Supplementary Data

Design and synthesis of a DNA intercalative half–Sandwich organoruthenium(II)–chromone complex: Cytotoxicity evaluation and topoisomerase Iα inhibition assay

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Table S1. Selected bond lengths and bond angles in complex **1**

Bond Lengths

Atom	Atom	Length/Å
Ru2	Cl2	2.4356(7)
Ru2	O6	2.072(3)
Ru2	O5	2.079(2)
Ru2	C34	2.199(4)
Ru2	C37	2.215(3)
Ru2	C38	2.174(3)
Ru2	C35	2.162(3)
Ru2	C39	2.161(4)
Ru2	C36	2.174(3)
Ru1	Cl1	2.4342(7)
Ru1	O1	2.080(2)
Ru1	O2	2.070(3)

Bond Angles

Atom	Atom	Atom	Angle/°
O6	Ru2	Cl2	82.88(7)
O5	Ru2	Cl2	85.21(6)
O5	Ru2	O6	88.28(9)
C34	Ru2	Cl2	116.42(9)
C34	Ru2	O6	160.49(11)
C34	Ru2	O5	90.46(12)
C37	Ru2	Cl2	120.50(9)
C37	Ru2	O6	91.08(12)
C37	Ru2	O5	154.00(10)
C37	Ru2	C34	81.62(14)
C38	Ru2	Cl2	93.88(8)
C38	Ru2	O6	115.08(11)
C38	Ru2	O5	156.38(12)
C38	Ru2	C34	68.78(14)
C38	Ru2	C37	37.35(13)

C35	Ru2	Cl2	154.55(10)
C35	Ru2	O6	121.94(12)
C35	Ru2	O5	89.70(12)
C35	Ru2	C34	38.56(14)
C35	Ru2	C37	68.73(13)
C35	Ru2	C38	81.02(13)
C39	Ru2	Cl2	92.38(9)
C39	Ru2	O6	153.01(13)
C39	Ru2	O5	117.90(12)
C39	Ru2	C34	37.26(14)
C39	Ru2	C37	68.45(14)
C39	Ru2	C38	38.49(14)

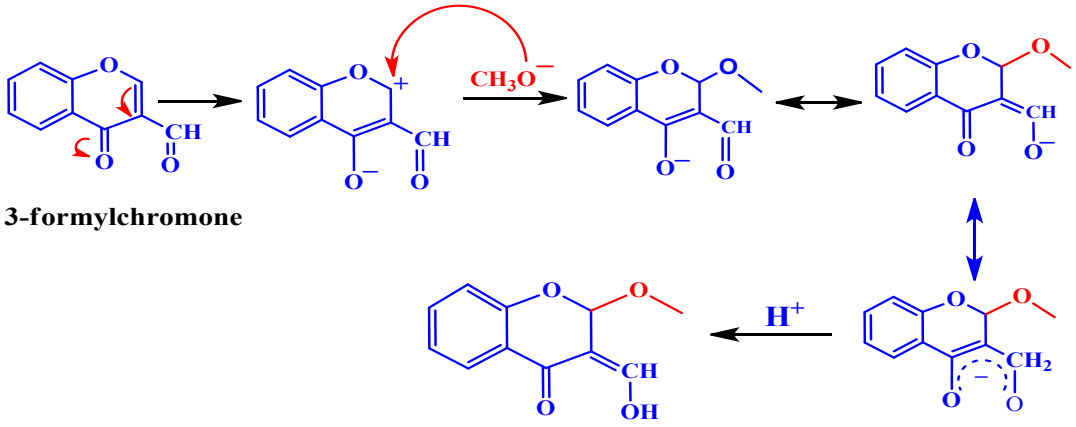
Table S2. IC_{50} (μM) values of the complexes **1** on topoisomerase I activities of some of the classical Topo-I inhibitors.

Drug/complex	**Inhibitory activity on Topo I (IC_{50}) (μM)**
Camptothecin	17
Topostatin	17
Etoposide	>1000
Hoechst 33258	30
Novobiocin	>100
Δ-$[Ru(bpy)_2(uip)]^{2+}$	~ 40
Λ-$[Ru(bpy)_2(uip)]^{2+}$	~ 40
Complex **1**	**20**

Table S3. *Summary of the screening data for in vitro antitumor activity of complex **1** (in μg/mL).*

Cell line		**A–498**	**Hep-G2**	**MIA-PA-CA-2**	**HeLA**	**MCF7**
GI_{50}	**Complex 1**	>80	>80	47.11	13.94	>80
	ADR	<10	<10	<10	<10	<10
TGI	**Complex 1**	NE	>80	22.4	64.39	NE
	ADR	<10	<10	<10	<10	<10

GI_{50} = growth inhibition of 50% (GI_{50}) calculated from [(Ti−Tz)/(C−Tz)] x 100 = 50, drug concentration that results in a 50% reduction in the net protein increase.
ADR = Adriamycin (taken as positive control compound).
TGI = tumor growth inhibition.



