Electronic Supplementary Material (ESI) for RSC Advances.

Design, synthesis and characterization of novel chromone based–copper (II) antitumor agents with *N,N*-donor ligands: comparative DNA/RNA binding profile and cytotoxicity.

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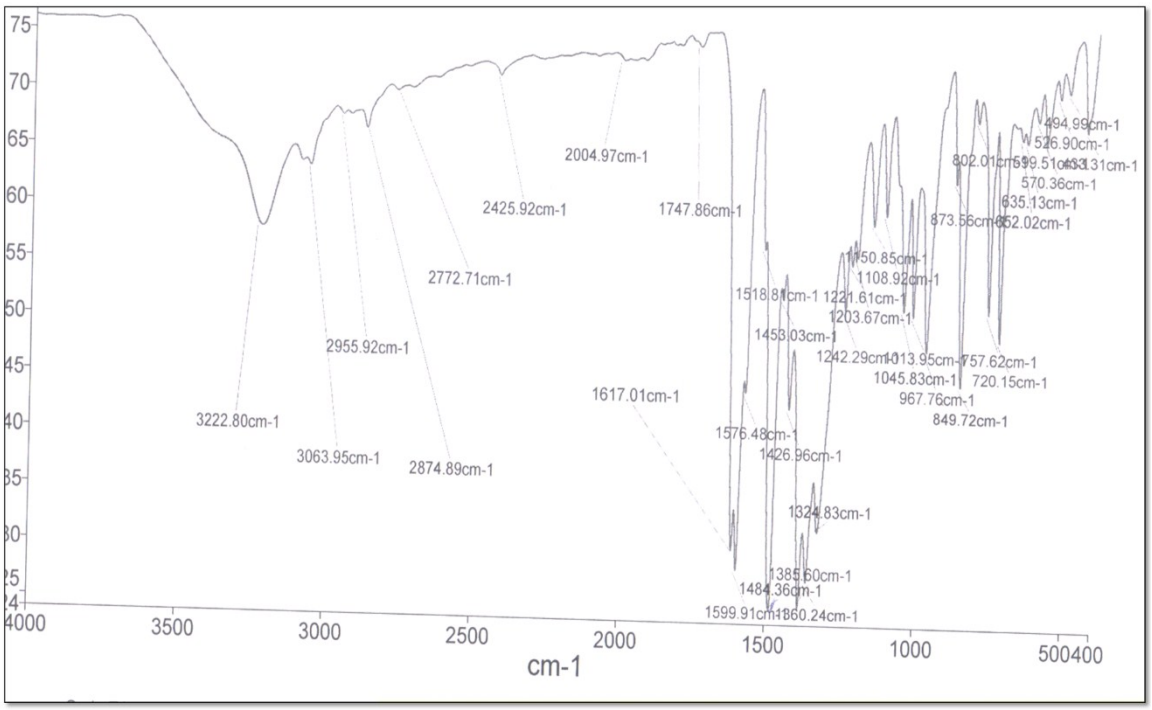
(a)



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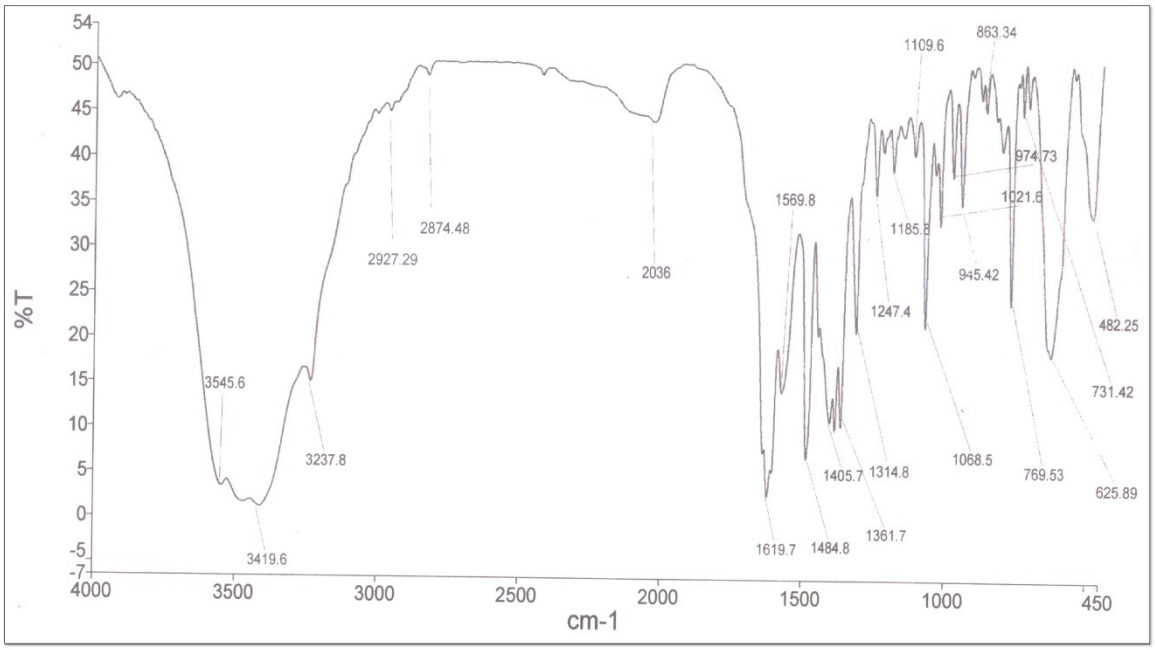


