Supplementary Information

Mixed-Ligand Copper (II) – maltolate complexes: Synthesis, characterization, DNA binding, DNA cleavage and cytotoxicity

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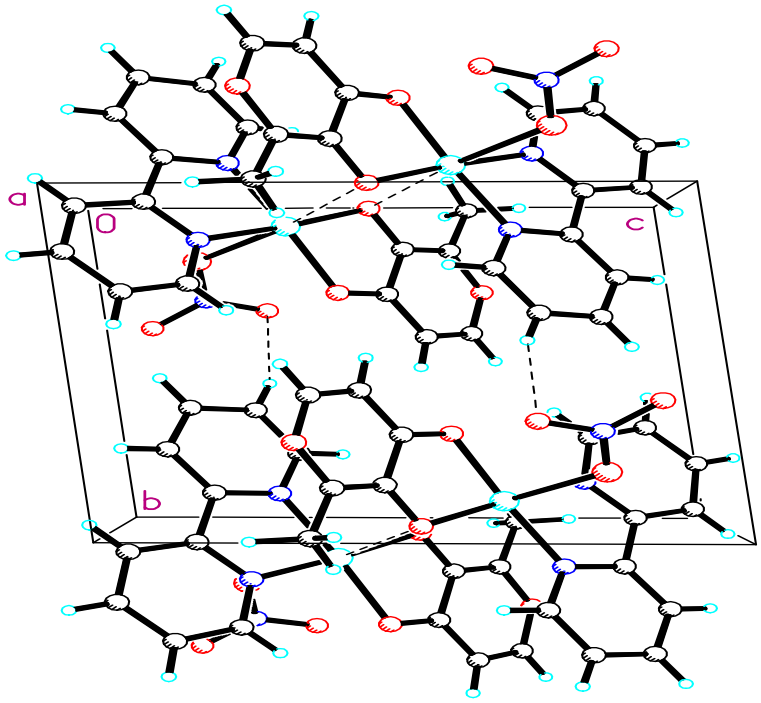
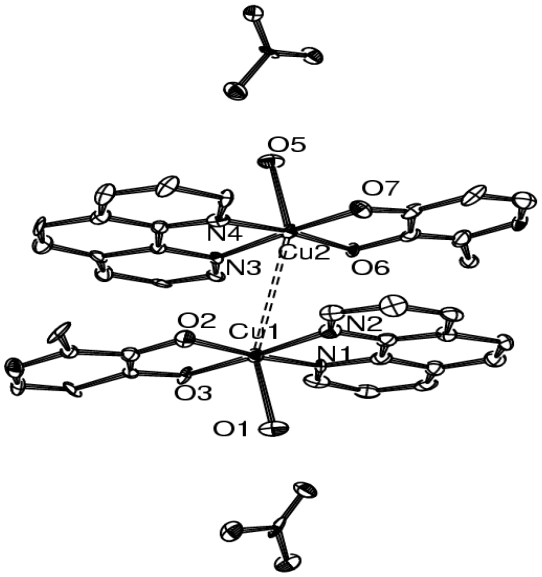


