Practical Information

All Fields are compulsory

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Diffusion of O_2 in cell membranes

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Around every cell and organelle in the human body, there is a membrane. Membranes consist of phospholipids which are composed of a hydrophilic head and two hydrophobic tails. In a bilayer membrane, the hydrophobic tails are facing each other (figure 1) [1].
In membranes, ordered domains can be found that are rich in cholesterol, sphingomyelin (a type of phospholipids) and saturated phospholipids. These nanoscale domains, called rafts, are surrounded by disordered domains. There are indications that rafts play a role in signal transduction and intracellular transport [2]. Oxygen must be transported through the cell membrane. It is important for the energy supply to the cell. Our research investigates whether rafts have an influence on the oxygen transport.
We studied oxygen diffusion in cell membranes using computational modeling. Three simple phospholipid bilayers were examined, each consisting of one specific type of phospholipid. The three studied phospholipids are phosphatidylcholines (PC) (figure 2), with the same hydrophilic head (phosphocholine bounded on the first hydroxyl group of glycerol), but they have different hydrophobic tails (fatty acids where each one is bounded on a hydroxyl group of glycerol). In dioleoyl-PC (DOPC) and dipalmitoyl-PC (DPPC), the hydrophobic tails are respectively two oleic acids and two palmitic acids. The third PC, palmitoyl-oleoyl-PC (POPC), contains a palmitic and an oleic acid. Oleic acid tails are unsaturated with a bent in the tail and are a model for disordered membranes. In contrast, palmitic acid tails are fully saturated and are a model for ordered membranes, such as the rafts.

Figure 1 Cell membrane

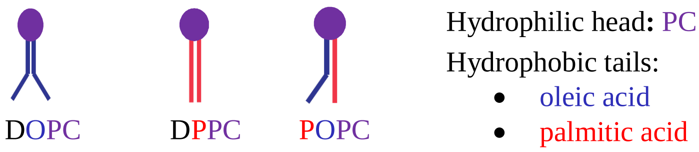

Figure 2 Representation of DOPC, DPPC and POPC

We investigated the influence on the oxygen diffusion of the different ordering patterns which are a consequence of the difference in saturation of the two acids.
Trajectories of the oxygen molecules in the cell membranes were created with molecular dynamics simulations with the software package CHARMM on the high performance computing infrastructure. A Monte Carlo analysis on these trajectories resulted in profiles of the free energy and of the position-dependent diffusion coefficient. We will discuss the effect of ordering and temperature on the oxygen diffusion profiles.

[1] Alberts, B.; Johnson, A.; Lewis, J.; Walter, P., Raff, M. and Roberts, K., Molecular Biology of the Cell (4th edition). Routledge, New York, 1616p (2002).
[2] Kupiainen, M.; Falck, E.; Ollila, S.; Niemelä, P.; Gurtovenko, A. A.; Patra, M.; Karttunen, M. and Vattulainen, I., J. Comput. Theor. Nanos. 2 (2005) 401-413.

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