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Probing the segmental mobility and energy of the active zones of a protein chain (aspartic acid protease) by a coarse-grained bond-fluctuation Monte Carlo simulation[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — A protein chain such as aspartic acid protease is described by a specific sequence of 99 residues each with its own specific characteristics. In a coarse-grained description, the backbone of a protein chain is described by nodes tethered together by peptide bonds where each node (the amino acid group) is characterized by molecular weight and hydrophobicity. A well-developed and somewhat mature computational modeling tool for the polymer chain such as the bond-fluctuation model is used to study such a specific protein chain with its constitutive amino groups and their sequence. The relative magnitude of hydrophobicity is used to develop appropriate interaction potentials for these amino acid groups in explicit solvent. The Metropolis algorithm is used to move each node and solvent constituent. Local energy and mobility of each amino group are analyzed along with global energy, mobility, and conformation of the protein chain. Effect of the solvent interaction and its concentration on these quantities will be presented.

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