Scheme S1: Mechanistic route for *insitu* metoxylation of 3–formylchromone ligand.

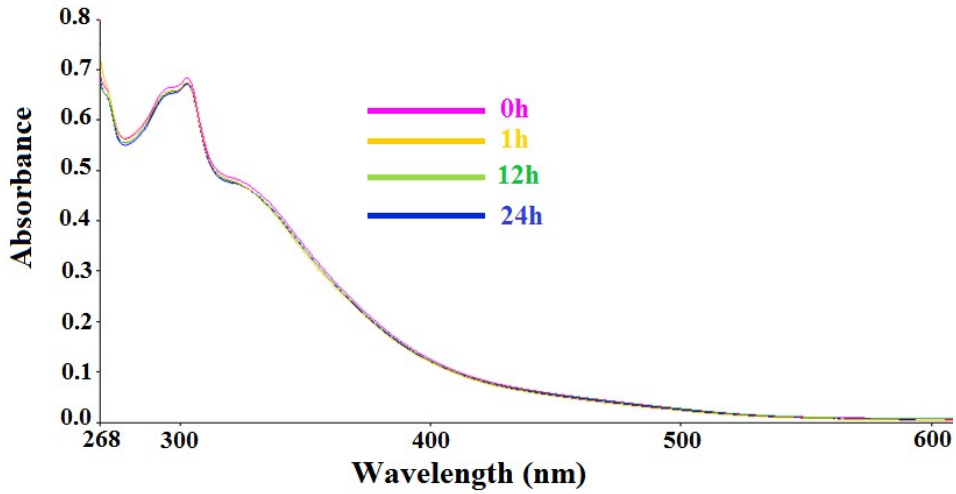


Fig. S1 UV–vis absorption spectra of complex **1** in Tris buffer at pH 7.4 and 310 K (physiological conditions) as a function of different time intervals (0h, 6h, 12h, & 24h).

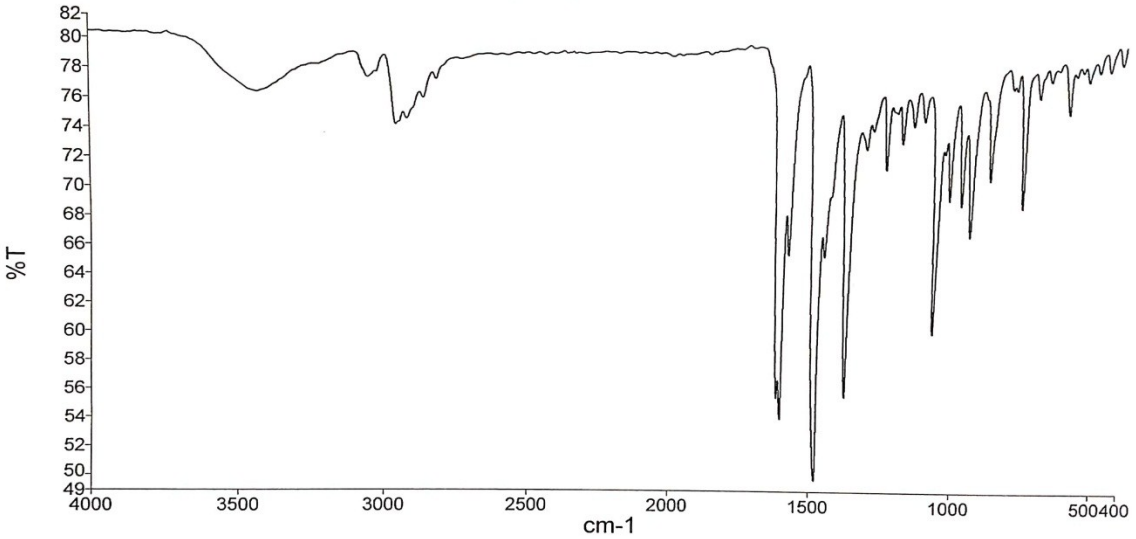


Fig. S2 FTIR spectrum of complex **1**.

