

Supporting information

Evaluating the substitution effects of Bis(β -iminoenolate)copper(II) complexes on their Photophysical, DNA binding/photocleavage, and cytotoxic activity

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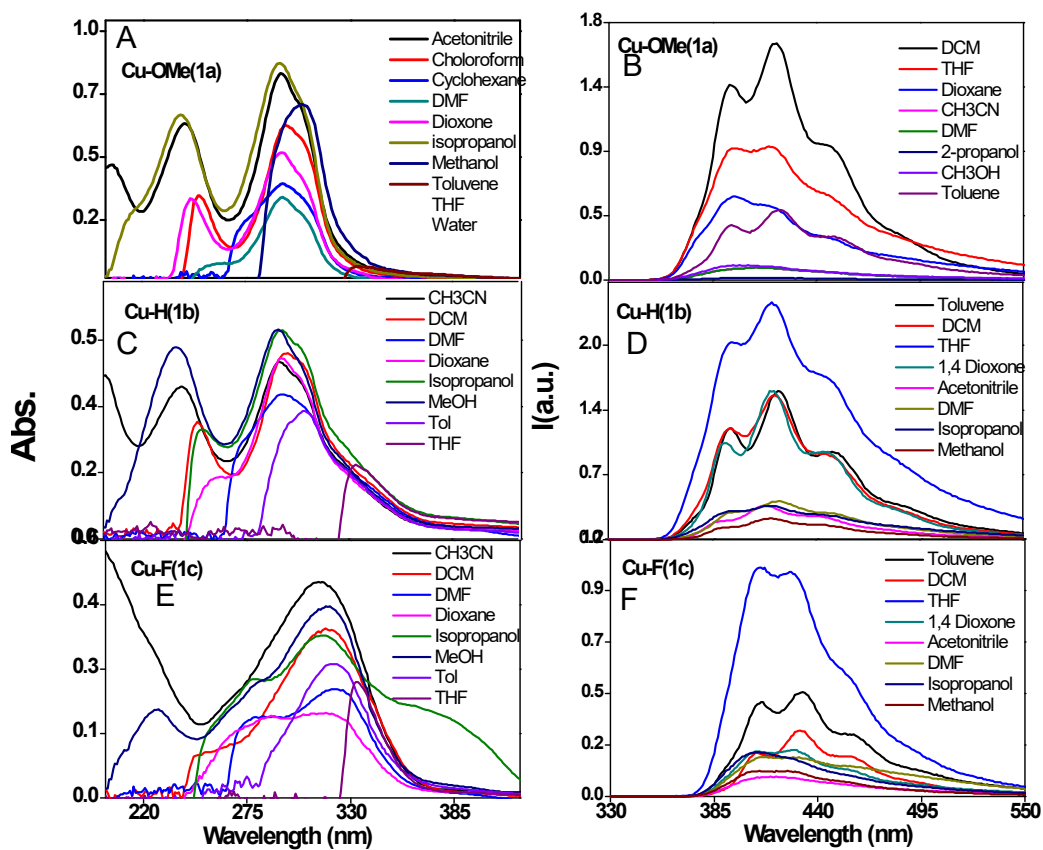


Fig. S1: Solvent dependent absorption (A, C, E) and emission spectra (B, D, F) for the compounds **1a-c**. For fluorescence spectra, 0.2 OD of the solution was prepared..

