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Abstract for an Invited Paper
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Computer Simulation of Membrane Permeation by Milestoning[1]

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Atomically detailed molecular dynamics trajectories in conjunction with Milestoning are used to analyze the different contributions of coarse variables to the permeation process of a small peptide (N-acetyl-L-tryptophanamide, NATA) through a 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC) membrane. Milestoning is a theory and algorithm that exploits the use of short trajectories between interfaces in phase space (milestones) to compute equilibrium and long time behavior. The permeation process takes hours, which makes it appropriate for a Milestoning study. Reasonable agreement between experiment and simulation is obtained. The peptide reverses its overall orientation as it permeates through the biological bilayer. The large change in orientation is investigated explicitly but is shown to impact the free energy landscape and permeation time only moderately.

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