

Utilizing computational resources to calculate the free energies associated with binding allose and glucose to the glucose/galactose binding protein

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The glucose/galactose binding protein (GGBP) plays a vital role in the transportation of the sugars galactose and glucose in addition to acting as a mediator of bacterial chemotaxis. The primary concern of this research was to discover GGBP's binding tendencies for sugars less common in nature. For this we used the molecular dynamics package known as GROMACS to simulate the interactions governing our systems and to also calculate the free energy associated with the binding and conversion processes. Initial results show that while GGBP will bind to allose (all), it is energetically less preferable than binding with glucose as shown by the ΔG (Couple allose + GGBP) and ΔG (Couple glucose + GGBP) values seen in figure 1. For clarification purposes, the (null) condition refers to a "dummy" molecule in which the van der Waal and charge interactions have been turned off. The simulations also suggest that the hydration of allose is less favorable than glucose, ΔG (all \rightarrow glu) in figure 1.

Figure 1: The thermodynamic cycle for the conversion of allose to glucose with GGBP

