P-1.166

Characterizing Synthetic Membrane Systems with Molecular Dynamics Simulations

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Nanodiscs and bicelles are popular model systems in the field of biophysics, and are considered native-like membrane mimics for membrane protein research. Although these mimetic systems provide an in vitro operating environment for proteins, it is uncertain how their biophysical properties correspond to the physiological conditions in which membrane proteins function in native tensionless bilayers and how these properties affect the conformational ensembles of the proteins. Using MD simulations, we study the biophysical properties of these membrane mimics and their effect on the membrane proteins that are embedded within. Our results indicate that even with simple lipid compositions, the biophysical properties of lipids in synthetic membranes that influence the conformational space of membrane proteins, differ significantly from the conditions in tensionless membranes. Based on a systematic deep learning based analysis of the simulation data, our results reveal that the conformational distribution of membrane proteins is highly dependent on their environment, giving rise to an intriguing picture of the complexity of membrane mimics that highlights both the good and the bad attributes of these synthetic membrane constructs.