Abstract

Investigation of the interactions of N-methyl-4-phenylpyridinium iodide (MPP⁺) derivatives and their 3-amino-2-phenylpropene (APP) combined compounds, 4-phenyl-1-(2-phenylallyl)pyridinium bromide (APP-MPP⁺) with cyclodextrin, bovine serum albumin (BSA), rats and several bacterial species (*Escherichia coli, Bacillus* species, *Staphylococcus aureus* and *Klebsiella* species) has been carried out under different conditions. The interaction of these compounds with BSA shows that there are conformational changes in the three dimensional structure of the protein. Spectroscopic analysis of complexes of BSA with derivatives of MPP⁺ and APP-MPP⁺ indicates that both ground state and excited state interactions are present. The effects of H⁺ ion concentration of the medium and the temperature were studied simultaneously in order to understand the mechanism of binding and the mode of interaction.

The binding modes, the binding constants and the changes that the protein structures undergo in the presence of those compounds in aqueous solutions at pH 5.50 and 7.45 have been evaluated using fluorescence and UV-Vis spectroscopy. The quenching constants k_{q} , k_{SV} and the association constant K were calculated according to the Stern-Volmer equation based on the quenching of the fluorescence of BSA. The analysis of fluorescence data indicates both dynamic and static quenching mechanisms are operating in binding. The thermodynamic parameters, the standard enthalpy changes (ΔH°) and the standard entropy changes (ΔS°) were estimated for each compound at each pH using the van't Hoff equation. The pH dependent experiments on binding of these quenchers with 4-hydroxyaryl moiety on BSA indicated that protonated structure has more affinity towards the BSA than it's deprotonated counterpart. The distance between the tryptophan residues in BSA and these quenchers were also estimated using Föster's method on the basis of fluorescence energy transfer. The interaction of APP-MPP⁺ compounds with rats showed that they have the potential to be developed as analgesic and sedative drugs. The studies continued with bacterial species demonstrated the use of these APP-MPP⁺ compounds as potential compounds to be used in the development of anti bacterial ointments.