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Synthesis, Characterization, and Interaction Studies of a Novel Schiff-Base Ligand with Human Serum Albumin (HSA): Spectroscopic and Molecular Docking Investigation

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Abstract

Schiff bases and their metal complexes are significant compounds in the medicinal and pharmaceutical fields. Their biological applications have gained traction due to their demonstrated antimicrobial, antifungal, antibacterial, antiviral, antipyretic, antidiabetic, and antitumor properties. Given their potential as anticancer agents, understanding how Schiff bases interact with Human Serum Albumin (HSA), the most prevalent plasma carrier protein, is of great interest. This can be explored through various spectroscopic techniques and molecular modeling. HSA has captured the pharmaceutical industry's interest because of its capacity to bind a wide array of metabolites and drugs, which can profoundly influence the pharmacokinetic characteristics of these drugs [1, 2].

In this research, a new Schiff-base ligand (L_2) has been synthesized and characterized using UV–Vis and FT-IR spectroscopy. The interaction between this ligand and HSA was investigated through fluorescence spectroscopy and cyclic voltammetry. The binding affinity of the ligand to HSA was assessed under conditions that simulate physiological relevance, utilizing both molecular docking (MD) and experimental methods. The findings indicated that the complex formation between HSA and the ligand led to the quenching of the protein's native fluorescence at 343 nm, which a static binding mechanism can explain.

Keywords: Schiff base, human serum albumin, anticancer potential, cyclic voltammetry, molecular docking.

References

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