Figure S1. Packing diagram of complex **(1)**



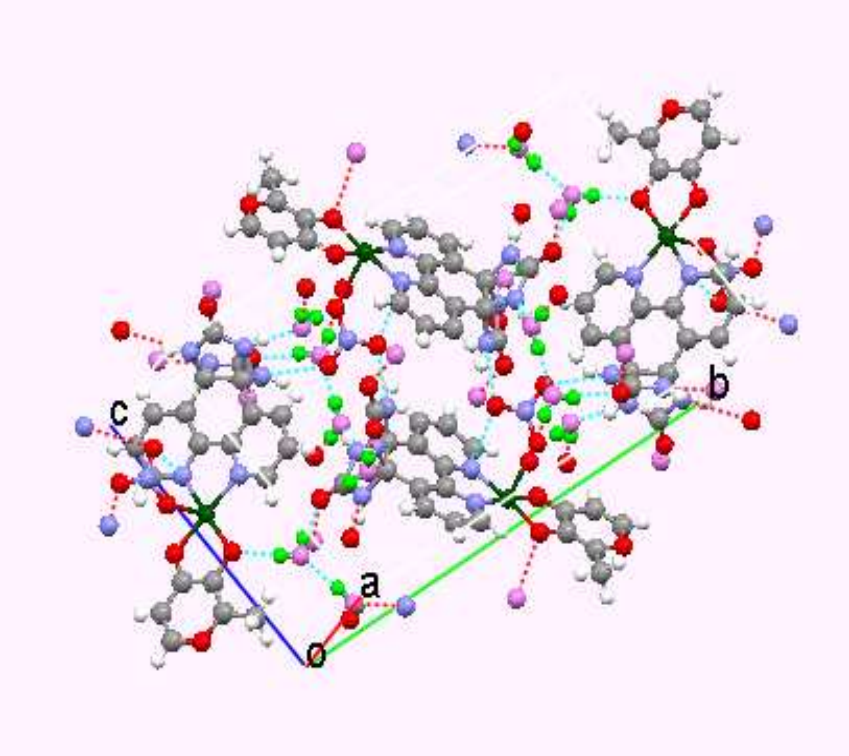


Figure S2. Packing diagram of complex **(2)**