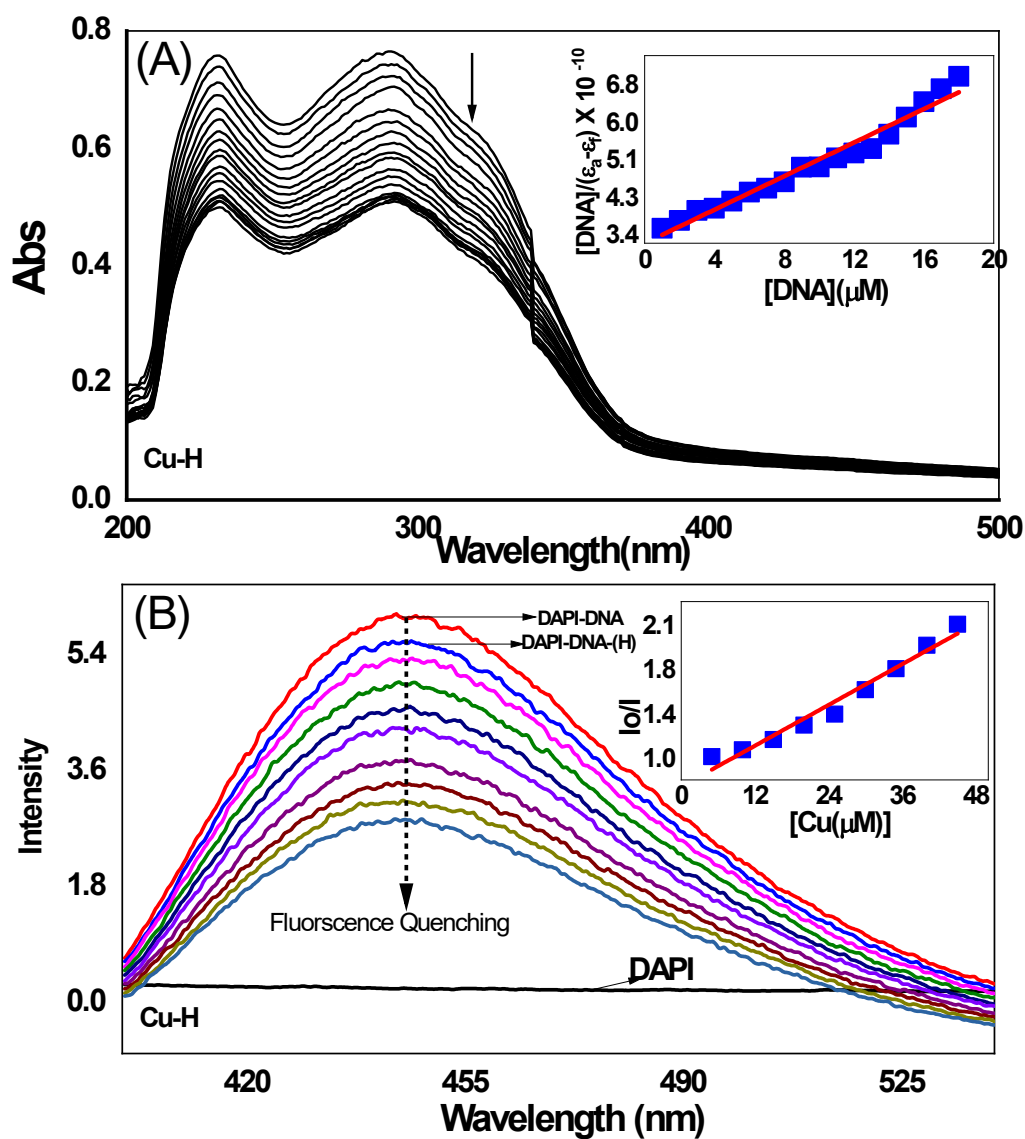


Fig. S2: (A) UV-Vis spectral titration of complex **1b** with CT DNA in Tris-HCl buffer (hypochromism) [**1b**]=10 μ M, [**DNA**_{NP}] = 0-100 μ M.. (B) Emission spectra of DAPI [50 μ M] bound to DNA in the presence of **1b** complex [10 μ M] with increasing concentration (0-50 μ M) in phosphate buffer.

