

Supplementary information

Synthesis of Ru(II)-benzene complexes containing aroylthiourea ligand, and their binding with biomolecules and *in vitro* cytotoxicity through apoptosis

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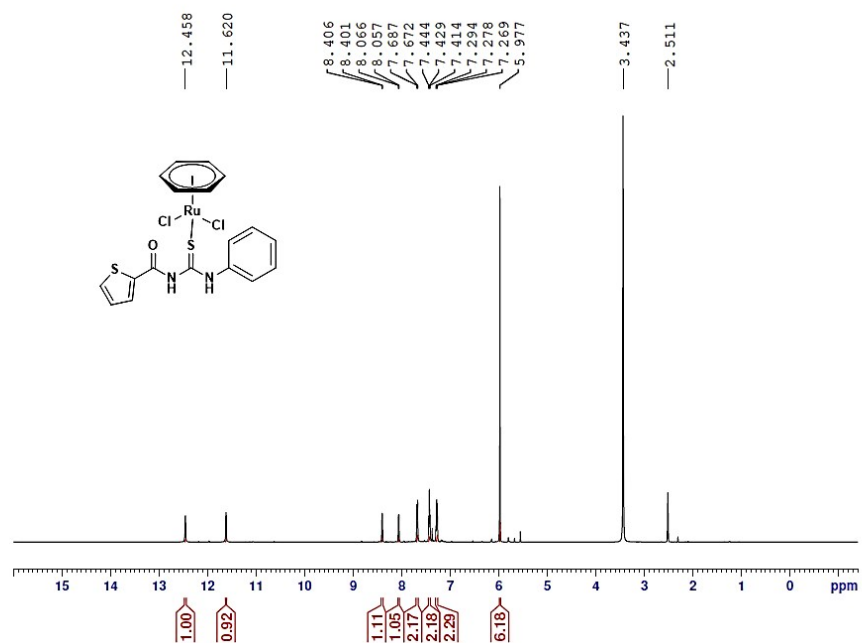


