

Interaction with DNA and different effect on the nucleus of cancer cells for copper (II) complexes of N-benzyl di(pyridylmethyl)amine

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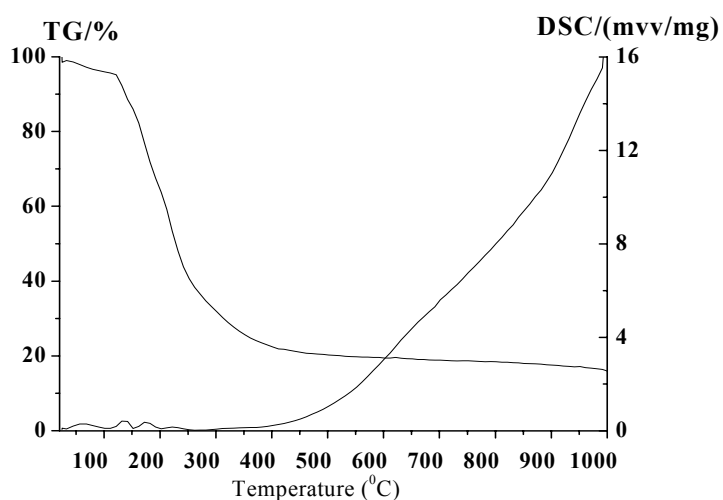


Fig S1 TG-DSC plot of the complex (1)

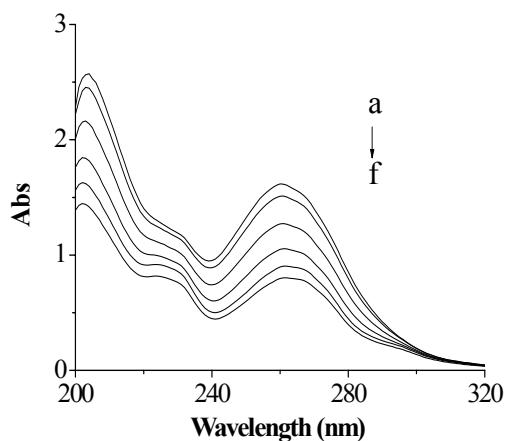


Fig S2 Electronic spectra of complex (3) (20 μM) in the presence of increasing amounts of CT-DNA (b–f); DNA concentrations are 0, 10, 20, 30, 40 and 50 μM for spectra (a–f), respectively. The arrow indicates the absorbance changes upon increasing DNA concentration

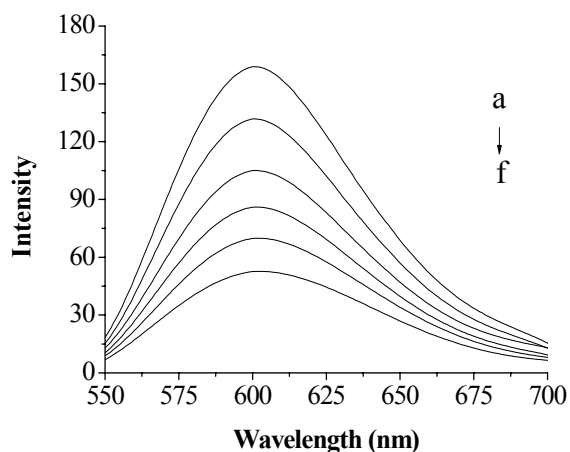


Fig. S3 Fluorescence spectra of DNA-EB in the presence of complex (2) at 0 °C. The total concentrations of the complexes are (a) 0, (b) 10.0, (c) 20.0, (d) 30.0, (e) 40.0, (f) 50.0 μM . EB and DNA concentration are 0.72 and 20 μM