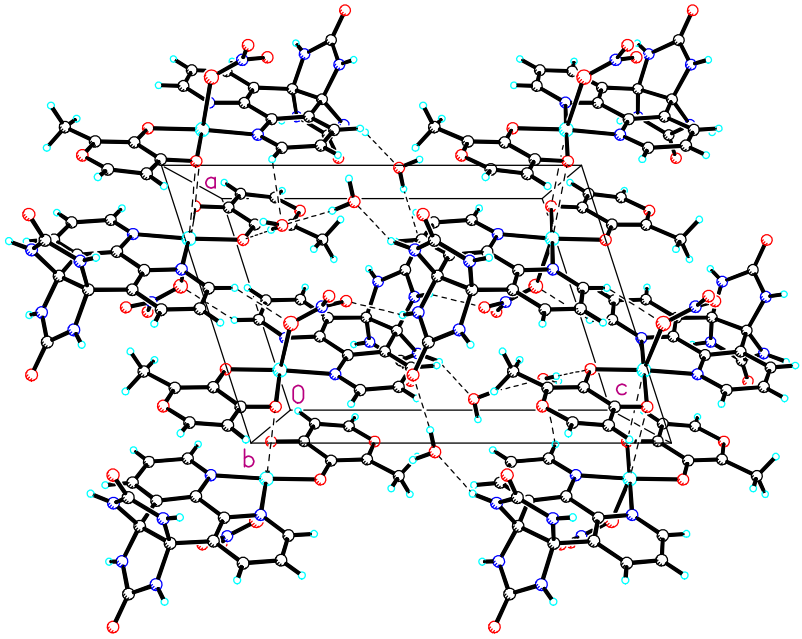


Figure S3. Packing diagram of complex **(5)**

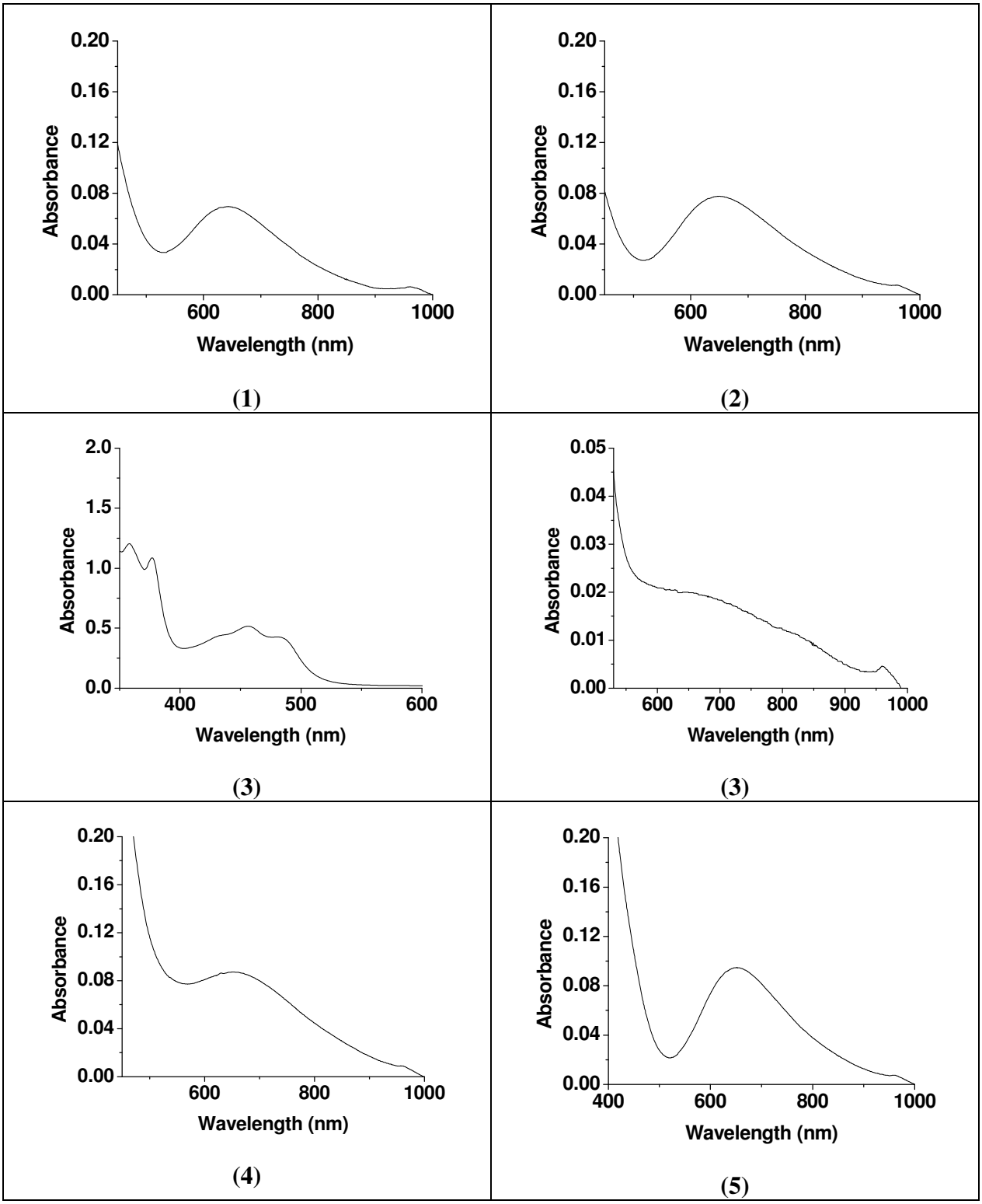


Figure S4. UV-Vis spectra of