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ISSN: 0743-7463 E-ISSN: 1520-5827

Subject area: Physics and Astronomy: Condensed Matter Physics | Chemistry: Spectroscopy | Materials Science: General Materials Science | Physics and Astronomy: Surfaces and Interfaces | View all

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Probing the Hydrogen Bond Involving Acridone Trapped in a Hydrophobic Biological Nanocavity: Integrated Spectroscopic and Docking Analyses

Brotati Chakraborty,* Chaitrali Sengupta, Uttam Pal, and Samita Basu

Cite This: *Langmuir* 2020, 36, 1241−1251 Read Online

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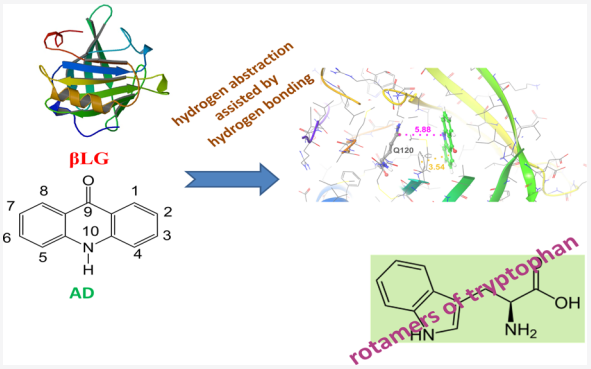
ABSTRACT: Spectroscopic analyses reveal that acridone (AD) penetrates through the structure and enters the hydrophobic cavity of the protein β-lactoglobulin (βLG). Although the protein contains two tryptophan (Trp) residues, AD interacts with only one (Trp-19), which is authenticated by the appearance of a single isoemissive point in TRANES. Alteration in the secondary structure of the protein while AD pierces through βLG is evident from the circular dichroism spectroscopic study. The ground-state interaction between AD and βLG is proven from the UV−vis spectroscopic study and the static nature of quenching of intrinsic fluorescence of the protein by the ligand. The steady-state fluorescence study in varied temperatures indicates the involvement of hydrogen bonding in the ligand−protein interaction. Further, the time-resolved fluorescence anisotropy study gives a hint of the presence of a hydrogen bond in AD−βLG interaction, which possibly involves the rotamers of Trp-19. In fact, the idea of involvement of rotamers of Trp-19 is obtained from the increase in fluorescence lifetime of βLG in the presence of AD. The docking study agrees to the involvement of hydrogen bonding in AD−βLG interaction. The direct evidence of hydrogen bonding between Trp and AD is obtained from the laser flash photolysis studies where the signature of formation of $ADH^{\bullet}$ and $Trp^{\bullet}$ through hydrogen abstraction between Trp and AD, loosely bound through hydrogen bonding, gets prominence. Thus, binding of AD to βLG involves hydrogen bonding in a hydrophobic pocket of the protein.



INTRODUCTION

β-Lactoglobulin (βLG) is a food-based biopolymer, which is the most abundant protein in the whey fraction of milk of cow, sheep, and other mammalians and responsible for transport of hydrophobic nutrients.[1−5] It is a small globular protein (molecular weight 18.3 kDa) containing 162 amino acid residues, folded into a calyx formed by eight antiparallel β-strands and an α-helix located at the outer surface of the β-barrel.[6] Several reports suggest that there are at least two hydrophobic binding sites in the βLG, one in the internal cavity and the other on the outer surface located between the β-barrel and the α-helix.[6] βLG serves as a model protein as its conformation, function, and physiological properties are well-defined. Further, it has two tryptophan (Trp) residues in varied microenvironments, viz. Trp-19 and Trp-61,[6] and thus, the intrinsic fluorescence of Trp may be utilized for the spectroscopic study of the protein.

