22nd Iranian Chemistry Conference, 23-25 August, 2023
University of Kurdistan

A new tetra-coordinated copper(II) complex: Synthesis, characterization, DFT studies and investigating interaction with Biomacromolecules

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In the present work, Reaction of $CuCl_2.2H_2O$ with 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol, (HEAC), in methanol in the presence of 4,4-bipyridine led to the $[Cu(HEAC)(Cl)_2(bipy)]$. The complex were identified by elemental analysis, FT-IR spectroscopy and DFT studies. As it is shown in (Fig.1), In the structure, the coordination number of the Cu(II) ion in the compound is four and Complex has a CuN_2Cl_2 environment. According to the τ value (τ =1.0), the geometry of the Cu is ideal square-planer. As well as, equation (Eq.1) illustrates Gibbs free energy changes (ΔG) at corresponding temperatures to determine the spontaneous or non-spontaneous process of the reaction([1]). The predicted free energy of the reaction is -0.157555 u.a. Molecular docking is done between a small molecule (complex) and a target macromolecule (protein and DNA) and is considered a key tool in drug design([2]). Docking calculation (Fig.2) showed that the complex has higher fitness scores with CatB, rHA and RNR proteins compared to doxorubicin (anticancer drug), thus we suggest that studying the anticancer activities of this compound could be interesting. $\Delta G_{reaction} = \Delta G_{products} - \Delta G_{reactants}$ (1)

***Keywords*:** Bio macromolecule, Geometry, DFT, Gibbs free energy

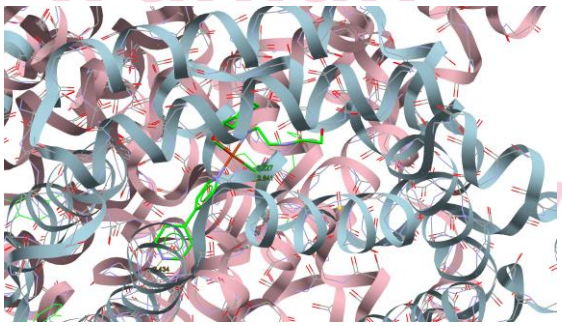


Fig.2. Docking study results, showing the interaction between the complex and rHA protein.

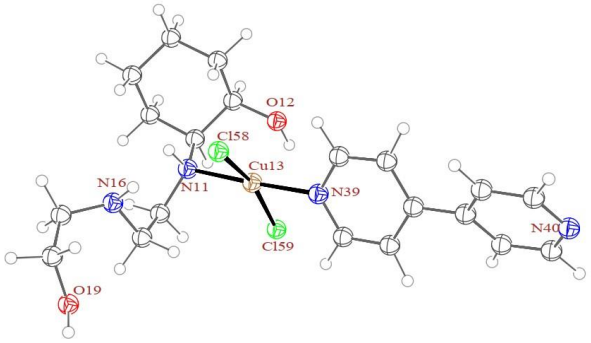


Fig. 1. The ortep diagram of complex.

References

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