complexes **(1-5)** in water

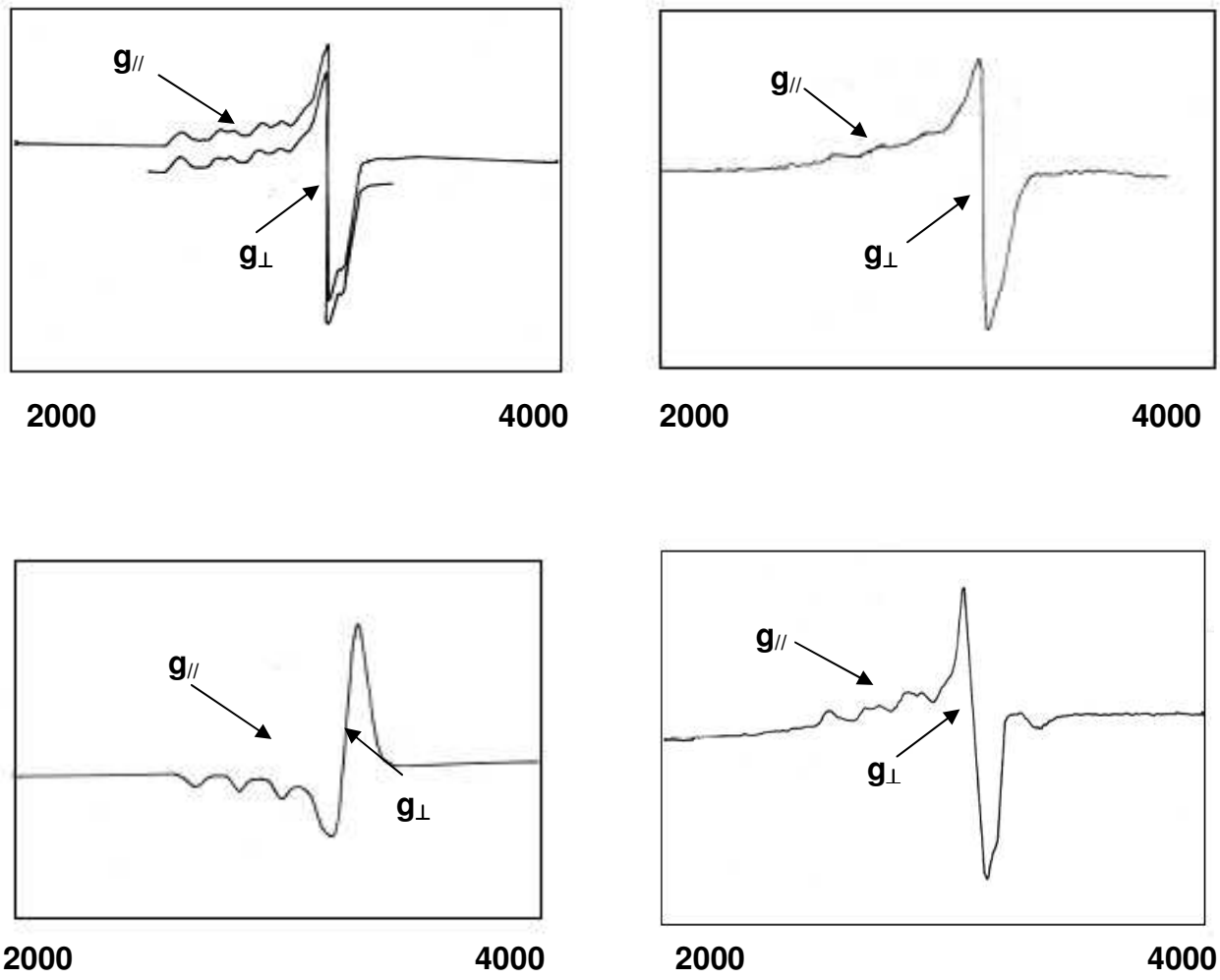
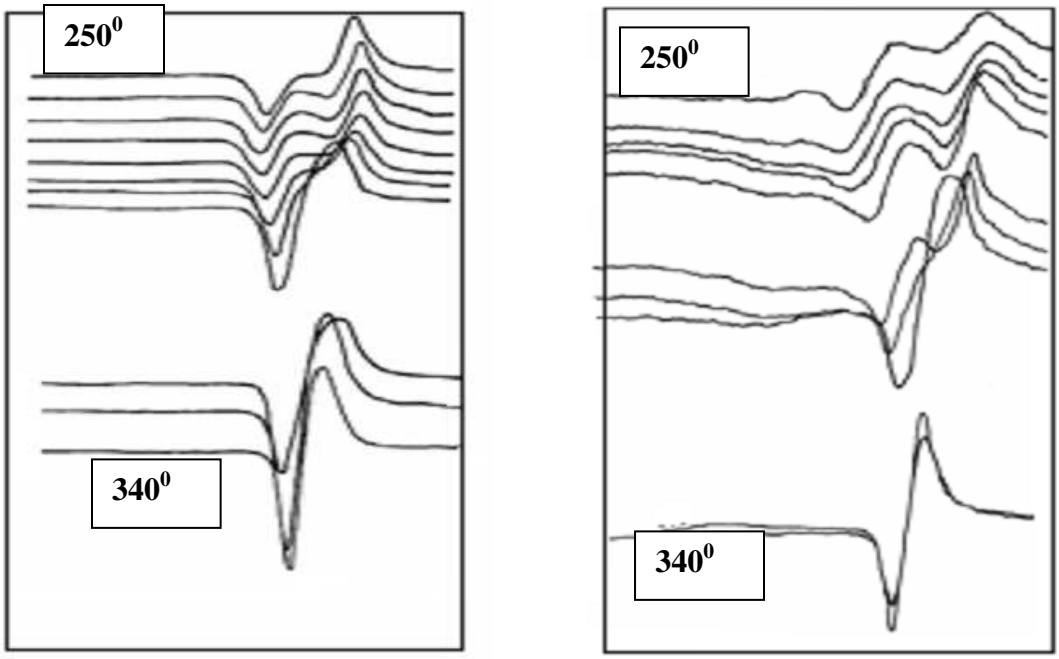
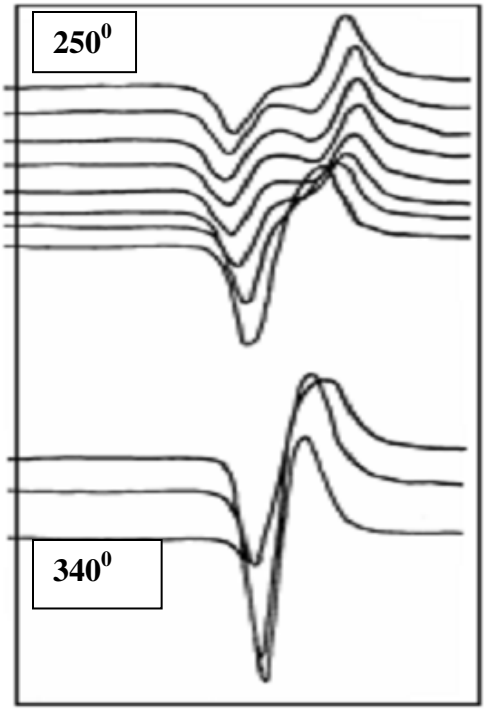


