Supplementary Information for

A study on the formation of the nitro radical anion by ornidazole and its significant decrease in a structurally characterized binuclear $Cu^{(II)}$-complex: impact in biology

by

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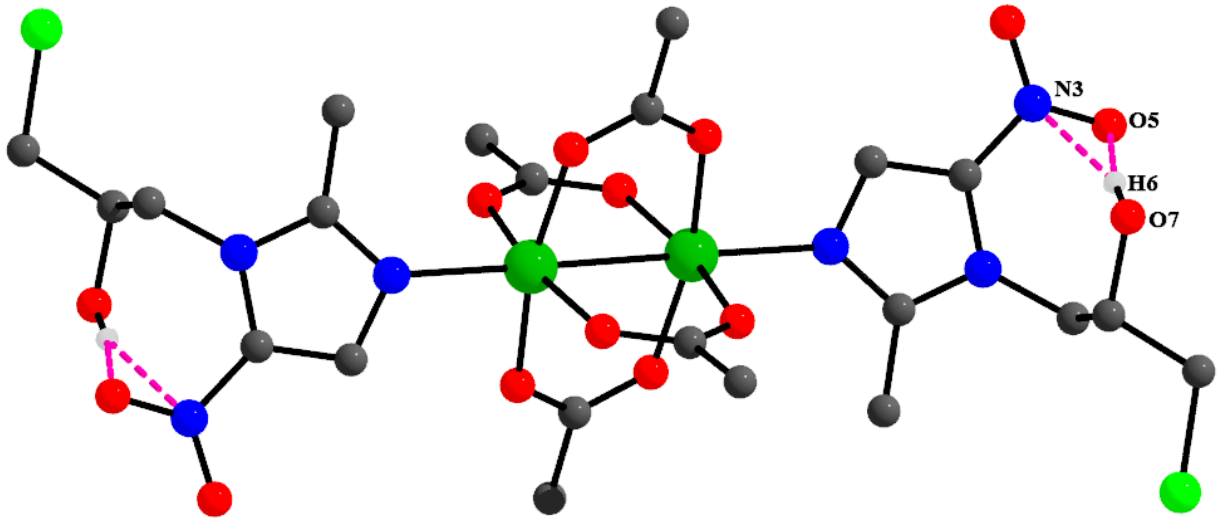

Figure S1: Hydrogen bonding interactions in $[Cu_2(OAc)_4(Onz)_2]$. Only the relevant hydrogen atoms are shown.

