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**Cell Penetration by Transportan** AMIR MOHSEN POURMOUSA ABKENAR, JIRASAK WONG-EKKABUT, MICHAEL PATRA, MIKKO KARTTUNEN, BIOLOGICAL AND SOFT MATTER GROUP-UNIVERSITY OF WESTERN ONTARIO TEAM — Translocation of peptides through cellular membranes is a fundamental problem in developing antimicrobial peptides and also in drug delivery. It is known from experiments that there are a number of very different classes of peptides, all known as cell-penetrating peptides, that are able to penetrate membranes and, for example, carry pharmacological compounds- thus a promising strategy for drug delivery. The common characteristics of these peptides is only their high charge density. It is not known, however, what are the physical mechanisms that facilitate the translocation. We have used large-scale Molecular Dynamics simulations to study the penetration of one of these peptides, namely Transportan, across Dipalmitoylphosphatidylcholine (DPPC) lipids. In particular, we have calculated the potential of mean force (PMF) by umbrella sampling. The energy profile has a deep minimum inside the the bilayer showing the tendency of peptide to go inside the bilayer. Our objective is to find the controlling mechanisms of translocation through a detailed analysis of peptide-lipid interactions and free energy analysis.

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