Figure S5. Liquid nitrogen temperature ESR spectra of complexes (1-5) in DMSO



(1) **(2)**



(5)

Figure S6. Single crystal ESR spectra of complexes **(1), (2)** and **(5)**

Table S1. Angular variations of g values in random plane

θ^0	**Complex 1** $g_{//}$	**Complex 2** $g_{//}$	**Complex 5** $g_{//}$
250	**1.91** **2.4** **2.66**	**2.10**	**2.13**
260	**1.91** **2.37** **2.71**	**2.15**	**2.10**
270	**1.91** **2.35**	**2.0** **2.24**	**2.11**
280	**1.91** **2.31**	**1.95** **2.2**	**2.11**
290	**1.91** **2.25**	**2.0** **2.23**	**2.11**
300	**2.3** **2.51**	**2.0** **2.24**	**2.08**
310	**2.07**	**2.0** **2.01**	**2.07**
320	**2.05**	**2.04** **2.25**	**2.07** **2.10**
330	**2.09**	**2.14**	**2.07** **2.24** **2.32**
340	**2.09**	**2.2**	**2.14** **2.33**

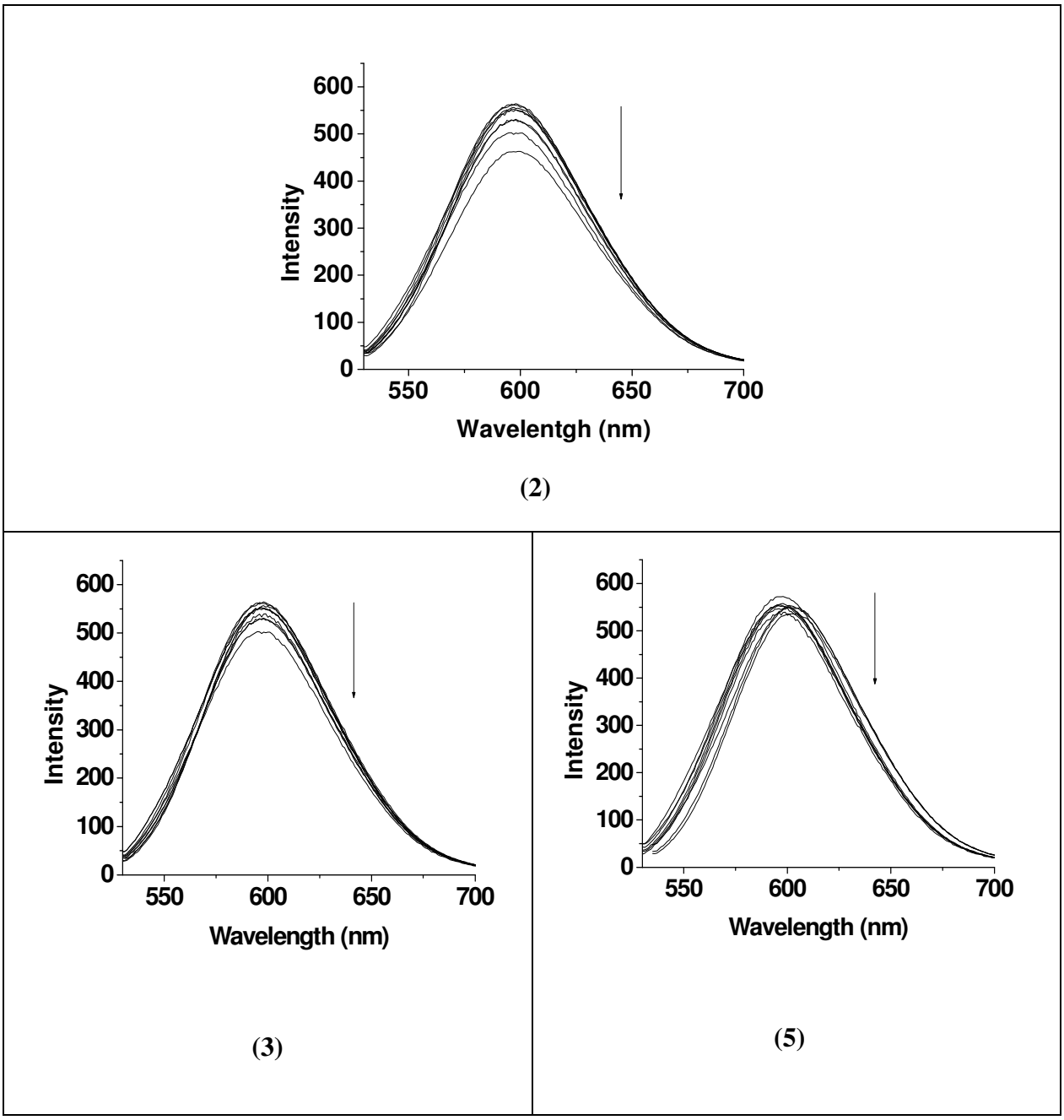


Figure S7. Fluorescence quenching curves of ethidium bromide bound to DNA by complexes (1) and (4), [DNA] = 20μM, [EBR] = 20 μM and [complex] 0 to 200 μM.

