

Abstract Submitted  
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**Identifying paths of allosteric communication in the protein BirA through simulations** GREGORY CUSTER, DOROTHY BECKETT, SILVINA MATYSIAK, University of Maryland — Biotin ligase/repressor (BirA) is a bifunctional enzyme which adenylates biotin and transfers the product, biotinyl-5-AMP (bio-5-AMP) to biotin carboxyl carrier protein (BCCP). In the absence of BCCP, bio-5-AMP promotes the dimerization of BirA. In dimer form, the BirAbio-5-AMP complex is able to bind to the biotin operator and prevents further synthesis of biotin. The bio-5-AMP binds away from the dimer interface, so it is acting as an allosteric activator. We perform all-atom molecular dynamics simulations with BirA to look at fluctuations within the protein at equilibrium. We simulate apoBirA, liganded BirA, as well as two mutants, M211A and V219A. In agreement with experimental observations, several loops of the protein become stabilized for the liganded BirA when compared to the apo protein. In addition, changes in the dimer interface are observed for the M211A and V219A mutations, which are located in the ligand binding region. Using inter-residue correlation coefficients and pair energies a communication network through the protein is constructed. With this network we have identified paths which have the potential to be important in allosteric activation of BirA. These paths and the methods we use to identify them will be presented.

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