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Supporting Information for Studies of Ruthenium(II)-2,2'-bisimidazole complexes on binding to G-quadruplex DNA and inducing apoptosis in HeLa cells

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Eq. (1)

$$(\varepsilon_a - \varepsilon_f)/(\varepsilon_b - \varepsilon_f) = (b - (b^2 - 2K_b^2 C_t [\text{DNA}]/s)^{1/2})/2K_b C_t \quad (1a)$$

$$b = 1 + K_b C_t + K_b [\text{DNA}]/2s \quad (1b)$$

where [DNA] is the concentration of DNA in nucleotides, ε_a is the molar absorptivity ($A_{\text{abs}}/[M]$) observed for the MLCT absorption band at a given DNA concentration, ε_f and ε_b are the molar absorptivity for the free Ru-complex and the molar absorptivity for the Ru-complex in the fully bound form, respectively. K_b is the equilibrium binding constant in M^{-1} , C_t is the total Ru-complex concentration, and s is the binding site size.

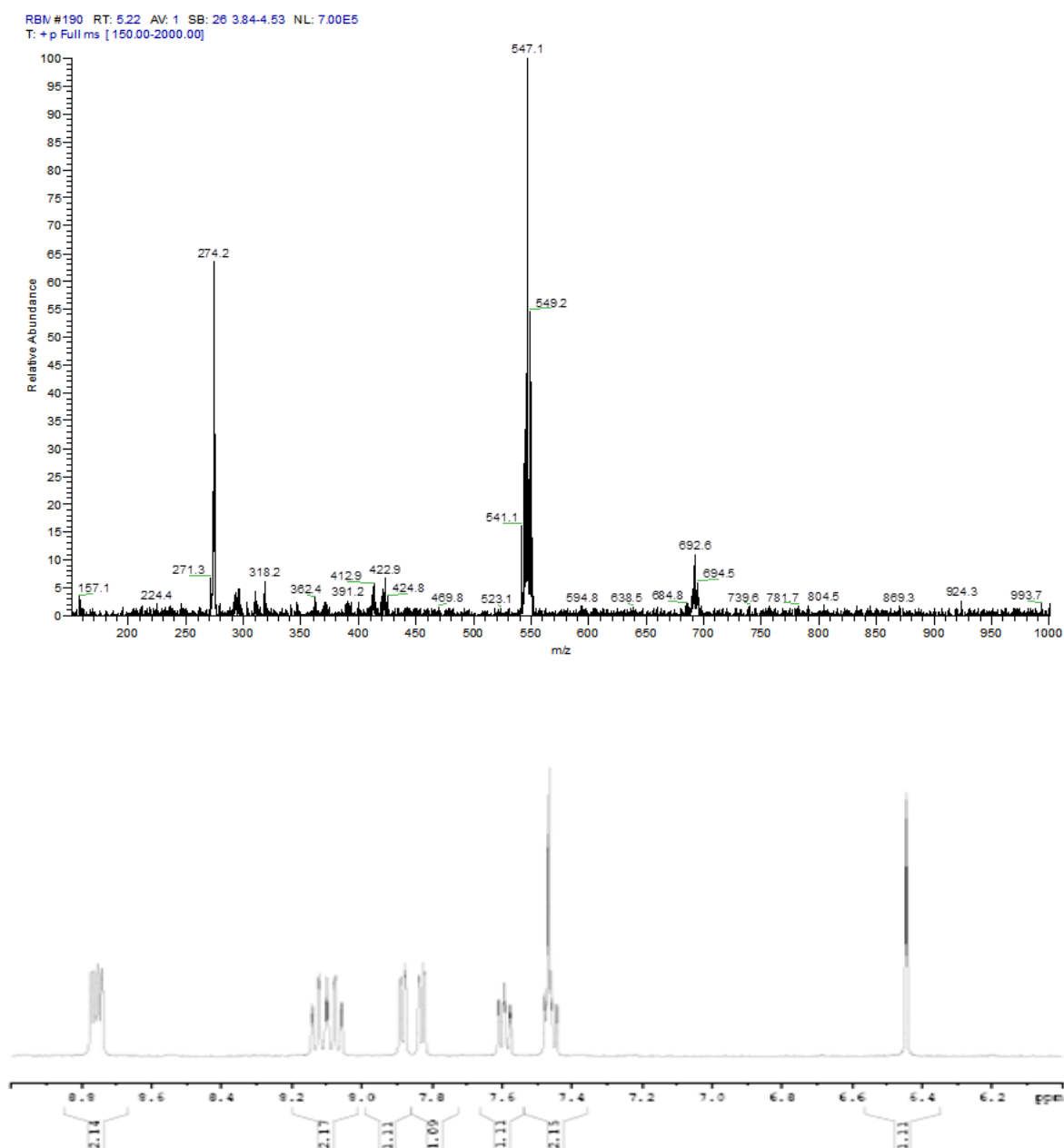


Fig. S1 ESI-MS and ¹H NMR spectra of complex 1.

