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Impact of the alkyl chain length on binding of imidazolium-based ionic liquids to bovine serum albumin

Mengyue Zhang [a], Ying Wang [a], Hongmei Zhang [a], Jian Cao [a], Zhenghao Fei [a,b], Yanqing Wang [a,b,*]

[a] Institute of Environmental Toxicology and Environmental Ecology, Yancheng Teachers University, Yancheng City, Jiangsu Province 224051, People's Republic of China
[b] Jiangsu Provincial Key Laboratory of Coastal Wetland Bioresources and Environmental Protection, Yancheng Teachers University, Yancheng City, Jiangsu Province 224051, People's Republic of China

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ABSTRACT

The effects of six imidazolium-based ionic liquids (ILs) with different alkyl chain length ([C_nMim]Cl, $n = 2, 4, 6, 8, 10, 12$) on the structure and functions of bovine serum albumin (BSA) were studied by multi-spectral methods and molecular docking. ILs with the longer alkyl chain length have the stronger binding interaction with BSA and the greater conformational damage to protein. The effects of ILs on the functional properties of BSA were further studied by the determination of non-enzyme esterase activity, β-fibrosis and other properties of BSA. The thermal stability of BSA was reduced, the rate of the formation of beta sheet structures of BSA was lowered, and the esterase-like activity of BSA were decreased with the increase of ILs concentration. Simultaneous molecular modeling technique revealed the favorable binding sites of ILs on protein. The hydrophobic force and polar interactions were the mainly binding forces of them. The calculated results are in a good agreement with the spectroscopic experiments. These studies on the impact of the alkyl chain length on binding of imidazolium-based ionic liquids to BSA are of great significance for understanding and developing the application of ionic liquid in life and physiological system.

1. Introduction

Ionic Liquids, ILs, are a kind of new materials with unique physical and chemical properties [1], such as low melting points, low or negligible vapor pressure, high thermal stability, and good catalytic properties [2,3]. Therefore, they have become increasingly attractive as green solvents for industrial applications [4]. At present, the application of ionic liquids in the field of biochemistry is also very broad, such as biocatalysis, biomass processing, drug delivery [5–7]. However, from an environmental viewpoint, the concomitant toxicological effects to various environments of them in the process of application should not be neglected if they are released into nature [8]. Accordingly, the negative environmental aspects of ILs should be characterized before their safe applications.

Numerous toxicity effects of ILs on the environment have been reported. There are some ionic liquids with low to high hazard potential for human being and the environment [9–14]. The toxicity of some ILs on *Vibrio fischeri* microorganism was found to be more toxic than toluene [15]. The toxicity of some imidazolium-based ionic liquids toward the Channel Catfish Ovary cell was chiefly related to the shape and hydrophobicity parameters of cations [16]. Some proteins have been highly denatured when exposed to ILs [17]. Incidentally, the distribution and metabolism of ILs in the body are correlated with their affinities toward serum albumin. The studies about ILs binding with albumin are of imperative and fundamental importance [18,19,20].

Bovine serum albumin (BSA) is selected as a model protein to study the interaction and its conformational damage induced by ILs because of their low cost, ready availability. BSA consisting of a single chain polypeptide chain of 583 amino acid residues is structurally similar to human serum albumin (HSA) [21]. It is indispensable in the transport and disposition of endogenous and exogenous ligands in vivo, and plays an important role in the life activities of organism [22–24].The interactions between ionic liquid and protein have been discussed in some articles [25–27], but the mechanism of action of globular protein and ionic liquid is still limited. In particular, there is a lack of research on the subsequent changes in protein structure and the ionic liquid tail chain length alters the different effects on protein conformation [28].

In this work, firstly, the intrinsic fluorescence quenching, UV–vis, and circular dichroism(CD) spectra have been used to study the effects of six imidazole-based ionic liquids ([C_nMim]Cl, $n = 2, 4, 6, 8, 10, 12$) with different tail length on the conformational changes of protein. CD signal changes of bilirubin-BSA system, 8-Anilino-1-naphthalenesulfonic acid

* Corresponding author at: Institute of Environmental Toxicology and Environmental Ecology, Yancheng Teachers University, Yancheng City, Jiangsu Province 224051, People's Republic of China.
E-mail address: wyqing76@126.com (Y. Wang).

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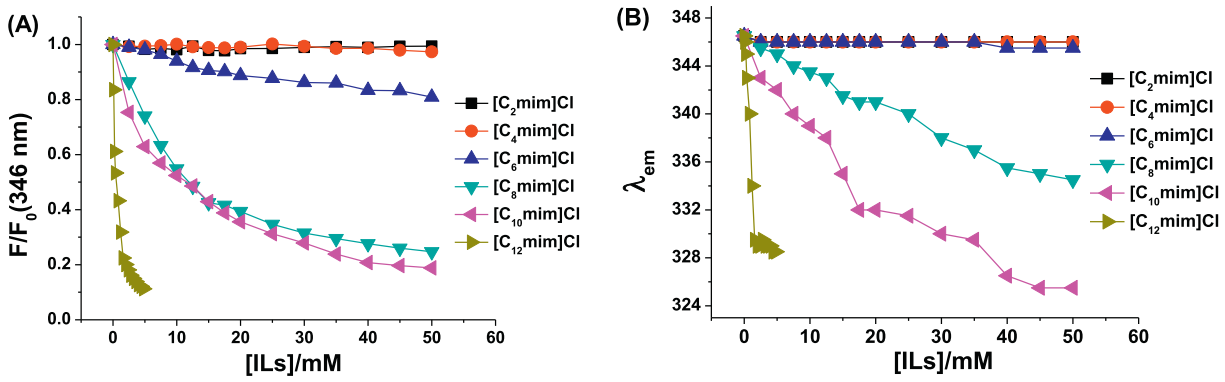

Fig. 1. The fluorescence quenching (A) and the maximum emission wavelength (B) of BSA in the presence of different concentration of ILs, c(BSA) = 5.0 μM, pH = 7.40, T = 298 K, λ_{ex} = 295 nm.

