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**Gramicidin Induce Local Non-Uniform Distribution of Lipids in Multi-Component Membrane Domains** YU MAO, FAZLE HUSSAIN, JUYANG HUANG, Texas Tech University — In lipid membranes, gramicidin form trans-membrane channels that are specific for monovalent cations. We performed Molecular Dynamics simulations of gramicidin in coexisting liquid-ordered (Lo) and liquid disordered (Ld) domains using GROMACS. The lipid compositions of Lo and Ld domains are DOPC/DSPC/Cholesterol = 6.5/52.6/40.9 and 74.4/10.6/15, respectively. In the Ld domain, the membrane thickness matches the hydrophobic length of gramicidin quite well, and water molecules can diffuse through the gramicidin channels. However, in the Lo lipid domain, the bilayer thickness is far greater than the hydrophobic length of gramicidin and majority of gramicidin do not form conducting channel. The simulation result explained our experimental finding that gramicidin partition favorably into the Ld domains. The calculated radial distribution functions of lipids indicate that gramicidin recruit a layer of short DOPC surrounding each protein and keep cholesterol and taller DSPC away from the protein-bilayer interface. Our result indicates that membrane proteins are capable of inducing non-uniform distributions of lipids and creating a local bilayer environment, which favors protein function.

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