Thermodynamic Free Energy Calculations for the Difference in Sugar Binding of the Glucose/Galactose Binding Protein

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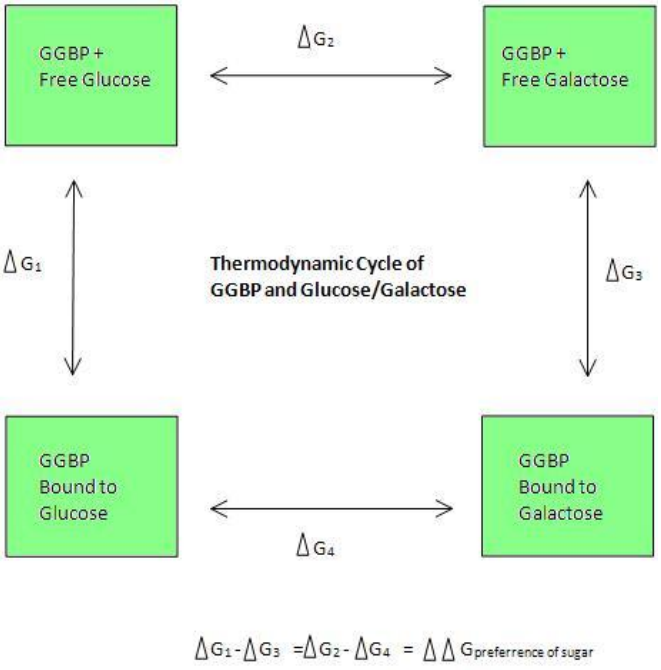
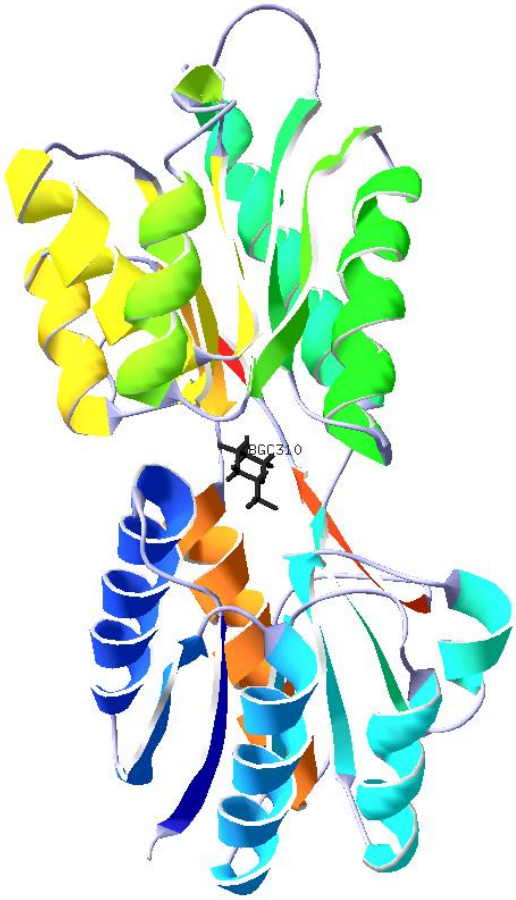
Glucose/galactose binding protein (GGBP) mediates chemotaxis in bacteria but also transports sugars, mainly glucose and galactose, through the membranes of cells. It binds around the sugar by using a "hinge feature" having two domains. *E. coli* is the main, known, bacteria that is associated with GGBP.

We were concerned with the free energy change for the binding of the protein to either glucose or galactose. We want to determine which sugar is more energetically favored in the binding process. We used molecular dynamic simulations in the 2 femtosecond time step, with a total simulation time on the order of nanoseconds, to convert glucose into galactose. Glucose does not naturally convert into galactose, but because it is mathematically possible to model this "alchemical" process, it became the easiest way to determine the difference in the free energy change between the bindings of the two sugars. Further molecular dynamic simulations will complete the thermodynamic cycle and tell us how much more one sugar was preferred over the other. GROMACS was used to carry out all of our simulations over the binding and folding process with regards to the sugars. Our research was based on the closed conformation of GGBP.





The closed form of GGBP with beta-glucose, BGC, bound to the center of the active site.