Electronic Supplementary Material (ESI) for Dalton Transactions

DNA binding, nuclease activity and cytotoxicity studies of Cu(II) complexes of tridentate ligands

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Ligand Characterization:

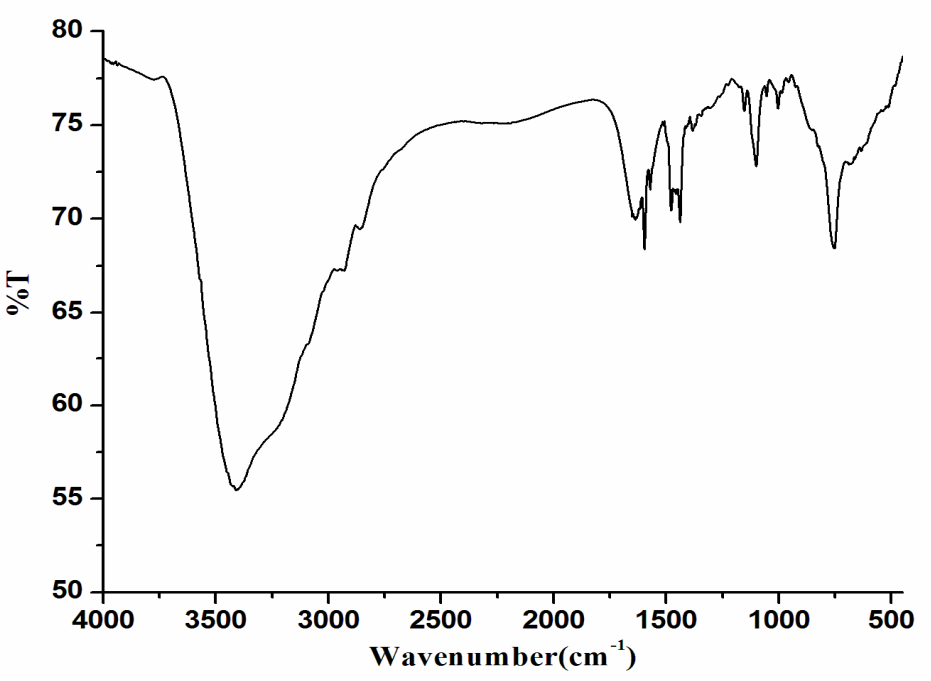

Figure S1. FT-IR spectrum of the $\mathbf{L_1}$ in KBr pellet.

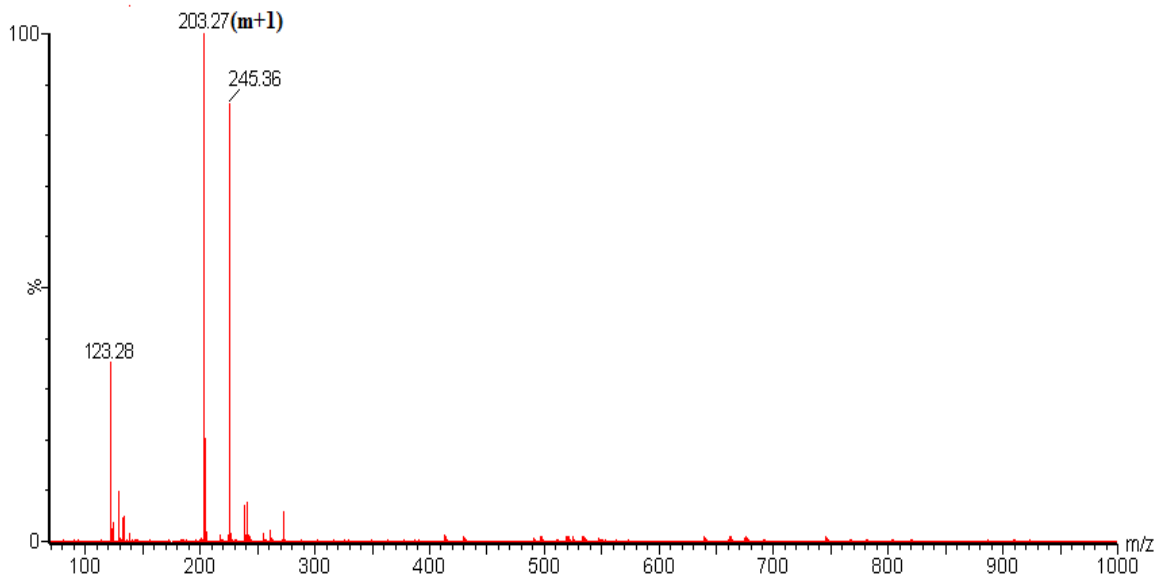

Figure S2. Mass spectrum for $\mathbf{L_1}$ in methanol.

