

Publication

A gate in the selectivity filter of potassium channels

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The selectivity filter of potassium channels is the structural element directly responsible for the selective and rapid conduction of K⁺, whereas other parts of the protein are thought to function as a molecular gate that either permits or blocks the passage of ions. However, whether the selectivity filter itself also possesses the ability to play the role of a gate is an unresolved question. Using free energy molecular dynamics simulations, it is shown that the reorientation of two peptide linkages in the selectivity filter of the KcsA K⁺ channel can lead to a stable nonconducting conformational state. Two microscopic factors influence the transition toward such a conformational state: the occupancy of one specific cation binding site in the selectivity filter (S2), and the strength of intersubunit interactions involving the GYG signature sequence. These results suggest that such conformational transitions occurring in the selectivity filter might be related to different K⁺ channel gating events, including C-type (slow) inactivation.

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