Diversity in lipid-protein interactions from coarse-grained simulations

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Abstract

Cell membranes function as physical barriers for the cell and control the exchange of ions, peptides, and small molecules between the interior and the exterior of the cell. The main constituents of cell membranes are lipid molecules, whose hydrocarbon tails provide the barrier-like properties, and membrane proteins, which carry out specific functions. Complex lipid-protein interactions take place in the membrane, where proteins and lipids affect each other, strictly regulating a wide range of cellular tasks. Here, we use coarse grained (CG) molecular dynamics (MD) simulations to characterize the lipid environment of ten membrane proteins, which include examples of receptors, transporters, channels, and enzymes. To provide a realistic lipid environment, the proteins are embedded in a model plasma membrane, where more than 60 lipid species are represented, asymmetrically distributed between upper and lower leaflet (JACS, 2014, 136, 14554-59). The simulations show in detail how each protein modulates its local lipid environment in a unique way through local lipid composition, thickness, curvature, lipid dynamics and other properties.