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Synthesis, characterization, DFT studies and molecular docking of Fe(III) complex containing *β*–amino alcohol ligand

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In this project, a new complex of Fe(III), $[Fe(L)(NO_3)(H_2O)_2]^{2+}$ (L: (2-((2-((2-hydroxyethyl)amino)ethyl)amino)cyclohexane-1-ol)), was prepared and identified by elemental analysis, FT-IR spectroscopy, and DFT studies. The L unit is a potentially tetradentate ligand that can be bound to the metal atoms through two N-atoms and two O-atoms but in this complex, the ligand acted as tridentate and formed two five-membered chelate rings. As shown in the structure of the compound (Figure 1), the complex has FeN_2O_4 environment, so the coordination number of the Fe(III) ion is 6 which proves that the geometry of the complex is octahedral. The structure was optimized with the Gaussian 09 software ([1]) and calculated for an isolated molecule using Density Functional Theory (DFT) ([2]) at the B3LYP/6-31G(d,p) and B3LYP/LanL2DZ level of theory for L and complex, respectively. However, since Gaussian provides the sum of electronic and thermal free energies, there is a shortcut: namely, to simply take the difference of the sums of these values for the reactants and the products. For example, using the information extracted from Gaussian, the Gibbs free energy of the reaction can be calculated simply by: $\Delta G = \Delta G_{products} - \Delta G_{reactants}$ = -0.136946 u.a([3]). Molecular docking showed that the complex has close fitness scores (In interaction with the CatB protein) compared to doxorubicin (anticancer drug) thus we suggest that studying the anticancer activities of this compound could be interesting (Figure 2).

***Keywords*:** Amino alcohol, Free gibbs energy, DFT calculation, Docking study

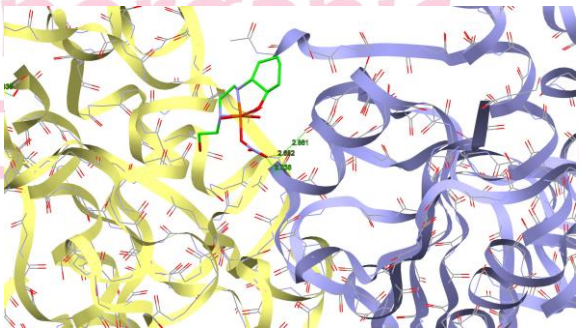


Figure 2. Docking study results, showing the interaction between the complex and CatB

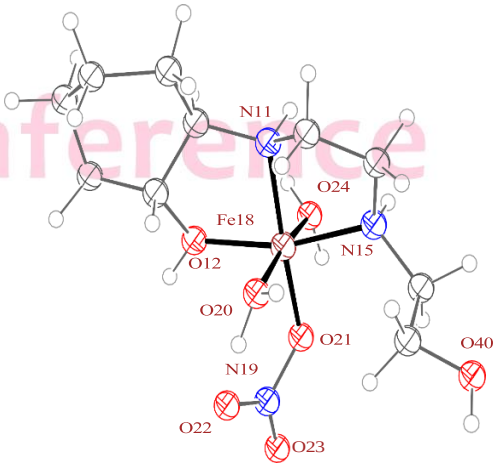


Figure 1.The ortep diagram of

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