

REPLICA-EXCHANGE SIMULATIONS OF THE PARTIALLY UNFOLDED STATE OF THE *LAC* REPRESSOR HEADPIECE Georgios Patargias and Arjan van der Vaart, University of South Florida, 4202 E. Fowler Ave CHE205, Tampa, FL 33620.

The binding of the lactose (*lac*) repressor headpiece with its natural operator is characterized by the folding of a small loop in the protein into an α -helix. To understand this unfolding/folding transition, we performed fully atomistic molecular dynamics simulations of the unfolded state. In order to achieve a better sampling of this large conformational space, we carried out the simulations in a new manner using a Tsallis-bias replica exchange scheme. The performance of the method will be assessed and preliminary data on the unfolded state will be discussed and compared with data from simulations of the folded state.