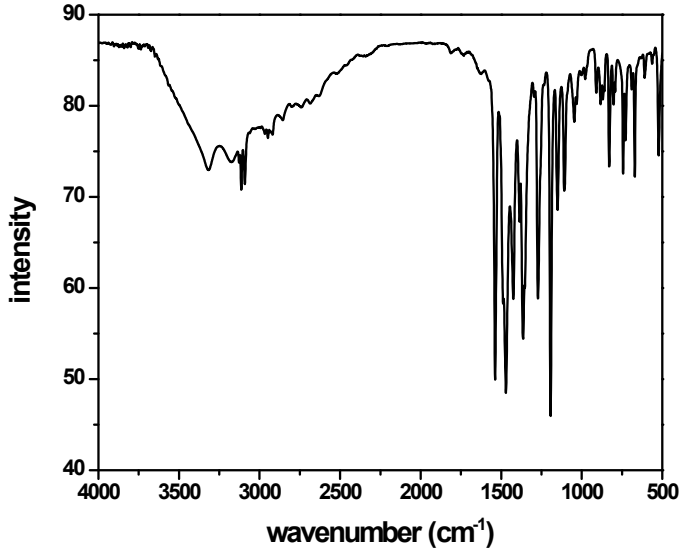

Figure S2: I R spectrum of Ornidazole

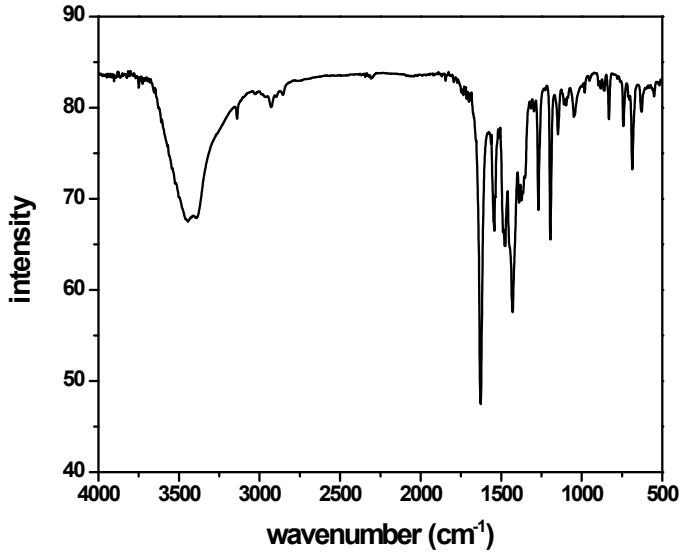

Figure S3: I R spectrum of $[Cu_2(OAc)_4(Onz)_2]$

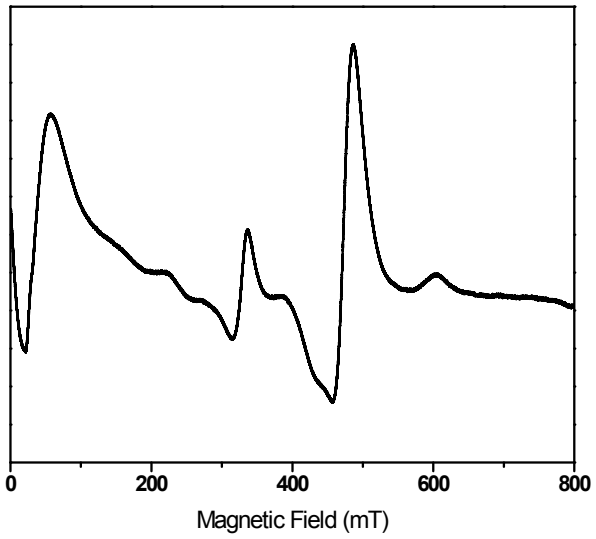

Figure S4: EPR spectrum of $[Cu_2(OAc)_4(Onz)_2]$

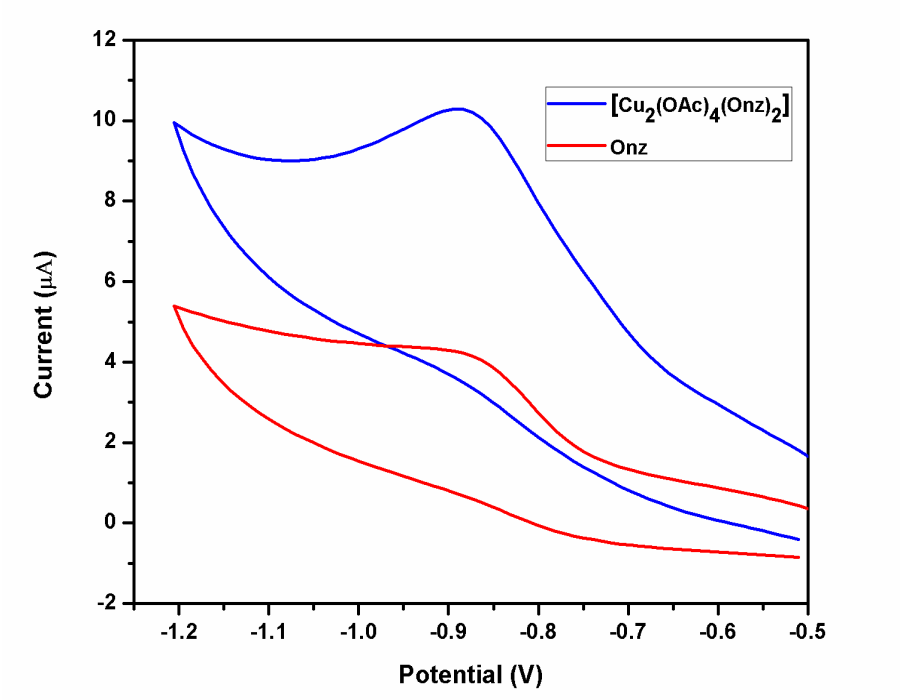

Figure S5: Cyclic voltammogram of 250 μM Onz and $[Cu_2(OAc)_4(onz)_2]$ at scan rate 0.1 V/sec in aqueous medium at pH = 7.4.

