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Acridone in a biological nanocavity: detailed spectroscopic and docking analyses of probing both the tryptophan residues of bovine serum albumin

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Spectroscopic and docking analyses reveal that acridone (AD) interacts with both the tryptophan (Trp) residues of bovine serum albumin (BSA) (both Trp 134 and Trp 212) in contrast to other organic ligands including other acridine derivatives which generally prefer to interact with Trp 212. The use of fluorescence spectroscopy, specifically the unusual time-resolved area normalized spectra depicting two isoemissive points with different times of evolution, confirms that AD "unusually" interacts with both the Trp residues present in the model protein. Upward curvature of the Stern Volmer plot suggests the interaction of AD with both the Trp residues present in varying microenvironments within BSA and possibly also indicates the denaturation of the protein. Ground state interaction of AD and BSA is explored using absorption spectroscopy, whereas strong perturbation in secondary and tertiary structures of the model protein on binding with the ligand is divulged from the observation of circular dichroism spectroscopy. Femtosecond fluorescence up-conversion kinetics implies that a photoinduced electron transfer reaction takes place from the Trp residue of the protein to AD, which has been authenticated using laser flash photolysis *via* identification of the radical ions. Binding as well as thermodynamic parameters associated with AD–BSA interaction are obtained from fluorescence studies. The prime deduction from the detailed spectroscopic and docking analyses is that AD initially interacts with Trp 212 present in the crevice of hydrophobic domain IIA of the protein and then perturbs the structure of BSA to bring about conformational changes such that it can gain access to Trp 134 housed in hydrophilic domain IB, which is possibly facilitated by hydrogen bonding.

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1. Introduction

The study of protein–ligand interactions finds immense applications in the study of biological processes like hormone action, enzyme–substrate recognition, signal transduction and cell communication.[1] In particular, the study of binding of drugs to transport proteins like serum albumins often attracts the interest of researchers as it yields information regarding modulation of drug solubility in plasma, their susceptibility to oxidation, toxicity and *in vivo* half-life.[2] Investigation of the behavior of probe molecules confined within nanocavities formed primarily within protein pockets is always interesting as the behaviors of these trapped molecules are drastically different from those free in solution. Furthermore, the binding ability of a drug to the serum albumins may significantly influence its distribution, free concentration and metabolism. Moreover, research on drugs which can be activated by photons is more appealing since light as an activating agent is more advantageous compared to other regulation methods, especially because irradiation can be easily controlled in space and time, thus confining drug activity to selected tissues with negligible side effects.[3] In this context, as photochemists our interest lies in whether photoinduced processes like energy transfer, excited state proton transfer, photoinduced electron transfer (PET) reactions *etc.* are taking place in systems which involve proteins and photoactivated drug molecules. Earlier we have resorted to a laser flash photolysis (LFP) technique to explore PET reactions in such protein–ligand systems *via* identification and characterization of radical/radical ion pairs which are formed as primary intermediates in such reactions.[4,5] Apart from optical spectroscopic tools like circular dichroism (CD), UV-vis absorption, FTIR, NMR *etc.*, fluorescence spectroscopy is mainly employed to gain information regarding the binding modes of drugs with proteins. The advantage of using fluorescence spectroscopy is that the early events of

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