

Non-steroidal anti-inflammatory drug-Copper(II) complexes: Structure and biological perspectives

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Supplementary material

Table S1.

Selected bond distances and angles for complex **5**.

Bond	(Å)	Angles	(°)
Cu - O(11)	1.972(2)	O(11) - Cu - O(11)'	180.0
Cu - N(1)	1.992(3)	O(11) - Cu - N(1)'	89.24(9)
Cu - Om	2.463(3)	O(11) - Cu - Om	95.80(8)
C(11) - O(11)	1.273(3)	O(11) - Cu - N(1)	90.76(9)
C(11) - O(12)	1.250(4)	N(1) - Cu - N(1)'	180.0
Cu...O(12)	3.242 Å	Om - Cu - Om'	180.0
		O(11) - Cu - Om'	84.20(8)

Symmetry operation to generate equivalent atoms: (') -x, -y, 1-z.

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Table S2. Crystallographic data for complex **5**.

5	
Formula	C ₄₂ H ₄₆ CuN ₄ O ₆
Fw	766.40
T	180 (2) K
Crystal system	Triclinic
Space group	$P\bar{1}$
a=	7.5765(1)
b=	8.5270(1)
c=	14.9018(2)
α =	100.793(1)
β =	90.666(1)
γ =	90.562(1)
Volume	945.56(2)
Z	1
D(calc), Mg m ⁻³	1.346
Abs. coef., μ , mm ⁻¹	1.247
F(000)	403
GOF on F ²	1.119
R1	0.0396 ^a
wR2	0.0908 ^a

^a2159 reflections with $I > 2\sigma(I)$

Figure S1. Stern-Volmer quenching plot of BSA for Hmef and complexes 1-5.

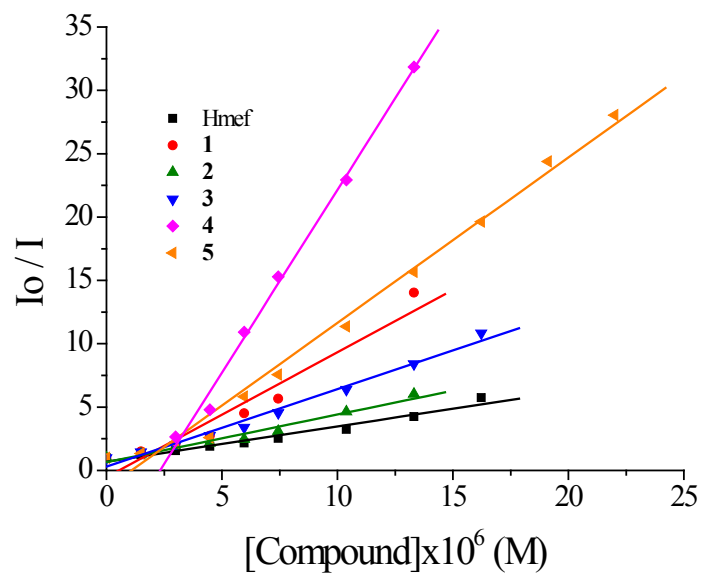


Figure S2. Scatchard plot of BSA for Hmef and complexes 1-5.

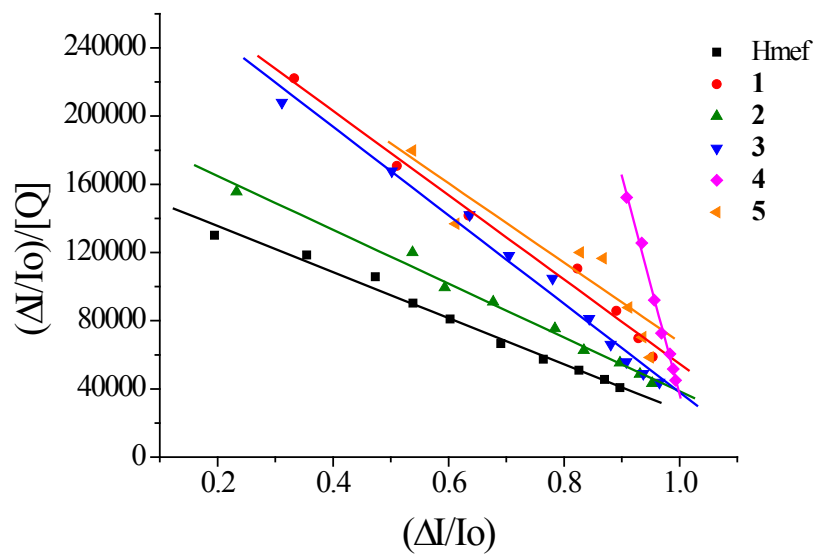


Figure S3. Stern-Volmer quenching plot of HSA for Hmef and complexes 1-5.

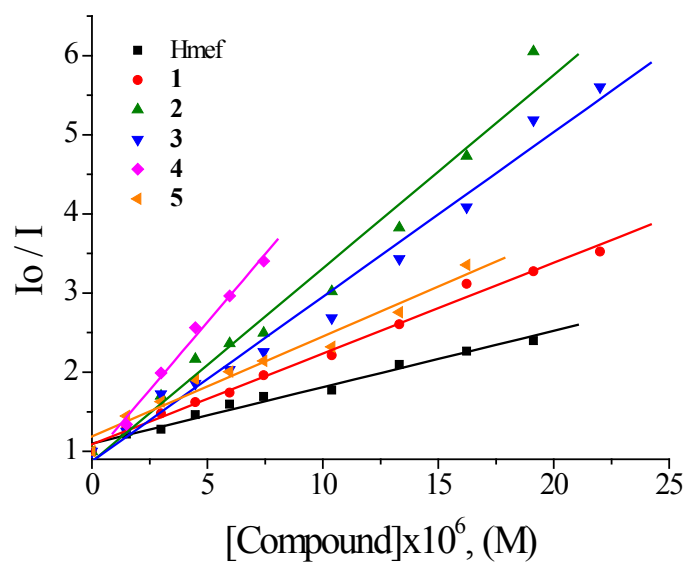


Figure S4. Scatchard plot of HSA for Hmef and complexes 1-5.

