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Potential of mean force of Glycophorin A alpha-helix dimerization LORANT JANOSI, MANOLIS DOXASTAKIS, University of Houston — Transmembrane proteins recognition and association plays a crucial role in their assembly and function. In spite of the extensive studies, these processes are only partially understood. We investigate the association of the model transmembrane alpha-helices by means of potential of mean force (PMF) calculations. The model system consists of a pair of alpha-helices of Glycophorin A, a system that experimentally exhibits dimerization in lipid membranes. Using established coarse-grained models, we developed a Monte Carlo methodology to overcome sampling limitations imposed by long characteristic times present in lipid membrane simulations. A combination of the Expanded Ensemble Density of States formalism and hybrid molecular dynamics allow for efficient and accurate calculations on the association of the helices. The methodology developed offers unique insight into the mechanism of dimerization and provides a means to evaluate the effect of lipid composition and temperature on the association of Glycophorin A.

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