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Shallow Free Energy Landscapes Remodelled by Ligand Binding[1]

TROY MESSINA, DAVID TALAGA, EMILIO GALLICHIO, RONALD LEVY, Rutgers University, Department of Chemistry and Chemical Biology — Glucose/galactose binding protein (GGBP) functions as part of a larger system of proteins for molecular recognition and signalling in enteric bacteria. Here we report on the thermodynamics of conformational equilibrium distributions of GGBP 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 GGBP has with cytoplasmic membrane proteins.

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