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Interaction of a New Schiff Base Ligand with Human Serum Albumin: Insights from Spectroscopy and Molecular Modeling

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Abstract

Research on the supramolecular interactions between drugs or organic compounds and biological macromolecules has greatly enhanced our understanding of the structures and functions of these bio-macromoleculesand various biophysical processes. Human serum albumin (HSA) plays a crucial role in this context, as it binds to most drugs, allowing them to circulate in plasma and reach target tissues. HSA primarily regulates the distribution of these drugs. Consequently, drug-protein binding is a key factor in pharmacokinetics, influencing the drug's in vivo half-life, unbound concentration, distribution, and elimination. HSA, the most abundant protein in human blood plasma, has a high affinity for numerous endogenous and exogenous compounds, acting as a solubilizer and transporter for drugs and other organic molecules to their intended targets. In this study, a new Schiff base ligand (H_2L), has been synthesized and characterized by UV–Vis and FT-IR. The interaction between this ligand and HSA was studied through fluorescence spectroscopy and circular dichroism. The intrinsic fluorescence of HSA was quenched by the ligand, which was rationalized in terms of the static quenching mechanism. The results show that this compound can obviously bind to HSA molecules. According to fluorescence quenching calculations, the bimolecular quenching constant (K_q), and apparent quenching constant (K_{SV}) at 27 °C were obtained. The binding constant, K_b, is 110.69 $L.mol^{-1}$ and the number of binding sites (n) is 1. Furthermore, the CD spectra show that the random coil and antiparallel parts of the secondary structure have trends inverse to the helix part in the presence of Schiff base ligand.

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

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