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COORDINATION COMPOUNDS

A Bowl-Shaped Zinc-Salen Complex: Structural Analysis and Molecular Docking Studies against Omicron-S and Delta-S Variants

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Abstract– A novel binuclear salen-Zn(II) complex has been prepared and structurally investigated by single-crystal X-ray crystallography, which reveals a distorted tetragonal pyramidal environment around one zinc atom and distorted tetrahedral geometry surrounding the second zinc atom. In order to further understand the structural aspects of the complex, additional research into its structure has been conducted using theoretical methods, such as DFT and TD-DFT. Furthermore, Hirschfeld surface analysis has been used to obtain quantitative descriptions of intermolecular interactions in molecules. A comparative molecular docking investigation for the title binuclear Zn(II) complex has been explored against the SARS-CoV-2 S-Delta (PDB ID: 7V8B) and the SARS-CoV-2 Omicron (PDB ID: 7T9K) variants, and the results indicated that the Omicron variation had higher energy for stabilization.

Keywords: Zn(II) complex, single crystal X-ray diffraction, TD-DFT, comparative molecular docking analysis

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INTRODUCTION

Schiff base ligands have become extremely popular due to their ease in synthesis, incredible versatility, and structural resemblance to natural biological molecules since their discovery in chemistry in the late 19th century [1–3]. In addition, Schiff bases have an imine group (–CH=N), which is essential in comprehending biological reactions [2, 3]. Furthermore, the chelating structures of Schiff bases give them numerous complexing possibilities and make it easy to change their electronic and steric properties [4]. Numerous studies have revealed that the presence of a lone pair of electrons in sp^2 of the nitrogen atom in the azomethine group causes significant chemical and biological effects [3]. When it comes to host-guest interaction, Geometric cavity control is a prominent feature of the Schiff base. A metal ion with modified lipophilicity becomes extremely stable, selective, and sensitive [4]. In order to contribute to the development of Schiff base chemistry, Schiff base ligands, and their metal complexes have been used to study a wide spectrum of organometallic compounds and bioinorganic chemistry [5]. In the last two decades, Schiff base metal complexes have attracted a lot of attention due to their useful properties in magnetism, material science, and catalysis of several reactions, including carbonylation, hydroformylation, reduction, oxidation, and epoxidation, as well as industrial applications [4]. A substantial correlation between metal ions and/or their complexes and potential ligands as anticancer [4, 6] and antibacterial agents [7] has also been investigated in many studies. Over the years, the Group 12 metal complexes with a stable d^{10} electronic configuration have received significant interest in inorganic chemistry, biology, and environmental chemistry [8].

Zinc is an essential trace element and the second most prevalent biocompatible metal in the body [9–11]. In addition, zinc is a redox inactive metal with a strong Lewis acid structure and a d^{10} electronic configuration and plays an important role in enzyme catalysis [10, 11] and protein functions, particularly zinc finger proteins [12]. Additionally, zinc is also essential for human growth and development [13]. Furthermore, Zn(II) exhibits a variety of fluorescence characteristics depending on the ligand [9, 10], as well