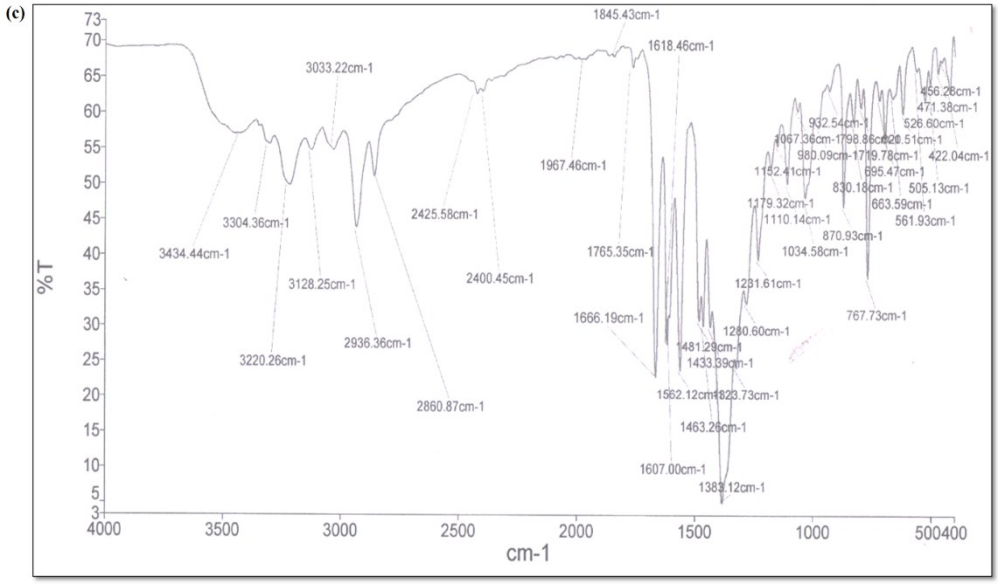
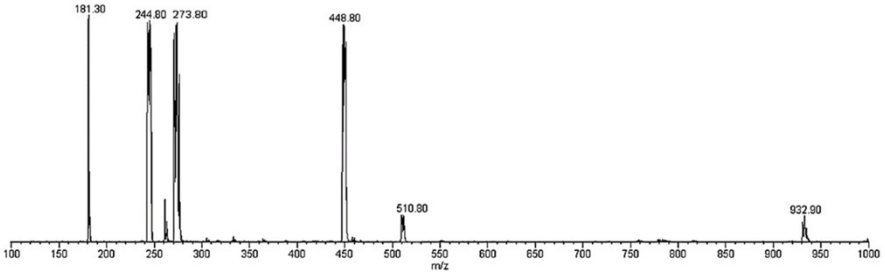
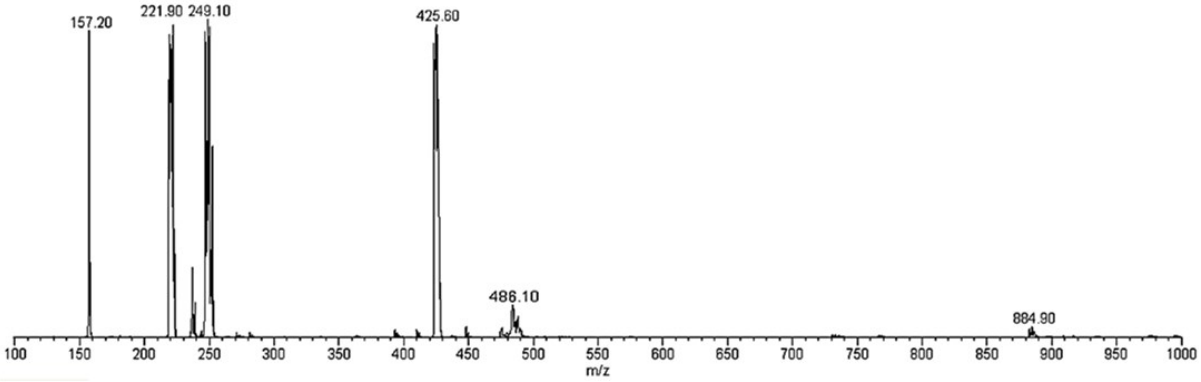


