

Abstract Submitted  
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**Permeation of anions through the central pore of human aquaporin 5**<sup>1</sup> THIERRY WAMBO, LIAO CHEN, Department of Physics & Astronomy, University of Texas at San Antonio — Aquaporin 5 (AQP5) plays an essential role in the physiology of saliva, tears and pulmonary secretion. We performed in silico experiments of the L51R mutant of the human Aquaporin 5 (PDB code: 3D9S) for which in vitro experimental data became available recently. Molecular Dynamic Simulations performed on the AQP5 tetramer embedded in a lipid bilayer reveal that the central pore of the AQP5 mutant lost the hydrophobicity of the wild type protein and becomes permeable to anions, but not to cations. This conclusion is in agreement with the in vitro experiments of Qin and Baron, 2013. Quantitatively, we compute the potential of mean force (PMF) of chloride and iodine anions along the permeation path through the central pore. We correlate the PMFs with the experimentally measured conductance of various anions, elucidating the atomistic details of ion conduction through AQP5 mutant.

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