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Molecular Simulations of Sequence-Specific Association of Transmembrane Proteins in Lipid Bilayers MANOLIS DOXASTAKIS, ANUPAM PRAKASH, LORANT JANOSI, University of Houston — Association of membrane proteins is central in material and information flow across the cellular membranes. Amino-acid sequence and the membrane environment are two critical factors controlling association, however, quantitative knowledge on such contributions is limited. In this work, we study the dimerization of helices in lipid bilayers using extensive parallel Monte Carlo simulations with recently developed algorithms. The dimerization of Glycophorin A is examined employing a coarse-grain model that retains a level of amino-acid specificity, in three different phospholipid bilayers. Association is driven by a balance of protein-protein and lipid-induced interactions with the latter playing a major role at short separations. Following a different approach, the effect of amino-acid sequence is studied using the four transmembrane domains of the epidermal growth factor receptor family in identical lipid environments. Detailed characterization of dimer formation and estimates of the free energy of association reveal that these helices present significant affinity to self-associate with certain dimers forming non-specific interfaces.

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