

Supplementary Information

Coumarin centered Copper(II) complex with Appended-Imidazole as Cancer Chemotherapeutic Agents against Lung Cancer: Molecular insight via DFT-based Vibrational Analysis

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Table S1. Selected bond lengths (Å) of complex **1**.

Bond lengths	(Å)
N1 Cu1	1.990(2)
N2 Cu1	1.943(2)
N3 Cu1	1.949(2)
O1 Cu1	1.918(19)
N5 O6	1.243(3)
N5 O4	1.250(3)
N5 O5	1.261(3)

Table S2. Selected bond angles of complex **1**

Bond Angle	[deg]
O6 N5 O4	121.0(2)
O6 N5 O5	119.1(2)
O4 N5 O5	119.9(2)
C19 O1 Cu1	127.7(2)
O1 Cu1 N2	92.83(9)
O1 Cu1 N3	88.58(9)
N2 Cu1 N3	171.91(10)
O1 Cu1 N1	159.69(9)
N2 Cu1 N1	83.67(10)
N3 Cu1 N1	97.69(10)

Table S3. Hydrogen bond metrics for **1**

$D - H \cdots A$	$H \cdots A$	$D \cdots A$	$\angle D - H \cdots A$	Symmetry operation
N(4) --H(4) ..O(5)	2.02	2.86(18)	167	$1/2-x, 1/2+y, 1/2-z$
C(5) --H(5) ..O(5)	2.52	3.40(2)	158	$3/2-x, -1/2+y, 1/2-z$
C(7) --H(7) ..O(3)	2.47	3.38(2)	164	$1-x, -y, -z$
C(10) --H(10) ..O(3)	2.45	2.78(17)	101	
C(10) --H(10) ..O(3)	2.49	3.41(2)	173	$1-x, -y, -z$
C(15) --H(15) ..O(4)	2.40	3.29(2)	161	$-x, 1-y, -z$
C(23) --H(23) ..O(5)	2.31	3.16(2)	153	
C(23) --H(23) ..O(6)	2.55	3.11(19)	120	$1/2-x, 1/2+y, 1/2-z$

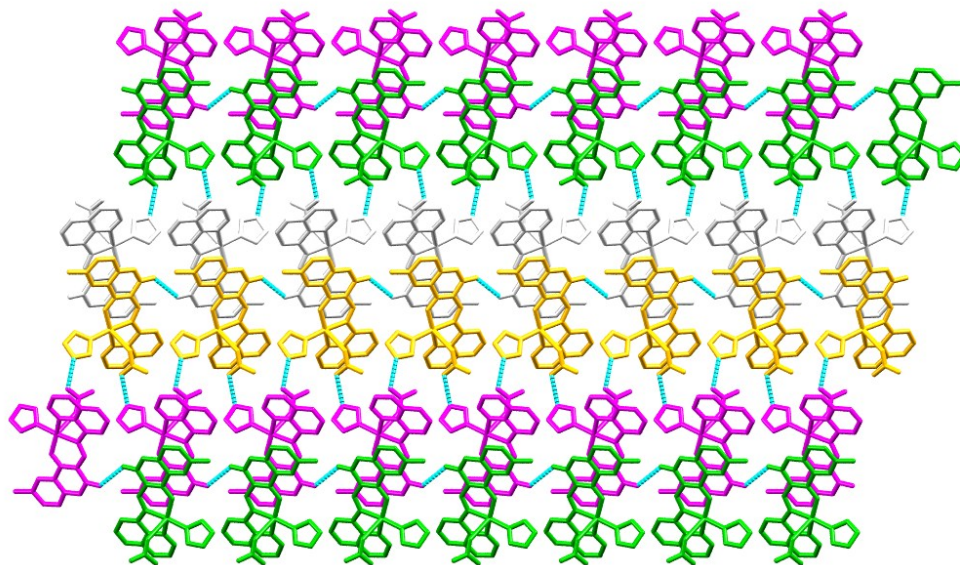


Fig. S1. Representation of 2D view along crystallographic a-axis of complex 1.

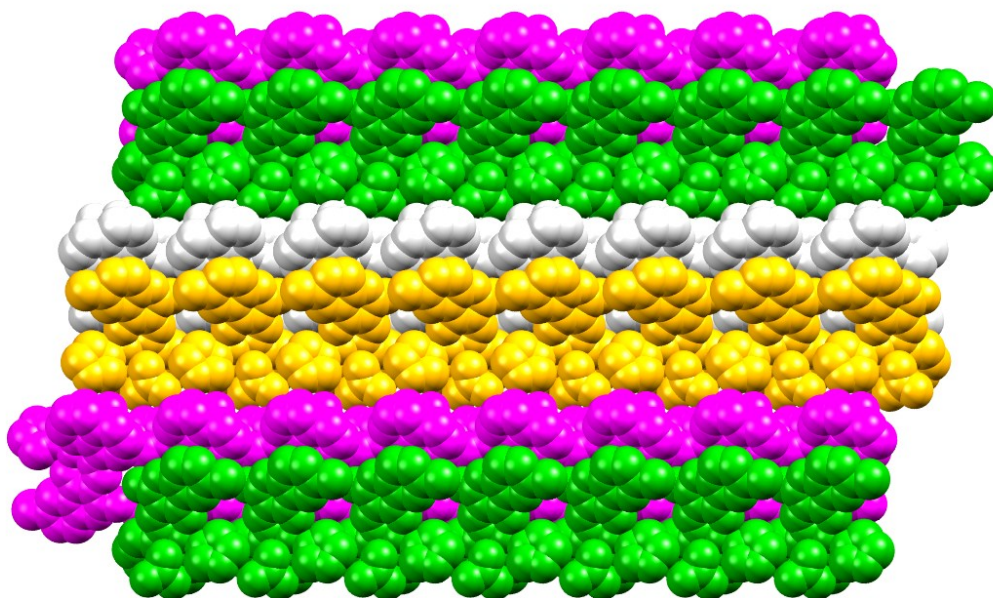


Fig. S2. 2D view in spacefill model of complex 1.

