Supporting Information

DMSO containing ruthenium(II) hydrazone complexes: *In vitro* evaluation of biomolecular interaction and anticancer activity

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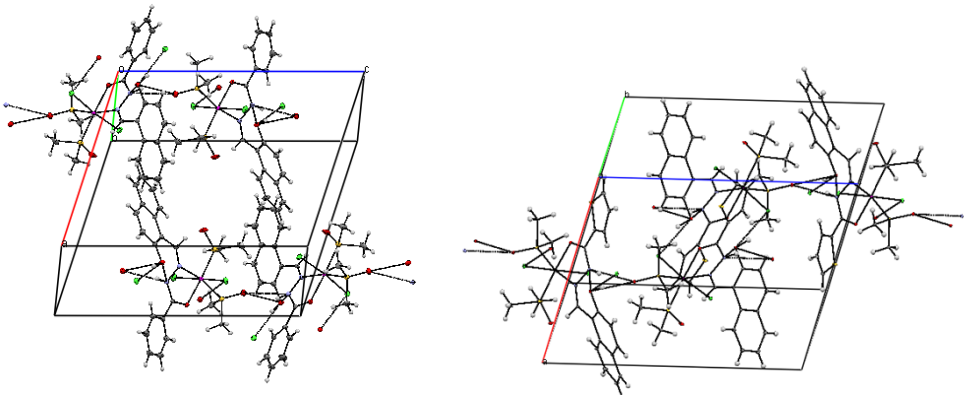
†Electronic supplementary information (ESI) available:

CCDC reference numbers 838986 and 852727 for complex 2 and 4. For ESI and crystallographic data in CIF or other electronic format see DOI:



Complex **1** Complex **4**

Figure S1 Packing diagrams of complexes **1** and **4** showing inter-molecular hydrogen bonding.