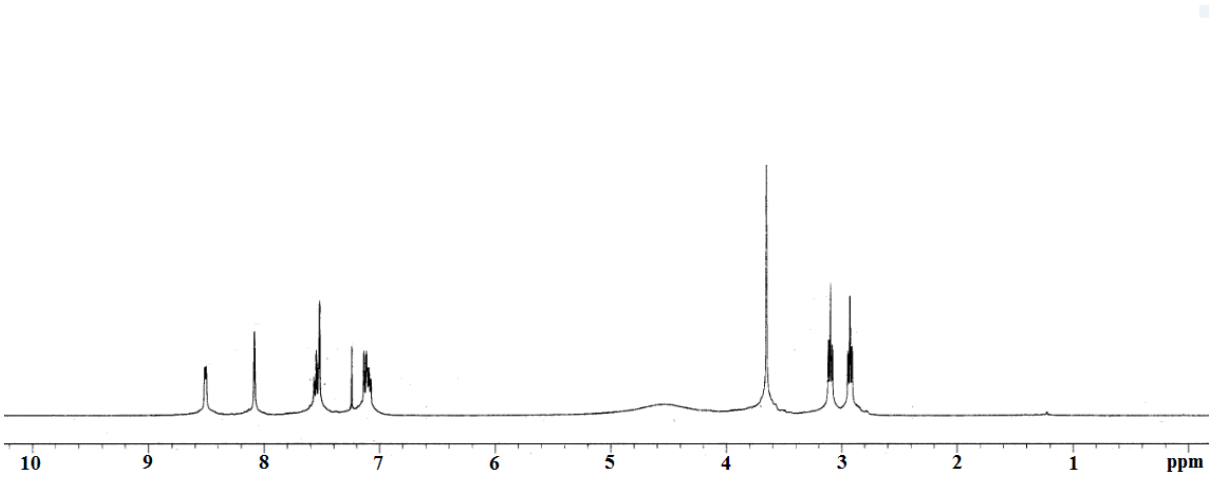

Figure S3. ^{1}H-NMR spectrum of $\mathbf{L_1}$ in $CDCl_3$.

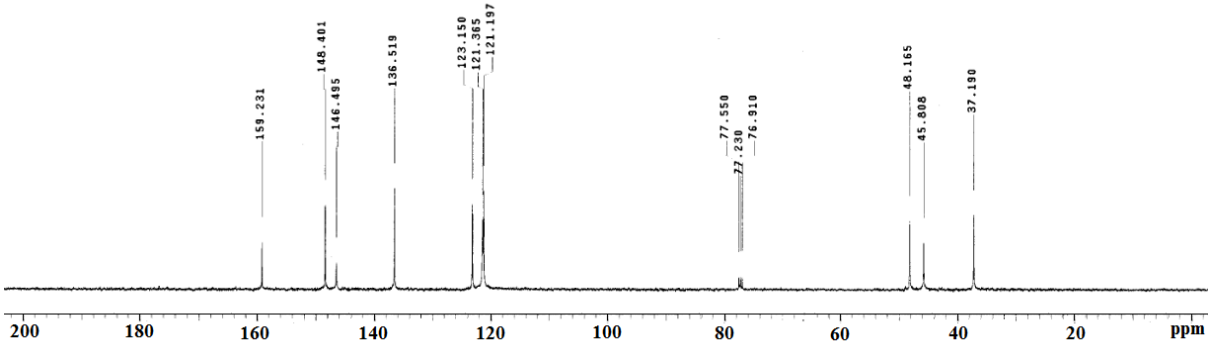

Figure S4. ^{13}C-NMR spectrum of $\mathbf{L_1}$ in $CDCl_3$.