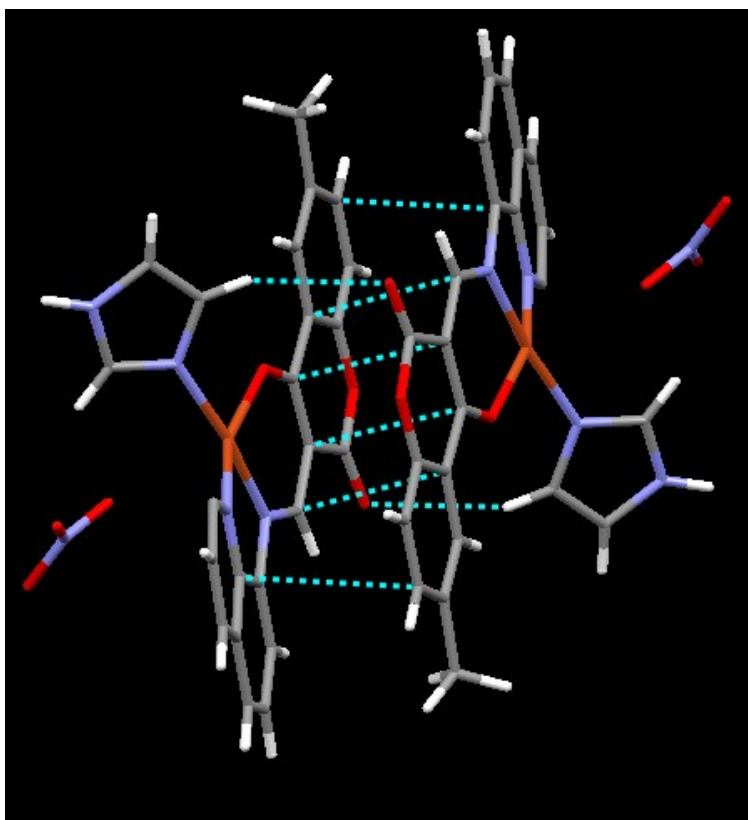


Fig. S3. Non-covalent ($\text{CH}\cdots\pi$, $\pi\cdots\pi$ and Hydrogen bonding) interactions of complex **1**.

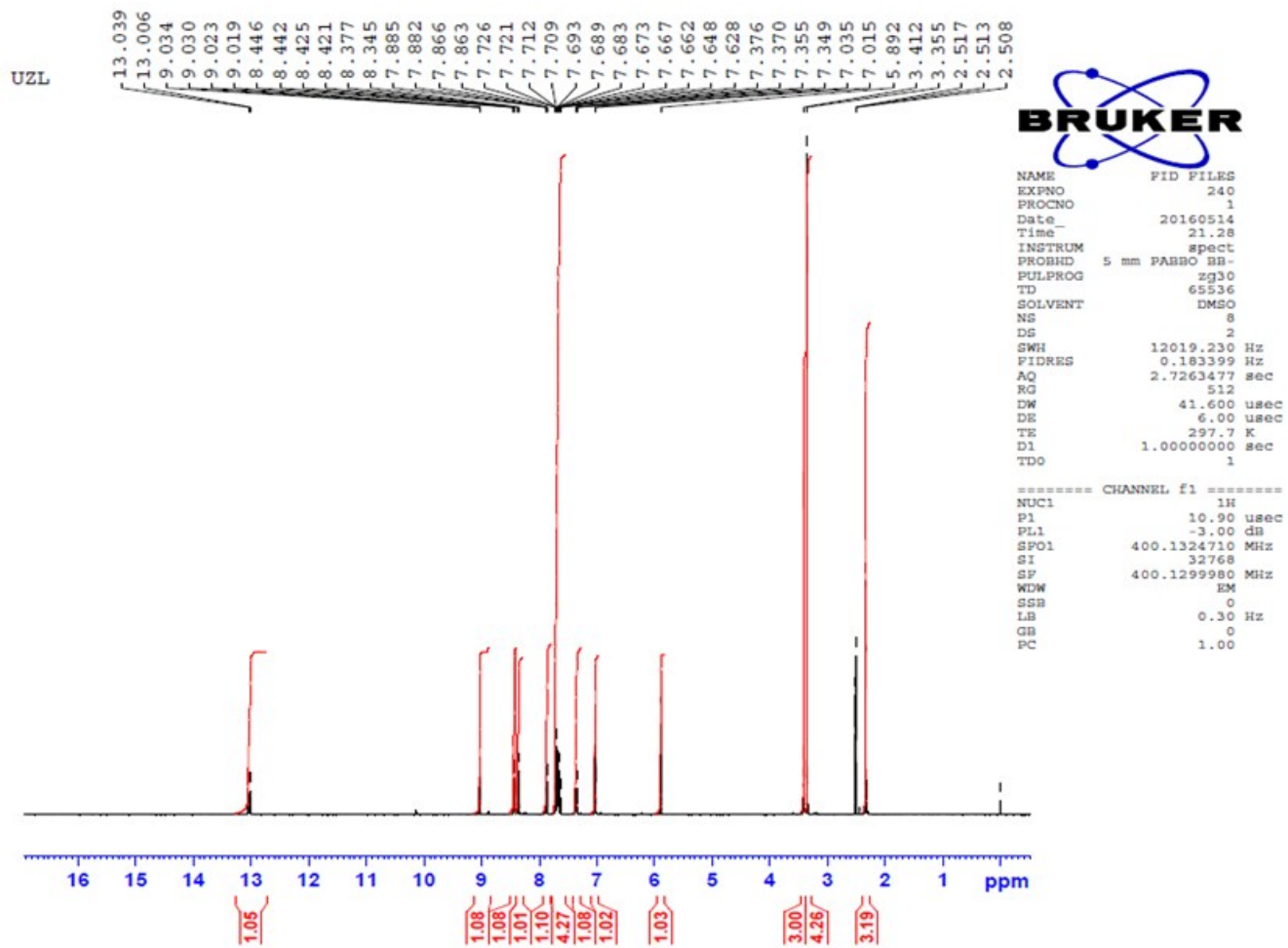


Fig. S4. ¹H NMR spectrum of ligand (HL).