Fig. S1 ^1H NMR spectrum of **1**

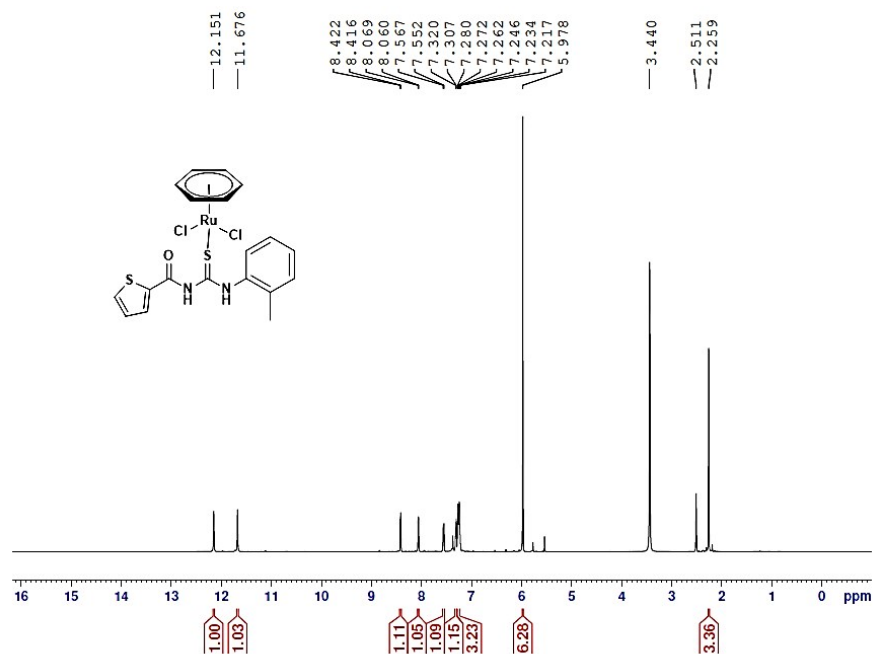


Fig. S2 ^1H NMR spectrum of **2**

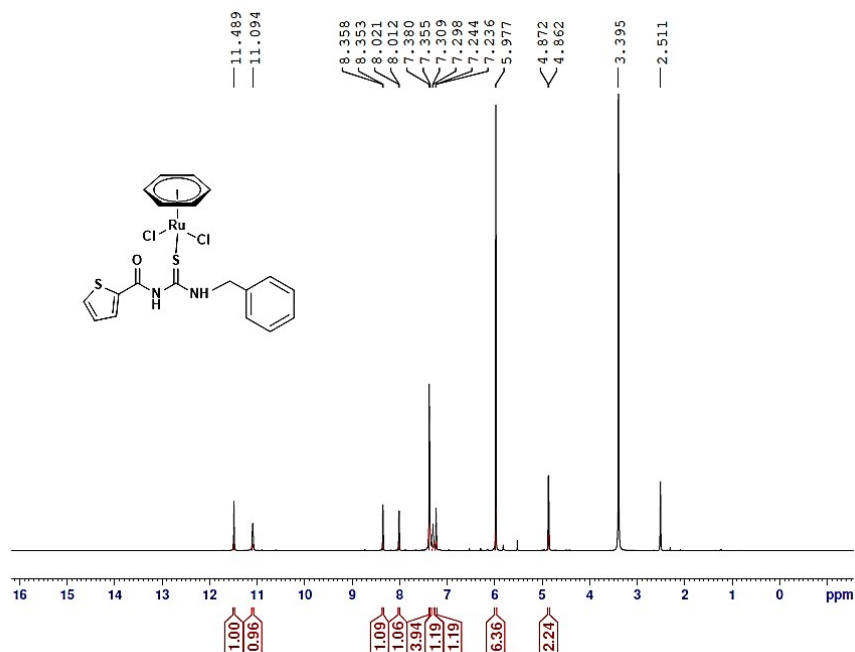


Fig. S3 ^1H NMR spectrum of **3**

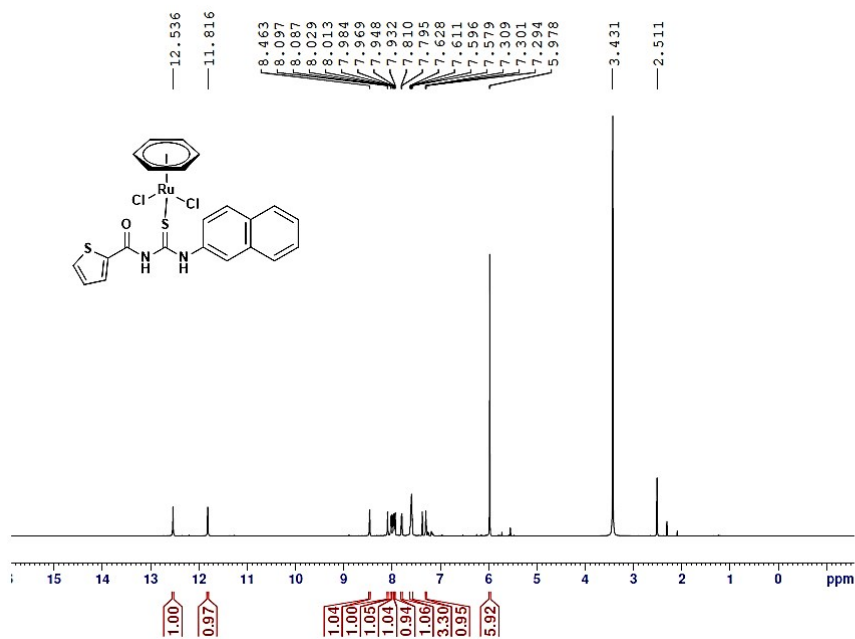


Fig. S4 ^1H NMR spectrum of **4**

