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PROBING THE INTERACTION OF ANTICANCER DRUG TEMSIROLIMUS WITH HUMAN SERUM ALBUMIN: MOLECULAR DOCKING AND SPECTROSCOPIC INSIGHT

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The binding interaction between temsirolimus, an important anti-renal cancer drug, and HSA, an important carrier protein was scrutinized making use of UV and fluorescence spectroscopy. Hyper chromaticity was observed in UV spectroscopy in the presence of temsirolimus as compared to free HSA suggests the formation of complex between human serum albumin (HAS) and temsirolimus. Fluorescence quenching experiments clearly showed quenching in the fluorescence of HSA in the presence of temsirolimus confirming the complex formation and also confirmed that static mode of interaction is operative for this binding process. Binding constant values obtained through UV and fluorescence spectroscopy reveal strong interaction; temsirolimus binds to HSA at 298 K with a binding constant of 2.9×104 M^{-1} implying the strength of interaction. The negative Gibbs free energy obtained through isothermal titration calorimetry as well as quenching experiments suggests that binding process is spontaneous. Molecular docking further provides an insight of various residues that are involved in this binding process; showing the binding energy to be -12.9 kcal/mol. CD spectroscopy was retorted to analyze changes in secondary structure of HSA; increased intensity in presence of temsirolimus showing changes in secondary structure of HSA induced by temsirolimus. This study is of importance as it provides an insight into the binding mechanism of an important anti-renal cancer drug with an important carrier protein. Once temsirolimus binds to HSA, it changes conformation of HSA which in turn can alter the functionality of this important carrier protein and this altered functionality of HSA can be highlighted in variety of diseases.

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