Free Energy Changes for Glucose binding to the Glucose/Galactose Binding Protein using Molecular Dynamics Simulations

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Abstract

Glucose/galactose binding protein (GGBP) meditates chemotaxis and is involved in active transport of sugars, mainly glucose and galactose, in a number of bacterial species. GGBP binds the sugar with hydrogen bonds in a site that is located between two domains of the protein. This research focuses on the change in free energy for glucose binding to GGBP by performing molecular dynamics simulations (GROMACS 4.6.1) using the umbrella sampling method. The reaction coordinate is along a line connecting the glucose to the GGBP binding site with a maximum separation of 5 nm. A series of 26 configurations with 0.2 nm intervals are selected from a pull trajectory. These starting configurations were run in independent umbrella simulation. The change in free energy was then calculated by using the Weighted Histogram Analysis Method (WHAM) to extract the Potential of Mean Force (PMF) and calculate $\Delta G_{binding}$.

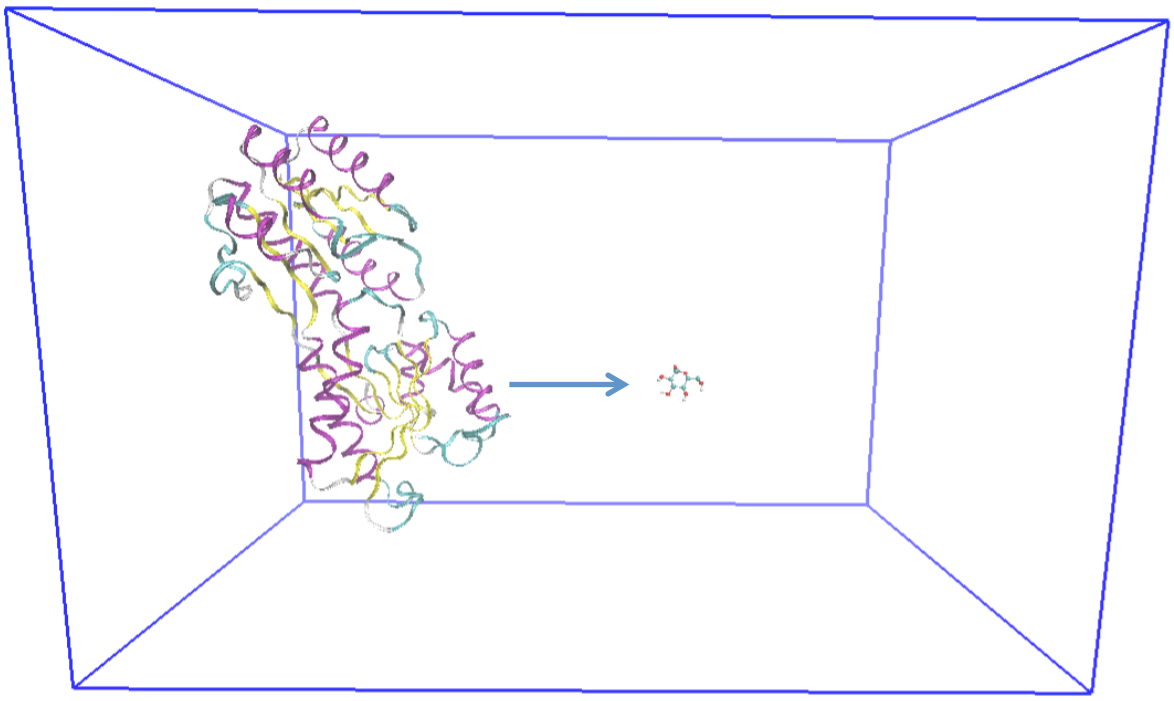

Figure 1: Reaction coordinate of glucose pulling away from GGBP