Modeling the Folding and Hydrogen Production of Clostridium Acetobutylicum and Clostridium Saccharobutylium Mutants Using Electrostatic Potential Surfaces and Molecular Dynamics

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Electrostatic potential surfaces (EPS) were used with molecular dynamics to model the folding mechanisms and kinetics of hydrogenase mutants from wild types Clostridium Acetobutylicum and Clostridium Saccharobutylium. The purpose of the EPS approach was to incorporate long range electrostatic forces between widely separated regions of the mutants which contain 575 amino acids. Also, it was demonstrated that the ratio of positive to negative EPS of unfolded mutants could be used to predict the production of molecular hydrogen from the folded mutants. Using the prediction model, mutant compositions were determined that should yield hydrogen of up to 40 times that obtainable from the wild type Clostridium Acetobutylicum. It is expected that the developed EPS techniques can be used to study the folding of other proteins and to predict the reactivity of the folded protein structures.