Investigation of DNA Cleavage Mechanism in Presence of Radical Scavengers

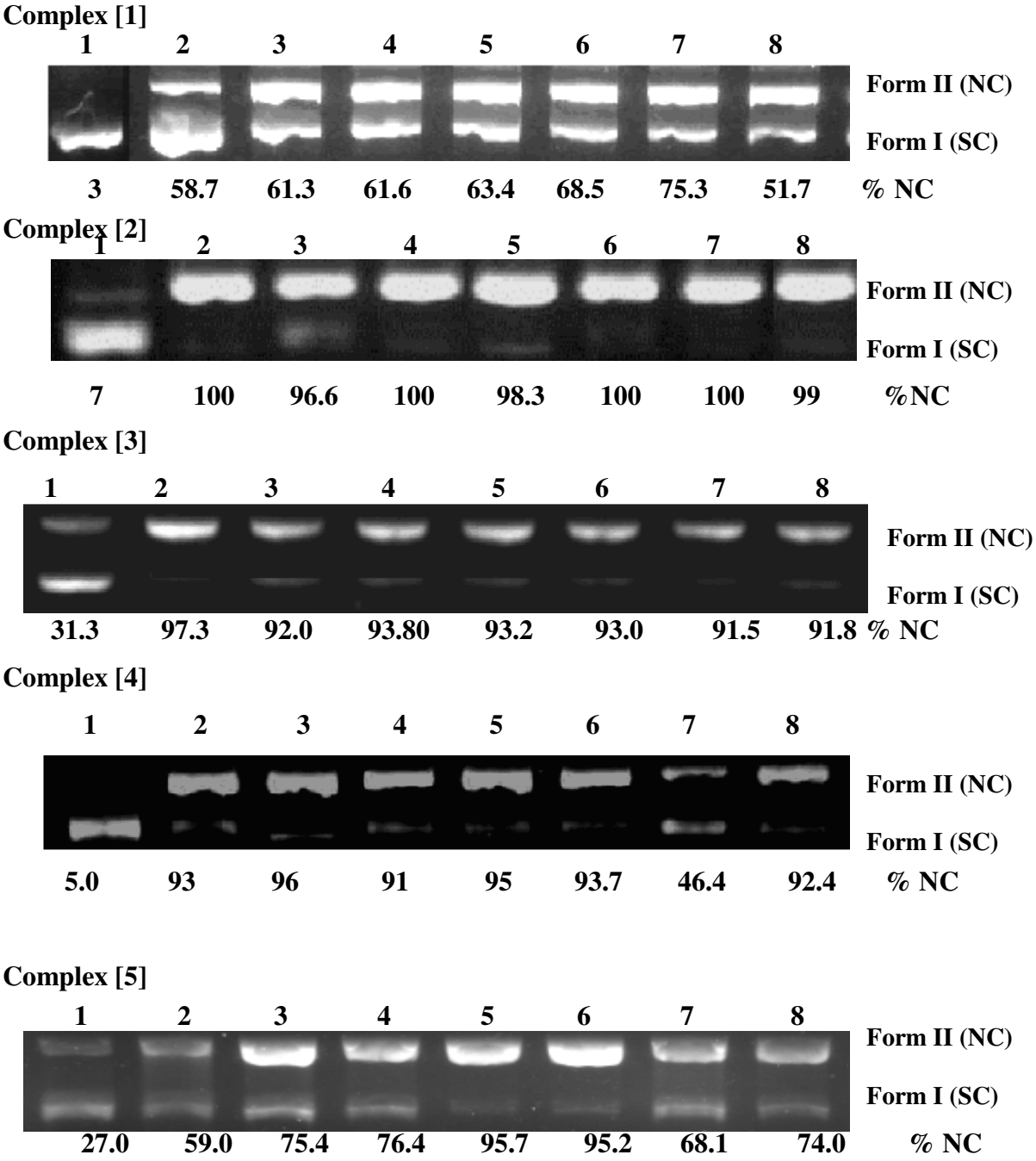


Figure S8. Effect of inhibitors on the activity of (500 μM) complexes **(1-5)** on (plasmid *pBR322* DNA 90 μM, in base pairs); 30 minutes incubation. Form I - supercoiled plasmid DNA; Form II - nicked circular plasmid DNA; lanes 1- untreated *pBR322*, lane 2 - DNA + D_2O + complex, lane 3 - DNA + complex + DMSO (1 mM), lane 4 - DNA + complex + mannitol (50 mM), lane 5 - DNA + complex + DABCO (10 mM), lane 6 - DNA + complex + NaN_3 (20 mM), lane 7 - DNA + complex + L-Histidine (20 mM), lane 8 - DNA + complex + SOD (15 units).

Distamycin assay

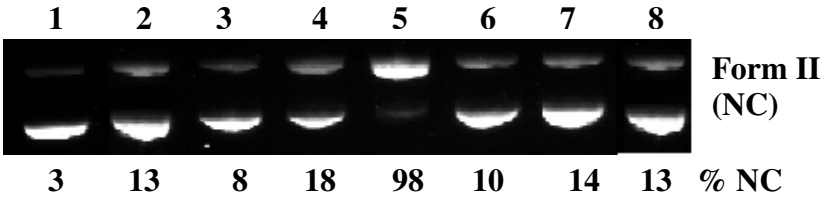
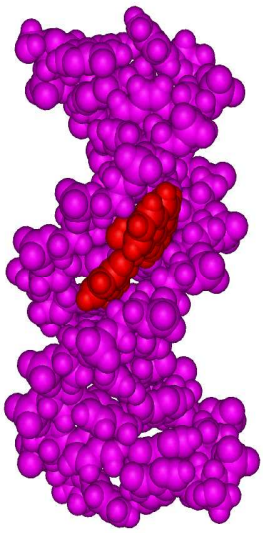
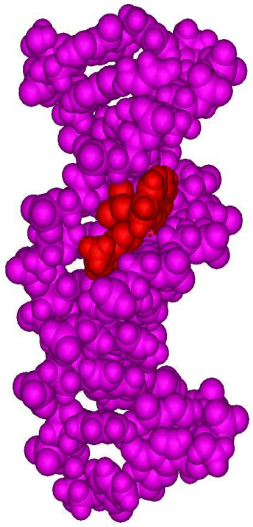


Figure S9. Ethidium bromide-stained agarose gel (1%) of 100 ng/mlpBR322 plasmid DNA in the presence of 100μM complex and 100μM minor groove binder Distamycin. lane 1 – DNA control, lane - 2 pBR322 + $[Cu(phen)_2]^{2+}$ + distamycin, lane - 3 pBR322 + **(1)** + distamycin, lane - 4 pBR322 + **(2)** + distamycin, lane – 5 pBR322 + **(4)** + distamycin, lane - 6 pBR322 + **(3)** + distamycin, lane - 7 pBR322 + **(5)** + distamycin, lane 8- DNA + distamycin

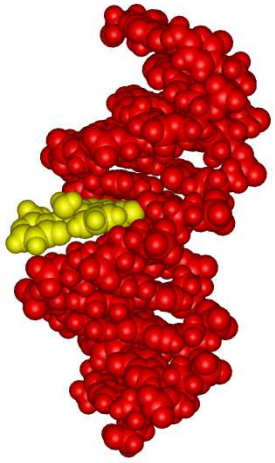
Molecular modeling studies



(1)



