

Abstract Submitted
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Exploration of Structural Changes in Lactose Permease on Sugar Binding and Proton Transport through Atomistic Simulations¹ JIN LIU, YEAD JEWEL, PRASHANTA DUTTA, Washington State University, Pullman WA — *Escherichia coli* lactose permease (LacY) actively transports lactose and other galactosides across cell membranes through lactose/H⁺ symport process. Lactose/H⁺ symport is a highly complex process that involves large-scale protein conformational changes. The complete picture of lactose/H⁺ symport is largely unclear. In this work, we develop the force field for sugar molecules compatible with PACE, a hybrid and coarse-grained force field that couples the united-atom protein models with the coarse-grained MARTINI water/lipid. After validation, we implement the new force field to investigate the binding of a β -D-galactopyranosyl-1-thio- β -D-galactopyranoside (TDG) molecule to a wild-type LacY. Transitions from inward-facing to outward-facing conformations upon TDG binding and protonation of Glu269 have been achieved from microsecond simulations. Both the opening of the periplasmic side and closure of the cytoplasmic side of LacY are consistent with experiments. Our analysis suggest that the conformational changes of LacY are a cumulative consequence of inter-domain H-bonds breaking at the periplasmic side, inter-domain salt-bridge formation at the cytoplasmic side, as well as the TDG orientational changes during the transition.

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