

Solute Sodium Symporters

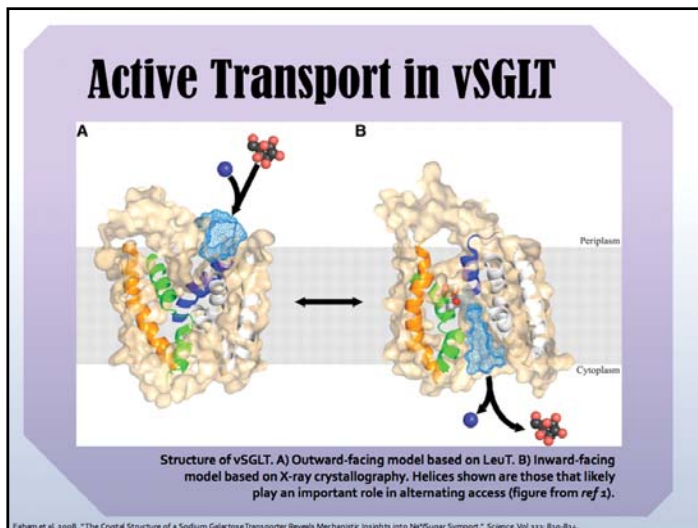
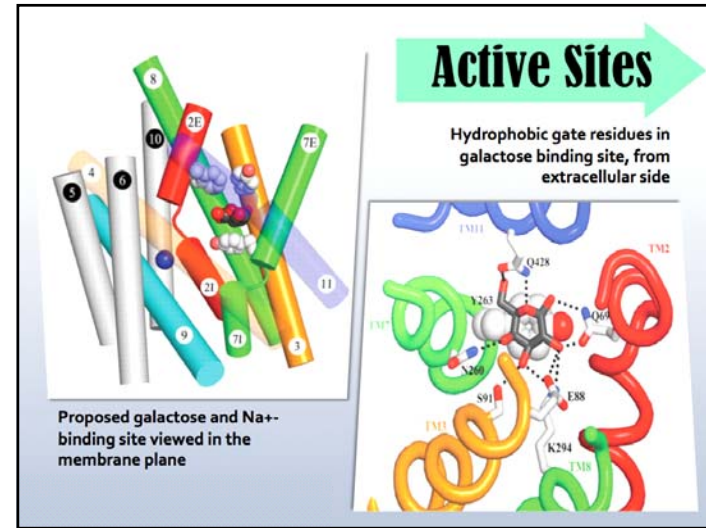
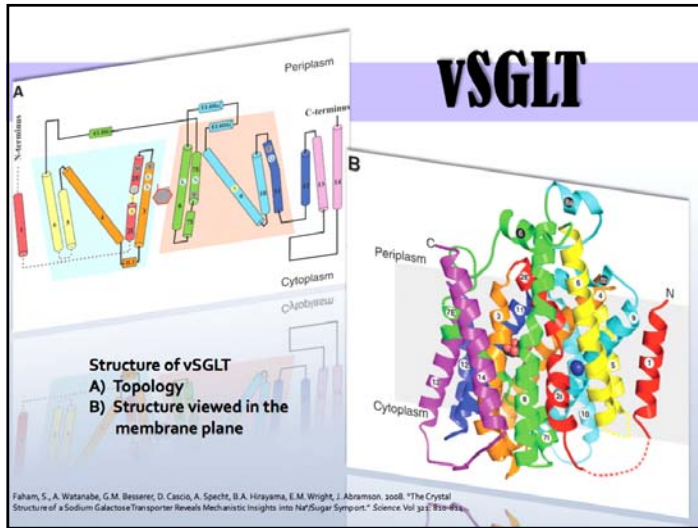
SSS

- Use electrochemical gradient of sodium
- Coupling ratio = number of sodium ions moved per substrate molecule
- Examples:
 - dopamine transporters (transmission of electrical signals)
 - sugar transporters (uptake of sugar required for diet of all mammals)
 - iodide transporters (uptake of iodide in thyroid, underexpressed in thyroid cancer patients)

