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Study on the mode and strength of DNA interaction with Thiamine and some of its metal complexes

Parnaz Nematifard[a], Farshid Hajibabaei[a] and Sadegh Salehzadeh[a]*

[a]*Department of Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran*
[*] *Corresponding author: saleh@basu.ac.ir*

DNA binding mechanism of molecules, especially metal complexes, has been studied in order to develop anticancer drugs for several decades. In order to reduce side effects and improve the effectiveness of treatments, researchers are trying to design and synthesize new biometal complexes [1-3]. In this project, three complexes of the thiamine chloride (ThmCl) with the proposed formula [M(Thm)Cl_3] (M= Zn(II), Cd(II), Co(II)) and also a new salt of thiamine chloride hydrochloride, with the chemical formula of [ThiamineClH][$CuCl_2$], were synthesized and characterized with elemental analysis (CHNS), FT-IR, and UV-Vis spectroscopies in all cases, and also with ^{1}H NMR, except in the case of Co(II) complex. In addition, the structure of the synthesized new thiamine chloride hydrochloride salt was characterized using X-Ray crystallography (Figure 1). The comparison of binding constants (K_b) measured from the UV–Vis absorption studies showed that the binding strength of the above compounds to ct-DNA is as follows: ThmCl·HCl > [Zn(Thm)Cl_3] > [Cd(Thm)Cl_3] > [Co(Thm)Cl_3]. The results of viscosity measurements indicated that the thiamine chloride hydrochloride and its complexes bind to ct-DNA via an intercalation binding mode. Moreover, the molecular docking simulation visualized that the thiamine and its complexes bind to DNA via an intercalation binding mode which is in agreement with the results of viscosity measurements studies.

Keywords: DNA interaction, Thiamine, Crystal structure, Intercalation.

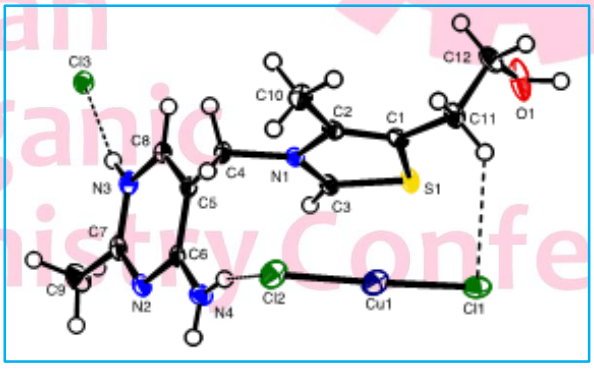


Figure 1. ORTEP diagram of [ThiamineClH][$CuCl_2$]. Ellipsoids are drawn at the 50% probability level.

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