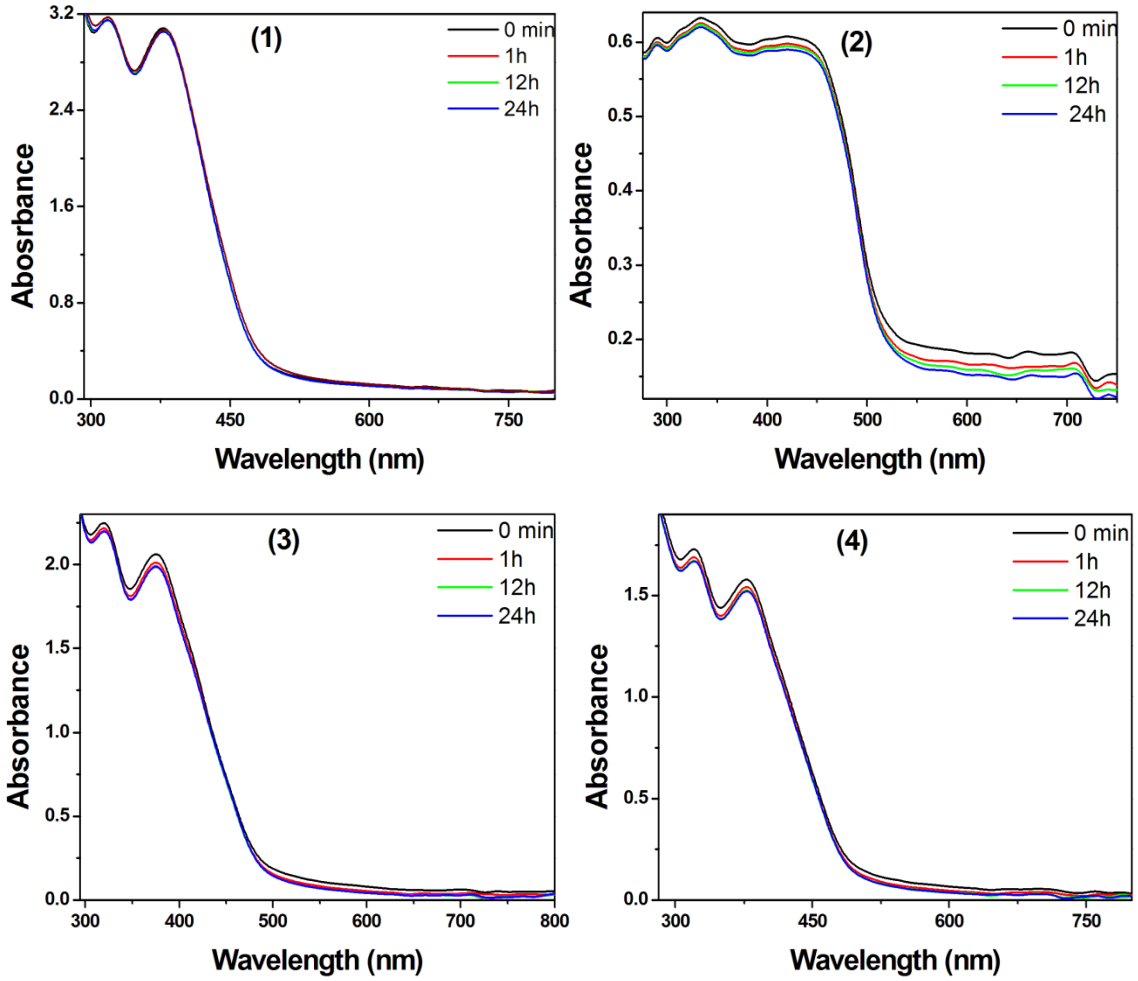


Figure S2 UV-visible absorption spectra of complexes **1**, **2**, **3** and **4** in aqueous PBS buffer at pH 7.4.

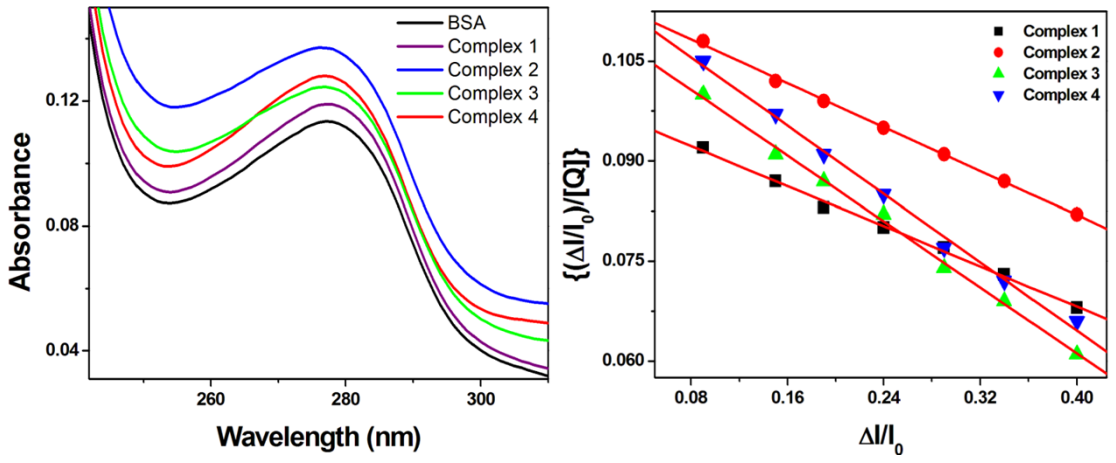


Figure S3 Electronic absorption spectra of BSA (10 μM), with ligands and complexes and Scatchard plots of the fluorescence titration of the complexes with BSA.