SGLT

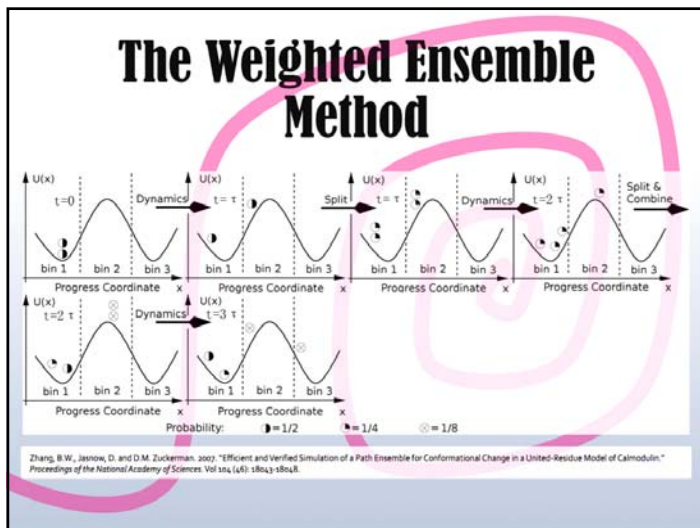
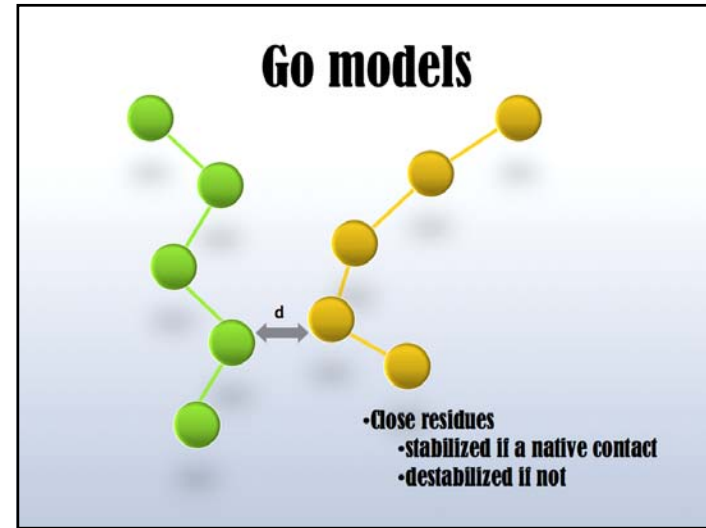
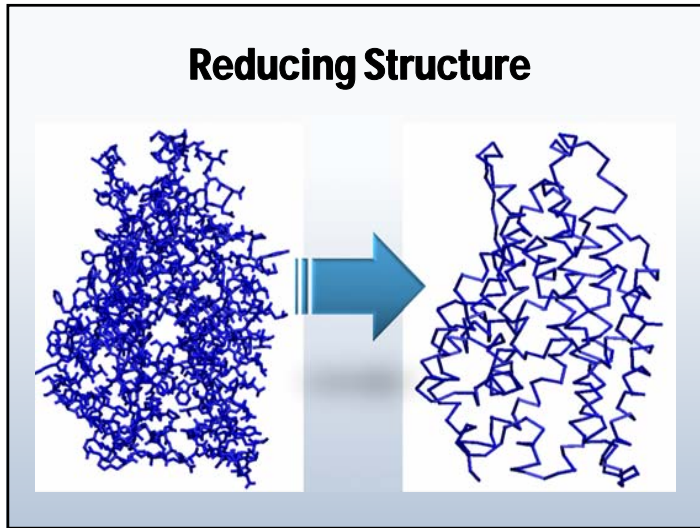
- Function**
 - Adsorption of carbohydrates in the gut
 - Readsorption of sugars in the kidneys
- Previous Research**
 - Cloned by Wright in 1987
 - Structure solved by Abramson and Wright in 2008
- Biomedical Significance**
 - Metabolism
 - Oral rehydration therapy
 - GGM/FGM
 - Possibly diabetes

Coupling ratio of human transporter SGLT: 1 sugar : 2 sodium
Coupling ratio of bacterial transporters: 1 sugar : 1 sodium