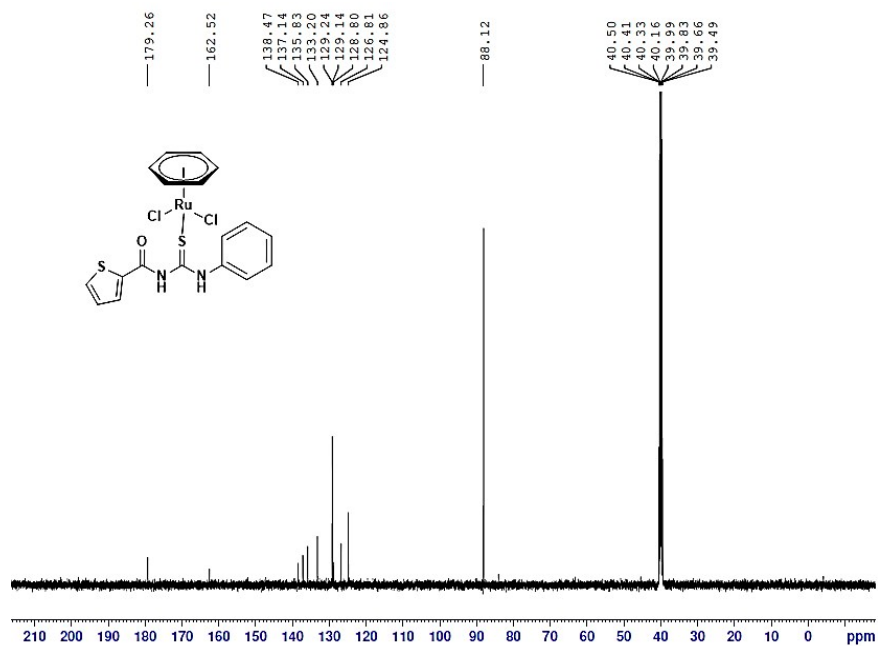


Fig. S5 ¹³C NMR spectrum of **1**

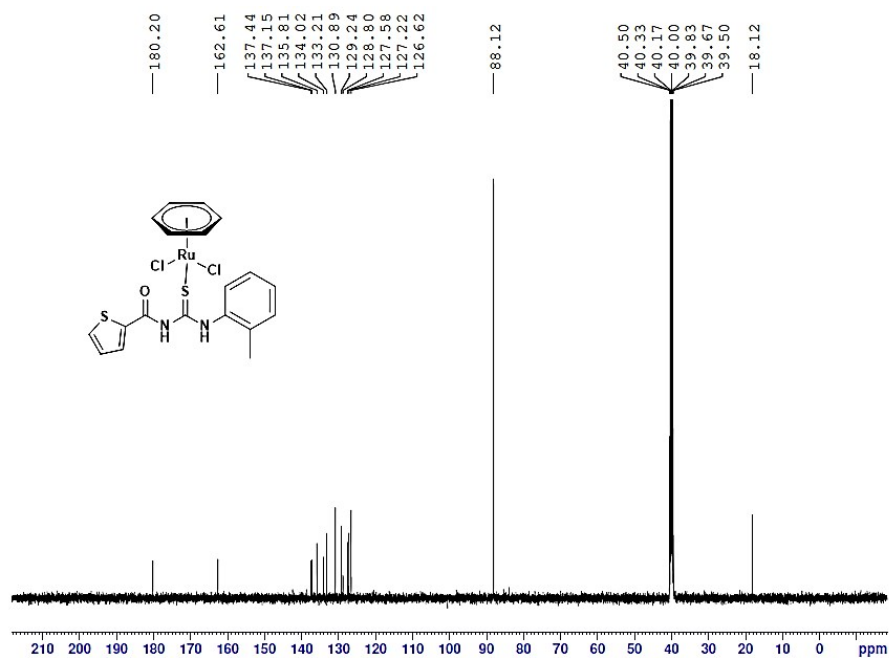


Fig. S6 ¹³C NMR spectrum of **2**

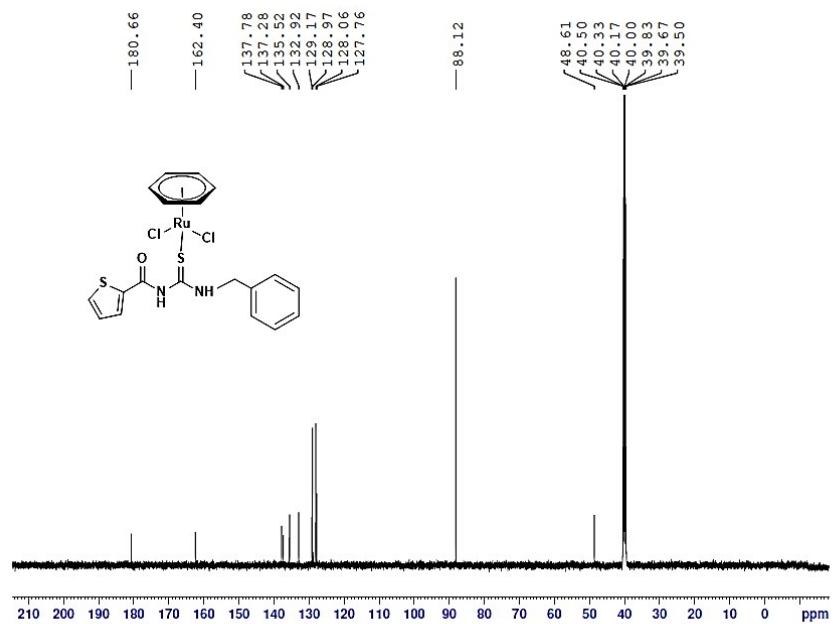


Fig. S7 ¹³C NMR spectrum of **3**

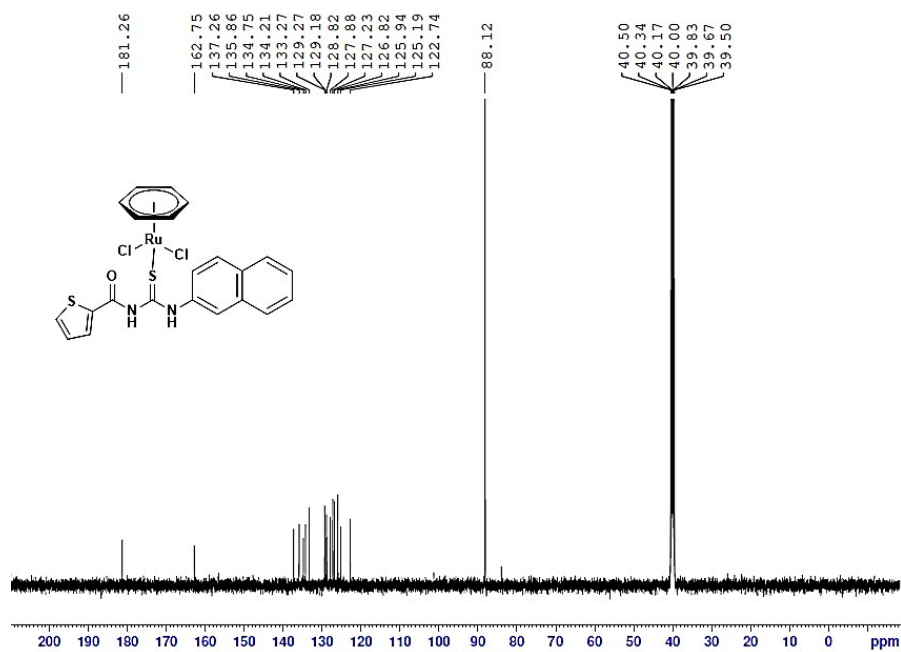


Fig. S8 ¹³C NMR spectrum of **4**