Acridine derivatives are known to interact with DNA,[7−11] and some of them are recognized as prospective candidates of photosensitizers in photodynamic therapy.[12−14] Thus, study of interactions of such acridine derivatives with exogenous and endogenous drug-delivery vehicles is of pharmacological importance. Previously, we have reported the interactions of an acridine derivative, acridone (AD), as depicted in Figure 1, with two model with two model proteins, human serum albumin (HSA)[15] and bovine serum albumin (BSA).[16] HSA consists of a single Trp (Trp-214) residue, which is housed in a hydrophobic cavity, whereas, BSA contains two Trp residues (Trp-212 and Trp-134) between which Trp-212 resides in a hydrophobic pocket while Trp-134 is solvent exposed. We have observed that in case of AD−HSA interaction, AD directly interacts with Trp-214 while in case of AD−BSA

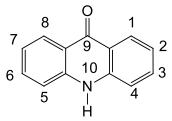


Figure 1. Chemical structure of AD.

Received: November 10, 2019
Revised: December 22, 2019
Published: January 17, 2020

https://dx.doi.org/10.1021/acs.langmuir.9b03506
Langmuir 2020, 36, 1241−1251

that the prime difference between the interaction of AD with serum albumins and βLG is that PET and FRET are the key phenomena involved in the interaction of AD with serum albumins, while hydrogen abstraction assisted by hydrogen bonding is prevalent in the case of interaction of AD with βLG. Both PET and hydrogen abstraction assisted by hydrogen bonding are confirmed using LFP technique. In fact, the manifestation of PET in AD−BSA and AD−HSA systems is exhibited by quenching of fluorescence lifetime of the serum albumins in the presence of AD. On the contrary, in the AD−βLG system, fluorescence lifetime of the protein is enhanced in the presence of AD, which gives an indication of the involvement of rotamers of Trp. The possibility of FRET is overruled in the AD−βLG system because of increase in fluorescence lifetime of Trp in the presence of AD. Moreover, in case of AD−BSA and AD−HSA systems, the mechanism of quenching of steady-state fluorescence of the proteins by AD is simultaneously static and dynamic, while in case of AD−βLG system, the nature of mechanism is exclusively static. The contribution of dynamic quenching accounts for the diffusion-controlled process in the system, may be related to PET for AD−BSA and AD−HSA systems, which is completely absent in the case of AD−βLG system. Finally, we feel that the extension of this work to study the interaction of AD with allied proteins/enzymes can possibly help in exploring and establishing its biological significance.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.langmuir.9b03506.

Available models of BLG in PDBe and PDB Redo databases and their quality, according to wwPDB validation report, plots of $\log(F_0 - F)/F$ versus $\log[Q]$ at 298, 303, and 308 K, and progressive quenching of intrinsic fluorescence of 10 μM βLG with rise in temperature (PDF)

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Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

Financial help from the Biomolecular Assembly, Recognition and Dynamics (BARD) project of Saha Institute of Nuclear Physics, Department of Atomic Energy, Government of India is greatly acknowledged. The authors are thankful to Dr. Soma Mondal, Saha Institute of Nuclear Physics, Kolkata, for her help.

■ REFERENCES

(1) Teng, Z.; Xu, R.; Wang, Q. Beta-lactoglobulin-based encapsulating systems as emerging bioavailability enhancers for nutraceuticals: a review. *RSC Adv.* **2015**, *5*, 35138−35154.

(2) Cho, Y.; Batt, C. A.; Sawyer, L. Probing the retinol-binding site of bovine beta-lactoglobulin. *J. Biol. Chem.* **1994**, *269*, 11102−11107.

(3) Kontopidis, G.; Holt, C.; Sawyer, L. The ligand-binding site of bovine β-lactoglobulin: evidence for a function? *J. Mol. Biol.* **2002**, *318*, 1043−1055.

(4) Narayan, M.; Berliner, L. J. Mapping fatty acid binding to β-lactoglobulin: ligand binding is restricted by modification of Cys 121. *Protein Sci.* **1998**, *7*, 150−157.

