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Voltage-gated K Channels - Gating I

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A potassium Channel Voltage-Sensing Domain in a Non-Phospholipid Bilayer

Harindar S. Keer, **J. Alfredo Freites**, Stephen H. White, Douglas J. Tobias. Non-phospholipid, cationic 1,2-dioleoyl-3-trimethylammonium propane (DOTAP) lipid based membranes fail to support the function of a voltage-dependent K⁺ channel due to the lack of phosphate groups (Schmidt et al., Nature 444, 775, 2006). However, the specific effects of the presence or absence of phosphate groups in the channel membrane environment on the voltage-sensing mechanism remain unknown. To characterize the conformational dynamics and protein-lipid interactions in the absence of lipid phosphates, we performed all-atom simulations of the KvAP channel voltage-sensing domain (VSD) in a DOTAP bilayer in excess water. We generated prolonged trajectories for an up-state (Krepkiy et al., Nature 462, 473, 2009) and a down-state (Schow et al., Biophys J 98, 2857, 2010) conformation of the VSD, and contrasted the results with simulations of the VSD embedded in a POPC bilayer. Pair interaction energies reveal differences in the way each VSD conformation interacts with the different components of the membrane environment in the presence and absence of phosphate groups, which result in significant changes to the system electrostatics. This work is supported by NIH grants GM74637 and GM86685 and NSF grant CHE-0750175. This research was supported in part by NSF through Teragrid resources provided by the TACC at UT Austin.