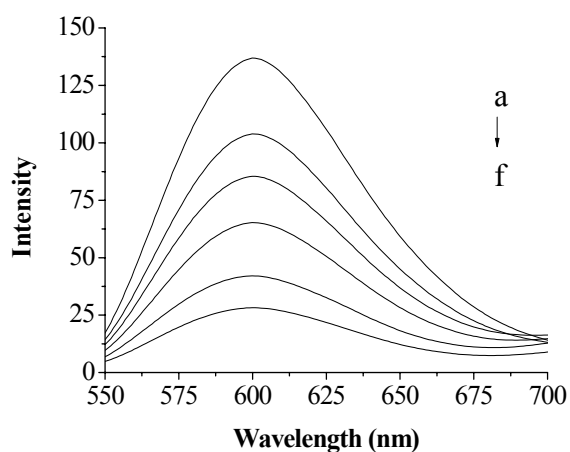


Fig. S4 Fluorescence spectra of DNA-EB in the presence of complex (3) at 0 °C. The total concentrations of complexes are (a) 0, (b) 10.0, (c) 20.0, (d) 30.0, (e) 40.0, (f) 50.0 μM . EB and DNA concentration are 0.72 and 20 μM .

Table S1

Partition coefficients of copper(II) complexes in 1-octanol/water

complexes	(1)	(2)	(3)
P _{OW}	0.12	1.53	2.36

Table S2

UV data of the copper complexes

Complexes	$\pi \rightarrow \pi^*$					$d \rightarrow d$	
	$\lambda_{\max}$ (nm)			$\epsilon \times 10^{-4}$ (L/mol · cm)		$\lambda_{\max}$ (nm)	ϵ (L/mol · cm)
(1)	254.0,	196	1.29	3.57	660.0	98.16	
(2)	253.0, 290.0, 210.0	1.73, 2.17, 3.79	597.0	125.87			
(3)	258.0, 308.0, 206.0	3.71, 0.38, 3.54	606.0	138.02			

Table S3

Crystal data and experimental data for the complex (2) and (3)

	Complex (2)	Complex (3)
Empirical formula	C ₃₁ H ₃₁ Cl ₂ CuN ₅ O ₈	C ₆₂ H ₆₀ Cl ₄ Cu ₂ N ₁₀ O ₁₉
Formular weight	768.05	1518.08
Crystal system	Monoclinic	Monoclinic
Space group	P2 ₁ /c	P2 ₁ /c
<i>a</i> (Å)	8.2186(16)	8.6111(17)
<i>b</i> (Å)	18.370(4)	21.793(4)
<i>c</i> (Å)	21.523(4)	19.306(4)
α (°)	90.00	90.00
β (°)	94.39(3)	96.29(3)
γ (°)	90.00	90.00
<i>V</i> (Å ³) / <i>Z</i>	3240.1(11) / 4	3601.2(13) / 2
Density (calc) (Mg/m ³)	1.575	1.400
Absorption coefficient (mm ⁻¹)	0.906	0.813
<i>F</i> (000)	1580	1560
Index ranges	-10 ≤ <i>h</i> ≤ 9; -18 ≤ <i>k</i> ≤ 22; -26 ≤ <i>l</i> ≤ 18	-9 ≤ <i>h</i> ≤ 10; -22 ≤ <i>k</i> ≤ 25; -15 ≤ <i>l</i> ≤ 22
Θ range (°)	2.20 - 26.38	2.83 – 25.00
Reflection collected	15849	16333
Independent reflections [<i>R</i> _{int}]	5304	5121
Data/restraints/parameters	6479/0/424	6305/0/442
Goodness-of-fit on <i>F</i> ²	1.133	1.063
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ =0.0876; <i>wR</i> ₂ =0.2406	<i>R</i> ₁ =0.0782; <i>wR</i> ₂ =0.2330
<i>R</i> indices (all data)	<i>R</i> ₁ =0.1055; <i>wR</i> ₂ =0.2572	<i>R</i> ₁ =0.0932; <i>wR</i> ₂ =0.2500
CCDC number	CCDC 766526	CCDC 782308

