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Protein Structure and Folding Pathway Prediction ROY CAMPBELL, ANDREW KRUGER, Department of Physics, Walla Walla College — We present *ab initio* predictions of the three-dimensional structures of the folded proteins Dictyostelium V4-lmcA and V4-lmcB. Beginning with linear sequences of amino acid residues, we use a Monte Carlo fragment insertion method for protein tertiary structure prediction (ROSETTA) merged with the I-SITES library of sequence structure motifs and the HMMSTR model for local structure in proteins available on a public server. These 160-residue proteins differ by just two residues but have significantly different predicted structures. We use the HMMSTR-CM contact map method to predict folding pathways and steered molecular dynamics (NAMD, VMD) to simulate the mechanical unfolding of the predicted structures.

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