Stability of proteins inside a hydrophobic cavity MITHUN RADHAKRISHNA, Columbia University, SUMIT SHARMA, Princeton University, SANAT K. KUMAR, Columbia University — Previous studies have shown that enclosing a protein in an athermal cavity stabilizes the protein against reversible unfolding by virtue of eliminating many open chain conformations. Examples of such confined spaces include pores in chromatographic columns, Anfinsen's cage in Chaperonins, interiors of Ribosomes or regions of steric occlusion inside cells. However, the situation is more complex inside a hydrophobic cavity. The protein has a tendency to adsorb on the surface of the hydrophobic cavity, but at the same time it loses conformational entropy because of confinement. We study this system using a simple Hydrophobic Polar (HP) lattice protein model. Canonical Monte Carlo (MC) simulations at different temperatures and surface hydrophobicity show that proteins are stabilized at low and moderate hydrophobicity upon adsorption. The range of surface hydrophobicity over which a protein is stable increases with a decrease in radius of the cavity.

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