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Quantitative Characterization of Protein-Lipid Interactions

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Understanding the delicate balance of forces governing protein-lipid interactions is central to understanding membrane structure and function. These membrane constituent interactions play an essential role in determining the structure and function of membrane proteins, and protein interactions in membranes, and thus form the basis for many vital processes, including transmembrane signaling, transport of ions and small molecules, energy transduction, and cell-cell recognition. In this talk, I will present our efforts toward quantitative characterization of protein-lipid interactions based on free energy simulations.