Interaction of Antimicrobial Peptides with Bacterial Membrane

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The antimicrobial peptides AMPs represent abundant and diverse group of molecules, which are evolved from many tissues and cells in the plant and animal kingdoms as protective reaction against infection organisms. They build a very strong first line of innate immunity [1]. Despite their enormous variety, most AMPs work directly against microbes, through a mechanism involving membrane disintegration or/and formation of pores, which allows easier passage of the ions and the basic nutrients. Molecular mechanisms, and the way of penetration through the membrane can be varied to various peptides, depending on the sequence of amino acids, the lipid composition of the membrane and the concentration of peptides, but for the beginning of their action, they must first be attracted to the bacterial surface. The objective of the present examination is namely the so called S-state, or an inactive state in which an AMP is oriented parallel before binding to the membrane. To this end we have conducted molecular dynamics studies. The conformational changes in the quaternary structure of one of the most popular antimicrobial peptides — magainin 2 (alpha-helical positively charged amphiphilic peptide) near to a charged lipid bilayer were examined. We have analyzed the behavior of peptides at their connection to the bilayers and their impact on the lateral organization of charged lipids. The system for MD simulation consists of a charged, equilibrated membrane (five uncharged POPE lipid molecules to three charged POPG lipid molecules) and eight copies of AMPs magainin 2 (located four on each side of bilayers), submerged in water.

References

[1] S. R. Dennison, J. Wallace, F. Harris and D. A. Phoenix, *Amphiphilic a-Helical Antimicrobial Peptides and Their Structure/Function Relationships*, Protein Pept.Lett. **12** 31–39, 2005.