

Lipid Composition and the Structure of Bacterial Outer Membranes

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Abstract: Bacterial resistance is a public health emergency, and in recent years there has been an increase in studies aimed at understanding the mechanisms of resistance. It is known that the outer membrane (OM) of Gram-negative bacteria plays a crucial role in the process of antibiotic resistance due to the presence of lipopolysaccharides (LPS).[1] The chemical composition of LPS units determines the structure and physical-chemical properties of the bacterial wall. In this work, we have investigated via atomistic computational simulations the role of lipid composition and spatial distribution on the structural properties of the Gram-negative bacterial membranes. We have performed molecular dynamics simulations of the Lipid-A moiety of the LPS and performed extensive structure characterization with the SuaVE code.[2] Lipid-A is the hydrophobic region of the LPS molecule responsible for the endotoxicity of the Gram-negative bacteria. We have simulated a total of six different bilayers by combining four distinct chemotypes. The systems exhibit different molecular packing and fluidity as shown by curvature analysis and area per lipids. Our preliminary results indicate that Lipid-A composition has an important role modulating the structural dynamics of the OM of Gram-negative bacteria.

Key-words: Gromos force-field, Number of acyl chains, Number of phosphorylation sites.

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References:

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