Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Simulation Model of Protein Transport and Stabilization APICHART LINHANANTA, Lakehead University — In a previous communication (Linhananta et al., Biophys. J., 2011, 100, 459), we reported results of a simulation model of a protein in solvents with protein-solvent contact energy parameter ε_{ps}, which mimics the effects of osmolytes ($\varepsilon_{ps} > 0$) and denaturants ($\varepsilon_{ps} < 0$). Here a model three-helix-bundle (THB) protein in solvents is confined in cylindrical cavity to mimic GroEL/ES. The interior wall is characterized by the protein-wall energy ε_{pw} , and solvent-wall energy, ε_{sw}. Simulations found a substantial increase in the folding temperature from $T^* = 4.2$, in scaled unit, for THB in vacuum, to $T^* > 6.0$ for confined THB in osmolytes. The model is generalized to THB and solvents confined in two connected cylindrical segments. The bottom segment represents the interior of a GroEL/ES, with the sidewall characterized by the parameters ε_{pw} and ε_{sw}. The upper segment represents the exterior surrounding the GroEL/ES, with periodic boundary condition on the sidewall. The protein and solvents can move through the channel connecting the two segments. Simulation data reveals new insights on the transport of unfolded proteins into GroEL/ES.

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Date submitted: 15 Nov 2013 Electronic form version 1.4