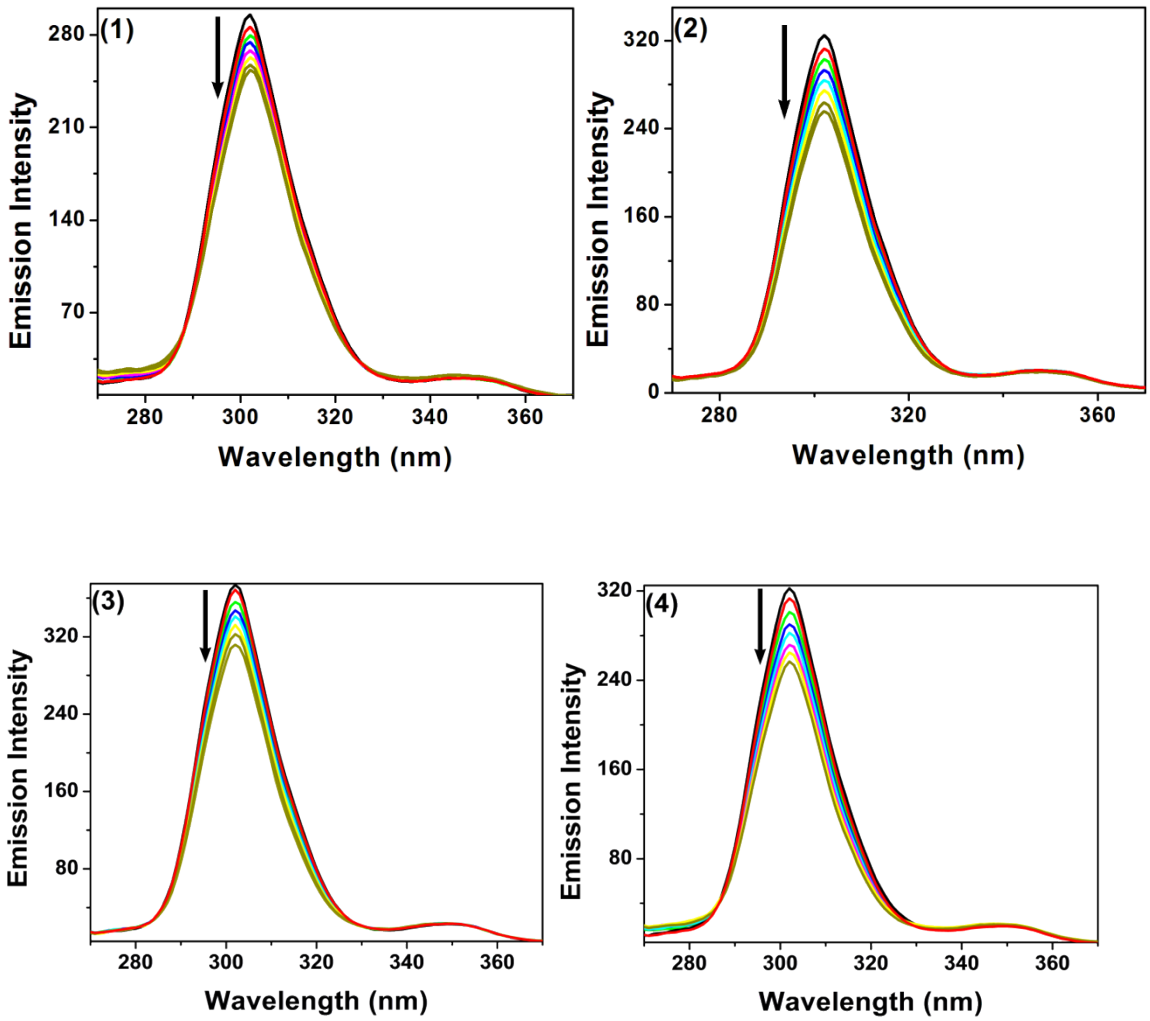


Figure S4 Synchronous spectra of BSA (1 μM) in the presence of increasing amounts of the complexes **1**, **2, 3** and **4 (**0-14 μM) at a wavelength difference of $\Delta\lambda$ = 15 nm. Arrow indicates the decrease of emission intensity as a function of increasing concentration of the compounds.