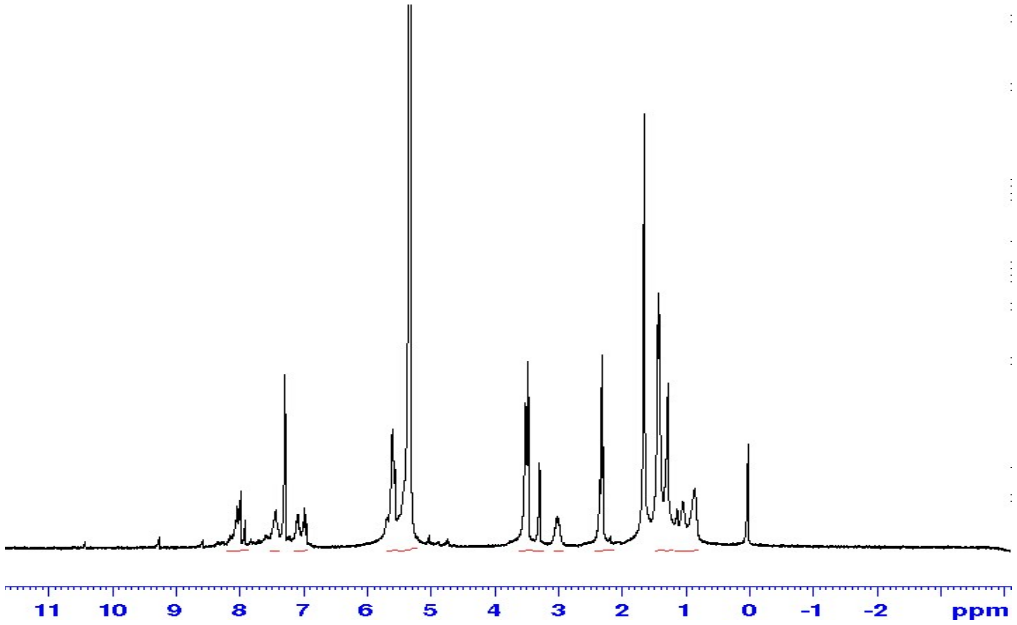


Fig. S3. ^{1}H NMR spectrum of complex **1**.

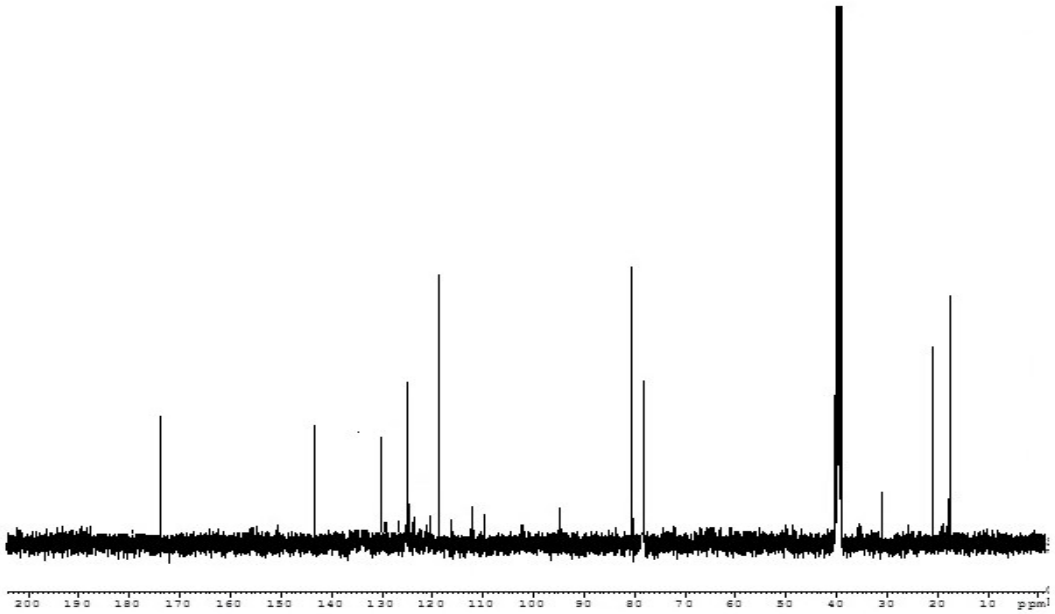


Fig. S4 ^{13}**C** NMR spectrum of complex **1**.