Fig S1. FT-IR spectra of complexes **1**(a), **2** (b) and **3** (c).

(a)



(b)



(c)

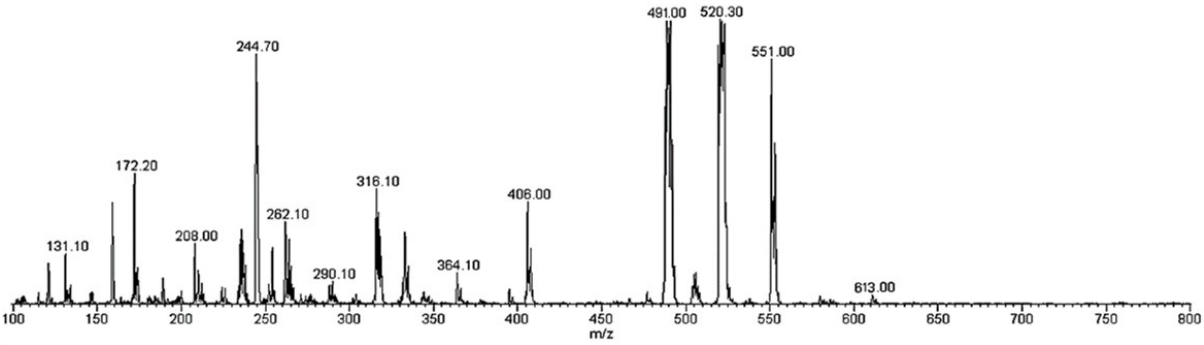


Fig. S2. ESI mass spectrum of complexes **1** (a), **2** (b) and **3** (c).

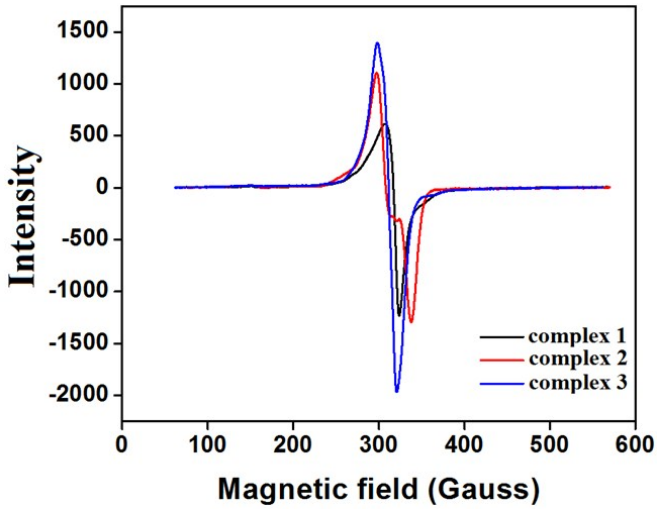


Fig. S3. X–band EPR spectrum of complexes **1** (a), **2** (b) and **3** (c) at room temperature.