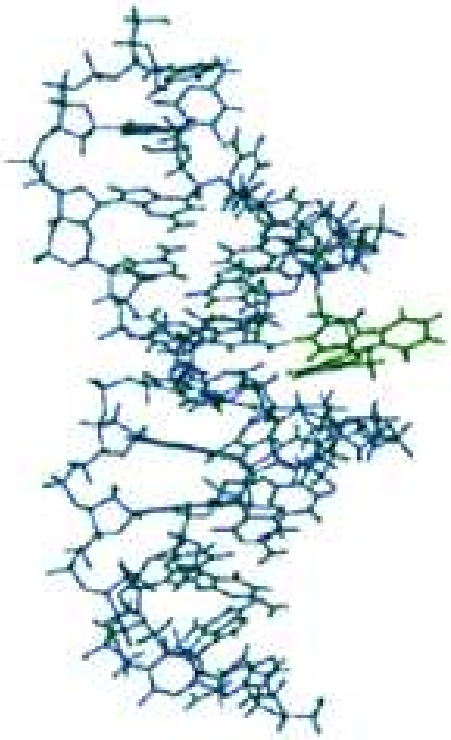
(2)



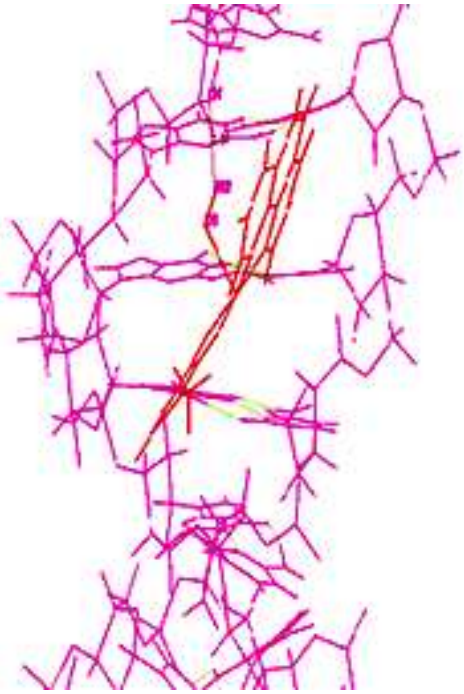
(3)

Minor groove binding of complexes (1) and (2) and partial intercalation of complex (3)

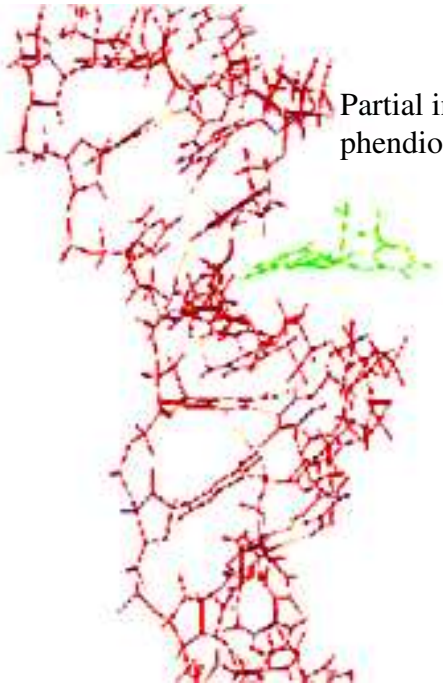
Hydrogen bonding interactions observed in complexes 1, 2, 5 with DNA



(1)

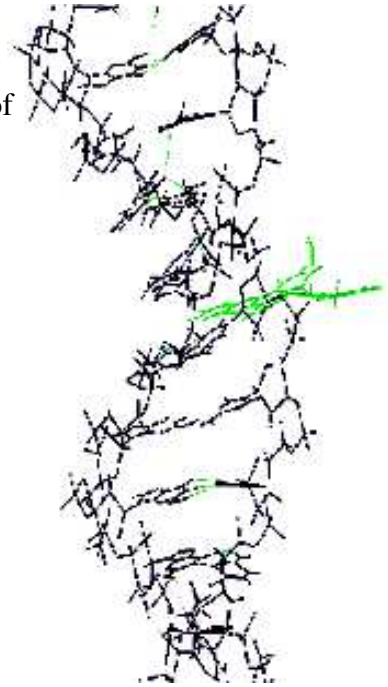


(2)

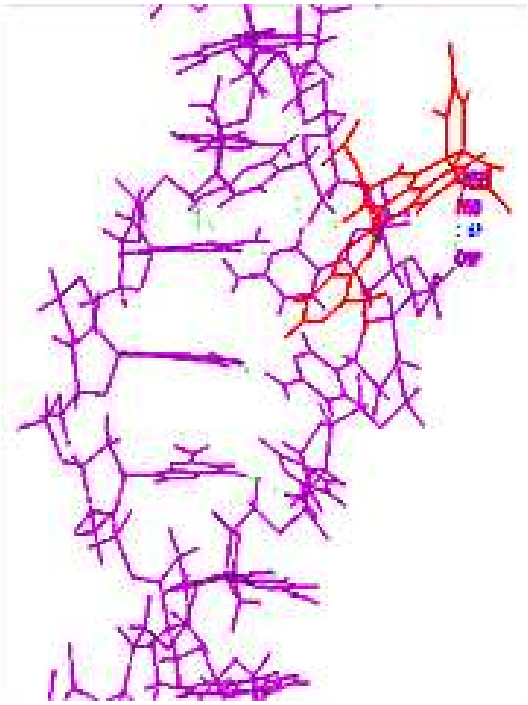


(3)