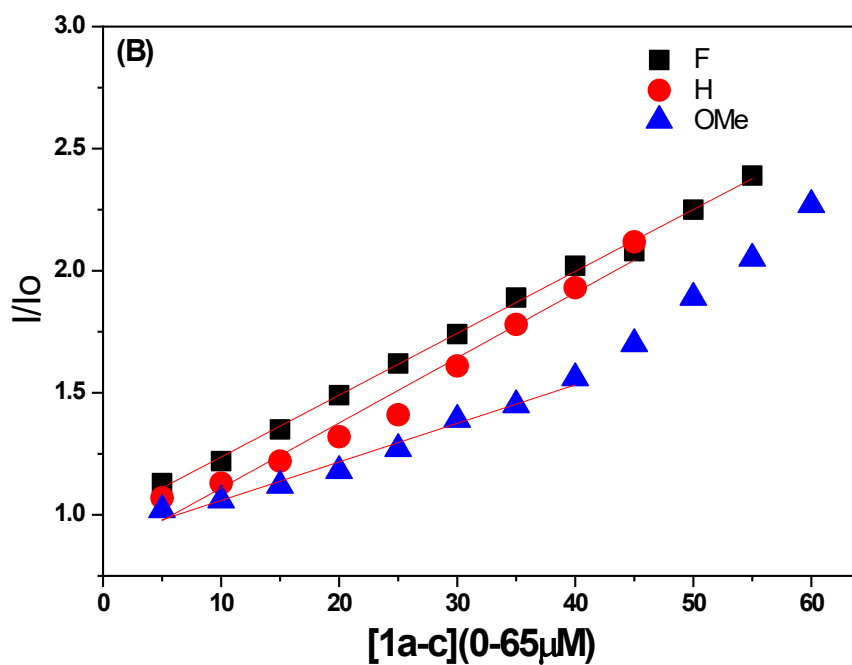
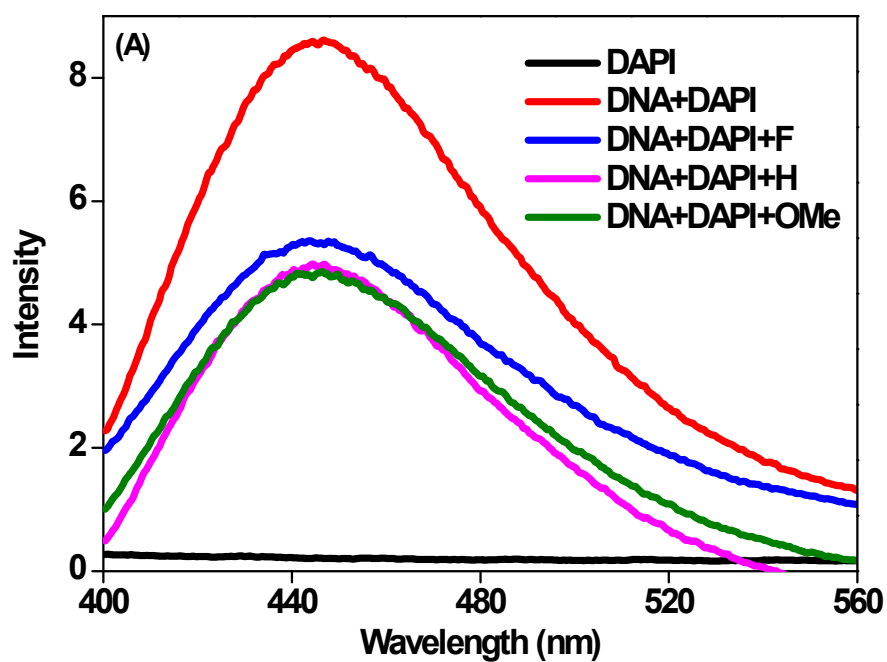


Fig. S3: (A) Emission spectral overlap of DAPI, DAPI with DNA and quenching spectra of complexes **1a-c** [10 μM] with the DAPI [50 μM] and DNA emission maxima mixture in phosphate buffer solution. (B) Curve fitting of the ratio between I/I_0 with the increase in the complexes **1a-c** concentration (0-65 μM).