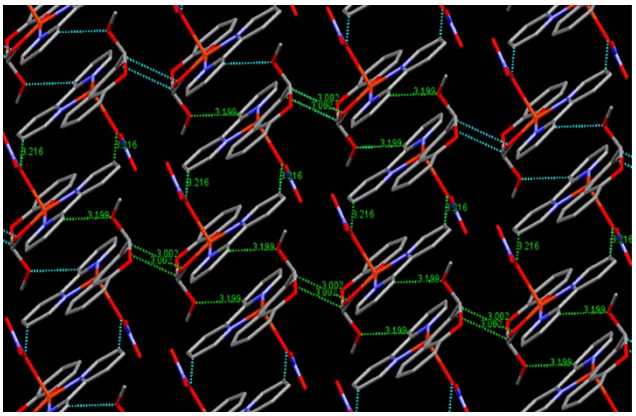


Fig. S4. Packing diagram showing possible intermolecular hydrogen bonding between C–O···H and N–O···H atoms.

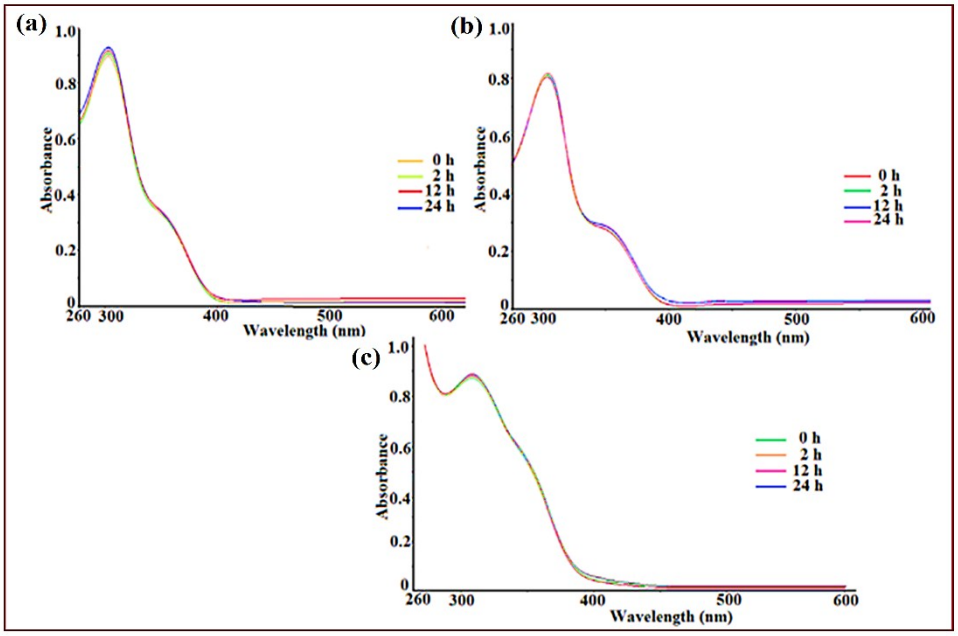


Fig. S5. UV–vis absorption spectra of complexes **1** (a), **2** (b) and **3** (c) in DMSO at different time intervals (0 h, 2 h, 12 h and 24 h).