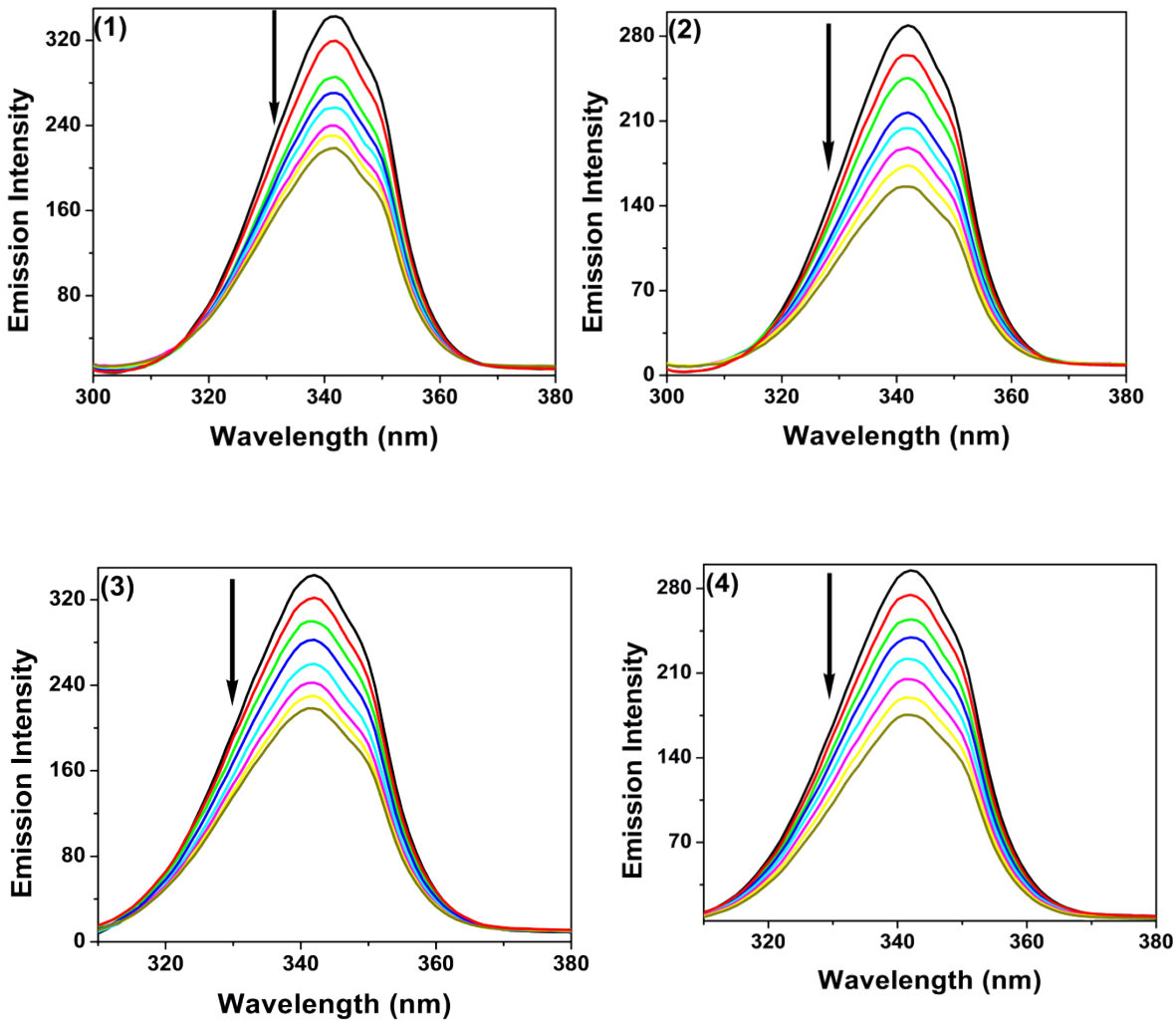


Figure S5 Synchronous spectra of BSA (1 μM) in the presence of increasing amounts of the complexes **1**, **2, 3** and **4** (0-14 μM) at a wavelength difference of $\Delta\lambda$ = 60 nm. Arrow indicates the decrease of emission intensity as a function of increasing concentration of the compounds.

