

Molecular dynamics study of gramicidin A in lipid bilayer: structure and energetics

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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, and recent spectroscopic approaches have highlighted the organization and dynamics of the channel in membrane. [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 should be an important modulator of membrane protein structure and function. It is becoming clear that subtle properties of the membrane environment such as membrane thickness and order, besides lipid composition, influence membrane protein function. [2,3] Thus, the understanding of these properties of lipid/protein in membrane should be a key subject to reveal the function of membrane protein system. In this study, we investigate the effects of lipid membrane on the structure and dynamics of the gramicidin A by molecular dynamics simulations. The changes of protein conformations by lipid-protein interactions, which are related to the function of ion channel in the membrane, are shown in detail. The channel structures and energetics of the gramicidin A are also investigated in several membrane conditions.

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