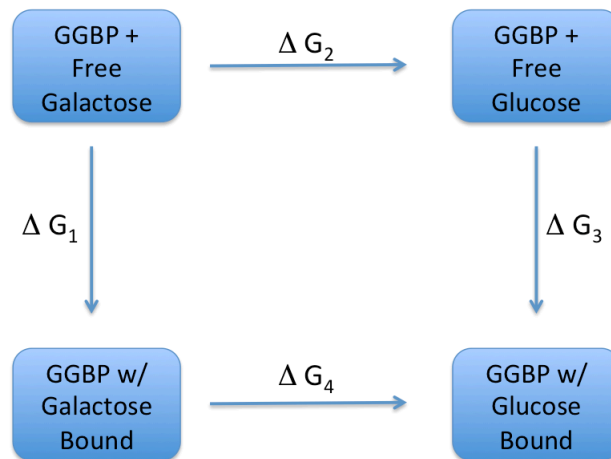


Reducing the Uncertainties of Calculated Free Energy Changes of Glucose/Galactose Binding Protein Binding to Glucose and Galactose

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The glucose/galactose binding protein (GGBP) found in the periplasmic space of *E. coli* is involved in chemotaxis and the active transport of sugars. Due to the different structures of the sugars, the degree of molecular complementarity upon binding will vary giving distinct binding affinities to each sugar. We wish to identify which sugar has the greater binding strength, specifically between glucose and galactose. The sugar with the greater binding affinity will be the most energetically favorable in the binding process, and relative affinities can be determined by comparing the Gibb's free energy changes for binding. The thermodynamic cycle shown below has been used to determine which sugar binds with greater affinity but preliminary results have yielded uncertainties that are too large for determining which sugar is preferred. Originally, we had sampled lambda (λ), our control variable for the free energy simulations, at intervals of 0.1 (e.g. $\lambda= 0.1, 0.2, \dots 0.9, 1.0$) and now we are more finely sampling by adding in runs to subdivide the intervals (e.g. $\lambda= 0.15, 0.25, 0.35, \text{etc.}$). This is being done with the molecular dynamics program GROMACS.



Thermodynamic cycle of sugar binding.