



Nano-Scale Property of Water and its Role in K-Ion Channel in Brain

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It is found in the recent experiments that the viscosity of water increases when the inner lining of nano-cavity is hydrophilic as well as hydrophobic. However, the viscosity increases dramatically in case of hydrophilic surface. In recent works [1,2] the present author along with his collaborators visualized this kind of situation within K-ion channel in brain. Ion channels are transmembrane proteins that include a pore-forming subunit that allows ions to flow between the extracellular and intracellular and interior of a cell. Ion channel pores present a narrow cross section of 100 Å and define a path of low dielectric constant across the membrane.

The ion channels play important role in understanding the information processing in the brain.

The channel pore presents a rather specific ion selectivity filter. The selectivity filter is about 12 Å long and hydrophilic lining with almost with no water molecules whereas the remainder of the pore is wider and has a hydrophobic lining, contains water molecules. Because of hydrophobic lining, the glue like viscous water molecules have mobility inside the basket region.

It is to be noted that the existence of glue-like viscous properties of water inside the pores are quite different from the water dynamics outside the channel.

The viscous properties of water in ion channel help us to understand the functioning of K-ion channel as discovered by McKinnon (who won Nobel prize for his works on structure and function of K-ion channel). Two types of modeling are usually done: Brownian Dynamics simulation and Molecular dynamic simulations. We used General Langevin equation in the framework of Brownian Dynamic simulation where Markovian approximation is supposed to be valid in the selectivity region and Non-Markovian approach is used in the basket region because of the dissipative character of glue like water molecules.

So, we have a system consists of two sub-systems – filter region where Markovian approximation is valid where as Non-Markovian approximation holds for the sub-system containing basket region. In this manner it is possible to understand the functioning of K-ion channel as found in the experiments. This result shed new light on the role of water in biological system.

Bibliography

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