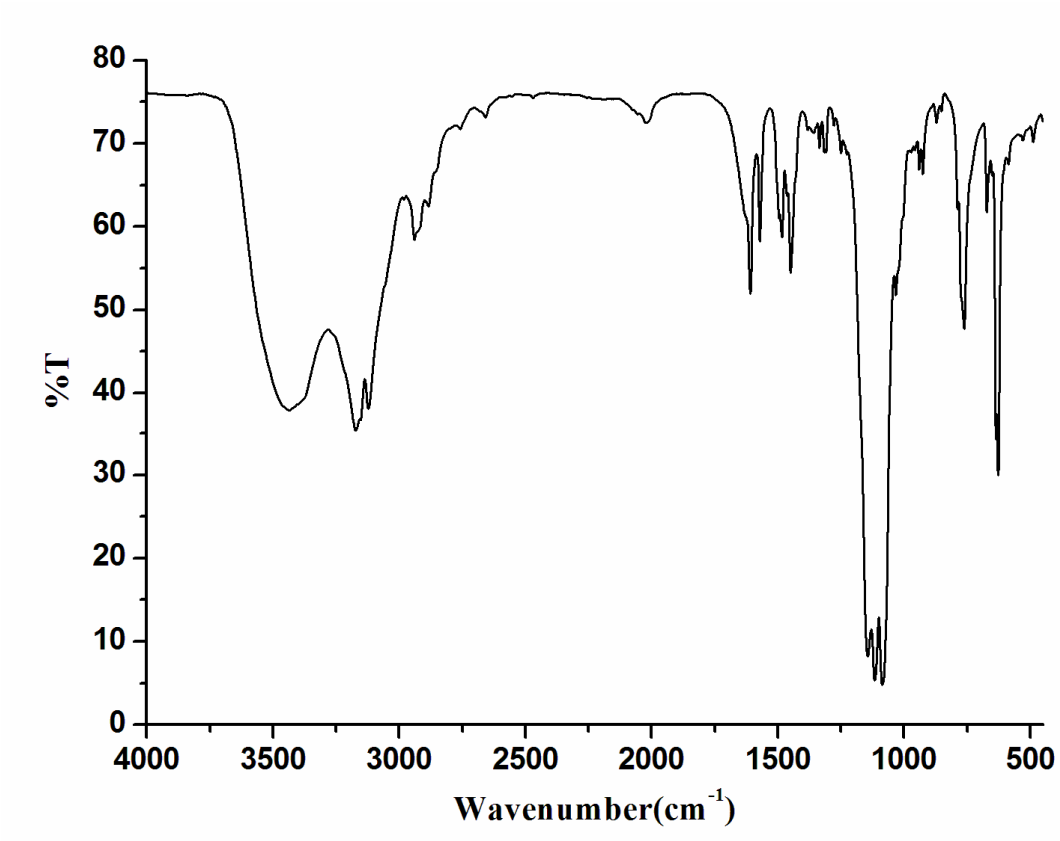

Figure S5. FT-IR spectrum of the complex **1** in KBr pellet.

