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

Synthesis and characterization of the copper(II) complex of a new *β*-amino alcoholic ligand in the presence of the 4,4-bipyridine supported by molecular docking

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In this work, 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol, L_1, was prepared in solvent by the ring opening of Epoxycyclohexane with 2-(2-amino-ethylamino)ethanol([1]). Reaction of $CuBr_2$ with L_1 in methanol in the presence of 4,4-bipyridine (L_2) led to the $[CuL_1L_2Br_2]$. we elucidated the structure of Cu(II) complex prepared and identified by elemental analysis and FT-IR spectroscopy. The L_1 unit is a potentially tetradentate ligand that can be bind to metal atoms through two N- and one O-atoms, but here, it is coordinated to the central metal through one N- atom. As it is shown in (Fig.1), the coordination number of the Cu(II) ion in the compound is 4 and according to the τ value (τ =1.0), the geometry of the compound is ideal square-planer. For the accurate evaluation of the located site of the synthesized complex on biomacromolecules, the docking analysis of the interaction was performed([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.

***Keywords*:** *β* -Amino alcohol, 4,4-bipyridine, Coordination Chemistry, Molecular docking

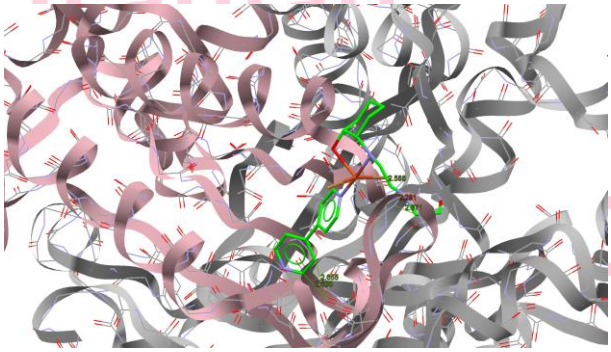


Fig.2. Docking study results, showing the interaction between the complex and RNR protein.

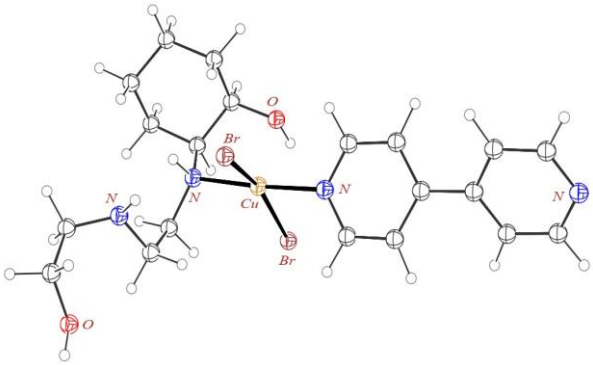


Fig. 1. The ortep diagram of complex.

References

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