Surface Tension Effect on Lipid Mobility and Transmembrane Channel Stability in a Model Membrane

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The effect of surface tension on the lipid bilayer membrane is a problem that has drawn considerable research effort. This interest has been driven both by the desire to determine the surface tension effects on the lipid bilayer, and from the observation that adding finite surface tension to a small membrane system may provide more realistic lipid properties in molecular dynamics simulations. Here,the effect of surface tension on a lipid bilayer membrane containing a 4-helix transmembrane alamethicin peptide bundle is investigated using molecular dynamics simulations. The lipid bilayer membrane contained 110 POPC lipid molecules and a peptide bundle of four alamethicin helices. Simulations of 10 ns were undertaken for two different ensembles, NPT and $NP_z\gamma T$ with a surface tension of 20 mPa/m per interface. The significance of differences between the tension-free and surface tension simulations was determined using non-parametric statistical analysis on replicate simulations with different initial conditions. The results suggest that when the membrane is under surface tension, the peptide helical structure is perturbed from that in the tension-free state, but the bundle conformational is more stable than in the tension-free state. The increased stability is apparently the result of better hydrophobic matching between the alamethicin bundle and the surface tension-thinned membrane. The lipid in the tension state is more mobile and the hydrocarbon tails have more freedom than those in the tension-free membrane, as determined from the mean square displacement and the deuterium order parameters. Additionally, surface tension counteracts the influence of the transmembrane helix bundle on nearby lipid order, making the lipid order parameter more uniform throughout the membrane in the tension-state.