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Presentation Abstract

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Abstract Title:	CONDUCTANCE AND CONCENTRATION RELATIONSHIP IN A REDUCED MODEL OF THE K CHANNEL

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Abstract Body: K^+ ions move rapidly through potassium channels more or less ignoring Na^+. The mechanism of selectivity is thought to depend on the solvation of K^+ and its electrostatic interactions with carbonyl dipoles of the channel wall, made of the side chains Thr Val Gly Tyr Gly TVGYG in many types of potassium channels. We calculate the conductance of the tetrameric KcsA prokaryotic K^+ channel measured in solutions of different K^+ concentration. The 3D model used here consists of two regions of different dielectric constant, one representing the protein and one representing a bath of implicit water. The geometry of the model is loosely based on the 'open' MthK crystal structure of Jiang's laboratory in which the intracellular half of the channel has a wide (~1.2 nm) pore radius. Ions are represented as hard spheres with Pauling radii. The surface charge on the protein is calculated using the induced charge computation method of Gillespie and collaborators. A Grand Canonical Monte Carlo approach developed by Boda maintains system neutrality while keeping bath concentrations fixed at values comparable to experiments. The Metropolis algorithm maintains a Boltzmann distribution to keep the system in thermodynamic equilibrium. The spatial density distribution of the ions allows an estimate of a characteristic slope conductance, for small driving force. Four

pairs of GLU71/ASP80 ionizable residues lie directly behind the K^+ selectivity filter and have a substantial effect on potential energy profile along the selectivity filter. The model will be used to investigate the relationship of the protonation state of the residues, the composition of the bathing solutions, and the slope conductance.

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