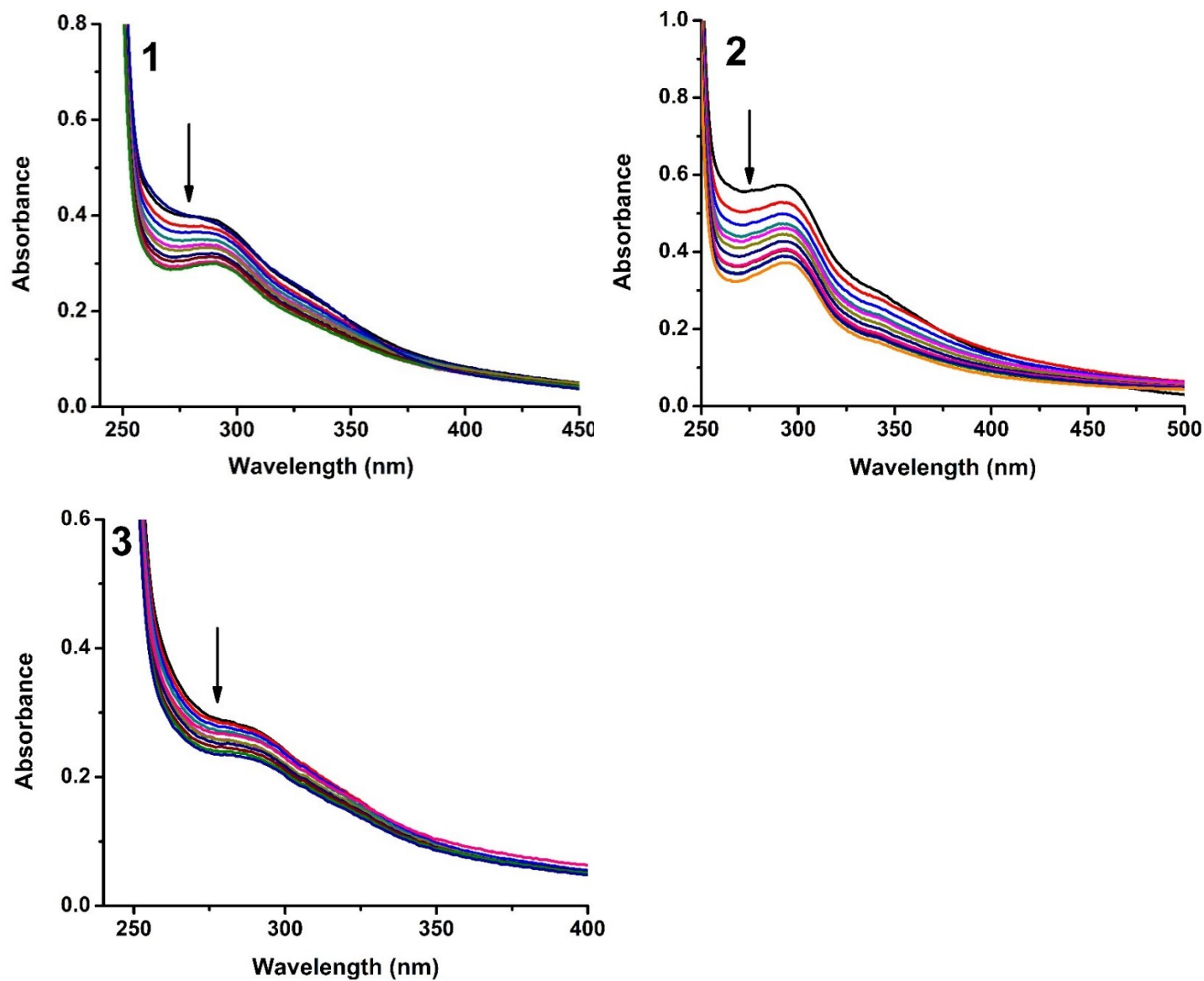


Fig. S9 Absorption spectra of complexes (**1-3**) in Tris-HCl buffer upon addition of CT DNA. [Complex] = 2.5×10^{-5} M, [DNA] = 0-50 μ M. The arrow shows that the absorption intensity decreases upon increasing the DNA concentration.

