Abstract Submitted
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Insights into the Opening and Closing Dynamics of Biotin Carboxylase[1] BRIAN NOVAK, DOREL MOLDOVAN, Mechanical Engineering, GROVER WALDROP, Biological Sciences, MARCIO DE QUEIROZ, Mechanical Engineering, Louisiana State University, Baton Rouge — Biotin carboxylase (BC) is a homodimer which catalyzes biotin carboxylation. A reaction is thought to occur in one monomer at a time (half-sites reactivity). BC can also function as a monomer. Evidence has shown that the B domain moves with hinge motion of 45 $^\circ$ between an unliganded form and one with bound ATP, suggesting that some of the energy from ATP hydrolysis might be harnessed to do useful work. The free energy along a closure angle for the B domain was calculated using MD simulations for a monomer and dimer with and without one bound ATP. We found that the monomer favors a closed state with or without ATP with mean times for opening much smaller than the reaction time, and the most stable structure for the dimer without ATP was with both monomers open. For the dimer with ATP, opening the B domain without ATP caused the other B domain to open, but hysteresis was observed when closing it, preventing an accurate calculation. The data suggest that the most stable state has both sides closed, supporting the idea of half-sites reactivity.

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