Molecular Dynamics Simulations of Interaction between Indolicidin and an Asymmetric Membrane

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Antimicrobial peptides (AMPs) are a component of the innate immune system. They are small proteins with broad spectrum antimicrobial activity against bacteria, viruses and fungi. As such, they must interact with pathogenic membranes, either through translocation or by disrupting their structural integrity [1]. To understand how this peptides permeabilize bacterial membrane, we performed coarse-grained simulation, using MARTINI force field. We studied the interaction between the 13-residue cationic peptide indolicidin, isolated from cytoplasmic granules of bovine neutrophils with different types of membranes. Indolicidin is an intensively studied antimicrobial peptide. This very efficient antimicrobial agent is the shortest natural AMPs and has a large proportion of tryptophan residues (39%) of any known protein. Furthermore, it exhibits activity against Gram-positive and Gram-negative bacteria, but it does not lyse the bacterial cells [2]. We investigated indolicidin interactions with both symmetric and asymmetric bilayers consisting of POPE and POPG lipids. In the former case, the peptide penetrate the membrane, but in the latter this process is faster and it induces reorganization of the bilayer, after forming a pore and crossing the membrane. We also examined the effect of indolicidin concentration on the morphology of the membrane.

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References

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