METHODOLOGY

Sampling Complex Reactions

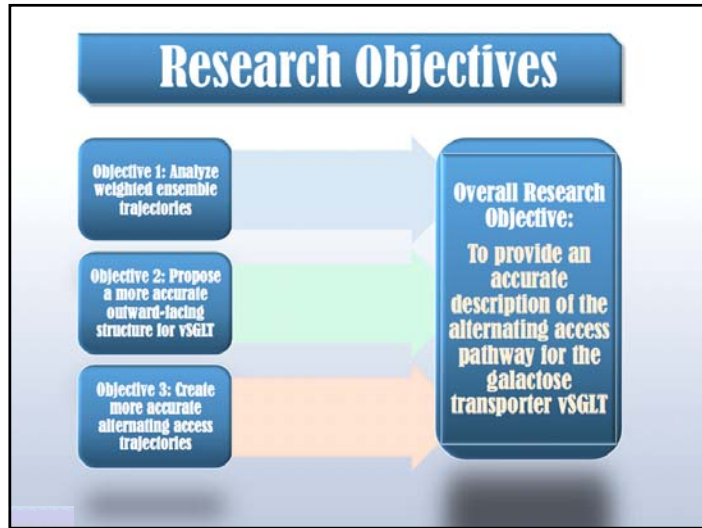


Homology modeling of the outward state

The screenshot shows a computer screen displaying sequence alignment results. The text on the screen includes:

- No outward-facing structure for vSGLT
- Model based on LeuT
- sequence alignment
- structural alignment

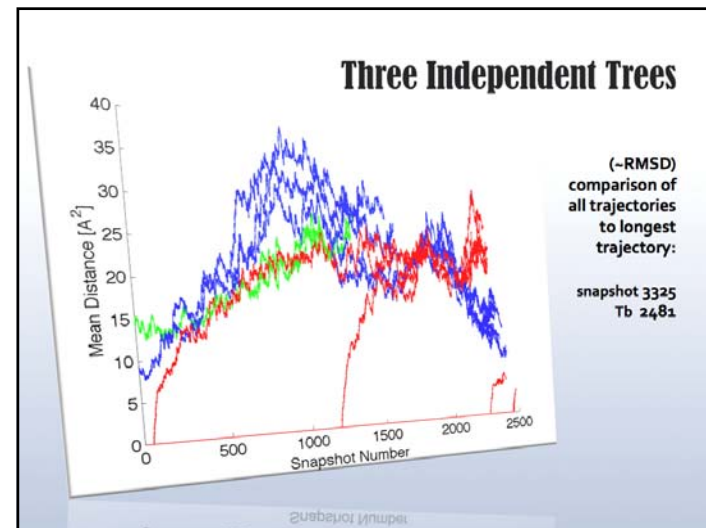
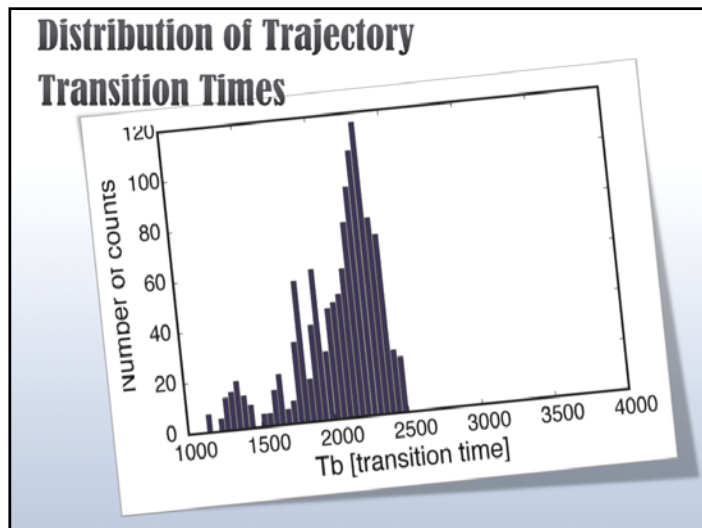
The screen also shows a table of sequence alignments for various proteins, including vSGLT and LeuT.