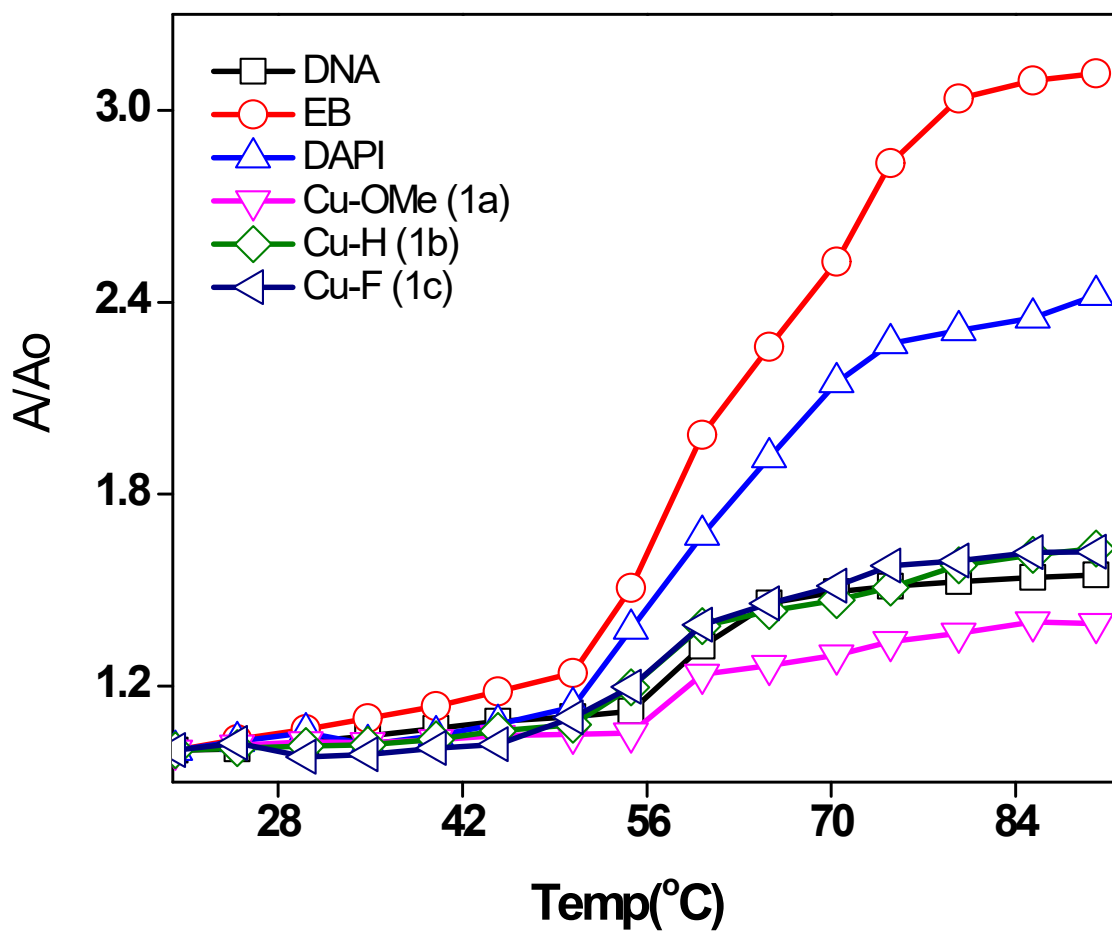


Fig. S4: Thermal melting profile curves of CT DNA alone and in the presence of complexes **1a-c** in buffer B [**1a-c**]= 10 μ M, [DNA]= 100 μ M

