Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Effect of solvent on the conformation and dynamics of Aspartic Acid Protease by a coarse-grained bond-fluctuating Monte Carlo simulation RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — In a coarse-grained description of a protein chain, all of the 20 amino acid residues can be broadly divided into three groups, hydrophobic (H), polar (P), and electrostatic (E). A protein can be described by tethered nodes in a chain with a node representing the amino acid group. Aspartic acid protease consists of 99 residues in a well-defined sequence. The specific sequence of H, P and E nodes tethered together by fluctuating bonds is placed on a cubic lattice where empty lattice sites constitute an effective solvent medium. The amino groups (nodes) interact with the solvent (S) sites with appropriate attractive (HS) and repulsive (PS) interactions with the solvent. Each node executes its stochastic movement with the Metropolis algorithm. Variations of the root mean square displacements of the center of mass and that of its center node of the protease chain, and its gyration radius with the time steps are examined for different solvent strength. The structure of the protease swells on increasing the solvent interaction strength which tends to enhance the relaxation time to reach diffusive behavior of the chain.

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Date submitted: 06 Nov 2006 Electronic form version 1.4