S2 segments) to the gating charge was then obtained by calculating the "electric" displacement of each amino acid side chain in the external field. The results show that the transmembrane electric field is focused inside the voltage sensor domains and that the gating charge arises mainly from the three positively charged residues located on the S4 segment.

989-Pos Board B868

Quantum Calculations on Potassium Channel Selectivity and Gating

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Selectivity: We have extended density functional (DFT) and Hartree Fock calculations **(1)** on sections of the KcsA K^+ channel selectivity filter. HF/3-21G calculations provided geometric optimization, starting from X-ray structures; single point DFT calculations (B3LYP/6-31+G**) were used for energy, charge, potential, and bonding, (techniques chosen to satisfy technical requirements). Calculations on K^+ and Na^+ at the middle and top of the ''cavity'' in the channel pore, and at the lowest (S4) position in the selectivity filter, show differences in solvation of the two ions: Na^+ depends on more water; K^+ in the S4 position has solvation mainly from threonine hydroxyls and backbone carbonyl oxygens. In the cavity Na^+ is asymmetrically placed, unlike K^+; as seen in geometry and electrostatic potential. Differences in weak covalent bonding to the ions seem responsible. Na^+ uses primarily 3s, K^+ the more extended 4s orbital, and small contributions from higher orbitals.

Gating: We also have an early-stage specific model of the voltage sensing domain of the $K_v1.2$ channel. A particular salt bridge switch, in response to proton movement initiated upon membrane depolarization, allows both S4 motion, and gating, as separate processes; gating appears similar to that in KcsA, not a response to S4 motion. As in KcsA, protons produce channel opening, and a ''nanocrystal'' composed of water plus the ion holds the channel closed until the protons place charge near one glutamine from each domain, separating them, destroying the nanocrystal, and allowing the channel to open **(2)**. Calculations are in progress on the model.

1) Kariev and Green (2008) J. Phys. Chem B, 112, 1293-1298.
2) Kariev, Znamenskiy, and Green (2007) BBA (Biomemb), 1768, 1218-1229.

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Using Molecular Simulation and Quantum Mechanics tools to answer unsolved questions about gating of plant voltage gated potassium channels

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Voltage gated potassium (Kv) channels are membrane proteins that allow voltage-driven potassium (K+) flux across cellular membranes. Kv channels in plants participate in multiple events, which include stomatal movements and ion uptake from the soil. Plant Kv channels show a similar topology as their counterpart in animals: four subunits with six transmembrane segments (S1-S6) each one; where S4 is the voltage sensor and S5-S6 constitute the pore.

Electrophysiology and structural bioinformatics tools have revealed partially the molecular mechanisms that regulate Kv channels gating in animals. To date, Kv channels in plants have been studied experimentally, but structural information about them does not exist.

We used Molecular Simulation and Quantum Mechanics methods to answer unsolved questions in plant Kv channels gating. Computational approaches helped to clarify the differences between KAT1 channel gating mediated by a membrane hyperpolarization and SKOR channel gating mediated by a membrane despolarization. We studied also the opening of KAT1 channel mediated by an apoplasm acidification of stomatal complex.

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Understanding gating transitions within K+ channels using Dynamic Importance Sampling

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Voltage-dependent potassium channels conduct potassium ions across the cell membrane by cycling between open and closed states. The transition between these well-defined states is driven by changes in the voltage drop across the bilayer. A growing dataset of K+ channel structures provides an opportunity to understand the molecular details of voltage-dependent gating. Determining the molecular details of gating is challenging because the x-ray structures are of either an open or closed state and of different sequence types. Thus, to gain an understanding of the molecular details of gating we are using dynamic importance sampling (DIMS) to create simulations of the transitions. Our starting point comes from the creation of a set of homology models for the full range of K+ channel sequences and structures that have been determined to date. Thus, we present simulations to suggest the transitions between open and closed states of four different sequences of K+ channels. The results suggest experimental alterations that influence gating and help to rationalize existing results. Furthermore the set of transitions suggests common modes to gating used in all K-channels.