



University of Zabol
Graduate school
Faculty of Science
Department of Chemistry

The Thesis Submitted for the Degree of M.Sc (in the field of Analytical
Chemistry)

**Experimental and theoretical study on the impact of a tri-
hetero metallic polymer on bovine liver catalase enzyme**

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Abstract

The binding of small molecules such as drugs to biological molecules plays an important role in their distribution and effectiveness in biological systems. Therefore, in this research trinuclear complex $[Cu_{0.152} Mn_{0.848}(\mu\text{-dipic})_2\{Na_2 (\mu\text{-H}_2O)_4\}]_n \cdot nH_2O$ (dipic = pyridine-2,6-dicarboxylato) was selected and its effect on the structure and function of bovine liver catalase (BLC) was evaluated using spectroscopic and molecular docking methods. In this study, various parameters such as binding constant, type of interaction, thermodynamic parameters and type of fluorescence quenching were investigated at three temperatures of 303, 310 and 317 K. The trinuclear complex could improve the catalytic activity of the enzyme. The results of spectroscopic studies confirmed that the complex is able to turn off the intrinsic fluorescence of protein through static mechanism and formation of hydrogen bonds and van der Waals interactions with catalase. Complex binding has led to some structural changes in catalase. Molecular docking studies were used to investigate the binding site of the complex in catalase. Finally, the antioxidant activity of the complex was investigated using the DPPH free radical and showed that the trinuclear complex has a higher ability to inhibit free radicals than many metal complexes.

Keywords: Polymeric Metal Complexes, Catalase, Metallodrugs, Interaction Mechanism, Molecular Docking