Water structure and proton conduction in protein channels

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In influenza virus A and B, the M2 protein serves as a proton-selective ion channel which can initiate viral replication under low pH conditions. This study investigates the shape of the pore passing through the ion channels of AM2 and BM2 proteins using HOLE.[1] A subroutine checks whether a spot is within the pore channel and water molecules are added to the pore at body temperature water density. Monte Carlo is used to find the equilibrium distribution of water in the channel as well as OO, OH, and HH radial distribution functions using a hard interaction between the pore surface and the water molecules and the Mahadevan and Garofalini (MG) diffused charge dissociative water potential between waters.[2] Hydrogen bonding is assessed to get a measure of pore proton conduction.

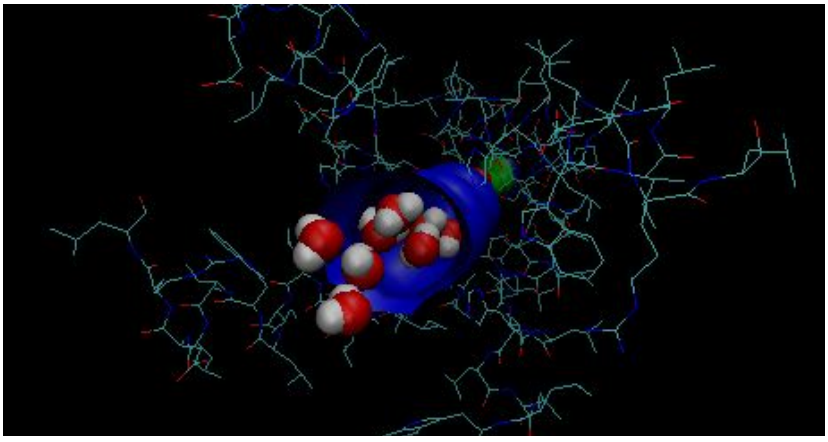

Figure 1: Water molecules inside the pore channel of AM2 protein

1. Smart, O.S., Goodfellow, J.M., Wallace, B.A. (1993). The pore dimensions of gramicidin A. Biophys. J., 65 : 2455-2460.
2. Mahadevan, T.S., and Garofalini, S. H. (2007). Dissociative water potential for molecular dynamics simulations. J. Phys. Chem., 111(30) : 8919–8927.