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Investigating Human Serum Albumin Interaction with H_2bpb: Spectroscopic Analysis and Molecular Docking Approaches

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Abstract

Human Serum Albumin (HSA), as one of the main plasma proteins, is crucial in transporting drugs and biomolecules throughout the body [1]. Its interactions with pharmaceutical compounds, such as carboxamides, can significantly impact the bioavailability and efficacy of these compounds. This study investigates the interaction between HSA and a specific Carboxamide. For this purpose, N, N'-(1,2-phenylene) dipicolinamide (H_2bpb), was synthesized via triphenylphosphite (TPP) and tetrabutylammonium bromide (TBAB) and characterized with Fourier-transform infrared (FT-IR) spectroscopy [2]. Spectroscopic techniques, including absorbance titration and Circular Dichroism spectroscopy, were employed to analyze this interaction and determine the binding mechanisms. Using Molecular Docking, the binding site on HSA was identified IIA. The results reveal that the bonding between HSA and the studied Carboxamide is primarily mediated by van der Waals forces and π-π stacking interactions, which lead to slight conformational changes in the protein's secondary structure. These findings offer valuable information for designing new drugs and optimizing existing ones, ultimately enhancing drug delivery methods mediated by HSA.

Keywords: Human Serum Albumin, Carboxamides, Binding Affinity, Molecular Docking.

References

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