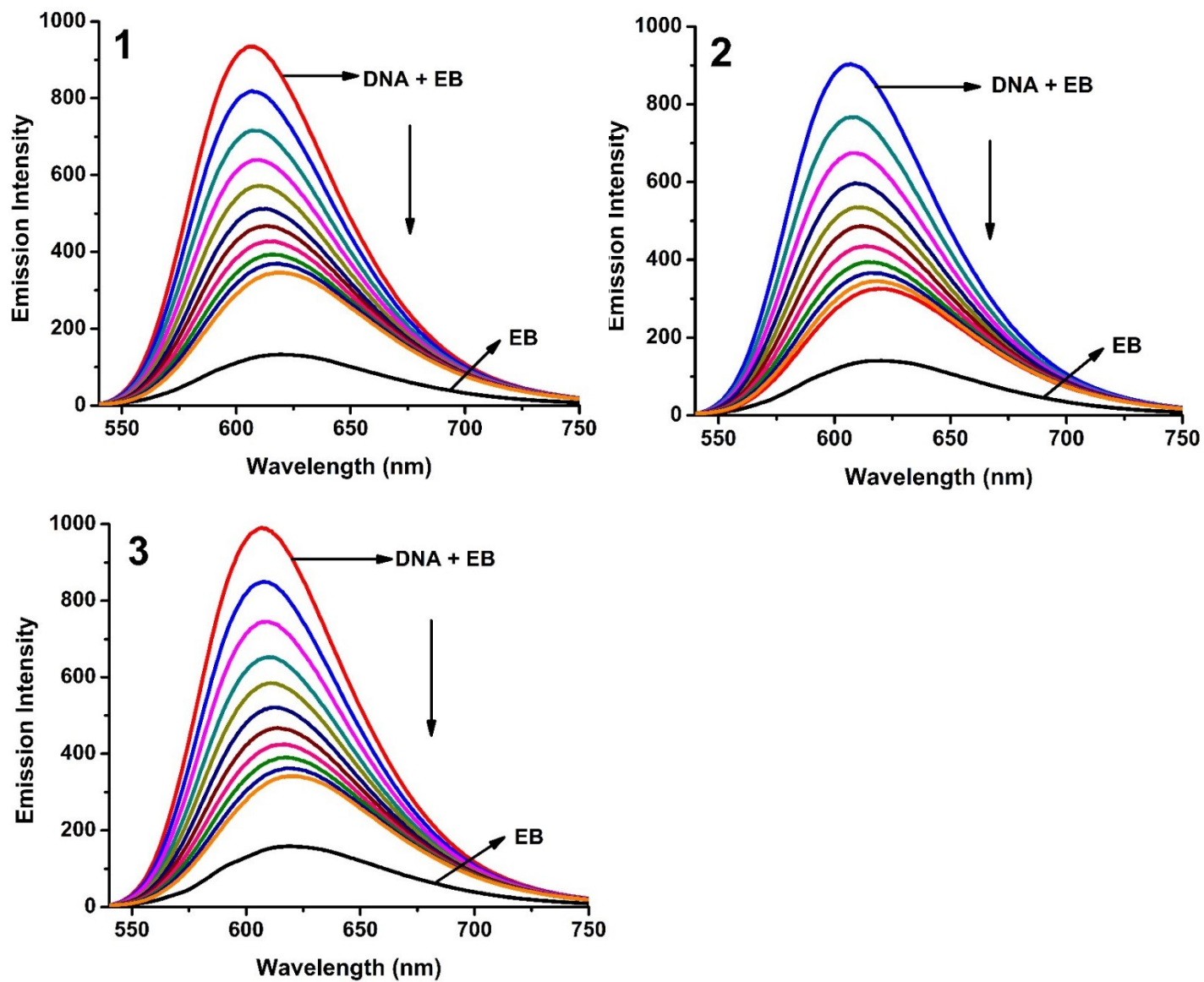


Fig. S10 Fluorescence quenching curves of EB bound to DNA in the presence of **1-3**. [DNA] = 5 μ M, [EB] = 5 μ M and [complex] = 0-50 μ M.

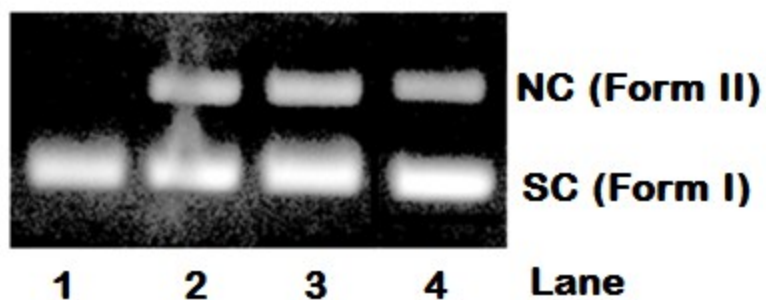


Fig. S11 (a) Cleavage of supercoiled pBR322 DNA (40 μ M) by complex **3** in a buffer containing 5 % DMF/5 mM Tris HCl/50 mM NaCl at pH = 7.2 and 37 $^{\circ}$ C with an incubation time of 4 h. Lane 1, DNA; lane 2, DNA + NaN₃ (0.2 mM) + **3** (50 μ M); lane 3, DNA + DMSO (2 μ L) + **3** (50 μ M); lane 4, DNA + **3** (50 μ M). Forms SC and NC are supercoiled and nicked circular DNA, respectively.