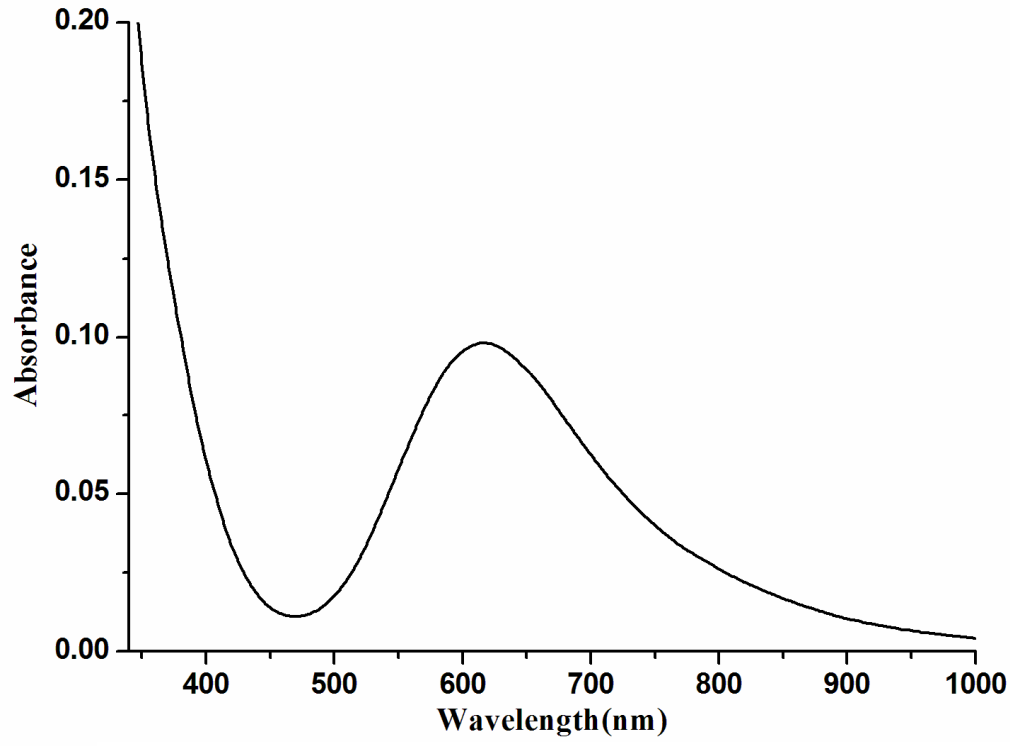

Figure S6. UV-visible spectrum of complex **1** in methanol.

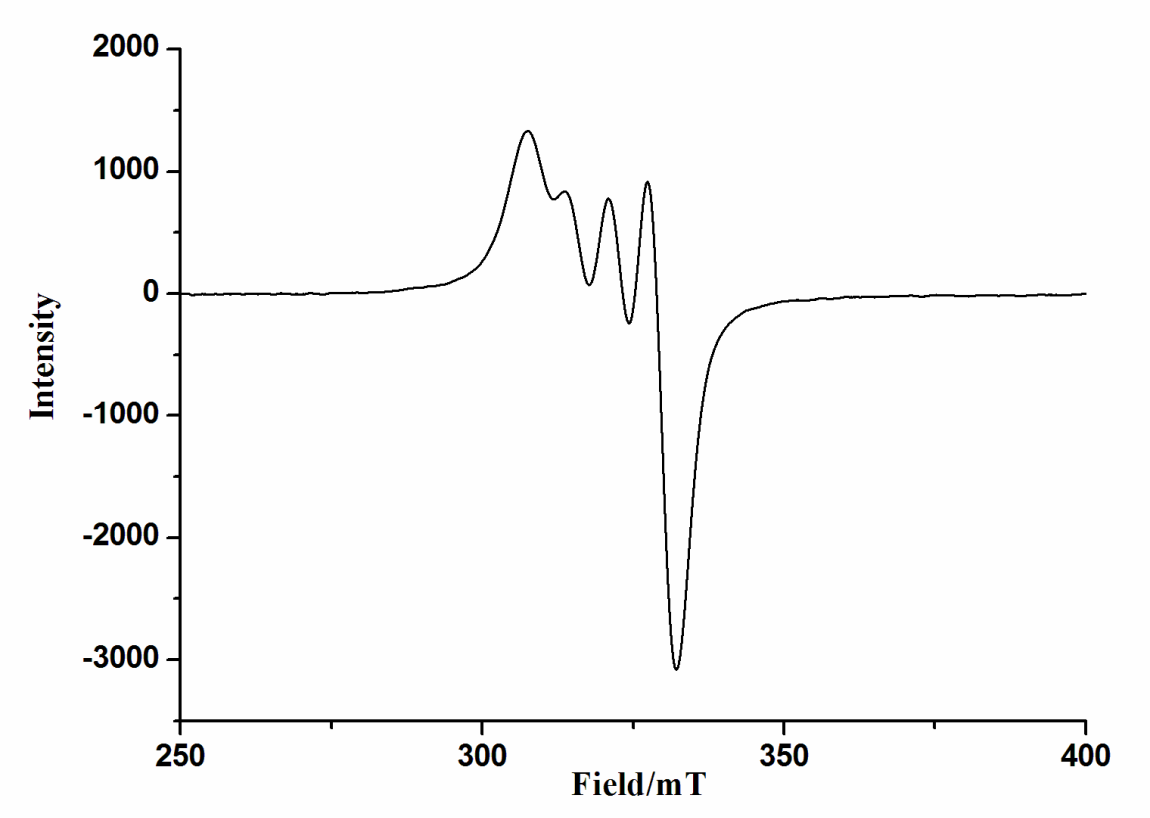

Figure S7. X-Band EPR spectrum of complex **1** in methanol at 298K.