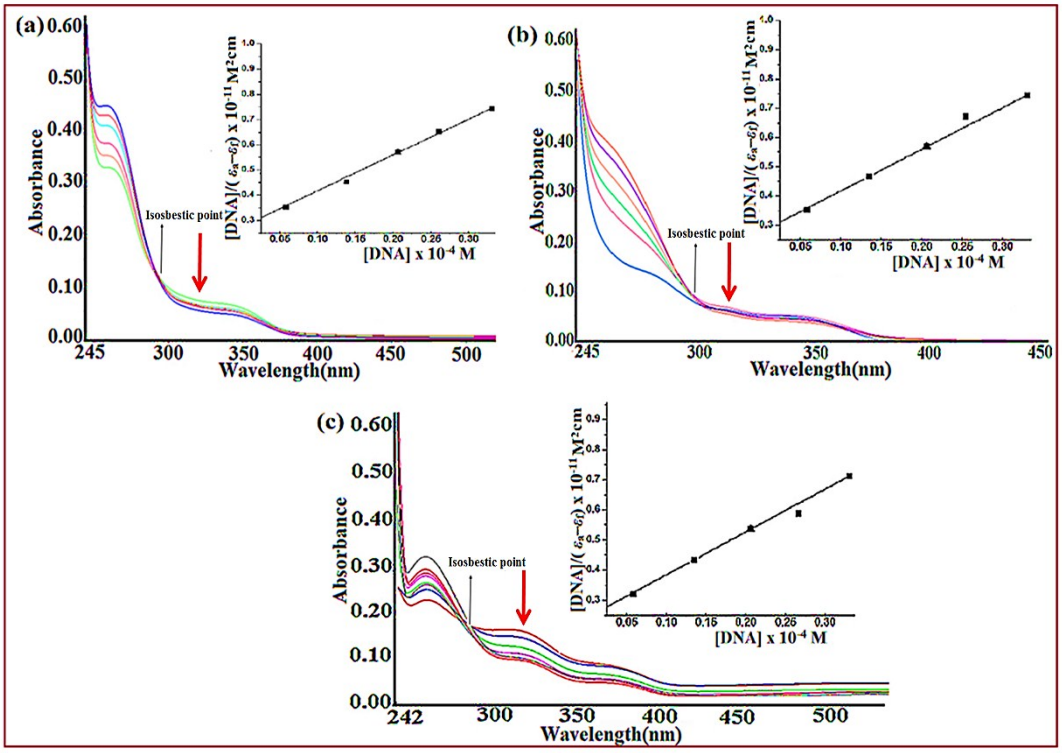


Fig. S6. Absorption titration curves of complexes **1** (a), **2** (b) and **3** (c) (2 ×10^{-4} M) with ct−DNA (0.0–4.0 ×10^{-5} M), in Tris–HCl buffer (pH 7.2). Arrows depicts the intensity change with increase in concentration of ct−DNA. Inset: Plots of [DNA]/ (εa–εf) (M^2 cm) vs. [DNA].

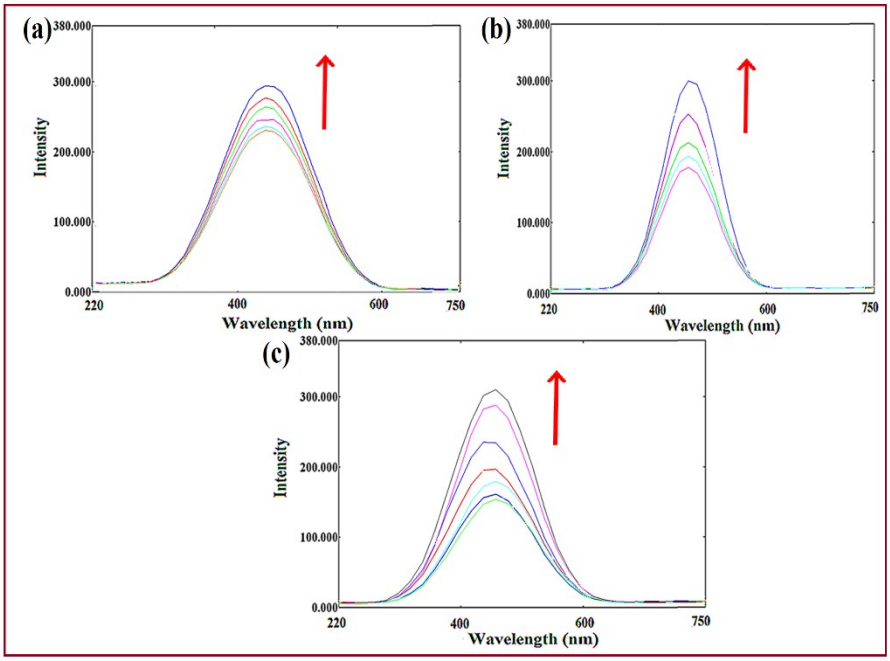


Fig. S7. Emission spectra of complexes **1** (a), **2** (b) and **3** (c) (2×10^{-4} M) with ct−DNA [DNA] = (0−4.00×10^{-5} M) in Tris–HCl buffer (pH 7.2). Arrows depicts the intensity change upon increasing concentration of ct−DNA.

