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Synthesis, Characterization, and Drug-Like Interaction Evaluation of Copper Schiff Base Complex with Human Serum Albumin: A Study on Structural Attributes and Therapeutic Applications

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Abstract

In this research, a novel Copper Schiff Base Complex was designed and synthesized, evaluated for its unique properties as a drug-like compound. Its molecular structure was confirmed using advanced techniques such as ¹H-NMR, IR, UV-Vis, and X-Ray, which collectively verified the integrity and accuracy of the molecular configuration. Understanding the interaction of potential drug candidates with target proteins in the body is critical in pharmaceutical development. Therefore, we focused on assessing the interaction of this complex with human serum albumin (HSA) using fluorescence spectroscopy and circular dichroism (CD) techniques. The results revealed a specific interaction between the complex and HSA, highlighting its potential therapeutic efficacy and safety profile. Furthermore, to gain deeper insights into the type and mechanism of molecular interactions, molecular docking simulations were employed. These simulations provided valuable information regarding the binding sites and interaction mechanisms of the complex with biological machinery, paving the way for further development of this complex as a potential therapeutic agent.

Key words: Copper Schiff Base Complex, human serum albumin, molecular docking circular dichroism, fluorescence spectroscopy

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