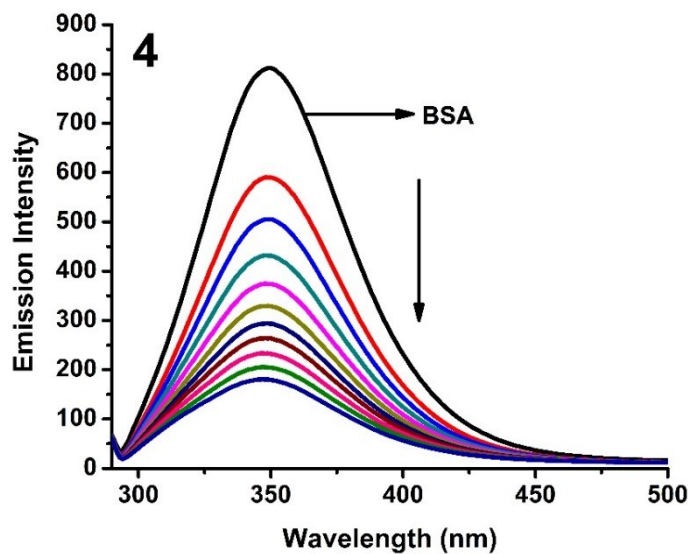
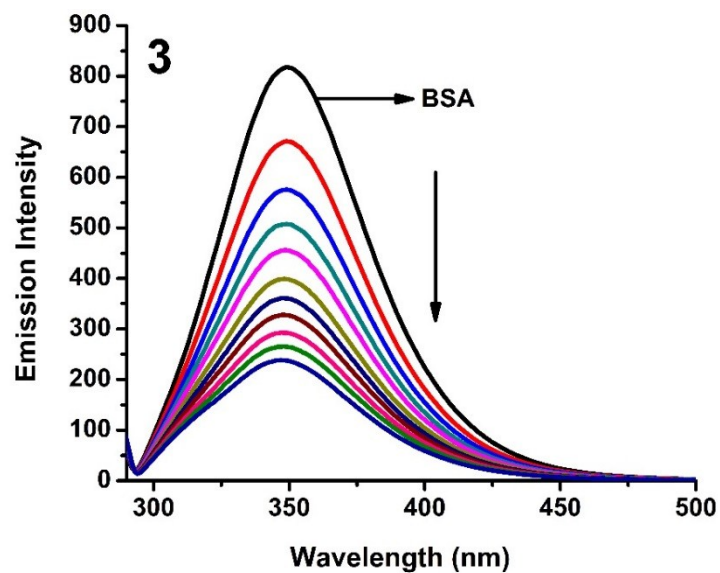
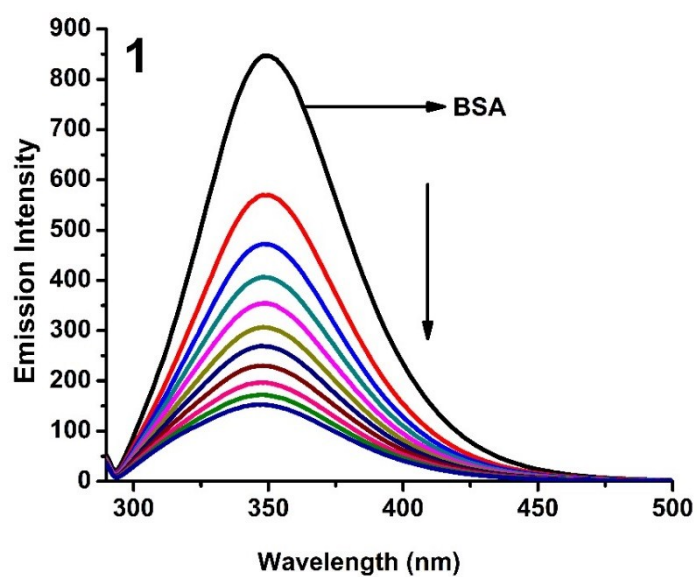


Fig. S12 Fluorescence quenching curves of BSA in the absence and presence of **1**, **3** and **4**.
[BSA] = 1 μ M and [complex] = 0-20 μ M.

