MAR09-2008-001548

Abstract for an Invited Paper
for the MAR09 Meeting of
the American Physical Society

Modeling Ion Solvation and Transport through Chloride Transport Proteins[1]

THOMAS BECK, Univ. of Cincinnati

Ion channels and transporters are membrane proteins that selectively conduct ions either passively (channels) or actively using a chemical gradient of one ion (transporters). The H+/Cl- transporter, first discovered in bacteria, has now been shown to also occur in animals and plants. This talk will discuss computational approaches aimed at understanding the ion transit pathways through the bacterial chloride transporter. A Monte Carlo method (TransPath) that uses the crystal structure as input and exhaustively searches the protein for open pore spaces and favorable electrostatic domains has been developed. The algorithm successfully predicted pathways for the motion of chloride ions and protons. In order to better understanding the free energies along the predicted transport pathways, we have developed a new statistical mechanical approach for computing absolute solvation free energies in restricted environments based on a quasi-chemical approach. Anion free energy results employing the new method will be presented.

[1]Support: DoD/MURI, NSF