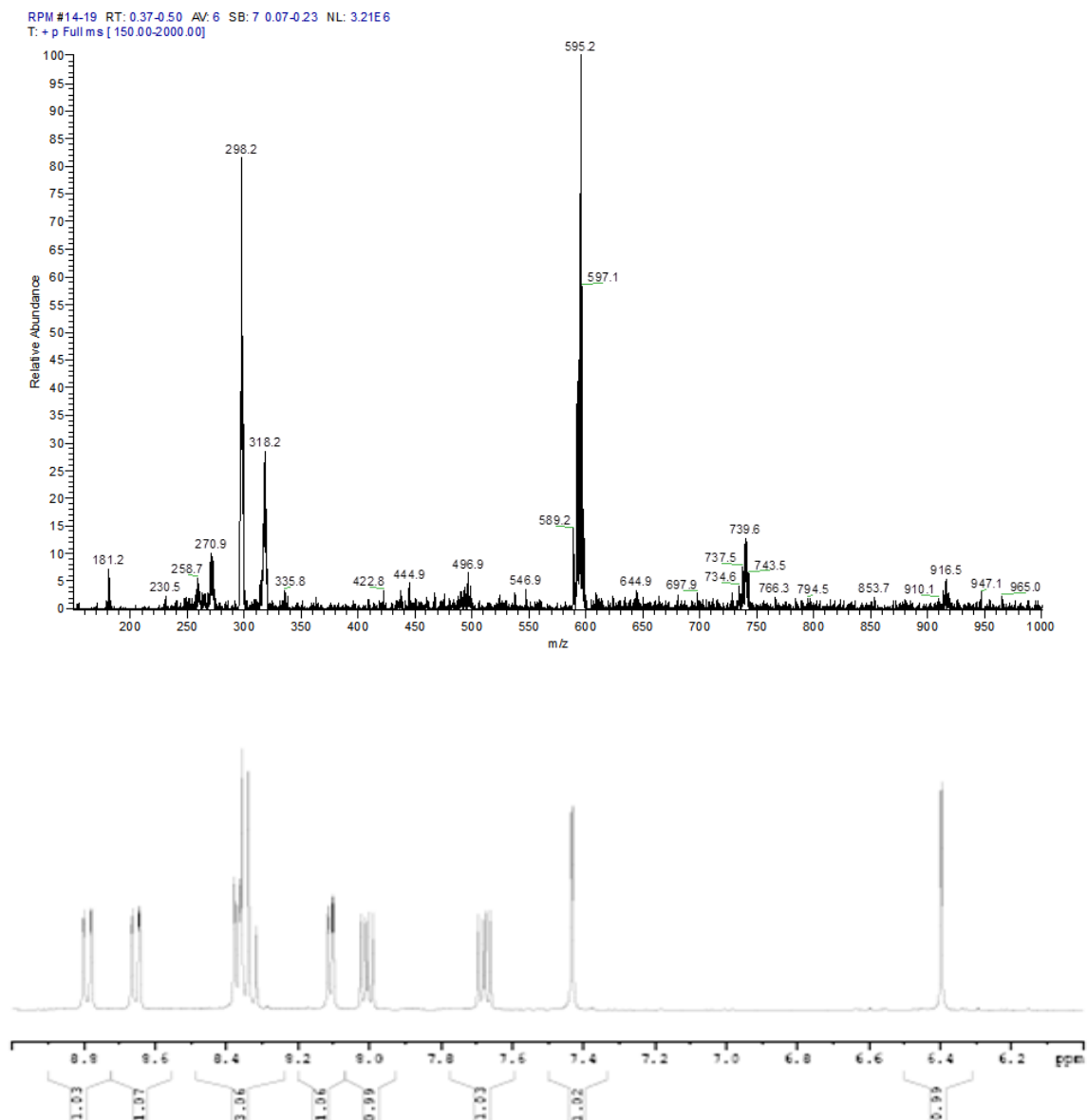


Fig. S2 ESI-MS and ¹H NMR spectra of complex **2**.

