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Influence of HSA on micellization of NLSS and BC: An experimental-theoretical approach of its binding characteristics $\stackrel{\text{theoretical}}{\to}$



Ishrat Fatma^a, Vivek Sharma^a, Nisar Ahmad Malik^b, Humira Assad^a, Plinio Cantero-López^{c,d,e}, Julio Sánchez^f, Roberto López-Rendón^{g,*}, Osvaldo Yañez^{h,i}, Ramesh Chand Thakur^{j,*}, Ashish Kumar^{k,*}

^a Department of Chemistry, Faculty of Technology and Sciences, Lovely Professional University, Phagwara, Punjab, India

^b Department of Chemistry, Islamic University of Science and Technology, Awantipora, J&K, India

^c Universidad Andres Bello, Facultad de Ciencias Exactas, Departamento de Ciencias Químicas, Viña del Mar, Chile

^d Center of Applied Nanoscience (CANS), Facultad de Ciencias Exactas, Universidad Andres Bello, Santiago, Chile

e Relativistic Molecular Physics Group (ReMoPh), PhD Program in Molecular Physical Chemistry, Facultad de Ciencias Exactas, Universidad Andres Bello, Santiago, Chile

^f Universidad de Santiago de Chile (USACH), Facultad de Química y Biología, Departamento de Ciencias del Ambiente, Santiago, Chile

^g Laboratorio de Bioingeniería Molecular a Multiescala, Facultad de Ciencias, Universidad Autónoma del Estado de México, Av. Instituto Literario 100, 50000 Toluca, México ^h Facultad de Ingeniería y Negocios, Universidad de las Américas, Santiago 7500000, Chile

ⁱ Center of New Drugs for Hypertension (CENDHY), Santiago 8380494, Chile

^j Department of Chemistry, Himachal Pradesh University, Summer Hill, Shimla, Himachal Pradesh 171005, India

^k NCE, Department of Science and Technology, Government of Bihar, India

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$A \hspace{0.1in} B \hspace{0.1in} S \hspace{0.1in} T \hspace{0.1in} R \hspace{0.1in} A \hspace{0.1in} C \hspace{0.1in} T$

Blood albumins play a very significant role in several biological operations and act as carriers for the transportation and circulation of various endogenous as well as exogenous materials. Experimental as well as computational studies have been carried out in understanding the major binding properties of the system. This investigation explains the interactions of Human serum albumin (HSA) with N-Lauroyl sarcosine sodium salt (NLSS) and benzethonium chloride (BC), which has been explored by means of conductometric, spectroscopic as well as computational studies. Phenomenon of micellization is hindered in several concentrations of protein (HSA) as well as by temperature. Binding ability of HSA with NLSS and BC has been obtained through UV-visible and fluorescence studies. Computational study revealed the presence of seven binding pockets in HSA, out of which the most stable binding pockets for NLSS and BC includes pocket1 and pocket2.

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1. Introduction

Interactions between surfactant and protein have been studied for years because of their extensive usage in pharmaceuticals, detergency, food and biological systems [1-3]. Studies on their interaction help us to recognize several types of interactions that include hydrophobic, electrostatic, van der Waals forces interaction, etc. [4]. These interactions serve as main forces for the association among various proteins and surfactant molecules in aqueous solutions [5,6]. It has been acknowledged from the previous studies that protein-surfactant interactions modify the molecular features of proteins by amending their binding capacities,

* Corresponding authors.

solubility and conformations [7,8]. Andersen et al. [9] explored the myoglobin-surfactant interaction, and suggested that enthalpy of interaction is exothermic and is indicator of the weak hydrophobic nature between myoglobin and SDS. Moreover, Hoque et al. [10] studied the interactions between SDS and BSA. The results demonstrated that three types of interactions exist between the protein and the surfactant molecules that includes hydrophobic, electrostatic as well as ion-dipole interactions. Additionally, Lal et al. [11] investigated the impact of BSA on cationic gemini surfactant via several techniques. The findings revealed that hydrogen bonding as well as van der Waals forces was mainly responsible for the spontaneous binding mechanism of the protein with the studied surfactant molecules. However, stabilization of proteins by surfactants occurs in two ways, firstly it inhibits the adsorption of proteins by controlling the interfacial properties and secondly it stops the coagulation of proteins by associating with them. In therapeutic preparations, the biotechnologists are inserting surfactants

 $^{\,^{*}}$ Dedicated to the memory of the recently deceased Professor Roberto López-Rendon.

E-mail addresses: drthakurchem@gmail.com (R. Chand Thakur), drashishchem-lpu@gmail.com (A. Kumar).