

Comparison of aerolysin modifications via molecular dynamics

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Comprehensive studies of nanopores are necessary for solving the problems facing humanity at the present time. There are protein sequencing techniques, however, there is always demand for cheaper faster methods when industry is involved. Nanopores act as natural biosensors in cells, so they can be used to analyze biomolecules of our choice [1]. Deoxyribonucleic acid (DNA) sequencing is already implemented on the industrial level. Protein sequencing, however, poses additional challenges [2]. Computer simulations of the protein translocation can help to understand the process of sequencing. However, straightforward simulation of the process is problematic due to its physical timespan. An approach to accelerate the simulations is suggested. Molecular-dynamical models of 4 aerolysin modifications are created in this work. Electrostatic maps for the systems are computed. They are used to compare the pores in terms of applicability to protein sequencing. This comparison also justifies the choice of a specific modification for the further analysis via steered dynamics and umbrella sampling.

[1] Deamer D, Akeson M and Branton D 2016 *Nat. Biotechnol.* **34** 518–524

[2] Alfaro J A, Bohländer P *et al* 2021 *Nat. Methods* **18** 604–617