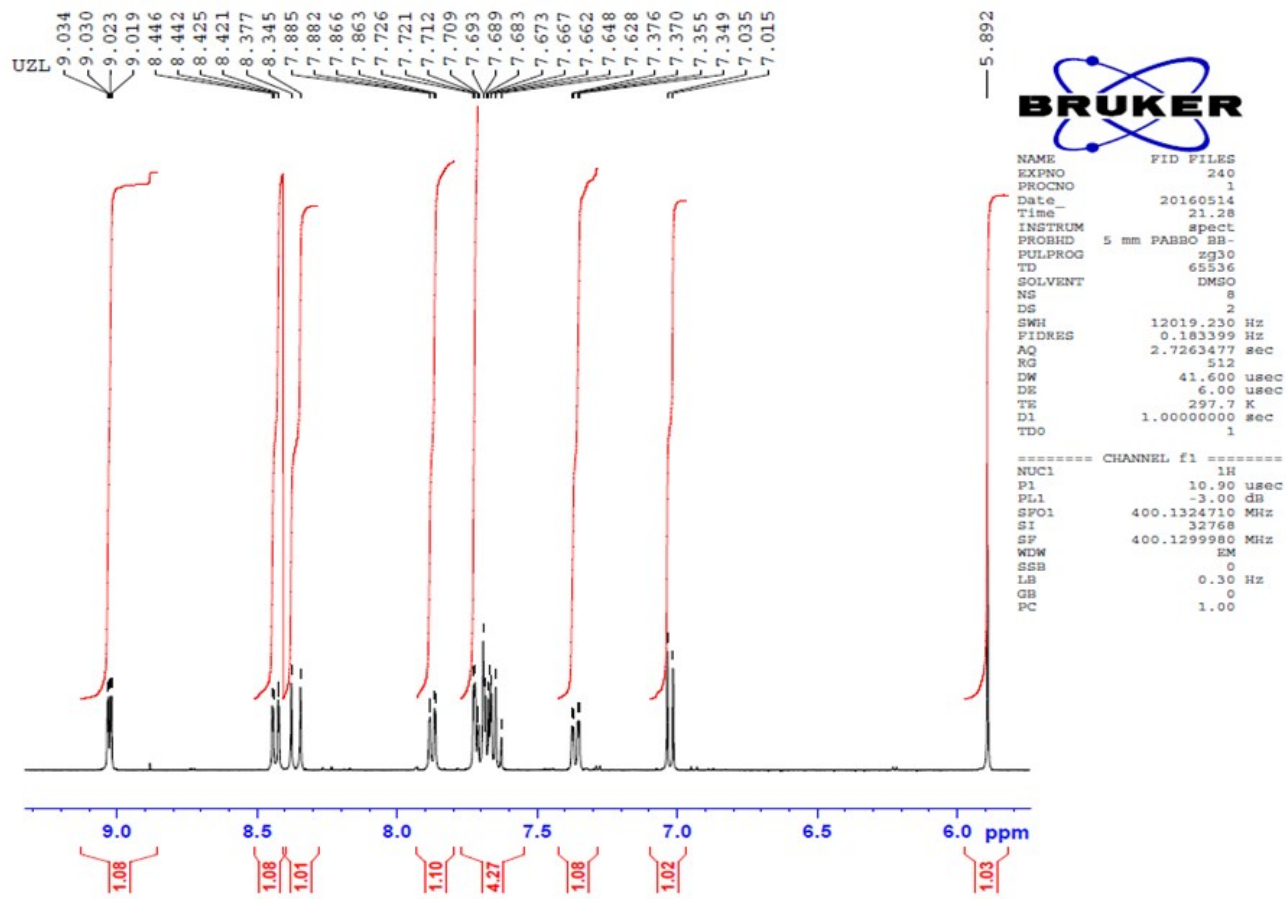
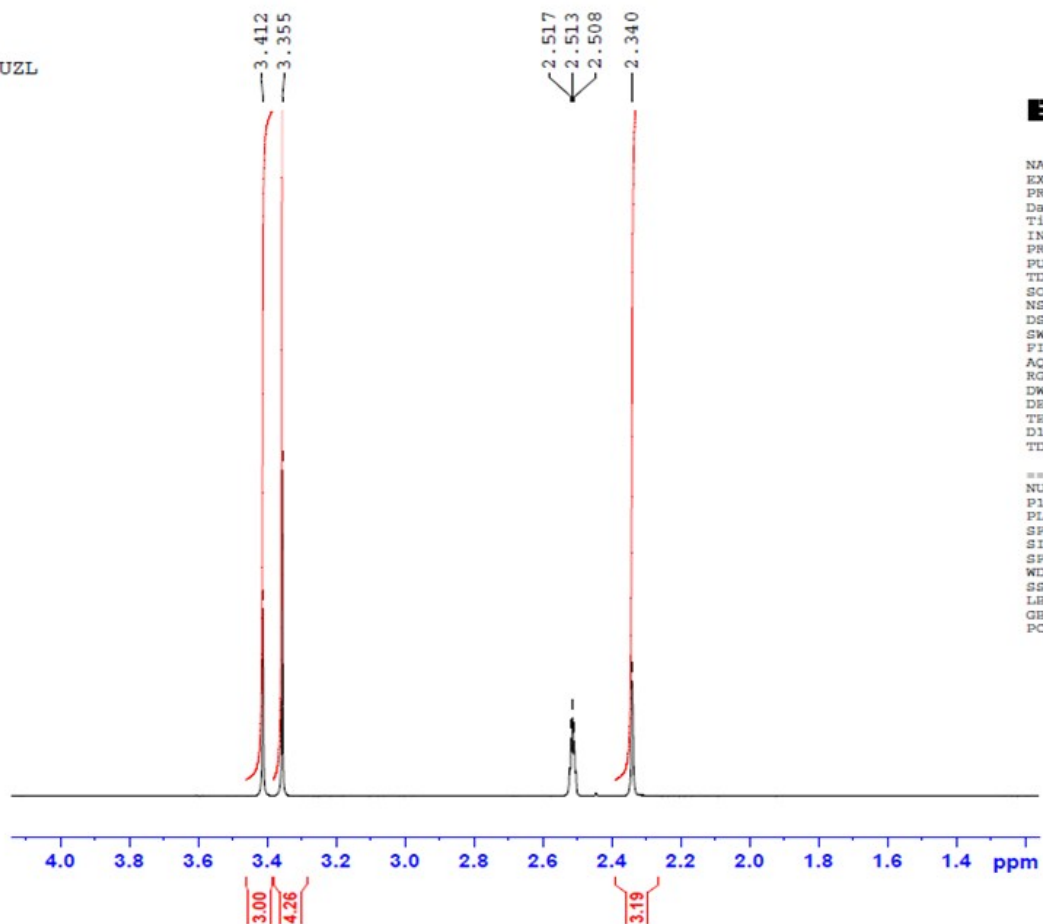


Fig. S5. ¹H NMR spectrum of ligand (HL).

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NAME          FID FILES
EXPNO         240
PROCNO        1
Date_         20160514
Time_         21.28
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            8
DS            2
SWH           12019.230 Hz
FIDRES        0.183399 Hz
AQ            2.7263477 sec
RG            512
DW            41.600 usec
DE            6.00 usec
TE            297.7 K
D1            1.00000000 sec
TDO           1

===== CHANNEL f1 =====
NUC1          1H
P1            10.90 usec
PL1           -3.00 dB
SFO1          400.1324710 MHz
SI            32768
SF            400.1299980 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
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Fig. S6. ¹H NMR spectrum of ligand (HL).

