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Supporting information for article:

Substrate binding in the bile acid transporter ASBTYf from *Yersinia frederiksenii*

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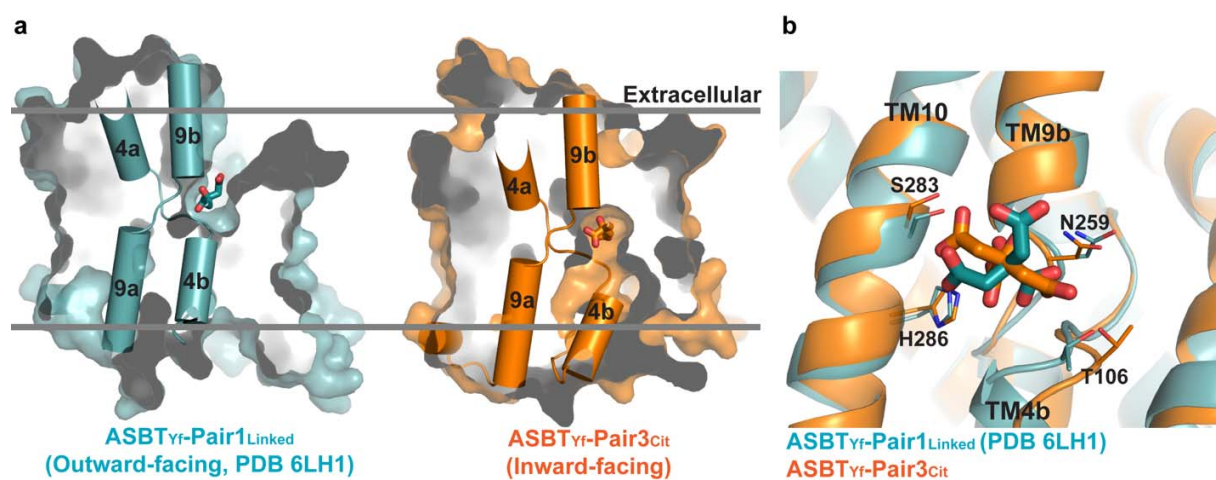


Figure S1 Binding of a citrate to the core domain of ASBT_{Yf} that fits an elevator-style alternating-access model. (a) Comparison of the outward-facing ASBT_{Yf}-Pair1_{Linked} (teal, left) and the inward-facing ASBT_{Yf}-Pair3_{Cit} (orange, right) structures in surface representation. TM4 and TM9 are displayed in cartoon, and the bound citrate is shown in stick mode. The relative position of cell membrane is indicated by two grey lines. (b) Superposition of ASBT_{Yf}-Pair1_{Linked} (teal) and ASBT_{Yf}-Pair3_{Cit} (orange) by aligning their core domains. The bound citrate molecules and interacting residues are shown in stick mode.

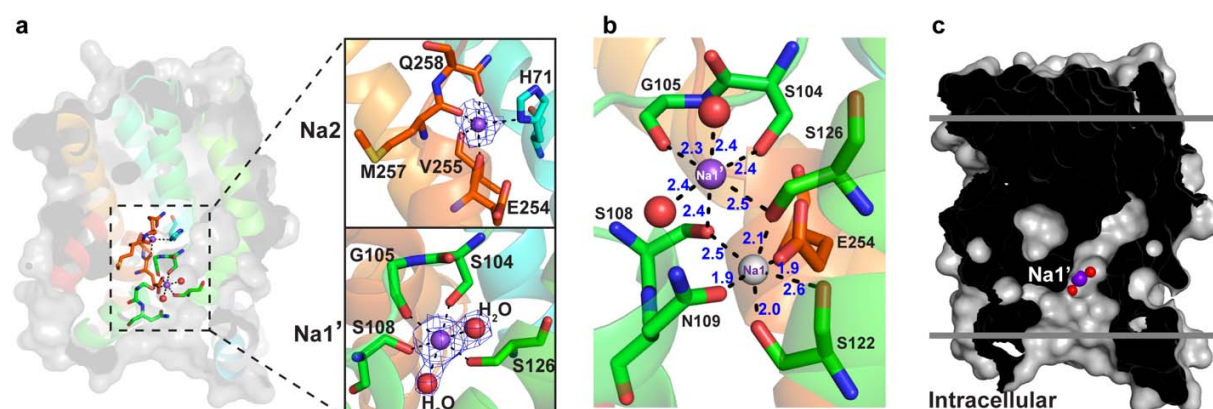


Figure S2 Binding of Na⁺ ions in the ASBT_{YF}-Pair3_{Gly} structure. (a) Coordination of two Na⁺ ions in the Na2 and Na1' sites. Na⁺ ions are displayed as purple spheres, and waters as red spheres. Coordinating residues are shown in stick mode. The distances from Na⁺ to its coordinating atoms are from 2.3 Å to 2.7 Å. The blue mesh shows the 2Fo-Fc map contoured at 1.5 σ level. (b) Coordination of Na⁺ in the Na1' site and the Na1 site. A pseudo-atom (grey sphere) is placed in the Na1 site. The distances from Na1' and Na1 to coordinating atoms are displayed in blue numbers. (c) Slab view of ASBT_{YF}-Pair3_{Gly} structure in surface representation showing the Na⁺ in the Na1' site in contact with intracellular solvent.