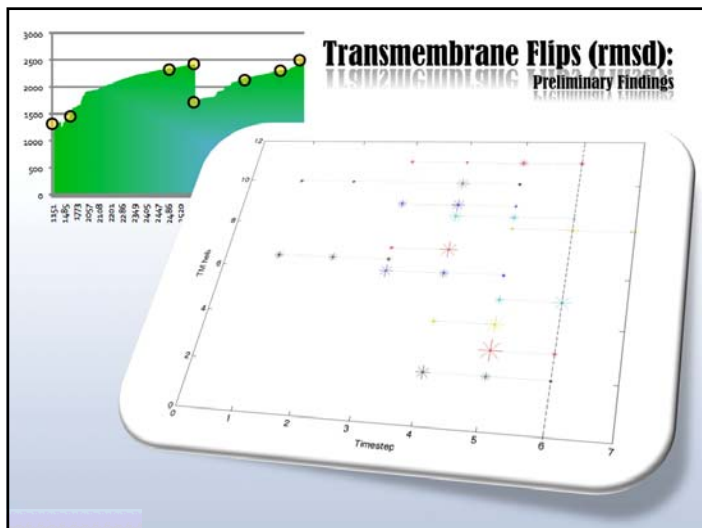
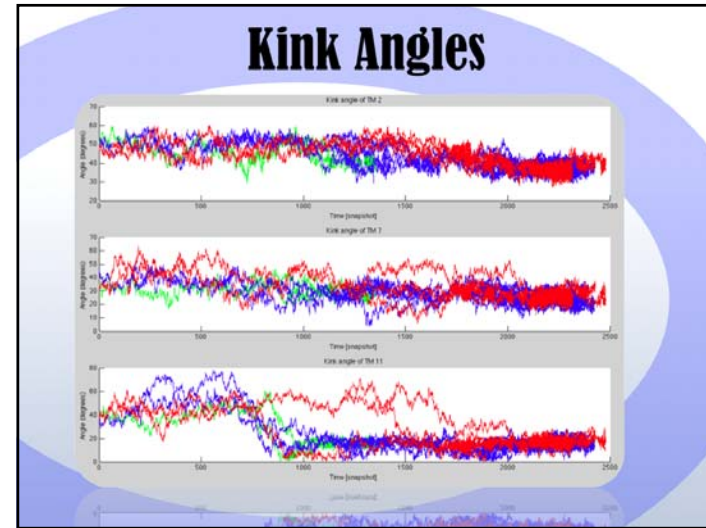
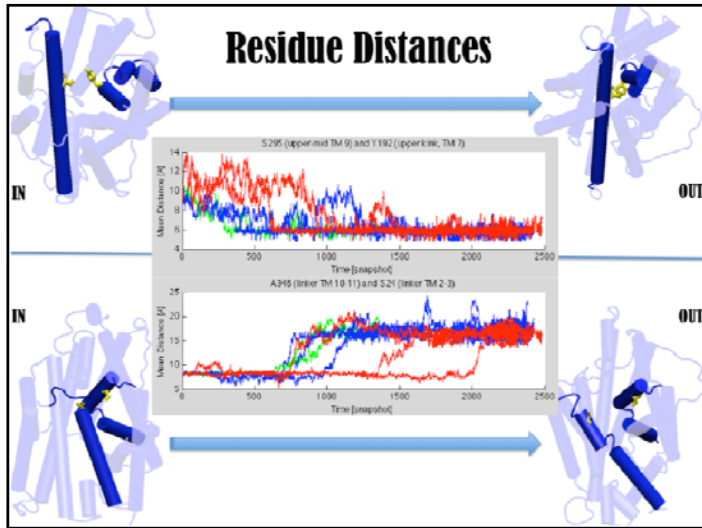


Results

Successful Trajectories


- ❖ 3 months on 8 cpus
- ❖ Generated 1154 trajectories





Future Research

- ❖ Improved code for kink angles
- ❖ Comparison of helix crossing angles
- ❖ RMSD calculations across all trajectories
- ❖ Consideration of hypotheses in literature (e.g., Forrest et al)
- ❖ Continuation of work on Mhp1 (NCS1)-based model



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