Conformational Changes for Glucose Binding to the D-galactose/D-glucose-Binding Protein using Molecular Dynamics Simulations

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Abstract:

D-galactose/D-glucose-binding protein (GGBP) works as an intermediate transport protein for glucose and galactose in bacteria, and participates in chemotaxis. As a periplasmic binding protein, it has two conformations: open without ligand and closed with ligand bound. The crystal structures for both the open and closed conformation of GGBP have been solved. Using the center-of-mass pulling algorithm found in the molecular dynamics simulation package GROMACS, the protein is pulled open. The hinge angle and the dihedral twist angle are monitored during the simulations as a way of following the conformational change. We are attempting to separate the sugar-protein interactions from the protein conformational changes to more fully understand the binding process. The free energy difference for the conformational change is determined by using umbrella sampling and the Weighted Histogram Analysis Method (WHAM) in GROMACS.

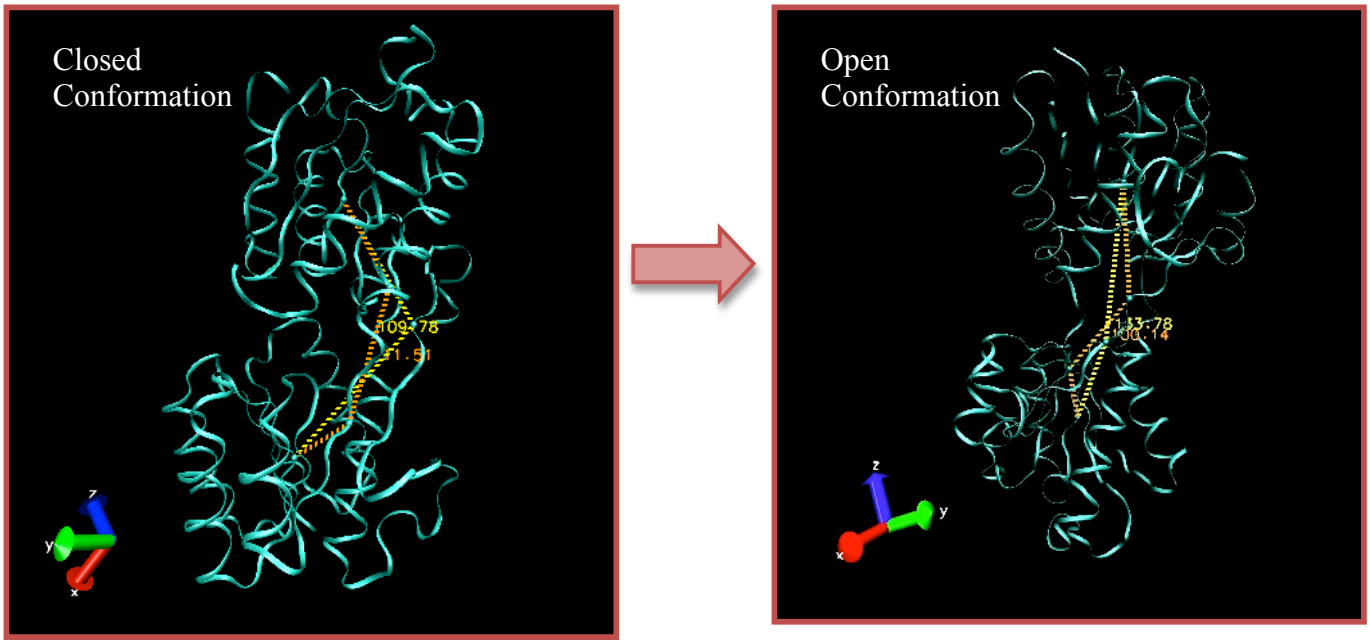

Figure 1. GGBP changes from closed conformation to open conformation (yellow: hinge angle; orange: dihedral twist angle)