(ANS) fluorescence probe and molecular modeling techniques were used to analysis the binding site of ILs in BSA. In addition, the non-enzyme esterase activity and fibrillation of BSA in the presence of ILs were also studied. It is hoped that the information obtained from this paper on

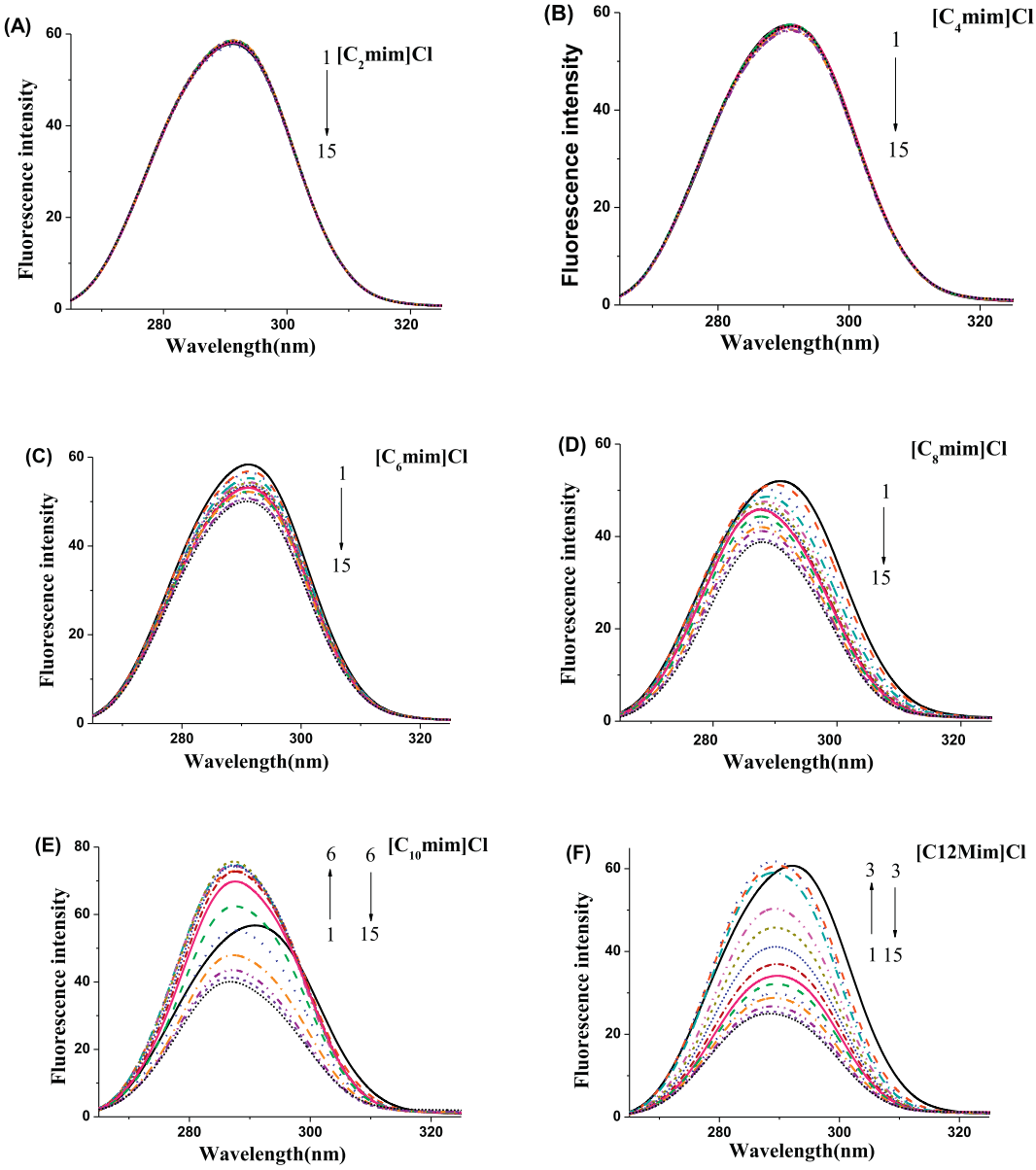

Fig. 2. Effects of ILs on the fluorescence intensity of BSA, Δλ = 15 nm, c(BSA) = 5 μM, pH = 7.40; T = 298 K;The concentration of ILs (A–E) (from 1 to 15): 0.0, 2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0, 50.0 mM; (F) (from 1 to 15): 0.0, 0.12, 0.24, 0.4, 0.8, 1.2, 1.6, 2.0, 2.4, 2.8, 3.2, 3.6, 4.0, 4.4, 4.8 mM.