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Synthesis and characterization of the new Cobalt(II) amino alcohol complex: A combined experimental, computational and docking studies

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In this work, a new complex of Co(II), $[Co(L_1)(L_2)(NO_3)(H_2O)]$, with 2-(2-aminoethylamino)ethanol (L_1) and 4,4-Bipyridine (L_2) was prepared and characterized by elemental analysis, molar conductivity and FT-IR spectroscopy. As it is shown in Figure 1, the coordination number of the Cobalt(II) ion in the compound is six and the geometry of the complex is octahedral. The L_1 unit which is based on Cambridge Structural Database(CSD) ([1]) is a potentially tridentate ligand that can be bind to metal atoms through two N-atoms and one O-atom.

In this structure, the ligand was fully coordinated and formed two five-membered chelate rings. The structure was optimized with the Gaussian 09 software and calculated for an isolated molecule using Density Functional Theory (DFT) at the B3LYP\6-31G(d,p) level of theory for ligands and B3LYP\LanL2DZ for the complex. The predicted free Gibbs energy of the reaction is -76.5366 u.a. For predicting the biological activities of the complex, interactions of this compound with macromolecule receptors, using Gold docking software ([2]), were studied. Docking calculation showed that the complex (interaction with CatB) worked better than the anti-cancer drug, Doxorubicin, thus we suggest that studying the anticancer activities of this compound could be interesting (Figure 2).

Keywords: Biological activity, Coordination chemistry, Docking study, Gaussian, DNA

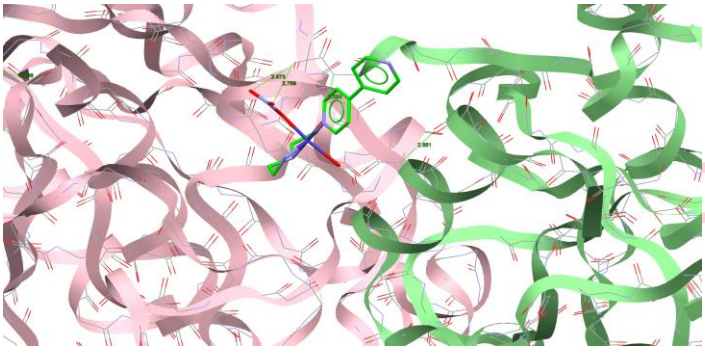


Figure2. Docking study results, showing the interaction between the complex and CatB

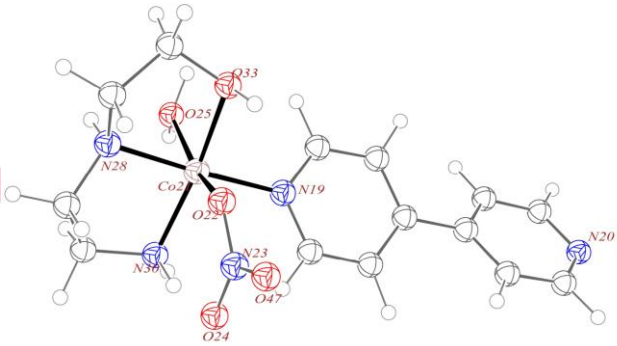


Figure1.The ortep diagram of complex.

References

[1] F. H. Allen, *Acta Crystallographica Section B: Structural Science*, **2002**, 58, 380.
[2] G. Jones, P. Willett, R. C. Glen, A. R. Leach and R. Taylor, *Journal of molecular biology*, **1997**, 267, 727.