University of Zabol
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Department of Chemistry

The Thesis Submitted for the Degree of M. Sc

In the field of Analytical Chemistry

Spectroscopic, chemometrics and molecular modeling approaches to investigate the interaction of a novel trinuclear iron complex with bovine liver catalase enzyme

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Abstract

The use of metal complexes with nitrogen and sulfur donor ligands is an important approach in medical studies due to their electronic properties and good solubility in common solvents, easy preparation and wide structural diversity of these compounds. Hence, in this research the tri-nuclear iron (II, III) complex ($[Fe(bpy)_3][Fe(dipic)_2]_2.7H_2O$; dipic= pyridine-2,6-dicarboxylate and bpy= 2,2′-bipyridine) was used for the study of its effect on the function and structure of bovine liver catalase (BLC). For this purpose, spectroscopic methods such as Ultraviolet-Visible (UV-Vis) spectroscopy, fluorescence quenching, and Circular Dichroism (CD) were used. The results of fluorescence spectroscopy showed that the interactions between the complex and the catalase lead to the quenching of the catalase fluorescence emission through the static quenching mechanism. Thermodynamic parameters showed that the predominant interactions between catalase and complex are hydrogen bond and van der Waals, and the process is exothermic and enthalpy-driven. Also, the results of synchronous fluorescence showed that no polarity change occurs around the tyrosine residue during the complex-catalase interaction while the polarity changes around the tryptophan. The study of circular dichroism spectroscopy also shows a decrease in the content of the alpha helix, which confirms the interaction of amino acids in the catalase chain and complex which leads to the change in the protein structure. Besides, the experimental data (Fluorescence and Uv-Vis spectroscopy) were analyzed using chemometrics. Finally, the accuracy of the results of spectroscopic methods was evaluated using molecular docking calculations. The results of docking and analysis of the active sites of catalse also confirmed the experimental results and showed that the interaction of the cationic part of the complex with catalase is mainly hydrophobic and van der Waals interactions, while the main interactions of the anionic part are hydrophobic, van der Waals and hydrogen bonding.

Keyword: Molecular Docking, Quenching, Bonding mechanism, Metal drugs