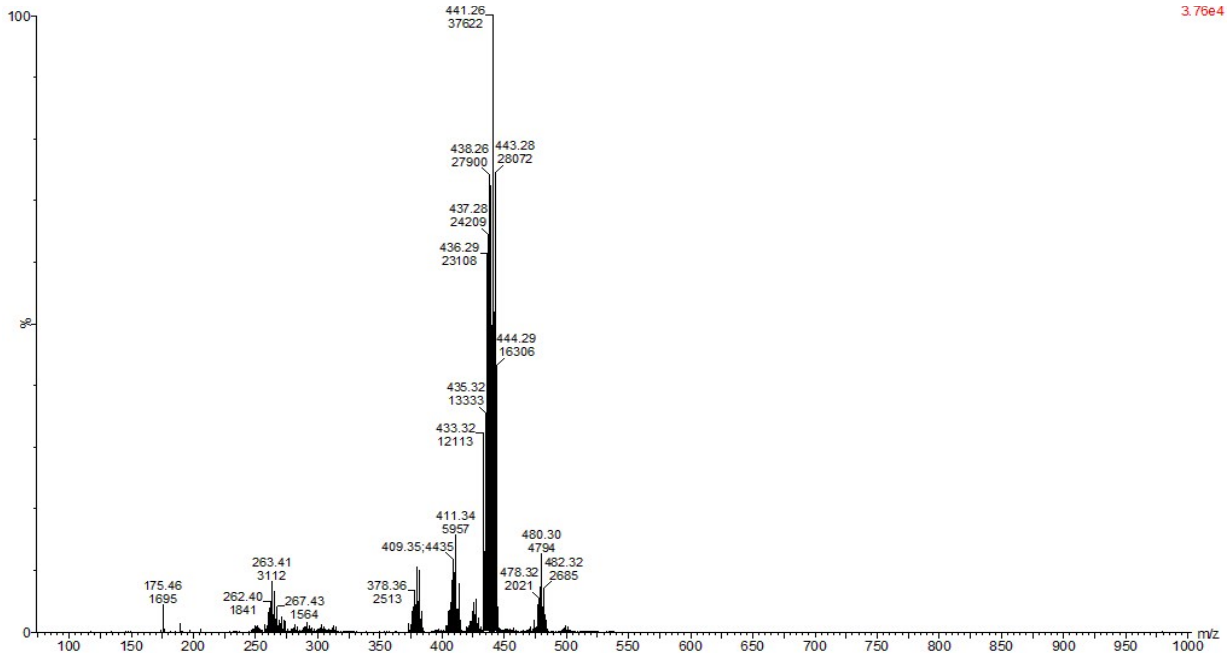


Fig. S5 ESI MS spectrum of complex **1**.

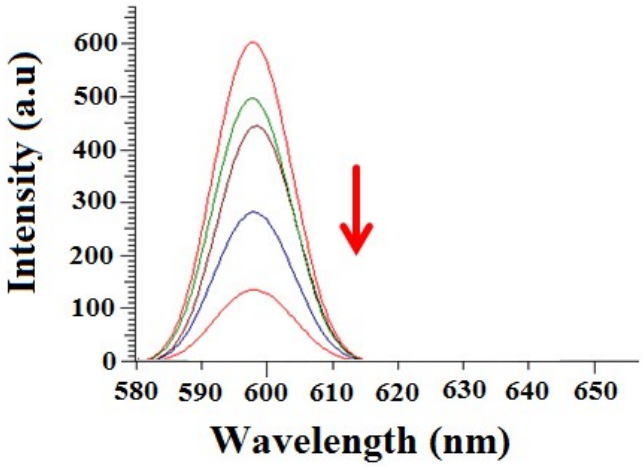


Fig. S6. Effect of increasing concentration of complex **1** on the emission spectra of EB–DNA system in Tris–HCl buffer at pH 7.2. [EB] = [DNA] = 1 x 10^{-5} M, [complex **1**] = 1 x 10^{-5} M Arrow shows change in intensity with increasing concentration of complex **1**.