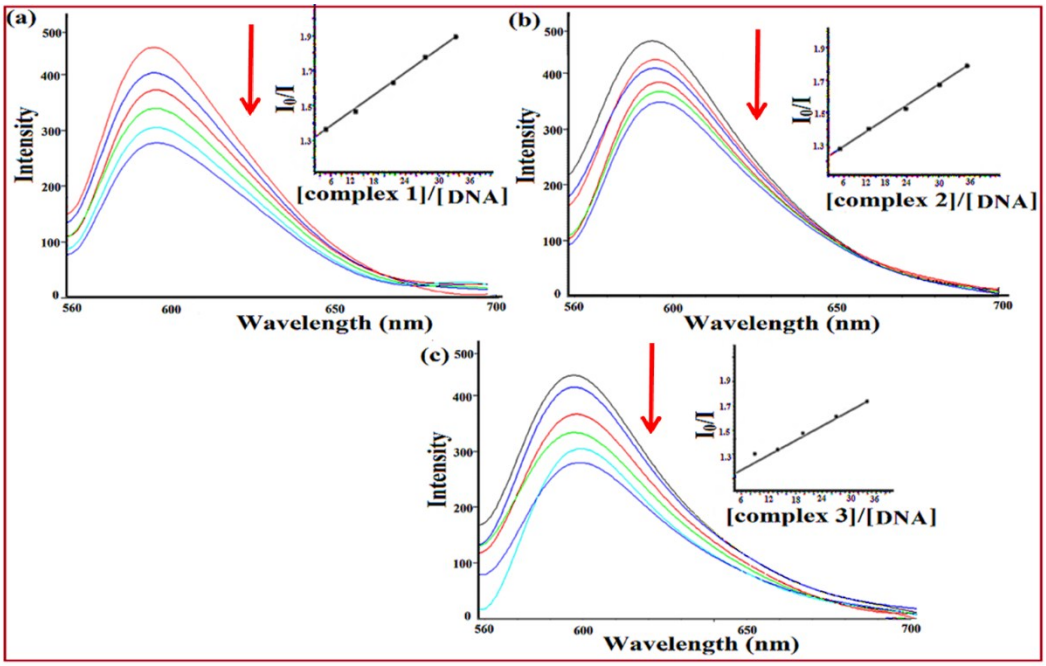


Fig. S8. Emission spectra of EB–ct–DNA in absence and presence of complexes **1** (a), **2** (b) and **3** (c) in Tris–HCl buffer (pH 7.2). [Complexes **1**–**3**] = [EB] = [DNA] = 1.11×10^{-4} M. Arrow depicts the intensity change with increasing concentration of complexes **1**–**3**.

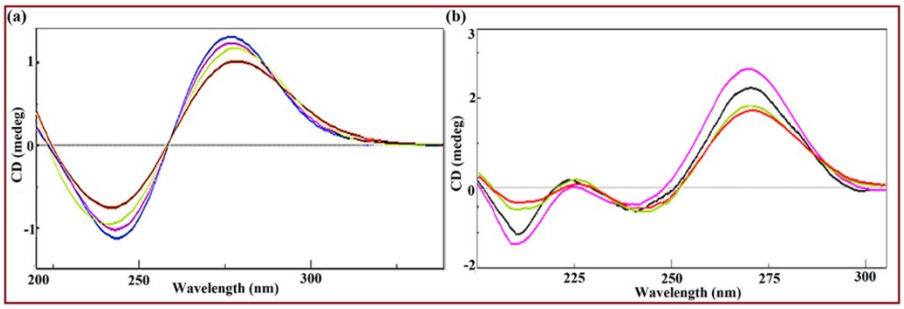


Fig. S9. CD spectra of (a) ct–DNA alone (blue), ct–DNA + **1** (brown), ct-DNA + **2** (pink) and ct–DNA + **3** (green); (b) tRNA alone (pink), tRNA + **1** (red), tRNA + **2** (black), tRNA + **3** (green) in Tris–HCl buffer (pH = 7.2).

