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Pioneering Insights into Warfarin-HSA Dynamics via Advanced Molecular Docking pharmacokinetics and therapeutic efficacy

Abstract : Human Serum Albumin (HSA), the most abundant plasma protein, is vital for the transport and distribution of endogenous molecules and exogenous drugs. Warfarin, a commonly prescribed anticoagulant, exhibits significant plasma protein binding, primarily to HSA, which profoundly affects its pharmacokinetics and therapeutic efficacy. This study employed molecular docking using AutoDock 4, in conjunction with Discovery Studio, to investigate warfarin's binding affinity and interaction profile with HSA.The methodology involved preparing the protein and ligand by adding polar hydrogens, assigning Kollman charges, and defining torsional flexibility, followed by generating a grid box around the binding region. Docking simulations, conducted via the Genetic Algorithm, yielded multiple poses and their corresponding binding energies. A lowest binding energy of -7.49 kcal/mol was obtained for warfarin, which indicates a strong and favorable interaction between warfarin and HSA. However, this binding affinity was less favorable when compared to that of 4,7-dihydroxycoumarin. Cluster analysis revealed that warfarin's primary binding site is stabilized by hydrogen bonds, electrostatic interactions, and aromatic contacts. Key interacting residues, including ARG117, ARG186, TYR138, TYR161, and GLY199, facilitate electrostatic stabilization, π–π stacking, and hydrogen bonding with warfarin's aromatic and acidic groups. Alternative clusters displayed weaker or secondary binding modes with reduced affinities. These computational findings align with previous experimental studies that identify HSA as warfarin's principal carrier in plasma. The reliability of AutoDock in predicting drug-protein interactions and offering structural insights into warfarin's pharmacokinetics highlights the significant value of such computational approaches in drug design, optimization, and understanding drug-protein dynamics.
Keywords: Human Serum Albumin (HSA),Molecular Docking,Drug-Protein Interaction,Pharmacokinetics, Binding Affinity

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