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Exploring Indole Ligand Interactions with Human Serum Albumin (HSA) via Spectroscopy and Molecular Docking Techniques

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Abstract

Indoles represent one of the most promising heterocyclic structures, noted for their distinctive properties attributed to the presence of an electron-rich pyrrole component. Heteroannulated indole derivatives have garnered significant interest due to their diverse biological and pharmacological activities [1,2]. This study reports the synthesis and characterization of an Indole ligand using UV–Vis and FT-IR spectroscopy. The interaction between this ligand and human serum albumin (HSA) was explored through fluorescence spectroscopy and cyclic voltammetry. Human serum albumin (HSA) has attracted considerable interest from the pharmaceutical industry owing to its capacity to bind a broad spectrum of metabolites and pharmaceuticals, which can significantly impact the pharmacokinetic profiles of these compounds [3]. Molecular docking and experimental techniques were employed to evaluate the binding affinity of the ligand to HSA under physiologically relevant conditions. The results demonstrated that the formation of a complex between HSA and the ligand resulted in the quenching of the protein's native fluorescence at 358 nm, which can be attributed to a static binding mechanism.

Keywords: Indole, HSA, Anticancer, Interaction, Molecular docking.

References

[1] Prakash, B., Amuthavalli, A., Edison, D., Sivaramkumar, M. S., & Velmurugan, R. (2018). Novel indole derivatives as potential anticancer agents: Design, synthesis and biological screening. *Medicinal Chemistry Research*, *27*, 321-331.

[2] Jafarpour, F., Ghasemi, M., Navid, H., Safaie, N., Rajai-Daryasarei, S., Habibi, A., & Ferrier Jr, R. C. (2020). Assembly of indole cores through a palladium-catalyzed metathesis of Ar–X σ-bonds. *Organic Letters*, *22*(24), 9556-9561.

[3] Dalal, M., Dubey, A., Antil, N., Tufail, A., & Garg, S. (2023). Synthesis, structural investigation of Schiff base endowed organyltellurium (IV) complexes: biological activities, molecular docking, quantum chemical computations and ADMET prediction. *Research on Chemical Intermediates*, *49*(7), 2889-2917.

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