Potassium ions in the cavity of a KcsA channel model

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Phys. Rev. E 2013

Ion channels are pore-forming proteins across the plasma membranes of cells that regulate the passage of ions, a crucial process in cell biology. Specifically, potassium ion channels represent an important class of ion channels that are responsible for the stabilization of the membrane potential. A most striking property of potassium channels is that they are able to achieve a high rate of ion flux at the order of 10-100 million ions per second while maintaining strong selectivity for potassium over sodium ions. To understand this key open question, we study the specific process of potassium ions entering the ion cavity using atomistic molecular dynamics (MD) simulation method complemented by arguments based on electrostatics. Our study reveals the important role of water molecules and the partially charged protein helices at the bottom of the cavity in overcoming the energy barrier and stabilizing the potassium ion in the cavity. The conclusions drawn from this study which are independent of specific atomic details of channels are applicable in generalized contexts, including the entry of ions in artificial ion channels and other confined geometries.

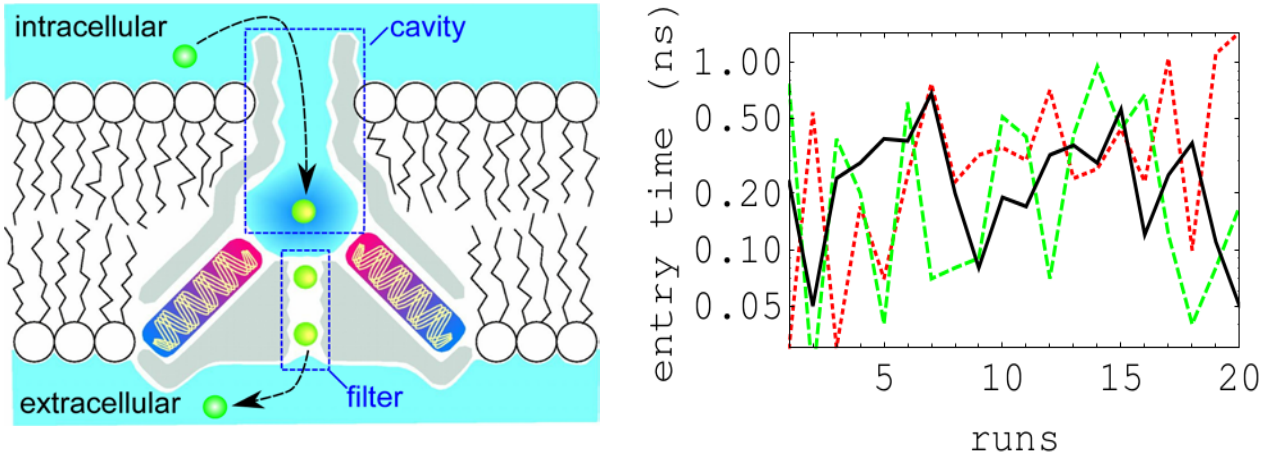

Figure *(left) Schematic plot of a KcsA channel in a cell membrane, as excerpted from Science 280, 69 (1998) with modifications. Reprinted with permission from AAAS. (right) The entry time for a potassium ion diffusing into the cavity at the electric field E = −80 mV/nm (dashed green), 0 (dotted red) and 80 mV/nm (solid black) for 20 independent simulations.*

Supported by the Office of the Secretary of Defense under the NSSEFF program award number FA9550-10-1-0167.