Abstract Submitted
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Study of ion transport in sodium/proton antiporter proteins by molecular dynamics simulations DAVID DOTSON, Arizona State University, CHIARA LEE, Imperial College London, DAVID DREW, Stockholm University, ALEXANDER CAMERON, University of Warwick, OLIVER BECKSTEIN, Arizona State University — Na+/H+ antiporters serve a vital role in cell homeostasis. New crystallographic X-ray structures for two antiporters exhibit two different conformations: a cytoplasmic-open one (NhaA from Escherichia coli) and a periplasmic-open one (NapA from Thermus thermophilus). NhaA and NapA show low sequence identity but high structural similarity, including a set of highly conserved residues at the sites considered to be vital for transport. The way in which these transporters operate at the molecular scale remains largely undetermined, but using molecular dynamics computer simulations to study the interaction of Na+ ions with the transport proteins affords us new insights. We identify likely ion binding sites in the inward and outward facing conformations, noting that Na+ binding is dependent on the protonation state of a conserved aspartate residue. We also identify a conserved salt bridge that can be destabilized by Na+ binding. Taken together, the combination of structural and simulation data suggests a new model for ion binding and transport for this class of antiporter.

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