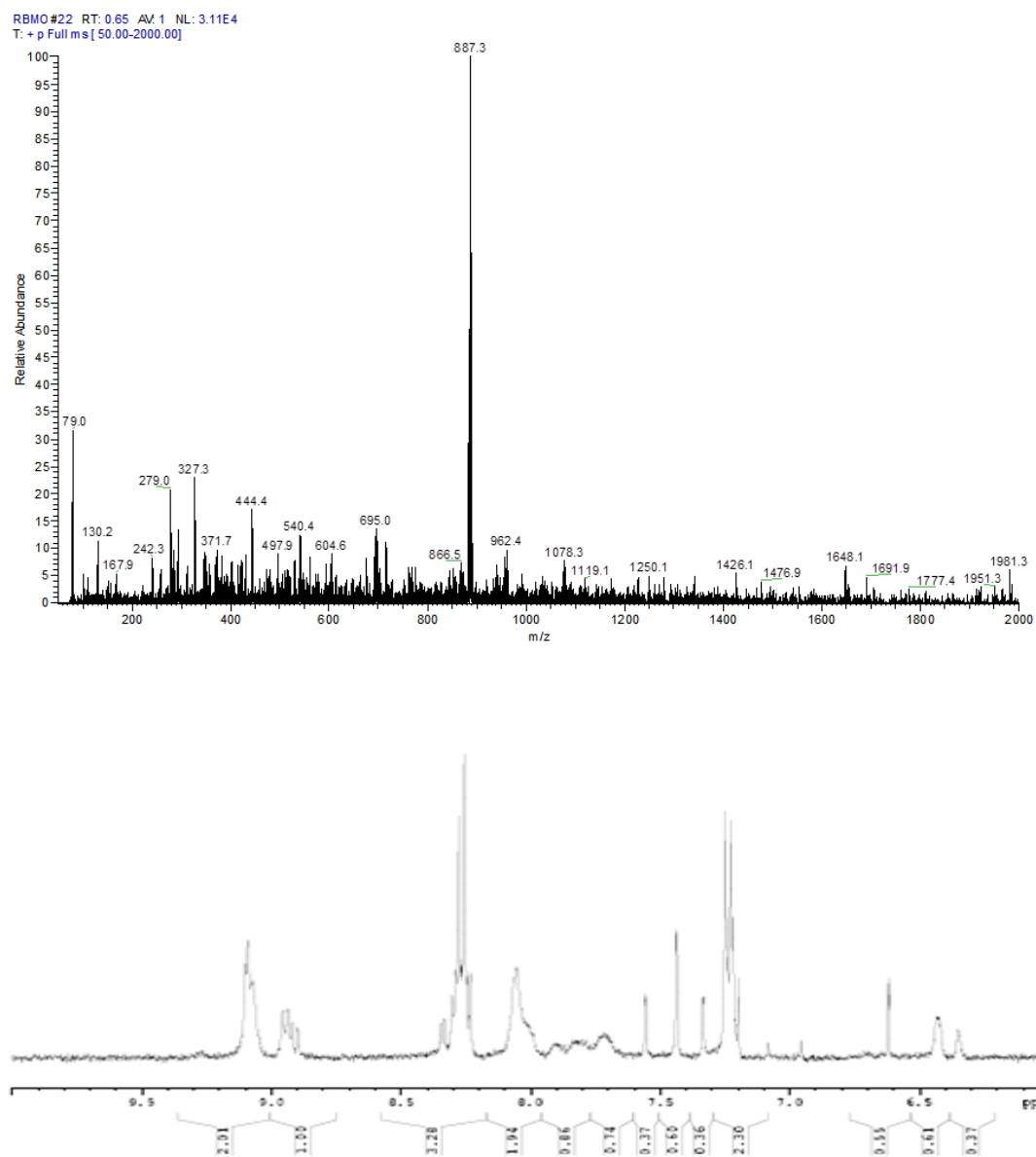


Fig.S3 ESI-MS and ¹H NMR spectra of complex **3**.

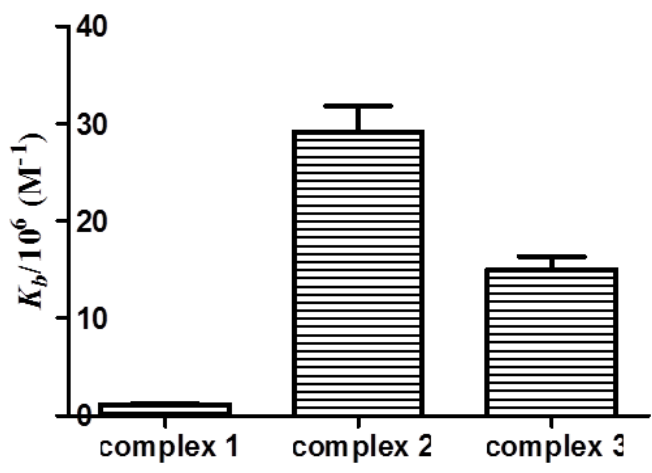


Fig. S4 DNA-binding constants K_b ($\times 10^6 M^{-1}$) of complexes **1**, **2** and **3**.

Table S1 Absorbance spectra (λ_{max}/nm) and DNA-binding constants K_b ($\times 10^6 M^{-1}$) of complexes **1**, **2** and **3**.

Complex	$\lambda_{max}/free$	$\lambda_{max}/bound$	$\Delta\lambda/nm$	H (%)	$K_b/10^6 (M^{-1})$
1	477	477	0	13	1.15 ± 0.14
	338	338	0	13	
	288	288	0	15	
2	471	474	3	29	29.11 ± 2.71
	420	424	4	31	
	263	266	3	33	
3	495	496	1	23	15 ± 1.35
	285	291	6	7	