Thermal Stability of Gramicidin A in Lipid Bilayer: A Free Energy Analysis

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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 this study, we thus carry out a series of MD simulations of GA in several lipid bilayers and evaluate the thermal stability of GA in the membranes by free energy calculations. The changes of protein/lipid conformations and dynamics in these system are investigated in detail. The contributing factors to the thermal stativity of GA in the membranes such as the hydrophobic matching with surrounding lipids, electrostatic interactions, and solvation energy will be discussed.

References

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