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Spectroscopic and computational evaluation on the binding of safranal with human serum albumin: Role of inner filter effect in fluorescence spectral correction

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A B S T R A C T

For determining the pharmacological properties of medicinal compounds, their binding with serum albumins is very crucial. Herein, we have selected safranal, a major constituent of saffron which is known to retain a number of medicinal properties including antioxidant, anti-inflammatory, tumoricidal, anti-genotoxic, and anti-aging activities; and studied its mechanism of binding with human serum albumin at physiological pH using various spectroscopic methods along with computational approach using molecular docking. A change in the difference UV-visible spectrum of HSA in presence of safranal was found which is due to the complex formation. Owing to the strong absorption of safranal at the fluorescence excitation wavelength of HSA (295 nm) and in the whole range of emission, the fluorescence spectra of HSA in presence of safranal were corrected for the inner filter effect. After the correction the spectra were free from the safranal absorption effect and it was found that addition of safranal causes the quenching of HSA fluorescence and a blue shift of the emission maximum which are attributed to the binding of safranal to the protein and dominance of hydrophobic forces in the interaction, respectively. It was evident from the comparison of observed and corrected fluorescence spectra that before correction there was a large red shift while after correction appearance of blue shift was occurred. The involvement of hydrophobic interaction was also found from the extrinsic fluorescence measurements using ANS dye as well as from the analyzed thermodynamic parameters. Safranal was found to partially induce the secondary structure of HSA as construed from the CD measurements. The size of the HSA was also decreased as evident from the DLS and RLS measurements. Both site marker studies and molecular docking simulations suggested that the primary binding site of the safranal in the HSA is Sudlow's site 1 located in the subdomain IIA. Hydrophobic interaction provides the major contribution to the binding forces along with a little amount of hydrogen bonding.

Keywords: Safranal; Human serum albumin; Fluorescence quenching; Molecular docking; Inner filter effect

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