

Abstract Submitted  
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**Residue mobility and energy profiles of an HIV-1 protease (1DIFA) chain by a coarse-grained Monte Carlo simulation**<sup>1</sup> RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — HIV-1 protease (1DIFA), an enzyme consists of two polypeptides, 99 amino acids each. Aspartic acid residue (Asp<sup>25</sup>) forms the active catalytic site. Specificities of residues are captured via an interaction matrix (residue-residue, residue-solvent) of the Lennard-Jones potential. Simulations are performed for a range of interaction strength ( $f$ ) with the solvent-residue interaction describing the quality of the solvent. Snapshots of the protein show considerable changes in the conformation of the protein on varying the interaction. From the mobility and energy profiles of the residues, it is possible to identify the active (and not so active) segments of the protein and consequently their role in proteolysis. Contrary to interaction thermodynamics, the hydrophobic residues possess higher configurational energy and lower mobility while the electrostatic and polar residues are more mobile despite their lower interaction energy.

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