COMPUTER SIMULATION OF A RECTIFYING ION CHANNEL

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EXTENDED ABSTRACT

Miedema et al. [1] modified the OmpF ion channel by point mutation and changed the amino acids lining the pore so that a p-n junction was formed inside the channel. They showed with electrophysiological experiments that this channel shows rectification; the current at positive voltage is much smaller than at negative voltage. The goal of this work is to build models for the rectifying ion channel and study them with computer simulation methods thus trying to reproduce the phenomenon and to explain the mechanism behind it. In modelling, we used two limiting approaches. In one approach, we used an all-atom model based on the known crystal structure of the OmpF porin and on well-established classical force fields and studied this model with the GROMACS molecular dynamics simulation package [2]. In this approach, we found selectivity, but we did not find rectification. Therefore, we also used a reduced model, in which we approached the problem from the other end; only the important degrees of freedom are built into this model. We model the ions and the charged protein side chains explicitly, while water, the rest of the protein, and the membrane is averaged into a dielectric background. We have studied this model with the Nernst-Planck transport equation coupled to the Local Equilibrium Monte Carlo method (NP+LEMC) [3]. In this model, we found clear rectification behavior.

REFERENCES

[1] H. Miedema, M. Vrouenraets, J. Wierenga, W. Meijberg, G. Robillard, B. Eisenberg, A biological porin engineered into a molecular, nanofluidic diode. Nano Letters 10/2007; 7(9):2886-91.
[2] D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A. E. Mark and H. J. C. Berendsen, GROMACS: Fast, Flexible and Free, J. Comp. Chem. 26 (2005) pp. 1701-1719
[3] D. Boda and D. Gillespie, Steady-State Electrodiffusion from the Nernst–Planck Equation Coupled to Local Equilibrium Monte Carlo Simulations, J. Chem. Theor. Comput. 8, 824 (2012)