

Title:

Poisson-Fermi Modeling of the Ion-Exchange Mechanism of the Sodium/Calcium Exchanger (NCX)

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Abstract:

The ion-exchange mechanism of the NCX crystallized by Liao et al. in 2012 is studied by using the Poisson-Fermi theory developed by Liu and Eisenberg in 2013. The theory considers the steric effect of ions and water molecules with different sizes and interstitial voids, the correlation effect of crowded ions with different valences, and the screening effect of polarized water molecules in an inhomogeneous aqueous electrolyte. We calculate the electrostatic and steric potentials of the four binding sites in NCX, i.e., three Na⁺ binding sites and one Ca²⁺ binding site, with protein charges provided by the software PDB2PQR. The energy profiles of Na⁺ and Ca²⁺ ions along their respective Na⁺ and Ca²⁺ pathways in experimental conditions enable us to explain the fundamental mechanism of NCX that extrudes intracellular Ca²⁺ across the cell membrane against its chemical gradient by using the downhill gradient of Na⁺. Atomic and numerical details of the binding sites are given to illustrate the ion-exchange mechanism.

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