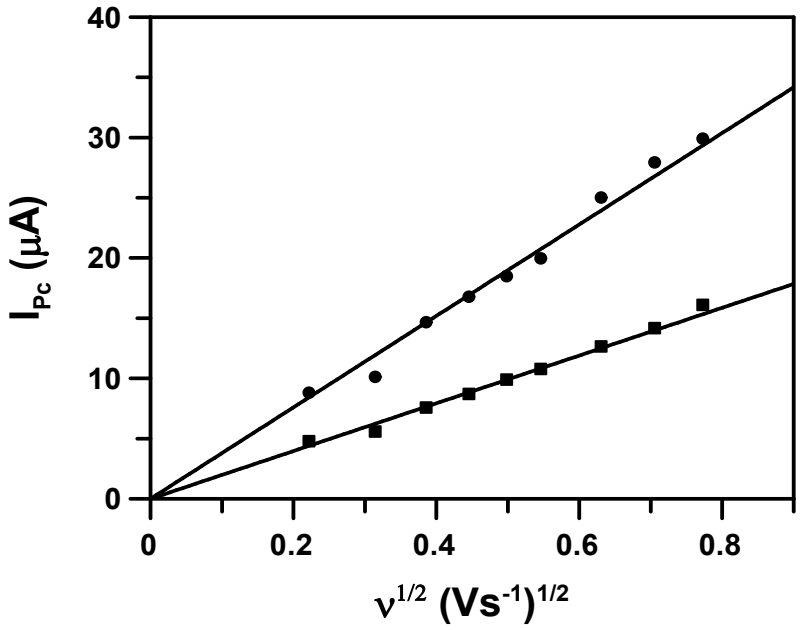

Fig. S6 Dependence of cathodic peak current on square root of scan rate for the reduction of onz (■) and $[Cu_2(oac)_4(onz)_2]$ (●) in pure methanol; T = 25 °C.