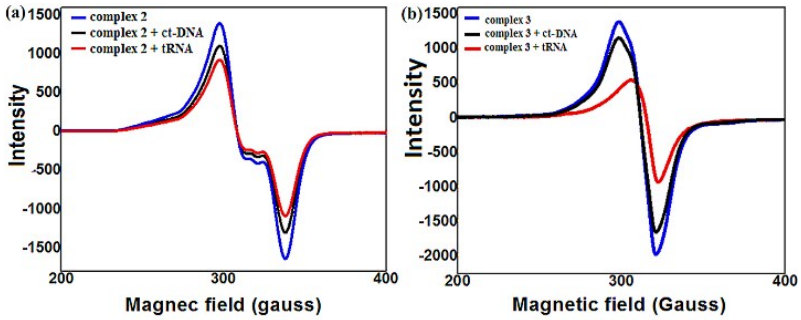
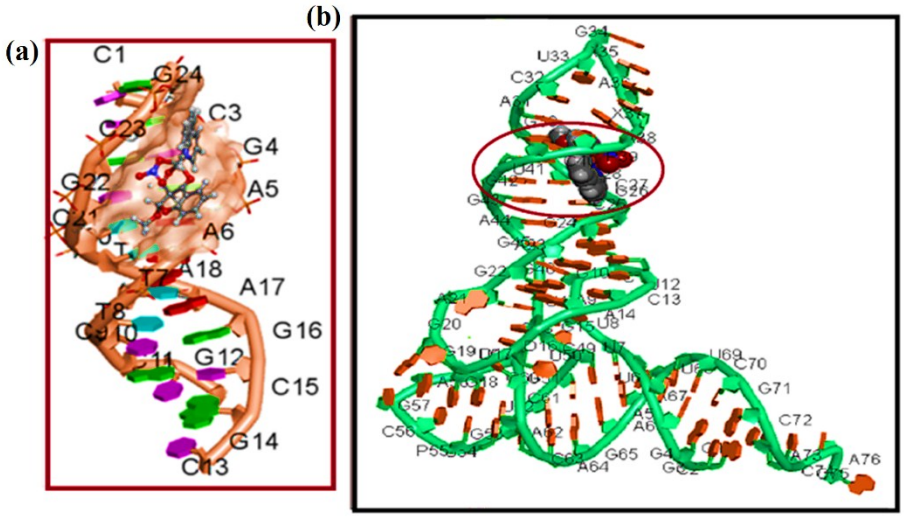


Fig. S10. X–band EPR spectra of (a) 0.3 mM complex 2 (red), 0.3 mM complex 2 + 1.4 mg mL^{-1} tRNA (black) and 0.3 mM complex 2 + 1.4 mg mL^{-1} ct–DNA (blue); (b) 0.3 mM complex 3 (red), 0.3 mM complex 3 + 1.4 mg mL^{-1} tRNA (blue) and 0.3 mM complex 3 + 1.4 mg mL^{-1} ct–DNA (black). Experimental conditions: T = 298 K; Microwave frequency = 9.46 GHz; microwave power = 20 mW; 10 G field modulation amplitude; time constant 81.92 ms; conversion time 81.92 ms; 3 accumulations.



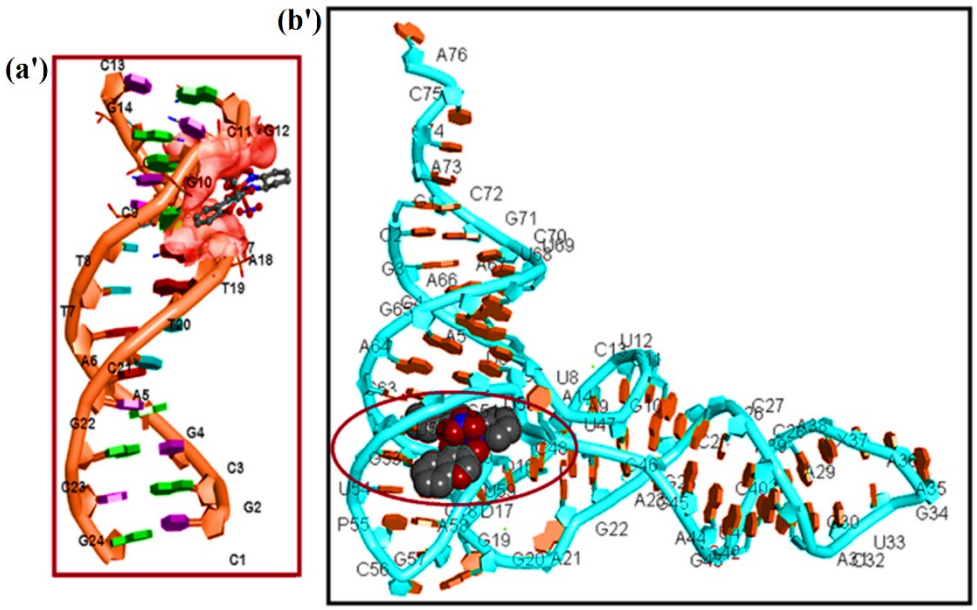


Fig. S11. Molecular docked model of complex **1** with (a) ct–DNA (PDB ID: 1BNA), (b) tRNA (PDB ID: 6TNA); complex **3** with (a′) ct–DNA (PDB ID: 1BNA) and (b′) tRNA (PDB ID: 6TNA).