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Water Mediated Non-Selective Conduction of K+ and Na+ in NaK Channel

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Summary

The NaK channel from Bacillus cereus, with properties of Na+ and K+ permeability and Ca2+ blockage, is the first structure of cation channels without high selectivity to K+ ion. Here, we investigate the mechanism for non-selective ion conduction in NaK channel by systematical molecular dynamics simulations. It is shown that K+ ions prefer to bind within the sites formed by two adjacent planes of oxygen atoms from the selectivity filter, while Na+ ions are inclined to bind to a single plane of four oxygen atoms. Meanwhile, we find four small grottos connecting with the vestibule of the NaK selectivity filter, which form a vestibule-grotto complex perpendicular to the filter pore with a few water molecules within it. Analysis of the simulation results indicate that two or more of the water molecules coming to the vestibule to coordinate the cation are necessary for conducting both Na+ and K+ ions, while only one water molecule in the vestibule will obstruct ion permeation. The complex with the aid of interior water movement forms a dynamic hydration valve which is flexible in conveying different cations through the vestibule. The investigation of the NaK channel will provide us an essential understanding of the underlying mechanisms governing ion conduction and Ca2+ blockage of the CNG channels, due to their similarity in the selectivity filter sequence and ion permeation properties. Similar exquisite hydration valve mechanisms are expected to be utilized by other non-selective cation channels, and the results should shed new light on the importance of water in neural signaling.