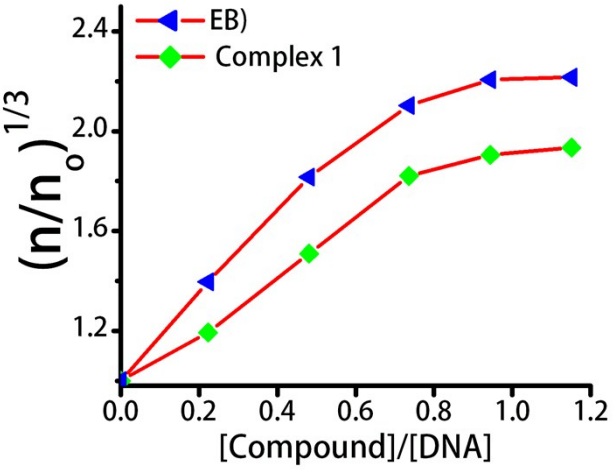


Fig. S7 The effect of increasing concentration of EB and complex **1**, on the relative viscosity of ct–DNA at 37.0 C in 5 mM Tris–HCl buffer at pH = 7.2. (η and η_0 are the specific viscosity of DNA in the presence and absence of the complex, respectively). [DNA] = 5.60 μM and the molar ratios of complex **1** or EB to DNA were varied from 0.2 to 1.0.

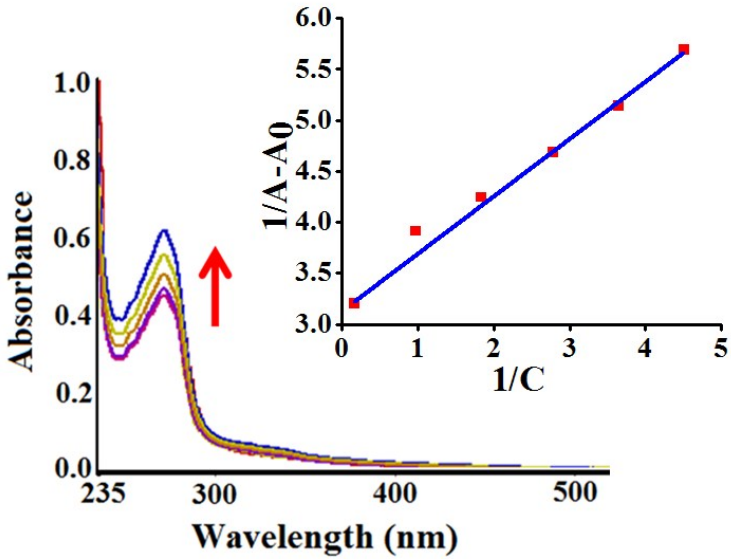


Fig. S8. UV–vis absorption spectra of HSA in presence of increasing concentration of complex **1** in 5 mM Tris–HCl/50 mM NaCl buffer at pH 7.4; [Complex **1**] = 1.50 x 10^{-5} M; [HSA] = 1.00 x 10^{-5} M. Inset: Plot of $1/A–A_o$ *vs* 1/[Complex **1**]. Arrows indicate changes in absorbance upon increasing concentration of the complex **1.**

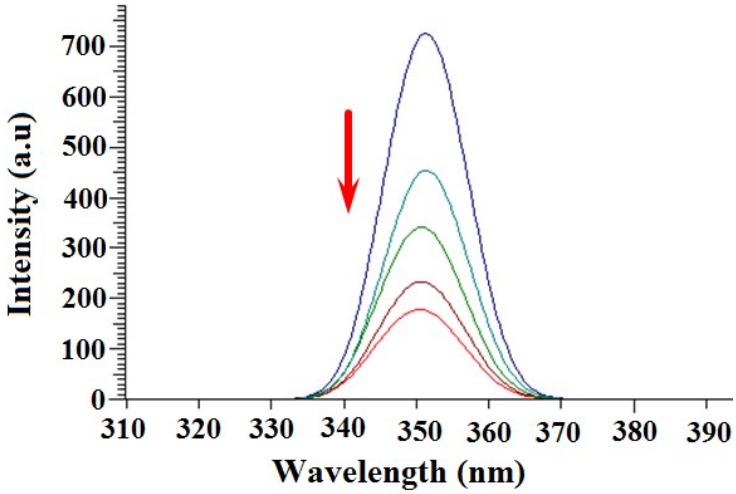


Fig S9. The fluorescence quenching spectra of HSA (Trp-214) upon titrating with different concentrations of complex **1** in 5 mM Tris–HCl/50 mM NaCl buffer, pH 7.4, at room temperature. [HSA] = 1.25 x 10^{-5} M, [Complex **1**] = 0.0–0.8 x 10^{-4} M. Arrow indicates intensity changes upon increasing concentration of the quencher (complex **1**).