Table S1 Selected bond lengths (Å) and angles (º) for the complex **1** and **4**

	Complex **1**	Complex **4**
Ru(1) – S(2)	2.236(10)	2.2368(8)
Ru(1) – Cl(2)	2.370(10)	2.4124(8)
Ru(1) – Cl(1)	2.401(11)	2.3703(8)
Ru(1) – O(1)	2.086 (2)	2.103(2)
Ru(1) – S(1)	2.250 (10)	
Ru(1) – S(3)		2.2467(8)
O(1)-Ru(1)-S(2)	175.94(8)	175.83(6)
O(1)-Ru(1)-Cl(2)	87.75(8)	88.14(6)
S(2)-Ru(1)-Cl(2)	91.49(4)	92.22(3)
O(1)-Ru(1)-Cl(1)	87.96(8)	87.79(6)
S(2)-Ru(1)-Cl(1)	92.48(4)	91.57(3)
Cl(2)-Ru(1)-Cl(1)	173.98(4)	174.43(3)
N(1)-Ru(1)-S(2)	99.32(8)	99.10(7)
N(1)-Ru(1)-Cl(1)	89.30(8)	84.75(7)
O(1)-Ru(1)-N(1)	76.66(1)	
O(1)-Ru(1)-S(1)	90.89(7)	
N(1)-Ru(1)-S(1)	167.53(8)	
S(2)-Ru(1)-S(1)	93.14(4)	
N(1)-Ru(1)-Cl(2)	85.60(8)	
S(1)-Ru(1)-Cl(2)	94.45(4)	
S(1)-Ru(1)-Cl(1)	89.85(4)	
S(2)-Ru(1)-S(3)		92.93(3)
O(1)-Ru(1)-N(1)		76.74(9)
O(1)-Ru(1)-S(3)		91.23(6)
N(1)-Ru(1)-S(3)		167.95(7)
S(3)-Ru(1)-Cl(1)		94.28(3)
N(1)-Ru(1)-Cl(2)		90.61(7)
S(3)-Ru(1)-Cl(2)		89.62(3)

Table S2 Results of interaction study of compounds **1**–**4** with DNA

Compounds	**Absorption wavelength (nm) (absence of DNA)**	**Shift of wavelength (nm) (presence of DNA)**	**Nature of shift**	**Change in intensity**
1	262	1	Red	26.57 (hyper)
	318	1	Red	8.69 (hypo)
	378	-	-	10.87 (hypo)
2	263	-	-	34.14 (hyper)
	331	1	Red	8.38 (hypo)
	383	-	-	11.72 (hypo)

	419	-	-	9.86 (hypo)
	447	-	-	6.73 (hypo)
3	320	-	-	13.28 (hypo)
	332	2	Red	11.79 (hypo)
	372	-	-	13.51 (hypo)
	451		-	10.40 (hypo)
4	259	-	-	25.44 (hyper)
	330	-	-	10.05 (hypo)
	379	-	-	10.95 (hypo)
	446	-	-	7.38 (hypo)

Table S3 Results of interaction study of compounds **1**–**4** with EB-DNA

	EB expt @ 605 nm	**DNA binding**	
Complex	**% hypochromism**	**K_q (M^{-1})**	**K_{app} (M^{-1})**
1	13.58	1.4758×10^3	7.4210×10^4
2	47.81	9.0270×10^3	4.5165×10^5
3	18.54	2.2401×10^3	1.1199×10^5
4	31.81	4.4309×10^3	2.2948×10^5

Table S4 Comparison of data related to interaction between compounds **1–4** and protein

Complex	**Protein binding experiment**			**Binding constants**		**Binding sites**
	Emission @345nm, (%hypo)	**S15@303 (%hypo)**	**S60@342 (%hypo)**	**K_{sv} ($\times10^5$ M^{-1})**	**K ($\times10^5$ M^{-1})**	**n**
1	38.27	14.12	36.14	4.287	0.5556	0.8835
2	42.76	21.29	46.08	4.823	2.0219	0.9465
3	40.98	16.54	36.40	4.512	1.4995	0.9191
4	41.25	20.38	40.54	4.800	1.8975	0.9406