Electroporation of a Native-like *E. Coli* Membrane Model

Katarina Šestić, Matej Kožić and Branimir Bertoša

katarina6ic@gmail.com

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, HR-10000 Zagreb, Croatia

Electroporation refers to the application of short, high-voltage electrical pulses designed to temporarily increase cell membrane permeability. Exposure of the cell to an external electric field leads to a reversible destabilization of the lipid bilayer, enabling the controlled uptake of molecules such as drugs or DNA [1]. The fundamental mechanism of electropore formation can be considered identical in both lipid bilayers and simple alkane systems (e.g. octane) in terms of the sequence of events. The process is initiated by the formation of "water wires," followed by the subsequent expansion of the pores [2]. However, the diversity of lipid types, their chemical structures and charges result in distinct physical properties of membranes depending on their composition [3]. Research has shown that during the translocation of a DNA molecule through a pore, interactions occur between the DNA and the polar lipid headgroups, leading to the formation of DNA/membrane complexes [4]. Therefore, for MD simulations to faithfully reproduce *in vitro* experiments and capture all relevant interactions, it is essential to simulate structurally complex systems and move away from simplified models. In this study, a native-like *Escherichia coli* membrane model consisting of 14 lipid components (the *Avanti* model [3]) was implemented using the CHARMM36 force field. A transverse electric field was applied along the z-axis. Several DNA molecules were positioned near the membrane. Preliminary results reveal membrane curvature under the influence of the external electric field, the emergence of water wires, and the formation of a pore.

References:

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