Partial intercalation of phendione and dppz



(4)



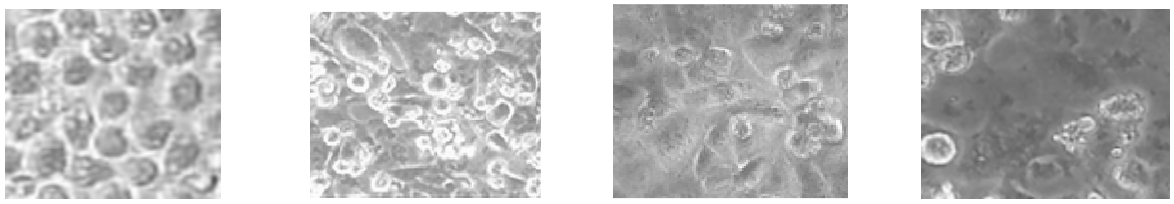
(5)

Figure S10. Core view model of complexes **(1, 2** and **5)** showing hydrogen bonding interactions and partial intercalation of complexes 3 and 4.

Complex 1

400 ug/ ml

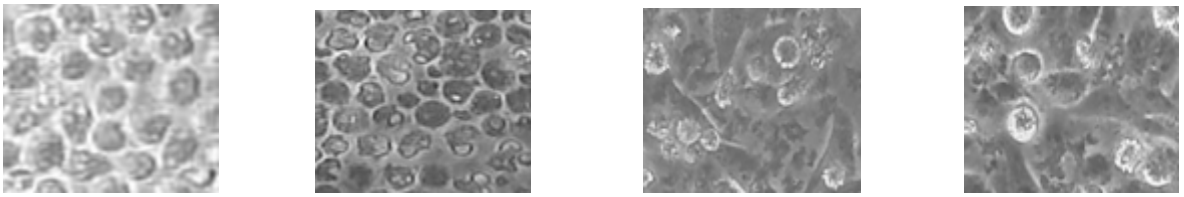
Control 24 hrs 48 hrs 72 hrs



Complex 2

400 ug/ ml

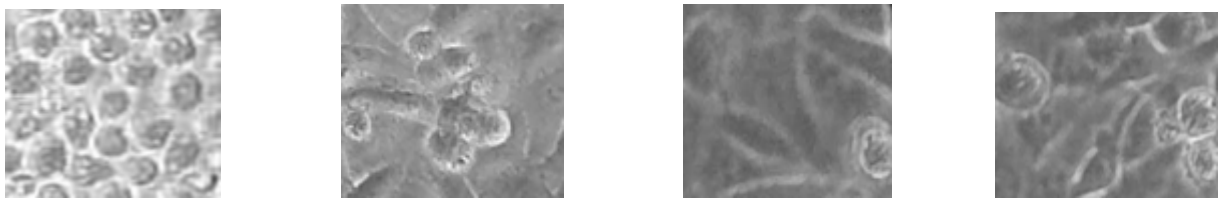
Control 24 hrs 48 hrs 72 hrs



Complex 3

400 ug/ ml

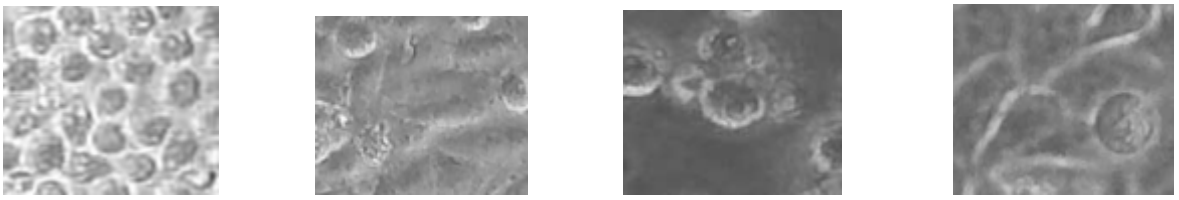
Control 24 hrs 48 hrs 72 hrs



Complex 4

400 ug/ ml

Control 24 hrs 48 hrs 72 hrs



Complex 5

400 ug/ ml

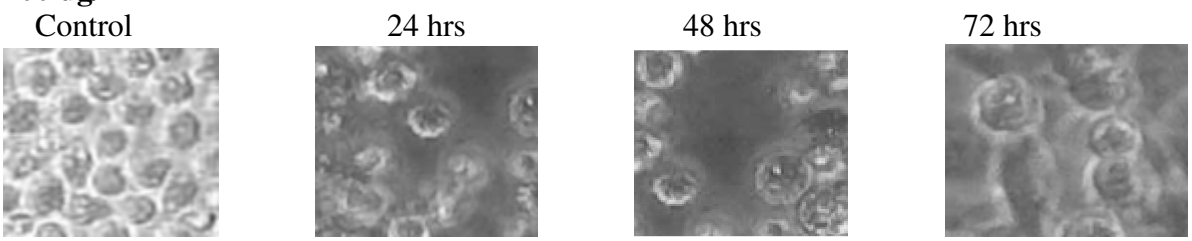


Figure S11. MTT assay of complexes (**1 -5**) (**400 ug/ ml)** against HeLa cell line