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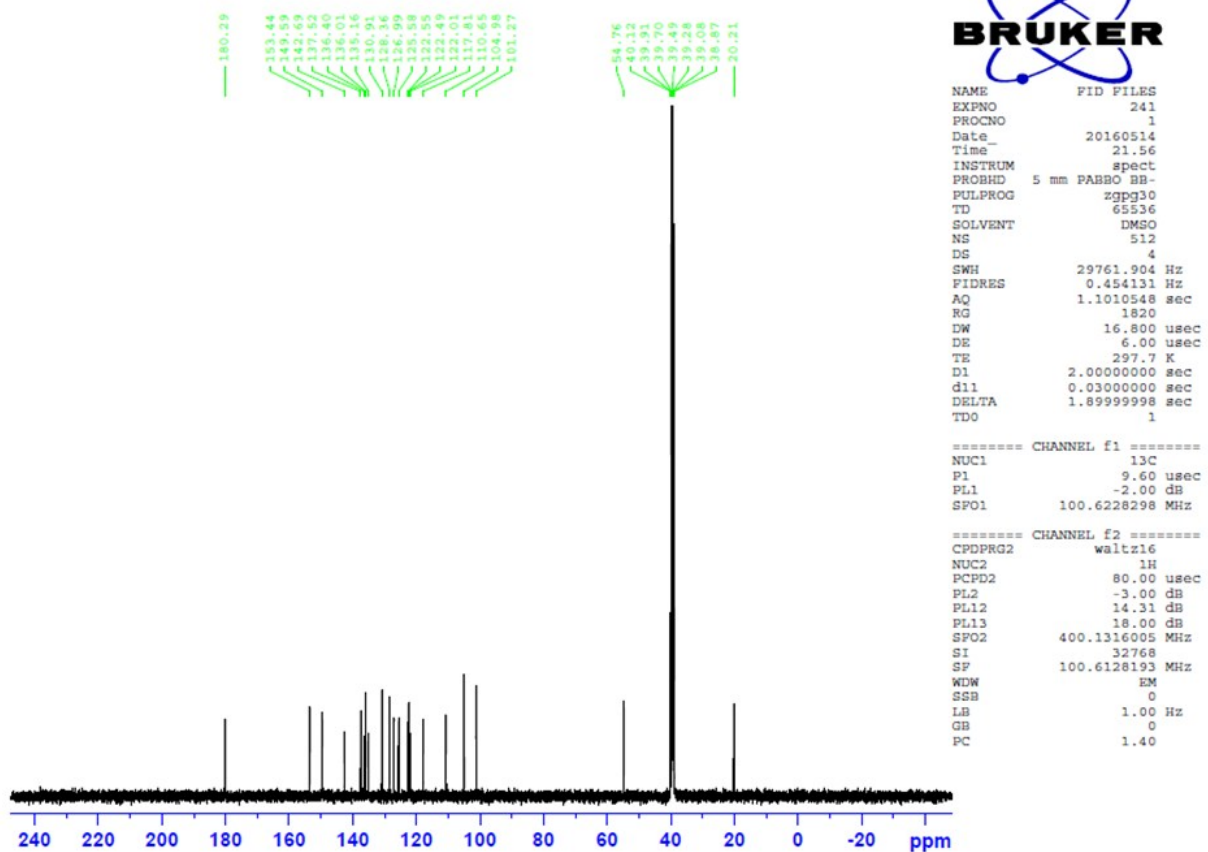


Fig. S7. ^{13}C NMR spectrum of ligand (HL).

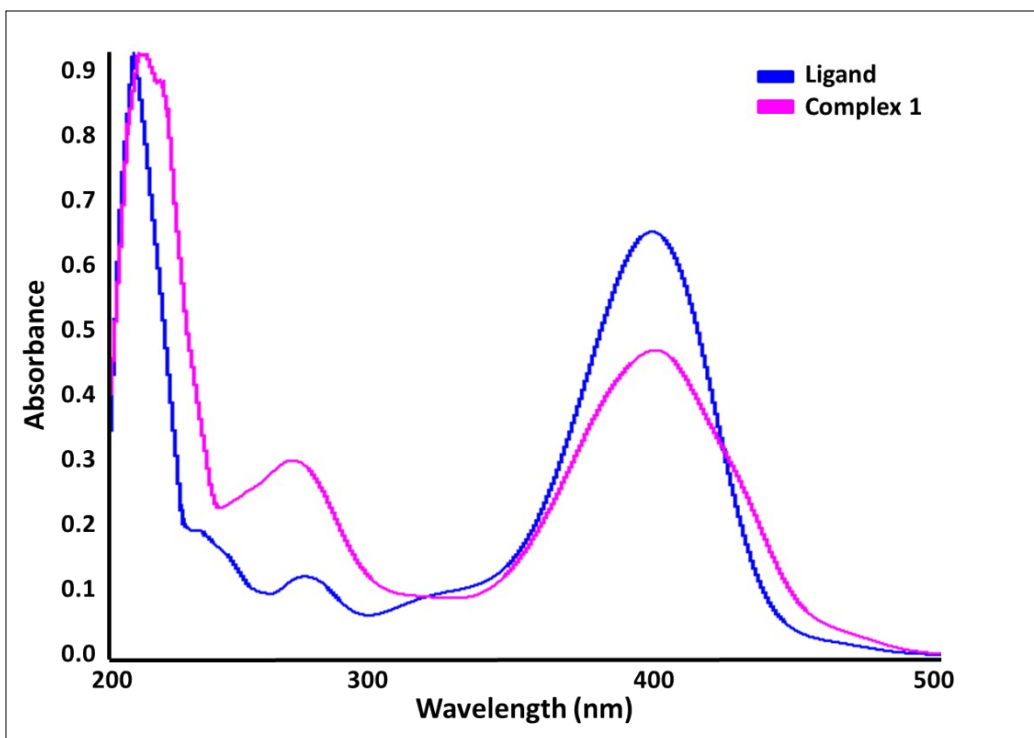


Fig. S8. UV-vis spectra in MeOH (1×10^{-4}).

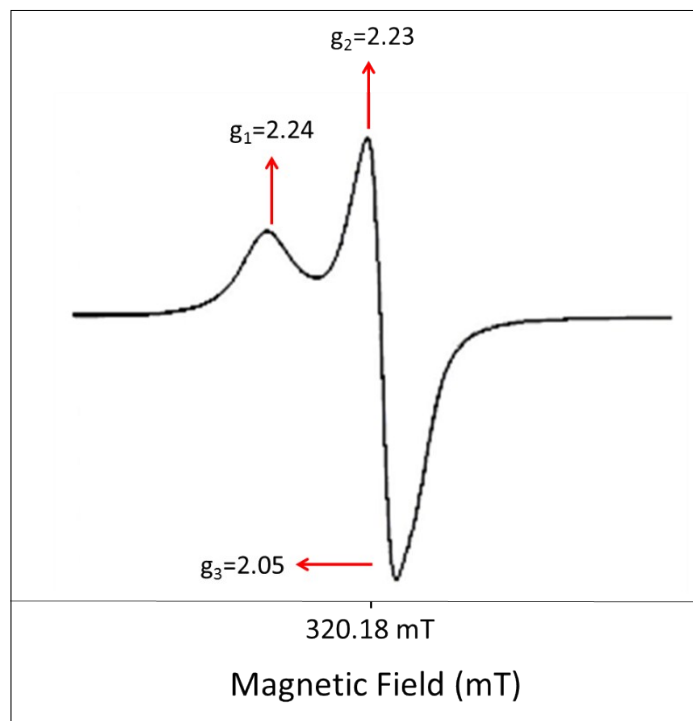


Fig. S9. X-band Polycrystalline EPR spectrum of complex 1 at 77K.