(5) Wang, Q.; Allen, J. C.; Swaisgood, H. E. Binding of vitamin D and cholesterol to β-lactoglobulin. *J. Dairy Sci.* **1997**, *80*, 1054−1059.

(6) Hasni, I.; Bourassa, P.; Tajmir-Riahi, H.-A. Binding of cationic lipids to milk β-lactoglobulin. *J. Phys. Chem. B* **2011**, *115*, 6683−6690.

(7) Armstrong, R. W.; Kurucsev, T.; Strauss, U. P. Interaction between acridine dyes and deoxyribonucleic acid. *J. Am. Chem. Soc.* **1970**, *92*, 3174−3181.

(8) Higashi, N.; Takahashi, M.; Niwa, M. Immobilization of DNA through intercalation at self-assembled monolayers on gold. *Langmuir* **1999**, *15*, 111−115.

(9) Read, M.; Harrison, R. J.; Romagnoli, B.; Tanious, F. A.; Gowan, S. H.; Reszka, A. P.; Wilson, W. D.; Kelland, L. R.; Neidle, S. Structure-based design of selective and potent G quadruplex-mediated telomerase inhibitors. *Proc. Natl. Acad. Sci. U. S. A.* **2001**, *98*, 4844−4849.

(10) Baruah, H.; Day, C. S.; Wright, M. W.; Bierbach, U. Metal−Intercalator-Mediated Self-Association and One-Dimensional Aggregation in the Structure of the Excised Major DNA Adduct of a Platinum− Acridine Agent. *J. Am. Chem. Soc.* **2004**, *126*, 4492−4493.

(11) Campbell, N. H.; Parkinson, G. N.; Reszka, A. P.; Neidle, S. Structural basis of DNA quadruplex recognition by an acridine drug. *J. Am. Chem. Soc.* **2008**, *130*, 6722−6724.

(12) Fritsch, C.; Goerz, G.; Ruzicka, T. Photodynamic therapy in dermatology. *Arch. Dermatol.* **1998**, *134*, 207−214.

(13) Varnell, E. D.; Kaufman, H. E. Photodynamic inactivation with proflavine: quantitative comparison with iodo-deoxyuridine. *Infect. Immun.* **1973**, *7*, 518−519.

(14) Satonaka, H.; Kusuzaki, K.; Matsubara, T.; Shintani, K.; Wakabayashi, T.; Nakamura, T.; Matsumine, A.; Uchida, A. Flash wave light strongly enhanced the cytocidal effect of photodynamic therapy with acridine orange on a mouse osteosarcoma cell line. *Anticancer Res.* **2007**, *27*, 3339.

(15) Chakraborty, B.; Mitra, P.; Basu, S. Spectroscopic exploration of drug-protein interaction: a study highlighting the dependence of the magnetic field effect on inter-radical separation distance formed during photoinduced electron transfer. *RSC Adv.* **2015**, *5*, 81533−81545.

(16) Chakraborty, B.; Sengupta, C.; Pal, U.; Basu, S. Acridone in a biological nanocavity: detailed spectroscopic and docking analyses of probing both the tryptophan residues of bovine serum albumin. *New J. Chem.* **2017**, *41*, 12520.

(17) Martins, P. A. T.; Gomes, F.; Vaz, W. L. C.; Moreno, M. J. Binding of phospholipids to β-Lactoglobulin and their transfer to lipid bilayers. *Biochim. Biophys. Acta* **2008**, *1778*, 1308−1315.

(18) Chakraborty, B.; Roy, A. S.; Dasgupta, S.; Basu, S. Magnetic field effect corroborated with docking study to explore photoinduced electron transfer in drug− protein interaction. *J. Phys. Chem. A* **2010**, *114*, 13313−13325.

(19) Koti, A. S. R.; Krishna, M. M. G.; Periasamy, N. Time-resolved area-normalized emission spectroscopy (TRANES): A novel method