

Supplementary Information

Zinc(II) complexes of carboxamide derivatives: crystal structures and interaction with calf thymus DNA

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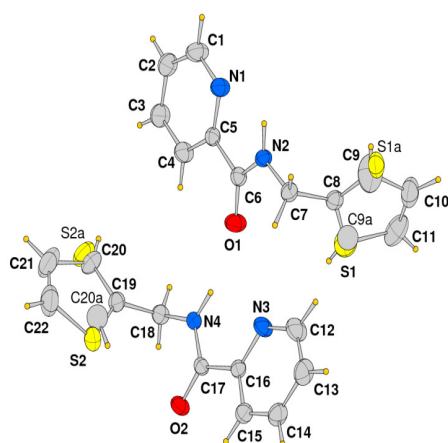


Figure s1. The two independent ligand molecules L2 (ORTEP view, 30% ellipsoid probability) with indication of the disorder of the thiophene rings (occupancy factors S1/C9 = 0.56; S1a/C9a = 0.44; S2/C20 = 0.69; S2a/C20a = 0.31)

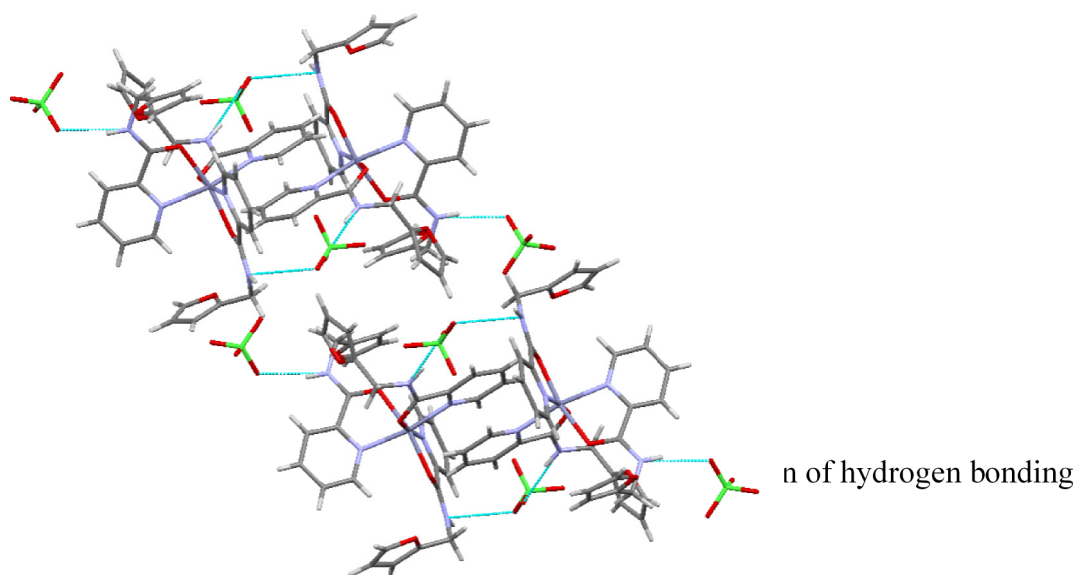


Figure s3. Optimized structure of complex **2**

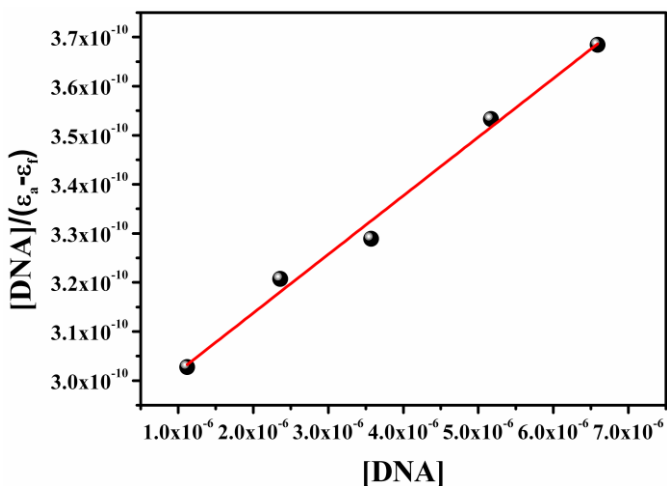
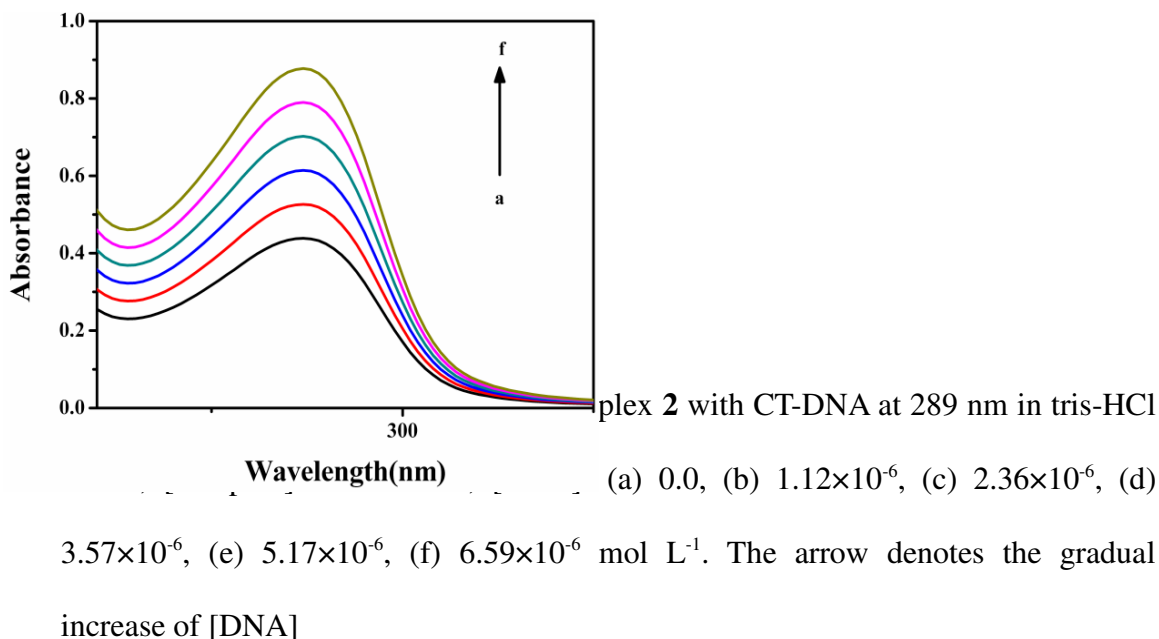