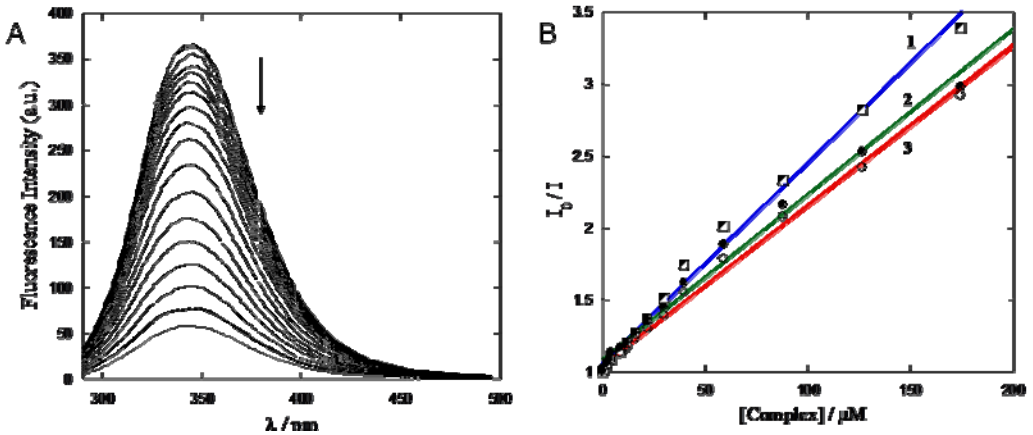

Figure S8: (A) Representative fluorescence emission spectra of BSA (2 μM) 5 mM Tris-HCl/NaCl buffer (pH 7.2) in presence of complex **1** at room temperature, with the increase in molar ratio of complexes to BSA (0-60). (B) The plot of I_0/I *vs.* [complex] for the Cu(II) complexes.