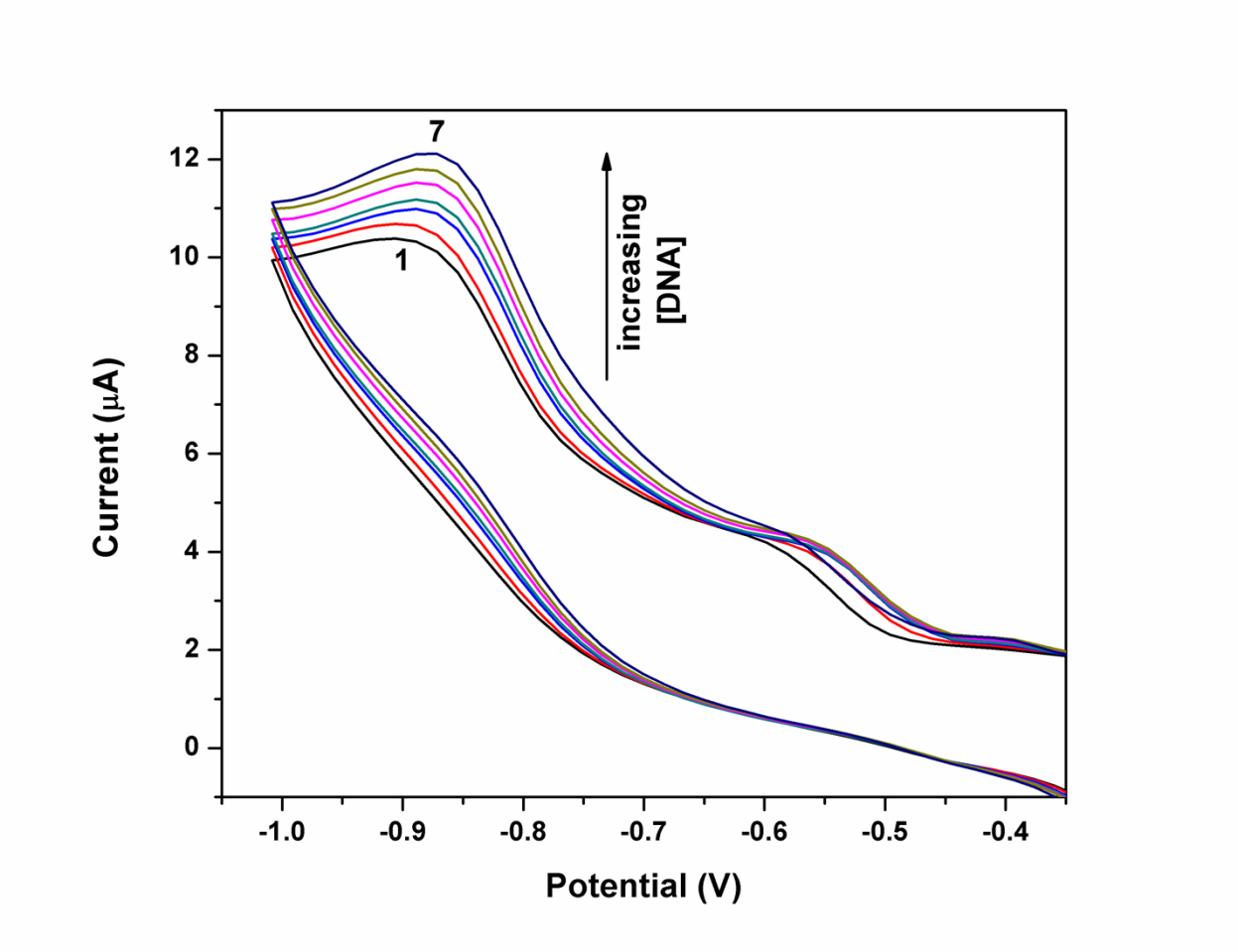

Fig. S7 Cyclic voltammograms for $[Cu_2(OAc)_4(Onz)_2]$ in the absence (1) and presence of different concentrations of c t DNA, 70.55 μM (2), 140.64 μM (3), 279.43 μM (4), 618.55 μM (5), 946.87 μM (6), 1783.26 μM (7). $[Cu_2(OAc)_4(Onz)_2]$ = 250 μM; [NaCl] = 120 mM; pH= 7.4; T = 25°C.

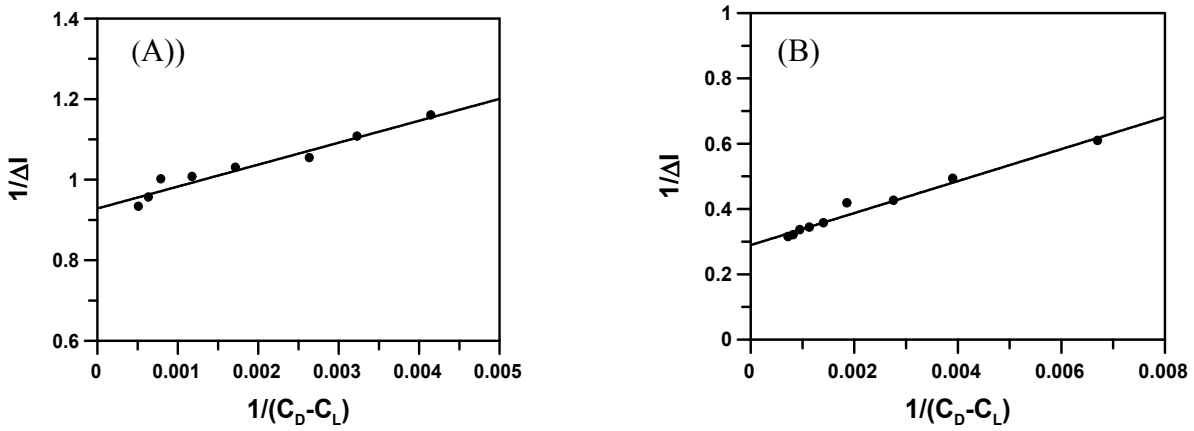

Fig. S8 Double reciprocal plots for the interaction of onz (A) and $[Cu_2(OAc)_4(Onz)_2]$ (B) with c t DNA; [Onz] = $[Cu_2(OAc)_4(Onz)_2]$ = 250 µM, [NaCl] = 120 mM; pH= 7.4; T = 25°C.

