Molecular dynamics study of gramicidin A in lipid bilayer: energetics of ion permeation

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The linear peptide gramicidin forms an ion channel specific for monovalent cation and has been extensively used to study the organization, dynamics and function of membrane-spanning channels. In these studies, the special emphasis has been given to the role and orientation of tryptophan residues in channel structure and function. [1] On the other hand, the membrane lipid environment is a strong modulator of membrane protein structure and function. A large portion of a membrane protein remains in contact with the membrane lipid environment. This raises the obvious possibility that the membrane is an important modulator of membrane protein structure and function. [2,3] Thus, the investigation of these properties of lipid/protein should be important to understand the function of membrane protein system. In our previous studies [4,5], we have studied the structure and lateral pressure properties of a gramicidin A in several lipid bilayers and have shown the effect of surrounding lipid bilayer on the channel structure of gramicidin A. In this study, we study the effects of lipid membrane on the energetics of ion permeation of the gramicidin A in lipid bilayer by molecular dynamics simulations. The electrostatic potential and the free energy profile of ion through the pore of gramicidin A are estimated in several membrane conditions, and the mechanism of ion permeation of the gramicidin A in lipid bilayer is discussed.

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