

Membrane Thickness and Charged Protein-Lipid Interactions

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Abstract

Charged amino acids are known to influence the functions of integral and peripheral membrane proteins, as well as cell disrupting peptides. Despite the fact that atomistic molecular dynamics studies have given light on the mechanics of charged protein group membrane binding and translocation, the impact of the full range of membrane Physio-chemical properties and topologies has yet to be addressed. In this research, we looked at how an Arginine (Arg) side chain analogue moved through saturated phosphatidylcholine (PC) bilayers with hydrocarbon tail lengths ranging from 10 to 18 carbons. The free energy profiles all exhibit sharp climbs as penetration into the hydrocarbon core increases, with predictable shifts between bilayers of various thickness, culminating in a barrier reduction from 26 kcal/mol for 18 carbons to 6 kcal/mol for 10 carbons.

Keywords: Proteins; Peptides; Atomistic; Membrane; Phosphatidylcholine; Lipids

Introduction

Biological membranes contain a range of proteins that play crucial roles, as well as protective shells that effectively prevent polar and charged molecules from permeating without being catalysed. This concept, which is based on the energetics of ion translocation through an oily membrane slab, has held sway for decades. According to new research, cell membranes aren't as impervious as previously imagined. Because charged protein groups such as Arginine (Arg) and Lysine (Lys) can affect protein structure and function, as well as the effects of a range of cell-perturbing peptides, it's vital to understand how charged protein groups interact with biological membranes at the molecular level.[1]

Bilayers of lipid molecules producing non-polar sheet-like regions are typically depicted as biological membranes. Due to the rigid slab model's large barriers, charged molecules (of several tens of kcal/mol) must dehydrate when passing over the membrane interface. This hypothesis has recently been challenged by the so-

called "paddle model" of voltage-gated ion channel activation, which predicted lipid-exposed movement of several charged Arg residues across the lipid membrane.[2] Cell biology tests using membrane protein synthesis's translocon machinery indicated low energy costs for inserting Arg during a transmembrane protein section, casting doubt on the theory. At a cost of only 4 kcal/mol, incorporating Arg on a host-barrel protein (OmpLA) in the midst of a 12-carbon Dilauroyl-PC (DLPC) membrane has recently been proposed. This apparent difference between theory and experiment has sparked a heated dispute about how to interpret these results, resulting in a slew of new study into the electromechanical behaviour of lipid membranes. In the lack of molecular-level descriptions of membrane charge transport mechanisms, the basic continuum concept of membranes remained stable for nearly half a century. All-atom molecular dynamics (MD) experiments, on the other hand, have revealed some unexpected (though predicted by A. Parsegian over 40 years ago) physico-chemical behaviour related to lipid bilayer deformability. The presence of charged molecules is now drawing water and lipid head groups towards the non-polar membrane core. The resulting free energy profile (or potential of mean force, PMF) for charge translocation differs significantly from earlier continuum models because the molecule never completely dehydrates but must pay the price of deforming the membrane. The lack of sensitivity of translocation energetics to the chemical identity of the charged molecule or protein group (Vorobyov et al., in preparation), the binding of a counter-ion of anionic lipid head group, and even the membrane's dipole potential are all serious implications of this unexpected result.[3]

Conclusion

The translocation of MguanH⁺, an Arg side chain analogue, over lipid membranes with varied hydrophobic thickness was investigated using atomistic simulations. According to our observations, MguanH⁺ generates equal membrane deformations in all bilayers by pulling water molecules and lipid head groups into their hydrocarbon cores. The solvation, H-bonding, and interaction energies of MguanH⁺ in both membranes are very equivalent, with the exception of a shift caused by the difference in bilayer hydrophobic thickness. When the data is plotted as a function of distance from the interface rather than the bilayer centre, the deformations and ion microenvironments in all bilayers are remarkably similar.

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