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Coarse-grained Simulations of Sugar Transport and Conformational Changes of Lactose Permease[1] JIN LIU, S M YEAD JEWEL, PRASHANTA DUTTA, Washington State University — *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 sugar translocation, H^+ transfer, as well as large-scale protein conformational changes. The complete picture of lactose/H^+ symport is largely unclear due to the complexity and multiscale nature of the process. 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 transport of a β-D-galactopyranosyl-1-thio-β-D-galactopyranoside (TDG) molecule across a wild-type LacY during lactose/H^+ symport process. Results show that the local interactions between TDG and LacY at the binding pocket are consistent with the X-ray experiment. Protonation of Glu325 stabilizes the TDG and inward-facing conformation of LacY. Protonation of Glu269 induces a dramatic protein structural reorganization and causes the expulsion of TDG from LacY to both sides of the membrane. The structural changes occur primarily in the N-terminal domain of LacY.

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