Abstract Submitted
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Computational Enzyme Design with Molecular Dynamics TALMAGE COATES, Brigham Young University — Enzymes catalyze reactions with lower environmental impact and often with greater efficiency than traditional chemical methods. Effective enzyme design is of industrial and academic relevance because many reactions are not catalyzed by known natural enzymes at appreciable rates. Computational enzyme design studies attempt to reduce the difference in Gibbs free energy between the transition state of the rate limiting reaction and the unactivated substrate. This energy difference is often calculated for a single state of the enzyme, even though enzymes exist in a thermodynamic ensemble of states. We use molecular dynamics simulations to account for dynamic effects in ranking designed sequences for the cyclization of ethyl-4,5,6-trihydroxy hept-2-enoate into ethyl 2-(2,3,4-trihydroxycyclopentyl) acetate using a radical S-adenosyl methionine enzyme.

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