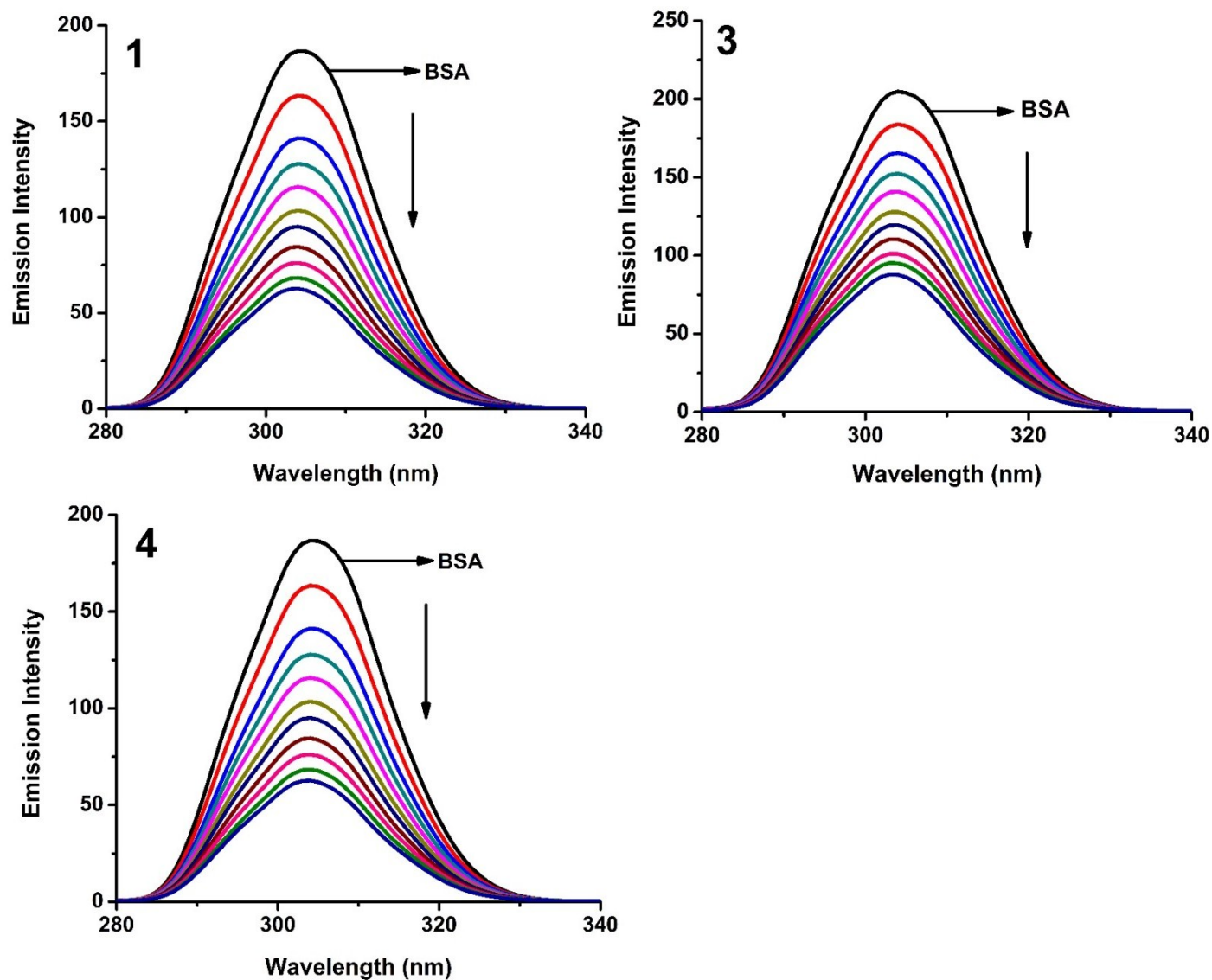


Fig. S13 Synchronous spectra of BSA (1 μM) as a function of concentration of **1**, **3** and **4** (0-20 μM) with $\Delta\lambda = 15$ nm.

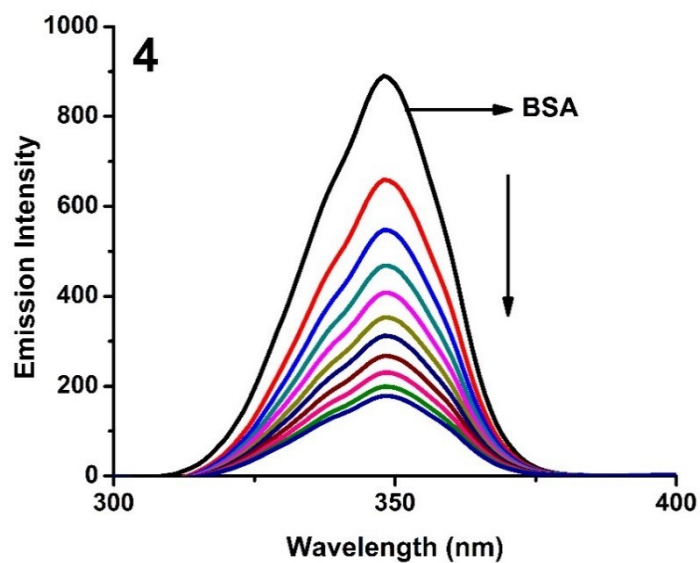
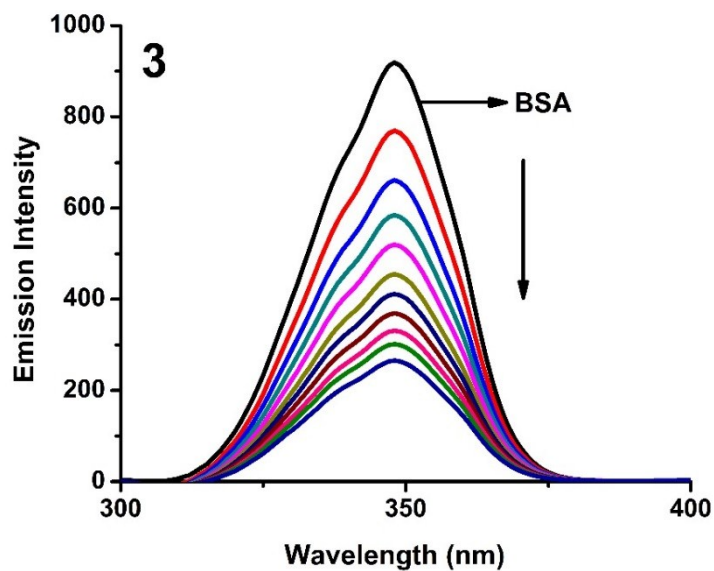
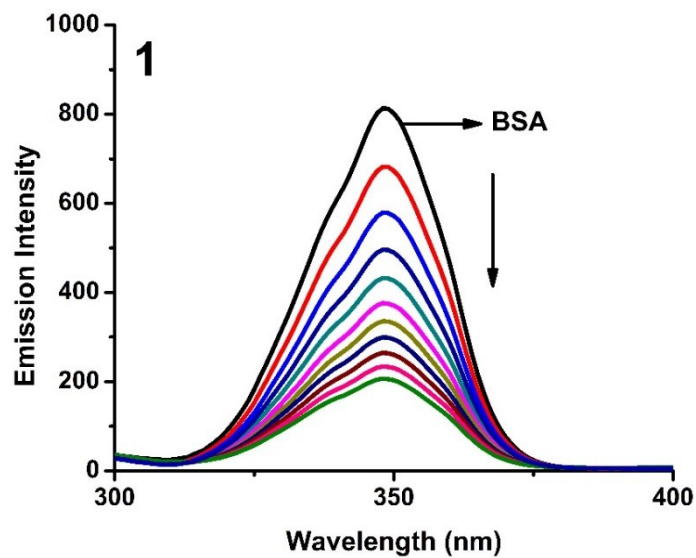


Fig. S14 Synchronous spectra of BSA (1 μM) as a function of concentration of **1**, **3** and **4** (0-20 μM) with $\Delta\lambda = 60$ nm.

