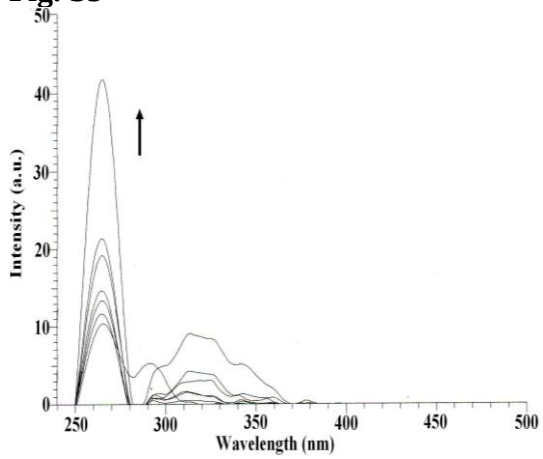


(a)



(b)

Fig. S5



(a)

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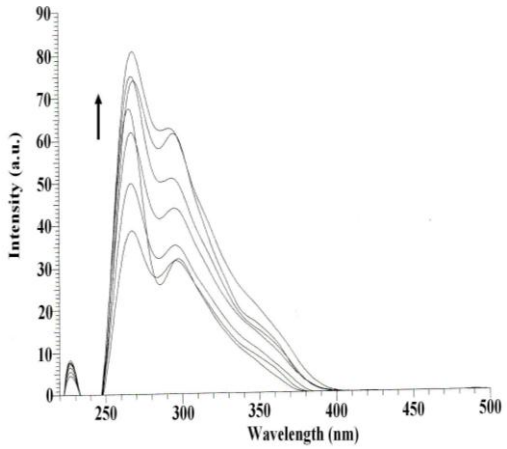
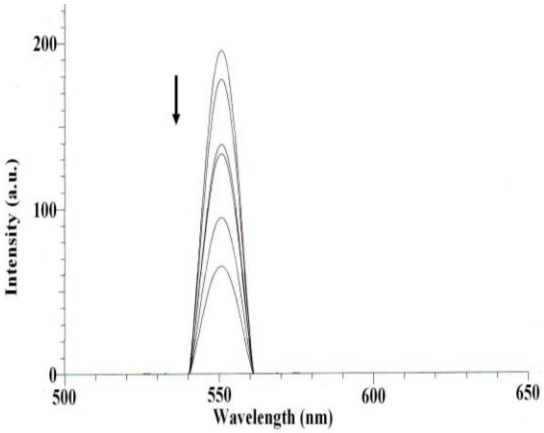


(b)

Fig. S6



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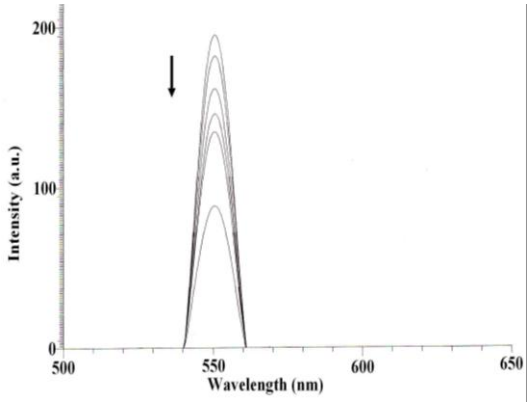

(b)

Fig. S7

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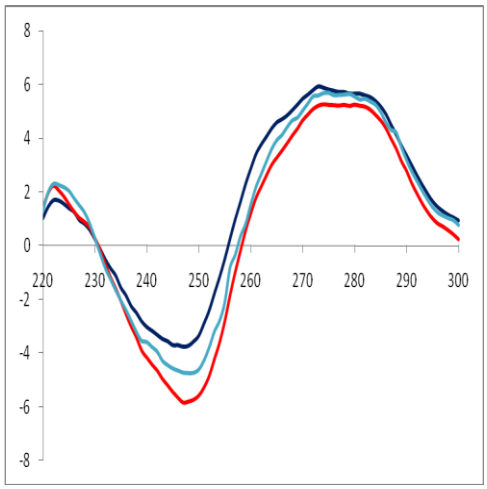

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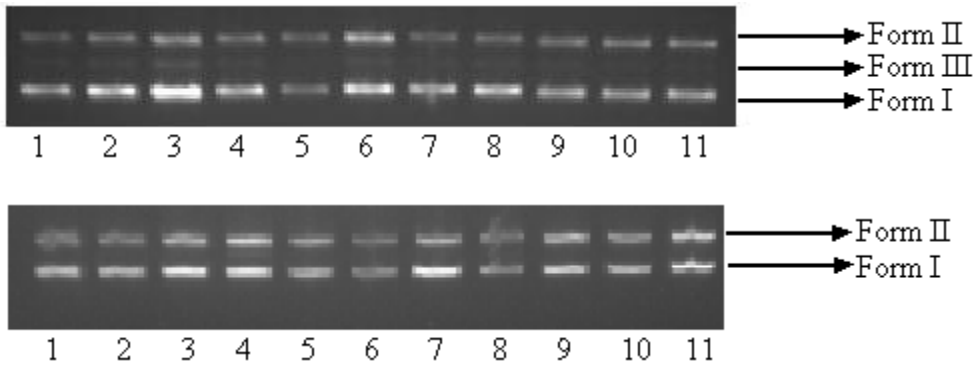

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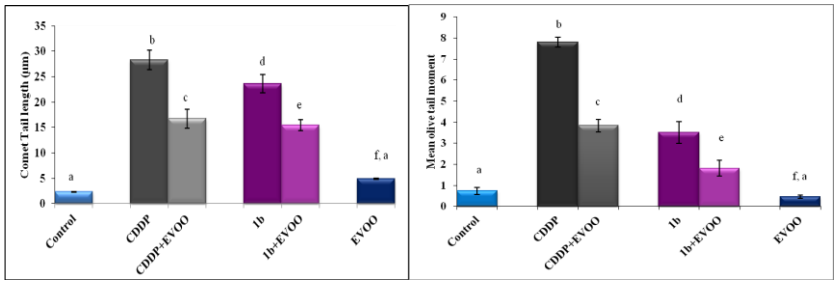

Fig. 10