

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ligand-Modulated Free Energy Landscapes of Glucose/Galactose Binding Protein¹ TROY MESSINA, Centenary College of Louisiana — Glucose/galactose binding protein (GBP) functions as part of a larger system of proteins for molecular recognition and signaling in enteric bacteria. Here we report on the thermodynamics of conformational equilibrium distributions of GBP from both time-resolved fluorescence experiments and computational umbrella sampling molecular dynamics analyzed by the weighted histogram analysis method (WHAM). Three conformations appear at zero glucose concentration and systematically transition to three conformations at high glucose concentration. Fluorescence anisotropy correlations, fluorescent lifetimes, thermodynamics, computational structure minimization and molecular dynamics, and previous work were used to identify the three components as open, closed, and twisted conformations of the protein. The existence of three states at all glucose concentrations indicates that the protein continuously fluctuates about its conformational state space via thermodynamically driven state transitions, and the glucose biases the populations by reorganizing the free energy profile. These results and their implications are discussed in terms specific and non-specific interactions GBP has with cytoplasmic membrane proteins.

¹NIH NRSA Ruth L. Kirschstein Post-Doctoral Fellowship and the Mattie Allen Broyle's Inaugural Year Research Chair

Troy Messina
Centenary College of Louisiana

Date submitted: 29 Nov 2007

Electronic form version 1.4