

Evaluating the Relative Binding Affinity of Galactose to Glucose for the Glucose/Galactose Binding Protein

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The glucose/galactose binding protein (GGBP) is found in enteric bacteria such as *E. coli* and is involved in chemotaxis and active transport. Presumably, the fact that glucose and galactose have different shapes causes them to bind with different strengths to the protein. By comparing the association constants for the reactions of the sugars binding to GGBP, the sugar with the higher binding affinity can be determined. One way to determine the association constants for the binding reactions is to find the changes in Gibb's free energy and use the equation $K_{assn.} = e^{-\Delta G/RT}$. The thermodynamic cycle shown below can be used to determine which sugar binds stronger because both $\Delta G_1 - \Delta G_4$ and $\Delta G_2 - \Delta G_3$ equal the difference in association constants, therefore giving the relative binding affinity. In this part of the project, the value of ΔG_2 was determined by performing molecular dynamics simulations of the conversion of free galactose to free glucose in a box of water and using a modified force field in accordance with the free energy perturbation method. The molecular dynamics program used was GROMACS. An error analysis was performed and the results were compared to the results of the reverse reaction to test the overall accuracy and precision of the simulations. The preliminary value for ΔG_2 is -0.7 ± 2.8 kJ/mol.

