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Exploiting the Properties of Aquaporin to Calculate Free Energy

HUGO ESPEJEL, LIAO CHEN, University of Texas at San Antonio — Aquaporins' (AQPs) main purpose is to facilitate the transfer of water molecules through a molecular membrane. We can calculate the free energy of the AQP system when water permeates through it. This is performed using the Visual Molecular Dynamics (VMD) and the Nanoscale Molecular Dynamics (NAMD) programs. In our first set of experiments, AQP is submerged in a body of water, in which case a water molecule near AQP is pulled through the protein. The data is then used to calculate the free energy using two different equations: the Jarzynski equality and the fluctuation-dissipation theorem. The values from both equations are then compared to examine their accuracy. The second set of experiments has the same set up, but now AQP is embedded in a lipid bilayer. We found that both equations give values that are much smaller than kT. This verifies that AQP is a channel for water molecules because the pulling of water gives constant values of free energy. We also found that the water molecules' negative poles were all pointing towards the center of the AQP channel. This means that the process of proton transport in AQP is overwhelmingly difficult.

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