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Simulations of water transport in membrane proteins

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Computer simulations are becoming an inevitable tool for describing the dynamics and function of biological macromolecules at various levels of resolution, in particular at the atomistic level. Among motions particularly important are those related to the transport processes. The complex topology of macromolecular channels and the transient nature of the penetrant passage pose difficulties in the modeling of the penetrant entry/escape pathways. We elucidate the basic physical factors influencing the water permeation in sodium glucose co-transporter SGLT1 including the channel opening as well as dynamic flexibility and its relationship with the domain motion.

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