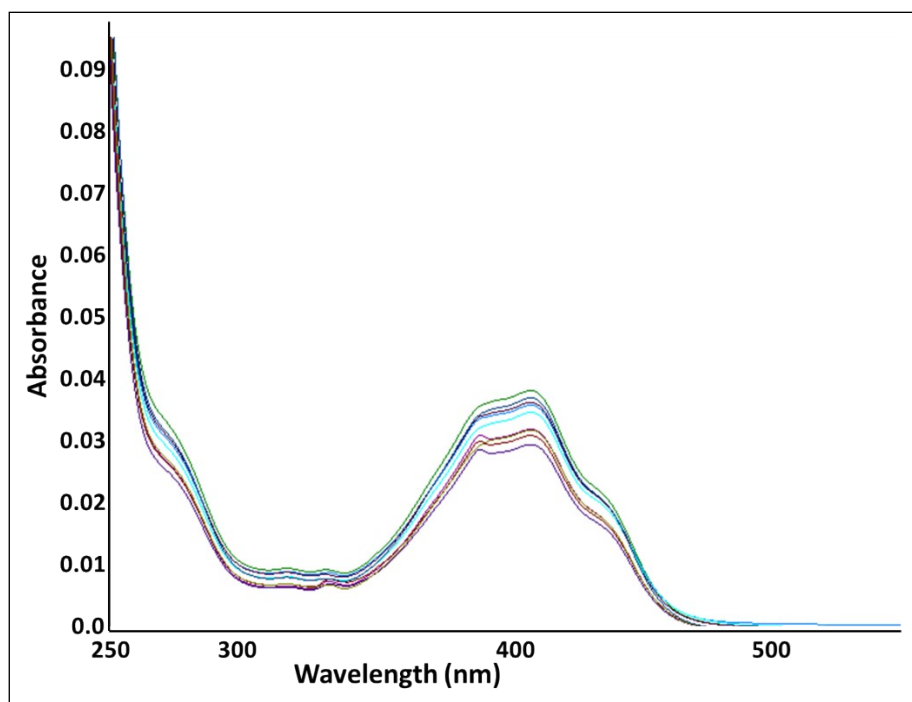
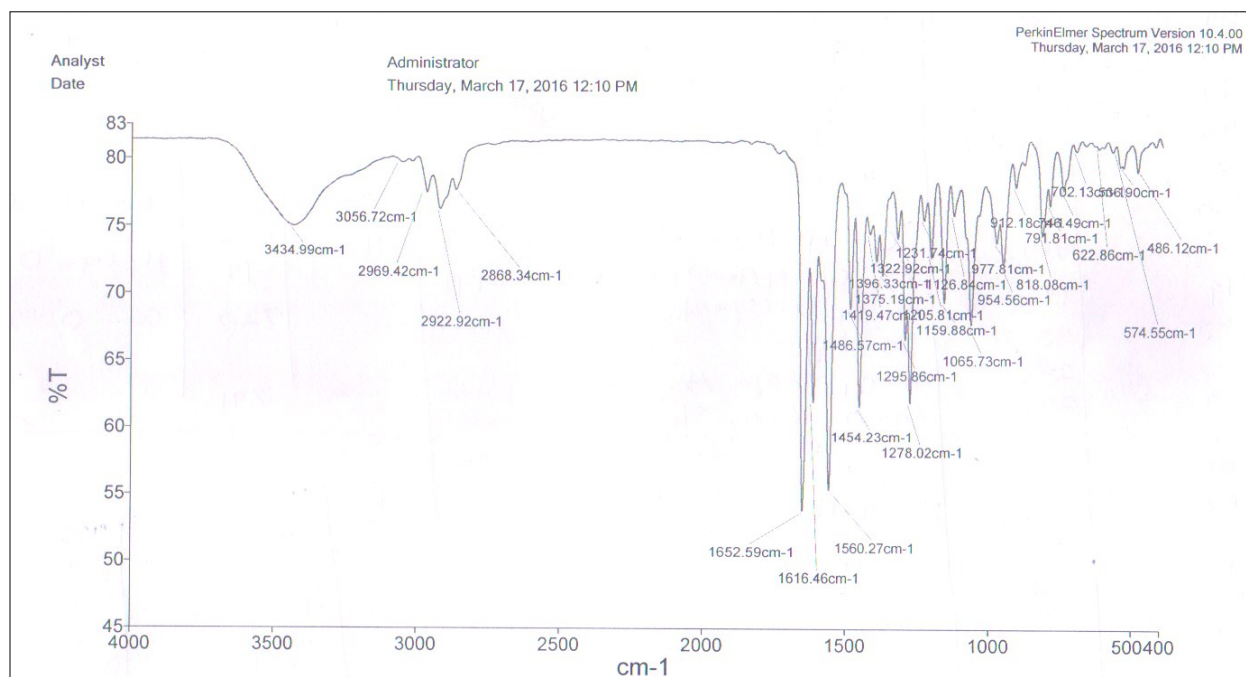
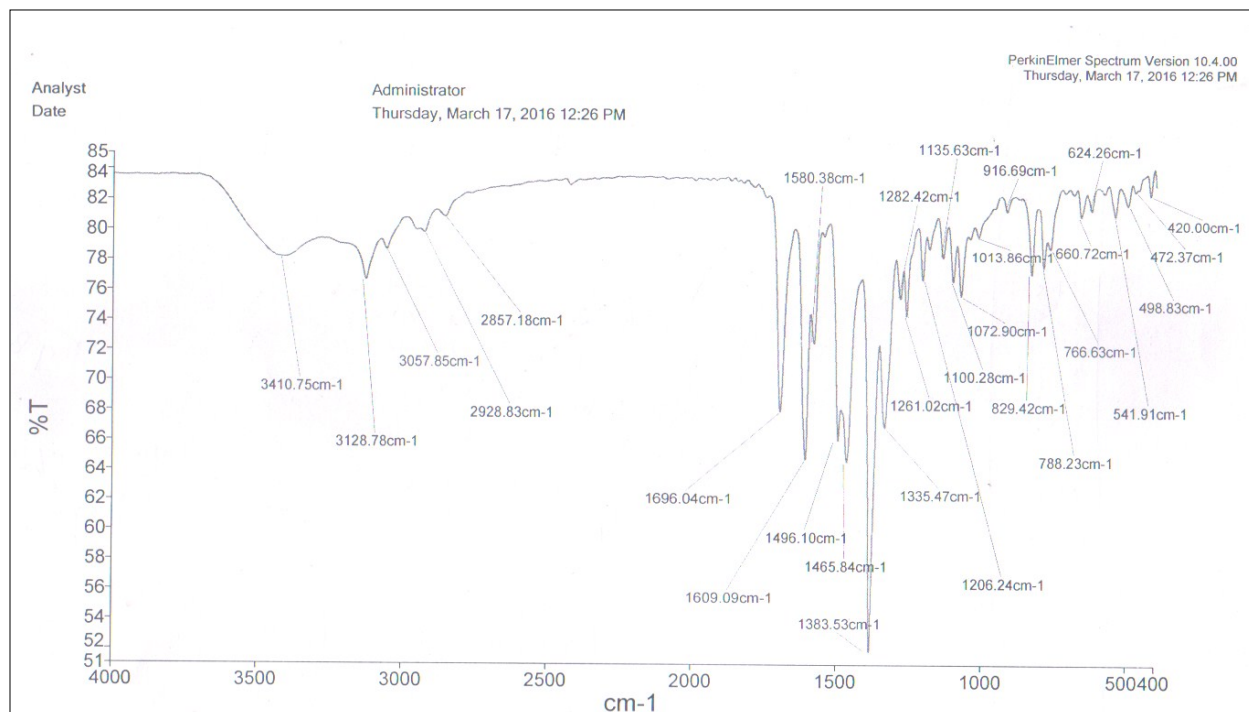


Fig. S10. Time-dependent stability studies of complex **1** in Tris-HCl buffer under physiological conditions (pH = 7.3 & T = 310 K) monitored by UV-vis absorption spectra.

