Pores, channels and transporters: computational studies of membrane transport

Peter Tieleman, Department of Biological Sciences, University of Calgary, 2500 Unniveristy Drive NW, Calgary AB, T2N 1N4, Canada.

A key function of biological membranes is to provide mechanisms for controlled transport of ions, nutrients, metabolites, peptides and proteins between a cell and its environment. We are using computer simulations to study several processes involved in transport. In model membranes, the distribution of small molecules can now be accurately calculated; we are making progress toward understanding the factors that determine the partitioning behavior in the inhomogeneous lipid environment, with implications for, e.g.. the energetics of arginine-lipid interactions in voltage-gated potassium channels. Computer simulations of complex membrane proteins such as potassium channels and ABC-transporters can give detailed information about the atomistic dynamics that forms the basis of ion transport, selectivity, conformational change, and the molecular mechanism of ATP-driven transport. I will illustrate this with recent simulation studies of the voltage-gated potassium channel KvAP and the ABC-transporter BtuCD.