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Department of Chemistry

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

Experimental and theoretical approaches to monitor the behavior of bovine liver catalase in the interaction with a binuclear Bismuth complex

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Abstract

Metal-based drugs, also known as metallodrugs, play a significant role in the treatment of diseases. Neutralizing free radicals can help in the prevention of conditions like cancer. Hence, the development and creation of antioxidant metallodrugs carry significant importance. This study reported the antioxidant properties and the interaction of a binuclear Bismuth complex, represented by the formula $[Bi2(\mu\text{-}ox)(dipic)_2(H2O)_2(taa)_2].H2O$, with bovine liver catalase (BLC). The Bi complex's antioxidant properties were assessed using a 1,1-diphenyl-2-picrylhydrazyl radicals (DPPH) assay, which revealed that the Bi complex effectively reduced DPPH radical activity in a 125 mg L^{-1} concentration. Reactive oxygen species are known to induce oxidative stress in living organisms, and catalase, being a valuable antioxidant enzyme, plays a protective role in mitigating this effect. The presence of the Bi complex substantially enhanced the catalytic performance of BLC. Spectral methods were employed to examine how the Bi complex influenced the structure and activity of bovine liver catalase. The fluorescence analysis showed that the BLC and Bi complex interaction follows a static quenching mechanism. This interaction occurred spontaneously, exothermic, and was primarily driven by van der Waals forces and hydrogen bonds. Through molecular docking simulation a stable binding arrangement was identified, aligning perfectly with the spectroscopic findings.

Key word: Catalase, Metal-based drugs, Binuclear Bismuth complex, Molecular docking, Antioxidant