(a)



(b)



(c)

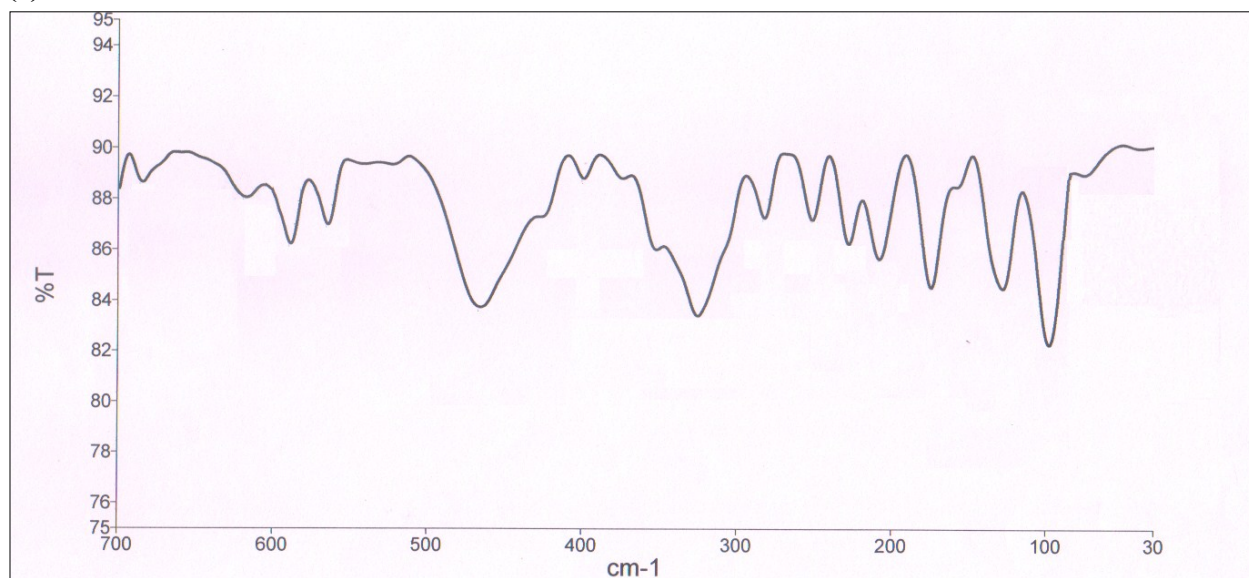


Fig. S11. (a) Experimental FTIR spectra of Ligand (b) complex 1 (c) Experimental Far-IR spectra of complex 1.

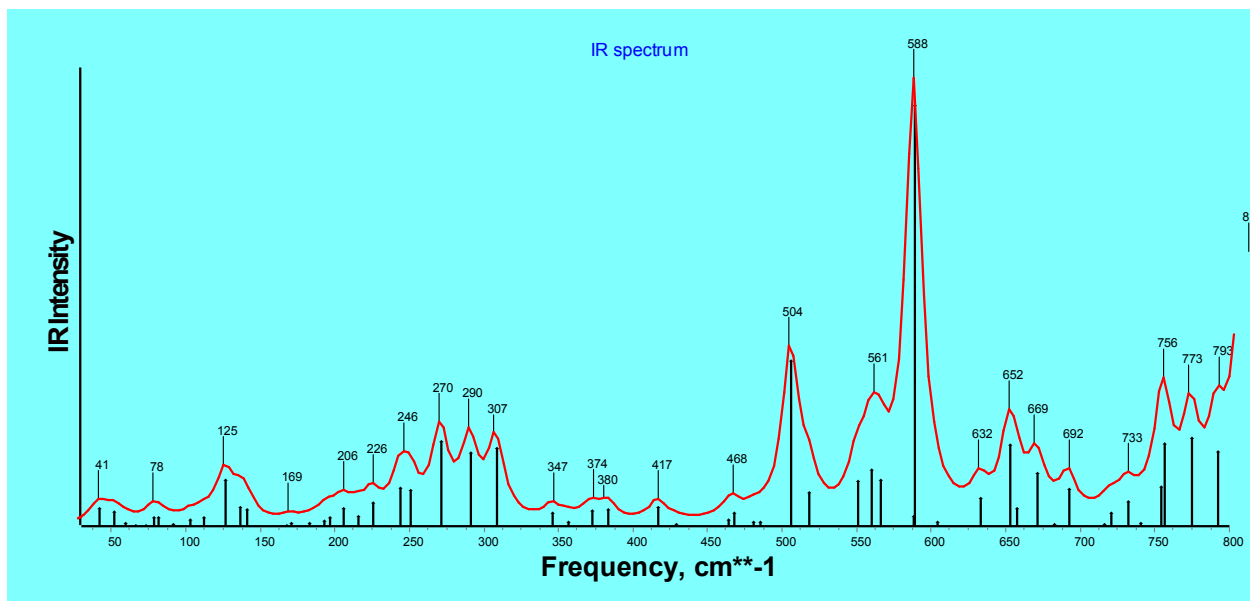


Fig. S12. B3LYP/DFT simulated IR spectrum of complex 1.

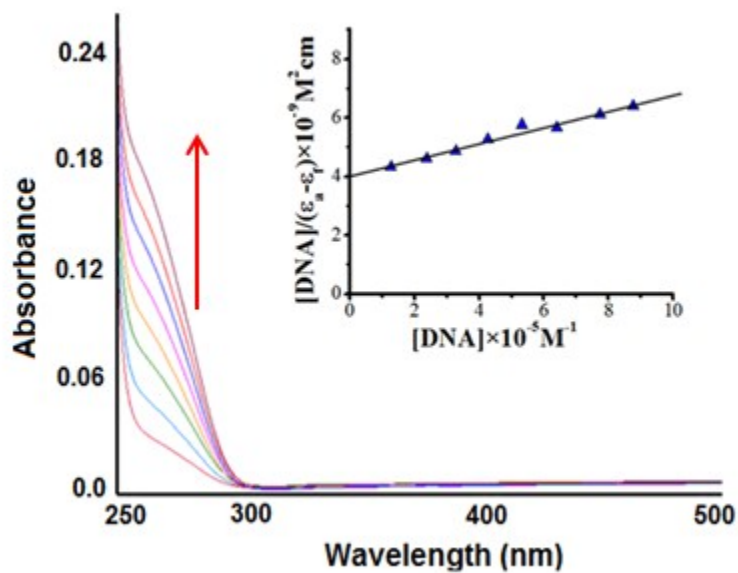


Fig. S13. Absorption spectra for ligand L (▲) interaction with CT DNA under the same condition for complex

