Membrane shredding, poration, and fusion studied with molecular simulations

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Abstract

Biological systems need to actively shape, maintain and remodel cellular and organellar membranes to maintain homeostasis. Despite using advanced imaging methods, direct visualization of dynamic processes at biological membranes remains challenging. Molecular dynamics simulations provide us with a detailed view of how protein-bilayer interactions are translated into specific membrane shaping and remodeling functions. This talk will discuss how molecular modeling and simulations complement cryoEM and AFM experiments. Using large scale atomistic and coarse-grained simulations, we demonstrate (1) how the reticulon-homology domain of FAM134B assists selective ER-phagy by inducing and sensing membrane curvature, (2) how protein-lipid interactions of pneumolysin rings induce membrane-pore formation, (3) and how carbon nanotubes induce spontaneous vesicle fusion. Molecular simulations and modeling provide us with tools to study large-scale membrane-shaping processes and help us bridge the gap between theory and experiment.

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