The University of Zabol
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Faculty of Science
Department of Chemistry

The Thesis Submitted for The Degree of M. Sc

In The Field of Inorganic Chemistry

Synthesis, antioxidant properties, enzyme inhibitions and molecular docking studies of Zn(II) complexesof acetohydrazide based Schiff base ligand

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Abstract

New Schiff base ligand N'-3-(hydroxyimino)butan-2-ylidene)acetohydrazide, HIBYA, and its Zn(II) complexes, $[Zn(HIBYA)_2]Cl_2$ (A), $[Zn(HIBYA)(bpy)]Cl_2$ (B), and $[Zn(HIBYA)(phen)]Cl_2$ (C) (bpy = 2 2'-bipyridine and phen = 1,10-phenanthroline) were synthesized and characterized. Antioxidant results showed that the ability of compounds to inhibit DPPH• is as follows: A > C > B > HIBYA. The interaction effects of A-C complexes on the activity and structure of the bovine liver catalase (BLC) were investigated by spectroscopic and molecular docking techniques. All complexes were able to change the performance and structure of BLC; A has a greater effect on BLC activity, so that at concentration of 0.17 µM, A, B and C improve initial BLC activity by 68%m 23% and 56%, respectively. The binding strength of the A-C complexes with BLC was almost similar and with the order of 10^4 M^{-1} (K_b = 11.74 × 10^4 M^{-1} for A, 10.23 × 10^4 M^{-1} for B, and 12.58 × 10^4 M^{-1} for C) .The interaction mechanism of three complexes with BLC was similar, A-C complexes interacted mostly with van der Waals interactions and hydrogen bonds. Docking studies confirmed the spectroscopic results and predicted the amino acids involved in the interaction.

Keywords: Schiff base complexes; Catalase; Interaction Mechanism, Antioxidant