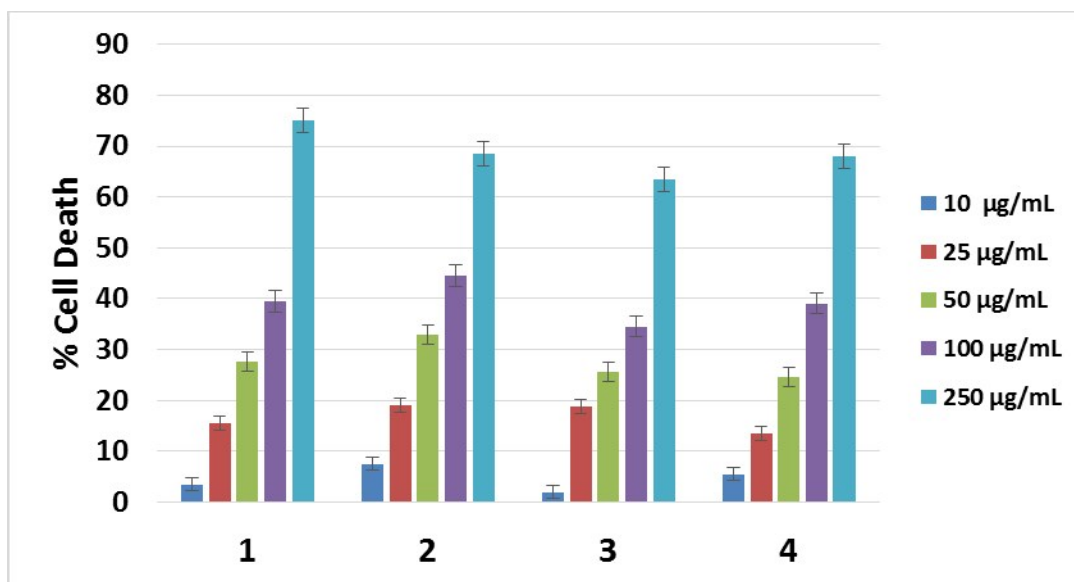


Fig. S15 Comparison of anticancer activity of synthesized complexes (1-4) against MCF7 cancer cells. Data are mean $\pm$ SD of three independent experiments with each experiment conducted in triplicate.

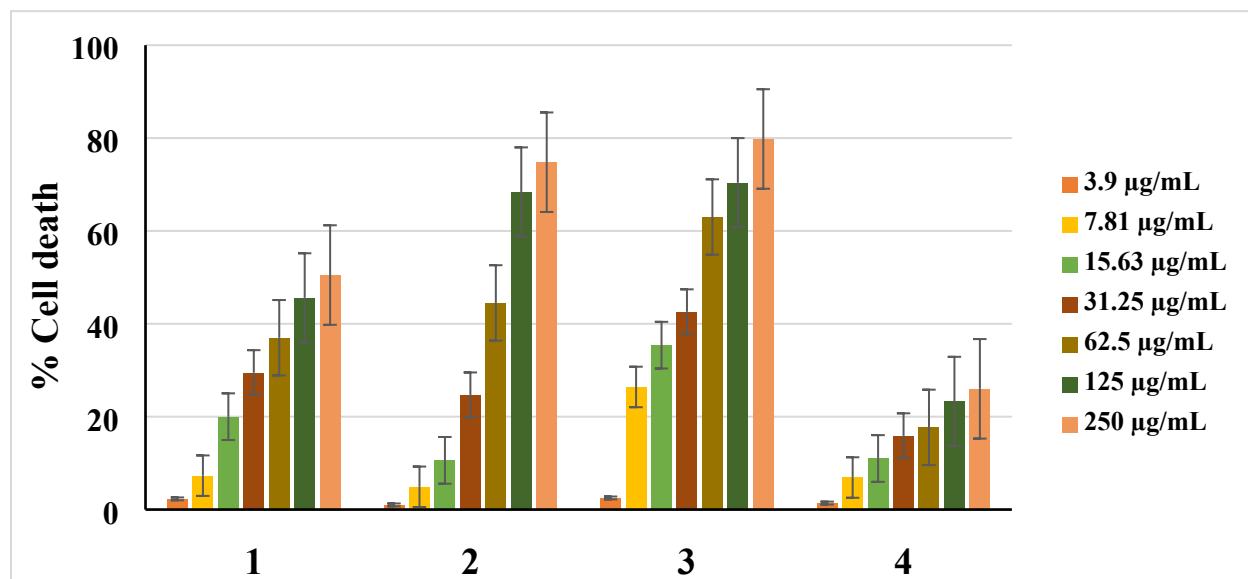


Fig. S16 Comparison of anticancer activity of the complexes (1-4) against SKOV3 cancer cells. Data are mean $\pm$ SD of three independent experiments with each experiment conducted in triplicate.