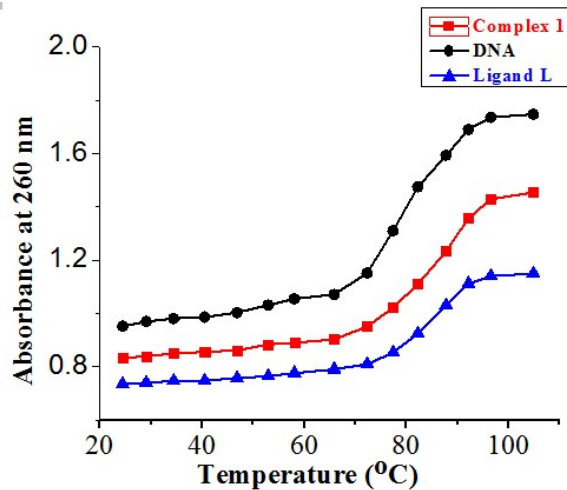


Fig. S14. Thermal melting profile for ligand L ▲ and complex 1 ■.

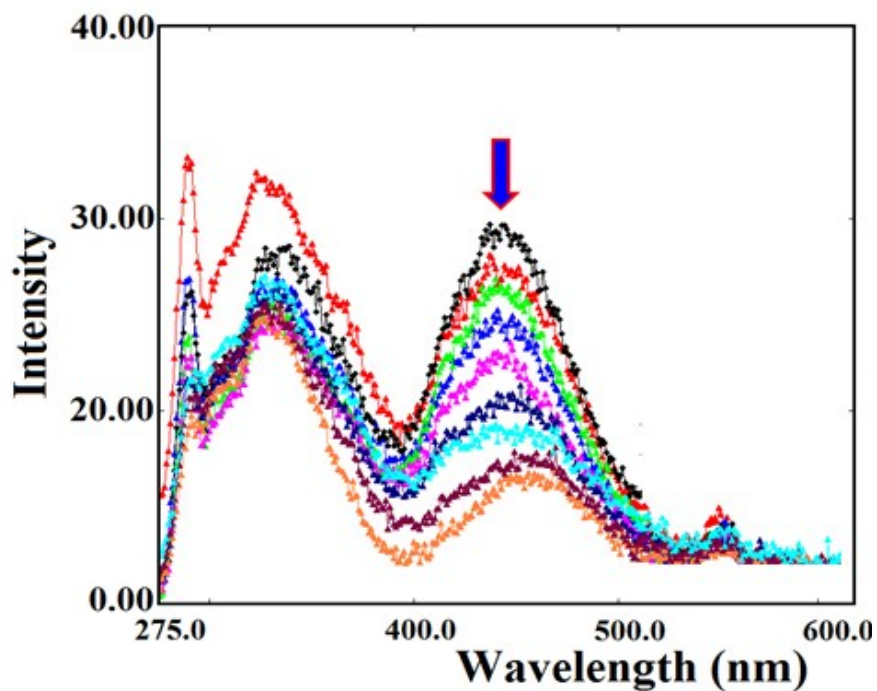


Fig. S15. Emission spectra of ligand (L) in Tris-HCl buffer (pH 7.2) with and without of CT DNA at room temperature. The arrow shows a change in intensity with increasing concentration of DNA.

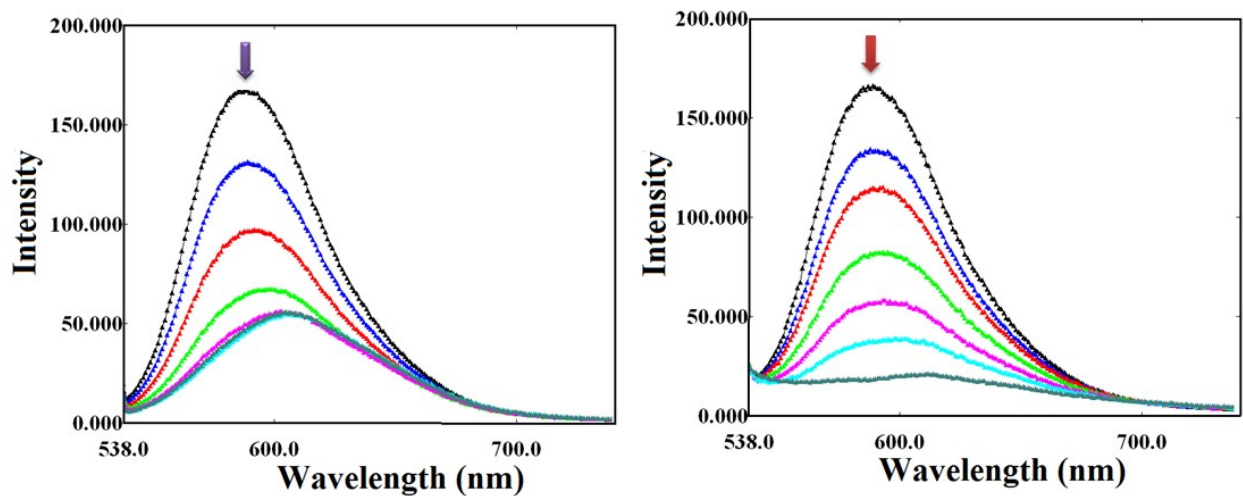


Fig. S16. Emission quenching spectra of CT DNA bound ethidium bromide in the presence of ligand **L** (left) and complex **1** (right) in buffer 5 mM Tris-HCl/50 mM NaCl, pH = 7.2 at 25 °C. Arrow shows change in intensity with increasing concentration of ligand **L**/complex **1**.