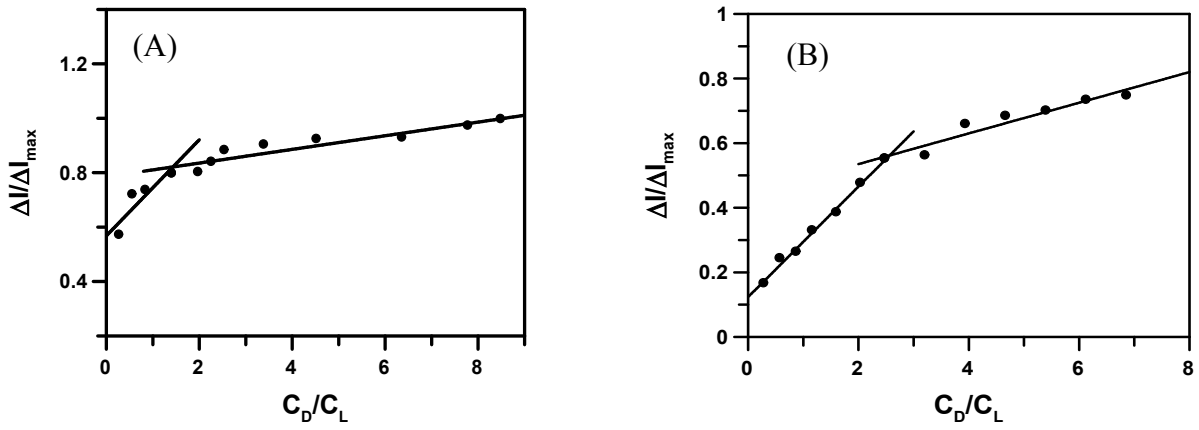

Fig. S9 Plot of normalized increase of peak current as a function of mole-ratio of c t DNA to Onz (A) and $[Cu_2(OAc)_4(Onz)_2]$ (B) respectively. [Onz] = $[Cu_2(OAc)_4(Onz)_2]$ = 250 µM, [NaCl] = 120 mM; pH= 7.4; T = 25°C.

Table ST1: Selected bond distances (Å)

Cu1	-O1	1.978(2)
Cu1	-O2	1.961(1)
Cu1	-O3	1.948(1)
Cu1	-O4	1.981(1)
Cu1	-N1	2.185(3)

Table ST2: Selected bond angles (º)

O1	-Cu1	-O2	88.72(7)
O1	-Cu1	-O3	91.42(6)
O1	-Cu1	-O4	167.91(11)
O1	-Cu1	-N1	93.39(11)
O2	-Cu1	-O3	167.55(9)
O2	-Cu1	-O4	90.37(6)
O2	-Cu1	-N1	94.08(7)
O3	-Cu1	-O4	86.90(5)
O3	-Cu1	-N1	98.34(7)
O4	-Cu1	-N1	98.70(8)

Table ST3: Hydrogen bond distances (Å) and angles (º)

D-H….A	**D-H**	**H…A**	**D…A**	**<D-H...A**
O7 -- H6 ... O5	0.85(4)	2.21(4)	3.032(5)	162(4)
O7 -- H6 ... N3	0.85(4)	2.31(4)	3.131(4)	162(4)

D, donor; H, hydrogen; A, acceptor.

Table ST4: MIC values of Onz, $[Cu_2(OAc)_4(Onz)_2]$ and different controls. The compounds were initially dissolved in DMSO and finally diluted to culture medium.

Compound	**Bacterial Strains**			
	***S. aureus* ATCC 29213**		***E. coli* ATCC 25922**	
	Run 1	**Run 2**	**Run 1**	**Run 2**
Onz	20.25 µM	40.5 µM	40.5 µM	20.25 µM
$[Cu_2(OAc)_4(Onz)_2]$	20.25 µM	40.5 µM	40.5 µM	20.25 µM
$Cu(NO_3)_2 \cdot 3H_2O$	>162.0 µM	>162.0 µM	>162.0 µM	>162.0 µM
1:1 mixture of Cu(II) & Onz	20.25 µM	40.5 µM	40.5 µM	20.25 µM
Na_2EDTA	81.0 µM	162.0 µM	81.0 µM	162.0 µM
Cu(II)-EDTA complex	81.0 µM	162.0 µM	162.0 µM	162.0 µM
$Cu(OAc)_2 \cdot H_2O$	>162.0 µM	>162.0 µM	>162.0 µM	>162.0 µM

$$\frac{1}{\Delta I} = \frac{1}{\Delta I_{max}} + \frac{K_d}{\Delta I_{max}(C_D - C_0)} \qquad (SE\ 1)$$

$$K_d = \frac{\left[C_0 - \left(\frac{\Delta I}{\Delta I_{max}}\right)C_0\right]\left[C_D - \left(\frac{\Delta I}{\Delta I_{max}}\right)C_0\right]}{\left(\frac{\Delta I}{\Delta I_{max}}\right)C_0} \qquad (SE\ 2)$$

$$C_0\left(\frac{\Delta I}{\Delta I_{max}}\right)^2 - (C_0 + C_D + K_d)\left(\frac{\Delta I}{\Delta I_{max}}\right) + C_D = 0 \quad (SE\ 3)$$

$$\frac{r}{C_f} = K_{(n - r)} \qquad (SE\ 4)$$