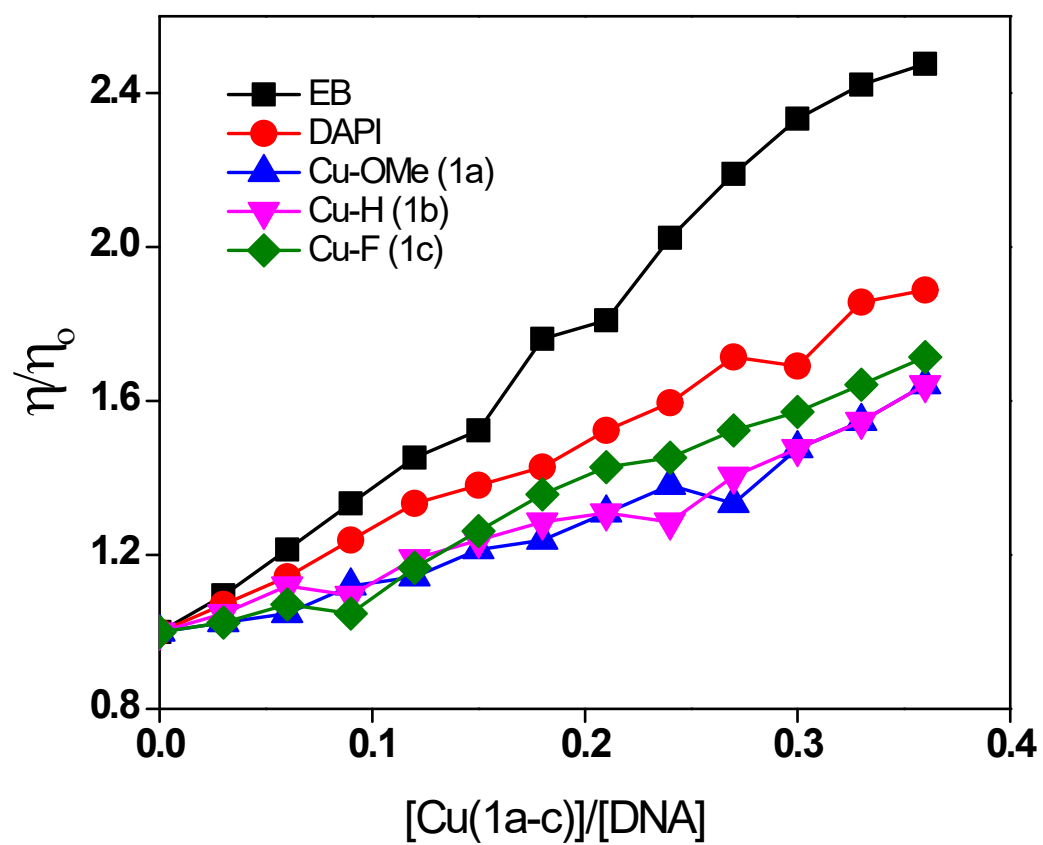


Fig. S5: Plot of relative viscosity versus $[1a-c]/[CT\ DNA]$ in in buffer C $[1a-c] = 10\ \mu M$, $[DNA] = 100\ \mu M$

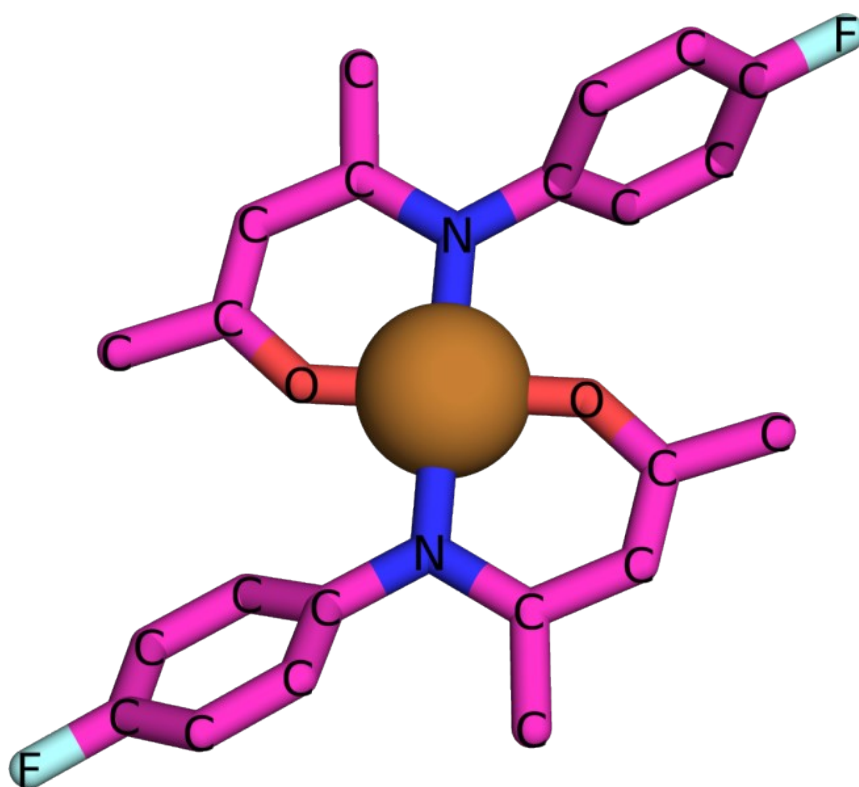


Fig. S6: DFT energy minimized structure of representative structure of the complex **1c**.

