

Supplementary Material

Superimposition of lactose onto TDG

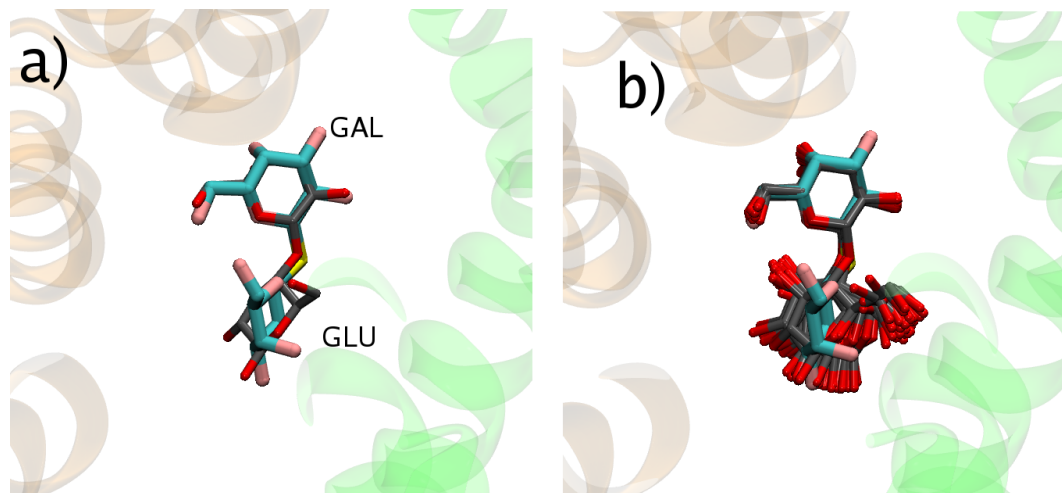


Figure S1: Superpositions of lactose onto TDG. Lactose is colored in red and gray; TDG is colored in pink, cyan and yellow. a) Initial position of lactose superimposed on the crystallographic position of TDG in the equilibration simulations of LacY (19). b) Snapshots of lactose from a reported simulation in (19) superimposed on top of the crystallographic position of TDG.

Movie Lactose steered across LacY from the cytoplasmic side (top) to the periplasmic side (bottom). The movie presents snapshots taken every 10 ps from simulation LacY(269^H/325⁻)_L. The galactosyl and glucosyl moieties of lactose are colored cyan/red and iceblue/red, respectively. Hydrogen atoms are omitted for clarity. The flexible helix segments at the periplasmic side of the N-domain, i.e., residues 28 – 37 (helix I), residues 89 – 100 (helix IV), residues 104 – 116 (helix III), kinked at Pro28, Pro89, and Gly111, respectively, are highlighted in purple. Possibly, these segments serve to facilitate passage of lactose across the tight periplasmic half-channel. The flexible, long loop connecting helices VI (N-domain) and VII (C-domain) at the cytoplasmic face is shown as a brown ribbon. Parts of helix I and VI of the N-domain have been omitted for clarity. Residues interacting with lactose during permeation appear temporarily in licorice representation with hydrogen atoms omitted for clarity.