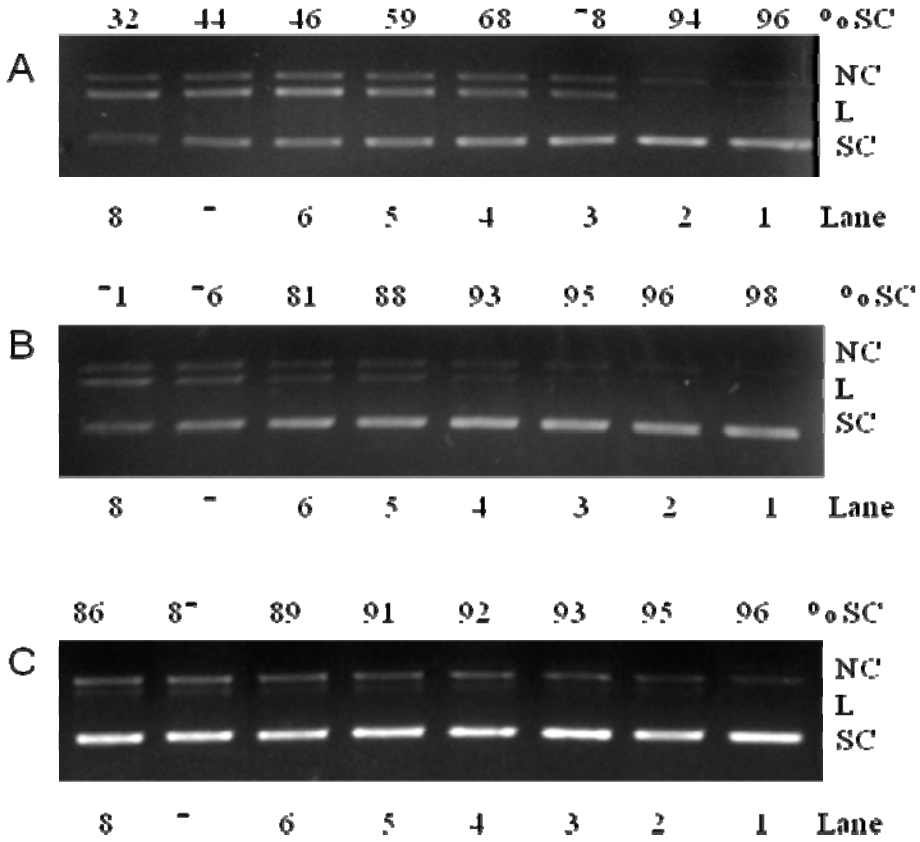

Figure S9: (a) Representative gel electrophoresis diagram showing the time dependent chemical nuclease activity of the complexes (150 μM) using SC pUC19 DNA (30 μM, 0.2 μg) in absence of external agents in 5 mM Tris-HCl/NaCl buffer (pH 7.2) at 37 °C: lane 1-8, DNA + complex (0, 0.5, 1.5, 2.5, 4, 5.5, 7, 9 h). The gel images from A-D are for complex **1**-**3** respectively.

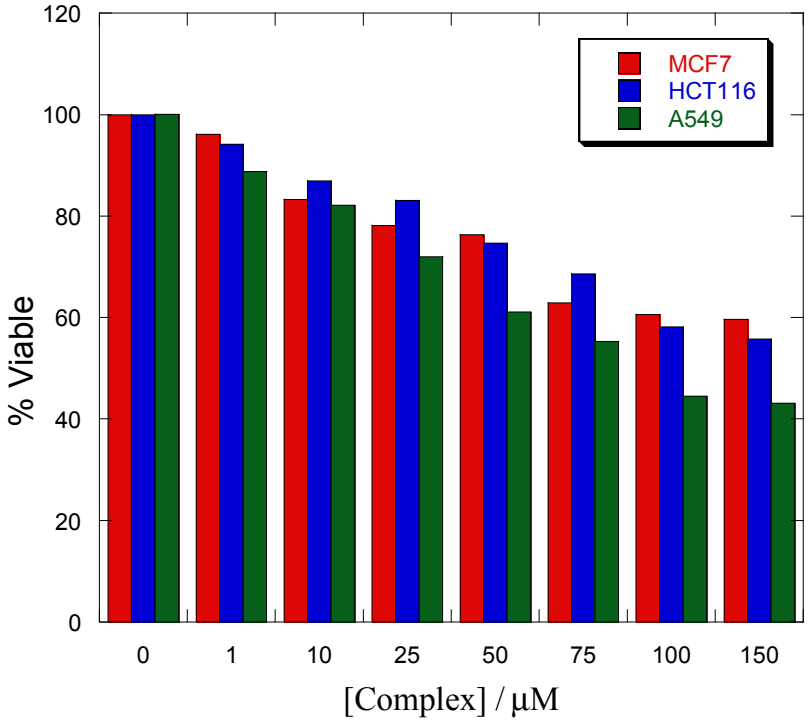

Figure S10: Representative plot of cell viability of complex **2** in a dose dependent manner in human breast (MCF7), lung (A549) and colon (HCT116) cancer cell lines.

Table S1: Observed rate constants for the cleavage of supercoiled pUC19 DNA by Cu(II) complexes.

[a]Complex	**1**	**2**	**3**
K_{obs}/s^{-1}	3.37 (±0.15) × 10^{-5}	1.02 (±0.053) × 10^{-5}	3.21 (±0.15) × 10^{-6}

[a][complex] = 150 µM. [DNA] = 30 µM

Table S2. Chemical nuclease activity of supercoiled pUC19 DNA by the complexes in presence of various additives.

Complex	% SC DNA							
	DNA Only	complex	complex + MPA	complex + H_2O_2	+DMSO[a]	+NaN3[b]	+KI[c]	+L-histidine[a]
1	82	67	6	25	96	61	19	8
2	86	83	2	64	92	57	32	40
3	96	86	3	46	59	4	21	6

[complex] = 50 μM. [a]DMSO = 6 μL. [b][NaN3] = 500 μM. [c][KI] = 500 μM. [d][L-histidine] = 500 μM.