Charge effects on polymer translocation through lipid bilayers

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Abstract

We study the effect of charges on the translocation behaviour of linear, amphiphilic polymers across lipid bilayer membranes using Monte Carlo simulations of a generic coarse grained model [1]. Understanding the interactions of such molecules with cell membranes has great scientific value. Cationic and anionic antimicrobial peptides (AMPs) are known to be an essential part of the immune system of many organisms, where they help fighting bacterial pathogens and other infections [2]. Inspired by this, researchers have been working on creating artificial AMPs, or synthetic AMP mimicking polymers, in the search for novel antibiotics, or treatment against drug resistant cancer cells [3].
It is commonly believed that the net positive charge found in many AMPs is a major determinant of the selectivity for the action of these molecules against pathogens *vs.* host cells. Our simulations show that positive charges on amphiphilic polymers can indeed facilitate a selective translocation across net negatively charged bilayers. However, also negatively charged polymers can display enhanced translocation across such membranes, if the balance of hydrophobic and negatively charged residues is chosen well.

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