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Investigating on the interaction of the new copper complex with DNA and proteins: synthesis and structural characterization

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A new complex of Cu(II), [Cu(AEAE)(L)Br], containing 2,2-aminoethylaminoethan-1-ol (AEAE) and 4,4-Bipyridine (L) as ligands were prepared and its spectral (IR), structural properties and molar conductivity were investigated. The AEAE ligand acts as an N2O- donor in this complex by forming two five-membered chelate rings. The Cu(II) ion has a CuN_3OBr environment which proves that the coordination number of the compound is 5 (Fig.1). The Geometry optimization was performed using Gaussian 09 software. The Protein Data Bank (PDB) files 4r5y, 3ai8, 5cdn, 3c0z, 2bx8, 1peo, 3qfa, 1njb, 4gfh for the nine receptors, BRAF kinase, CatB, DNA gyrase, HDAC7, rHA, RNR, TrxR, TS, Top II, respectively, used in this research were obtained from the PDB ([1]). The Hermes visualizer in the Gold Suite was used to further prepare the metal complex and the receptors for docking. The optimized complex was used for the docking studies. The results are reported in terms of the values of fitness which means that the higher fitness the better the docked interaction of the compound (Fig.2). The fitness score of the complex with CatB(Protein) is higher than the fitness score of doxorubicin([2]).

Keywords: Protein, Copper, Structural characterization, Doxorubicin

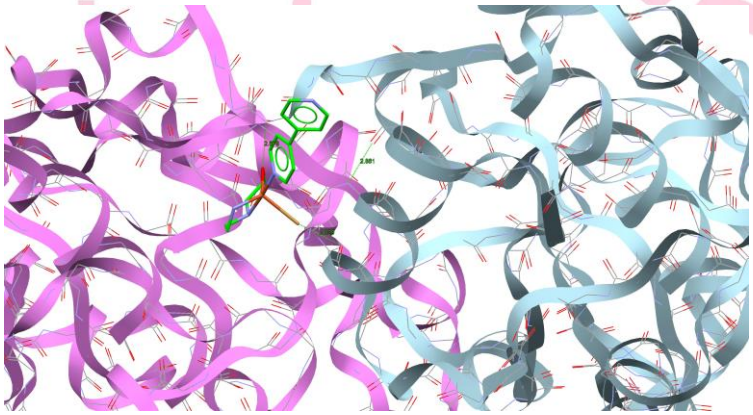


Fig.2. Docking study results, showing the interaction between the complex and CatB protein.

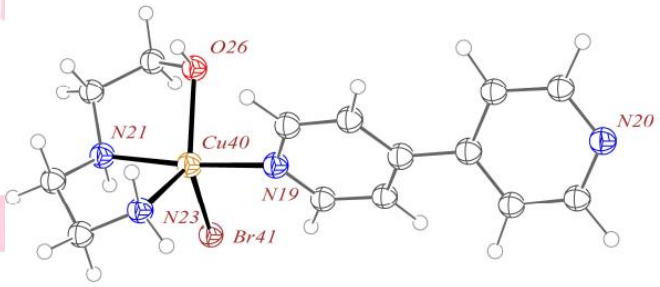


Fig.1. The ORTEP-III diagrams for the complex.

References

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