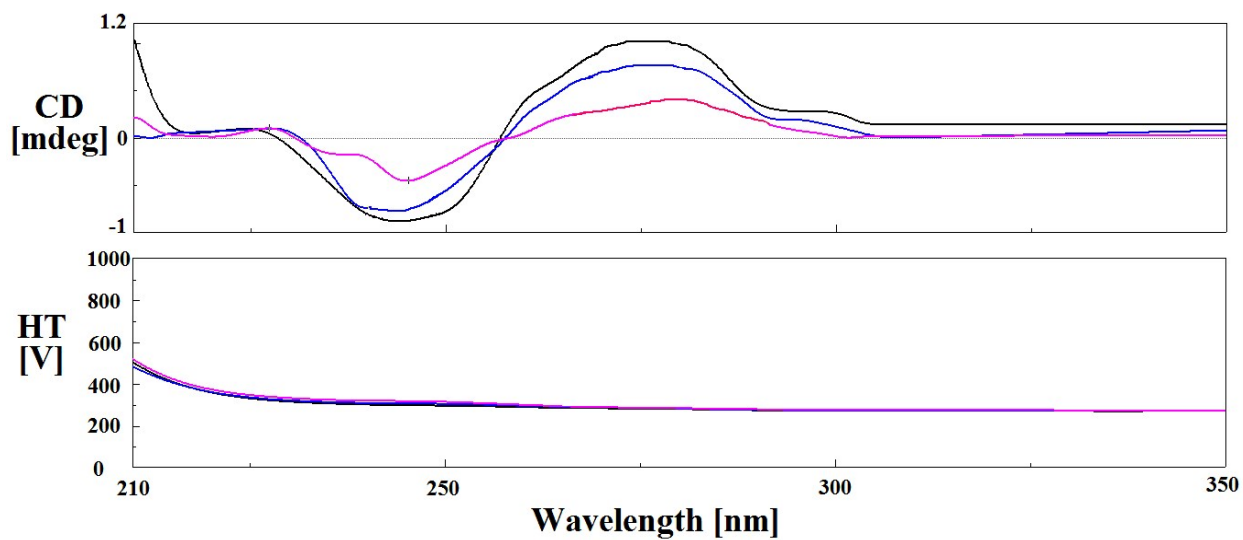


Fig. S17. CD spectra of CT DNA alone in black line (—) and with ligand **L** in blue line (—) Complex **1** in red line (—) in 5 mM Tris-HCl/50 mM NaCl buffer at 25 °C. [Ligand/Complex] = 35 μ M, [DNA] = 140 μ M.

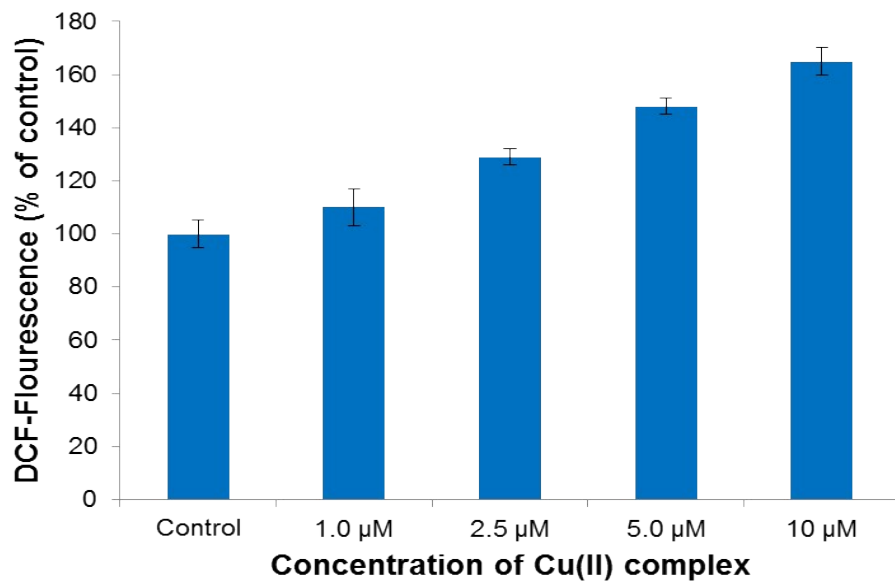


Fig. S18. ROS generation in A549 cells following the exposure of 20 μM for 24 h.

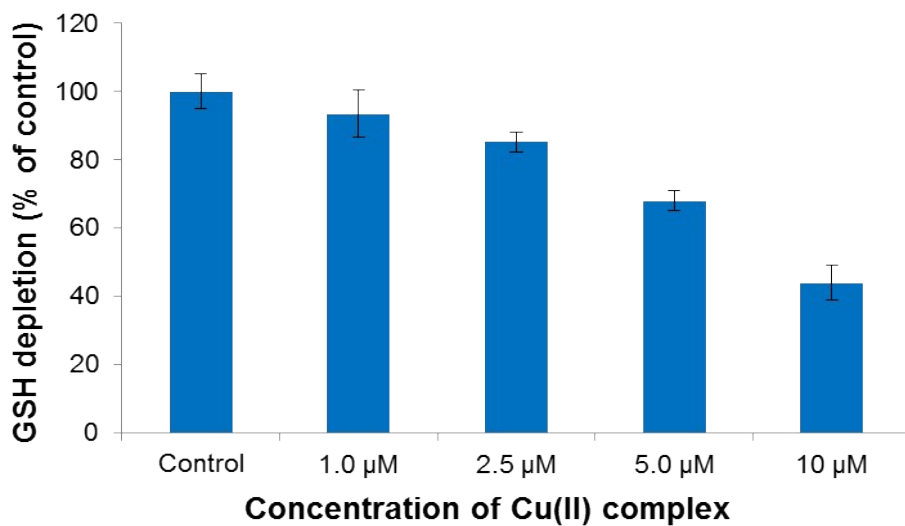


Fig. S19. Glutathione depletion in A549 cells exposed to complex 1 for 24 h.

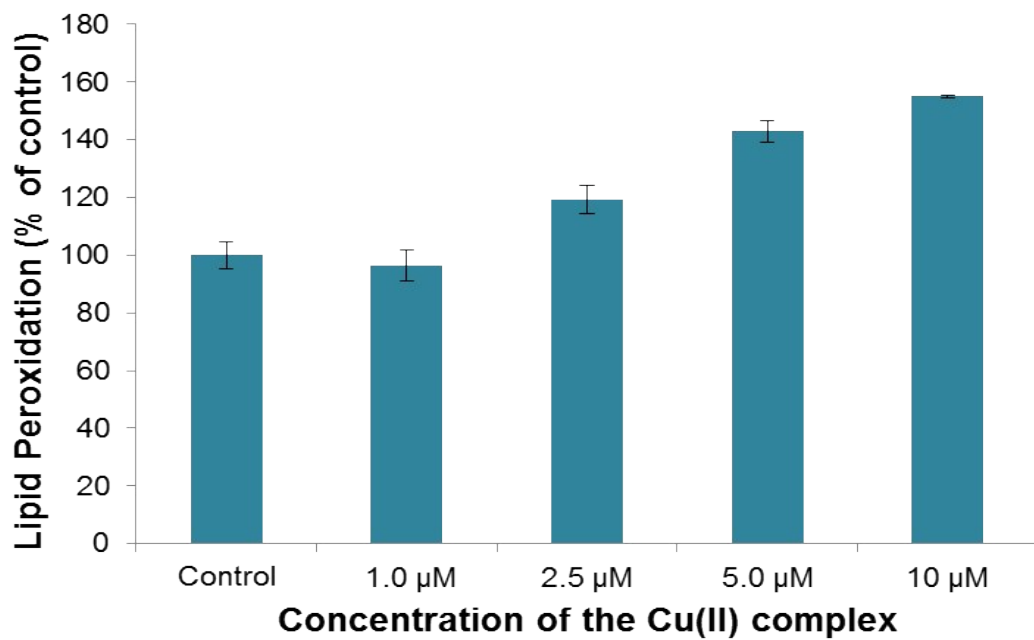


Fig. S20. Lipid peroxidation level in A549 cells exposed to complex 1 for 24 h.