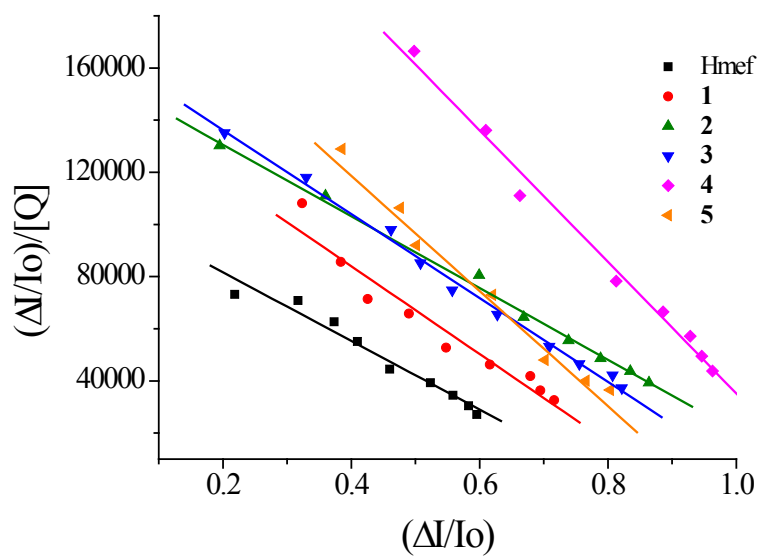


Figure S5. Cyclic voltammogram of 0.4 mM dmsol solution of **3**. Scan rate = $100 \text{ mV} \cdot \text{s}^{-1}$.
Supporting electrolyte = TEAP, 0.1 M.

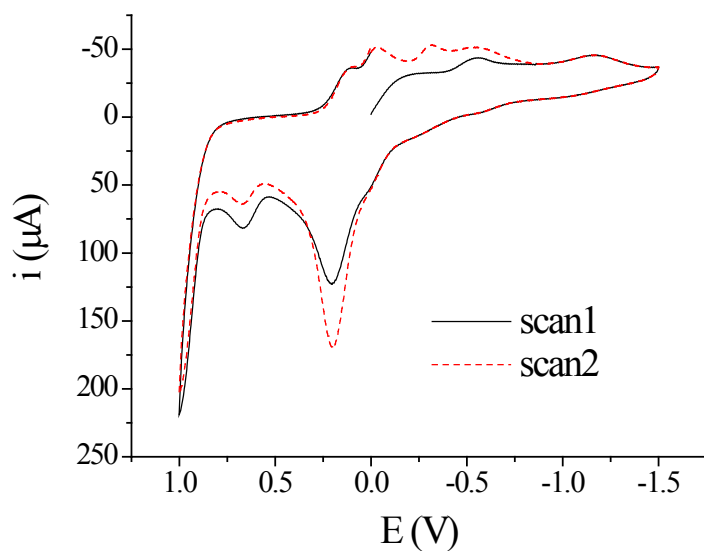


Figure S6. Cyclic voltammogram of 0.4 mM 1/2 dmsol/buffer (containing 150 mM NaCl and 15 mM trisodium citrate at pH=7.0) solution of $[\text{Cu}(\text{mef})_2(\text{py})_2(\text{MeOH})_2]$, **5** in the absence or presence of CT DNA. The arrows show the changes upon addition of CT DNA. Scan rate = 100 mV s^{-1} .
Supporting electrolyte = buffer solution.

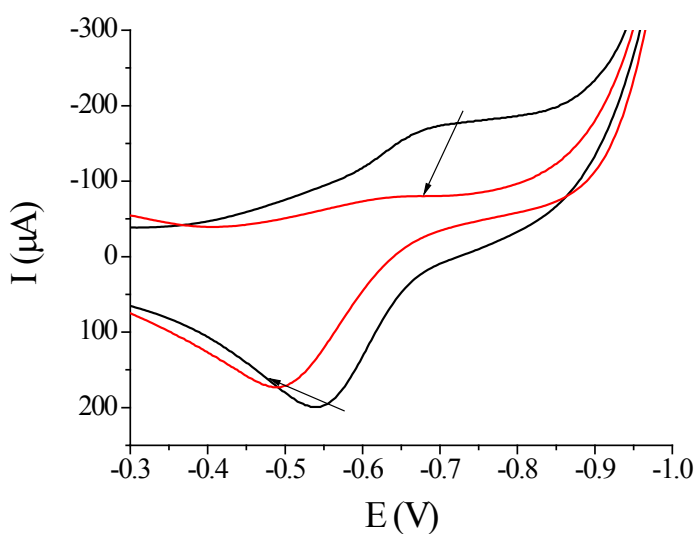


Figure S7. Stern-Volmer quenching plot of EB bound to CT DNA for Hmef and complexes **1-5**.

