Molecular Dynamics Study of Ion-Mediated DNA-Membrane Interactions

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Interaction of DNA and membranes are crucial for understanding basic cellular processes. Depending on the membrane content and properties of the DNA molecule, representative native-like systems for studying mentioned interactions can be constructed *in silico*. Novel *in silico* model of *Avanti* lipid membrane provides a platform for conducting realistic computational research. It consists of 14 different lipids and presents one of the most complex and most realistic *in silico* models of membranes [1]. *Avanti* membrane represents *Escherichia coli* polar lipids extract used *in vitro* and it was proved to maintain stable membrane properties across a physiologically relevant temperature range.

For this study, using *Avanti* membrane, a system of two lipid bilayers enclosing two DNA molecules of different sizes and structures was constructed. Linear double stranded DNA promotor region of 78 bp and a homohexameric assembly of 50 bp per subunit were generated in *silico*. The membrane patches were expanded four times their original size to reduce artefacts of boundary effects and the DNAs were oriented for the optimal fit between the opposing membrane surfaces. The system was solvated with TP3P water model molecules and neutralized with Na^+ and Cl^- ions reaching a concentration of 0.1 M. In this study, we examine the effect of temperature, pressure and ionic strength on the sandwich-like system. Temperature is raised to 320 K and subsequently to 500 K while pressure is raised to 10, 50 and 100 bar. In a neutralised system, ionic strength is increased by adding various cations, namely Ca^{2+}, Mg^{2+} and K^+. The properties of bilayer and DNA, DNA-bilayer distance and potential insertion of DNA molecules into the bilayer were studied.

References:

[1] K. Pluhackova, A. Horner, *BMC Biol.* **19** (2021) 1-22.