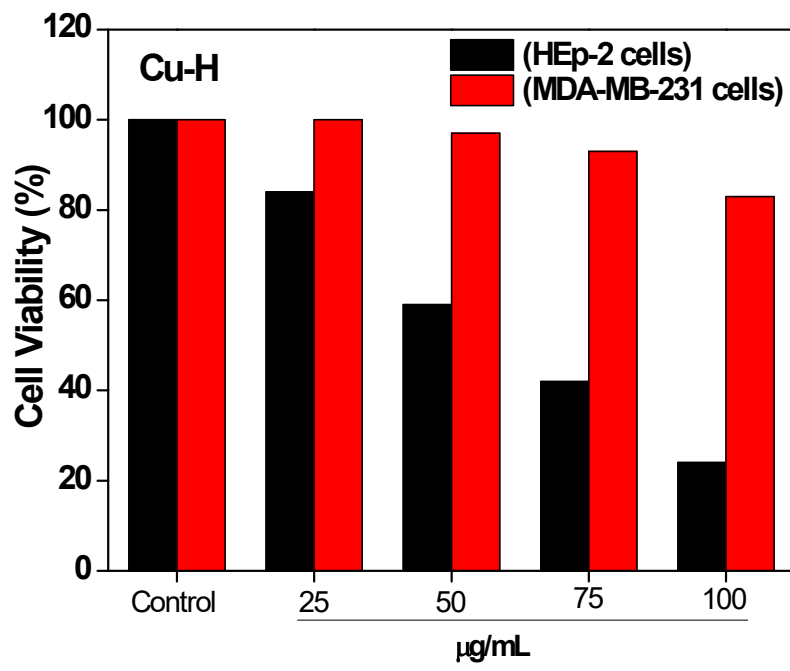


Table S1: Molar conductivity data for the complexes recorded in methanol.

Conductivity of Cu (II) complexes

S.No	Samples	200 m Ω	2 m Ω	200 $\mu\Omega$	20 $\mu\Omega$
1	H	Nil	.001	2.0	2.25
2	F	Nil	.002	2.3	2.54
3	OMe	Nil	.001	2.1	2.35

Complexes concentration; 1 mM in 10 ml MeOH

Table S2: Redox potential data of compounds 1a-c in CH₃CN

Compound	Oxidation^b E_{1/2} (V vs SCE)	Reduction^b E_{1/2} (V vs SCE)
Cu-OMe	+1.03	-1.21, -1.48
Cu-H	+0.96	-1.35, -1.76
Cu-F	---	-1.45, -1.91

Error limits: E_{1/2}, ± 0.02 V, 0.1 M TBAPF₆

Table S3: Binding and quenching constant (K_b , K_{app} , K_{SV}) and Melting temperature data for the reference and studied complexes 1a-c.

<i>Compound</i>	K_b (M^{-1})	K_{SV} (M^{-1})	K_{app} (M^{-1})	T_m ($^{\circ}C$)	ΔG ($kJmol^{-1}$)
DNA	--	-	-	57.4	-
EB	$> 10^7$	-	-	67.8	-44.86
DAPI	5.64×10^5	-	1.69×10^5	64.1	-34.23
Cu-OMe	1.29×10^4	2.12×10^4	1.98×10^4	58.1	-23.44
Cu-H	0.58×10^5	2.43×10^4	1.26×10^5	59.3	-27.15
Cu-F	1.57×10^5	2.97×10^4	1.74×10^5	61.6	-29.48

a) Error limits: K_b , $\pm 5\%$; T_m , ± 1 $^{\circ}C$