Figure s5. Plot of $[DNA]/(\epsilon_a - \epsilon_f)$ vs $[DNA]$ for the absorption titration of CT-DNA with complex **2** in tris-HCl buffer. Association constant $K_b = 4.12 \times 10^4$ M⁻¹ ($R = 0.9887$, $n = 5$ points)

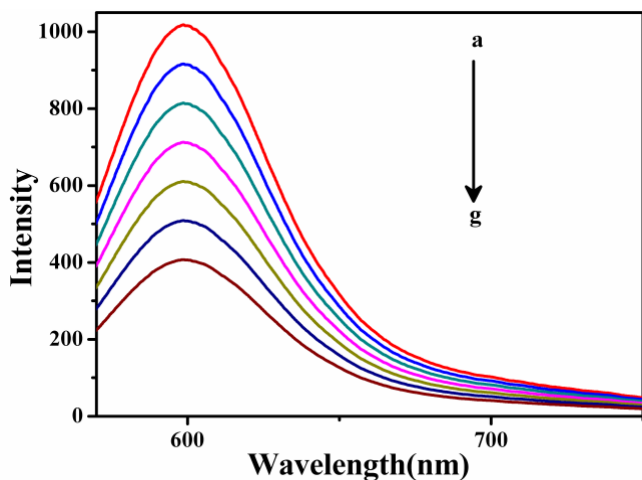
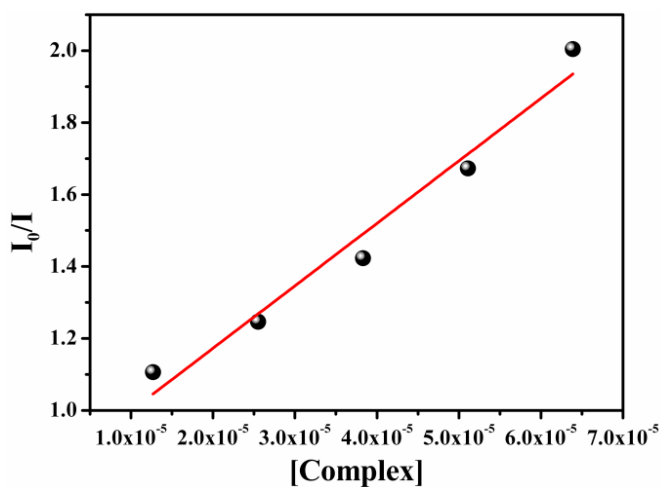


Figure s6. (A) Emission spectrum of the CT-DNA-EB system in tris-HCl buffer upon titration with increasing concentration of complex **2**. $\lambda_{\text{ex}} = 522 \text{ nm}$; $[\text{EB}] = 1.3 \times 10^{-6}$, $[\text{DNA}] = 1.58 \times 10^{-5}$; $[\mathbf{2}] =$ (a) 0.0, (b) 1.27×10^{-5} , (c) 2.55×10^{-5} , (d) 3.83×10^{-5} , (e) 5.11×10^{-5} , (f) 6.39×10^{-5} , (g) $7.72 \times 10^{-5} \text{ mol L}^{-1}$



of complex **2** to CT-DNA-EB system;

Table s1. K_b , K_{SV} and K_{app} values of DNA binding study

Complex	K_b	K_{SV}	K_{app}
1	1.34×10^5	3.52×10^5	9.2×10^5
2	4.12×10^4	2.103×10^4	2.03×10^5