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Life in a Crowd: Macromolecular Crowding and Confinement Effects on Protein Interactions in Living Systems MARGARET CHEUNG, Department of Physics, University of Houston — Biological polymers carry out their functions in living systems where the environment is very concentrated or crowded by macromolecules. Physically, the composition of a cell is more than "a sack of water"; its consistency is closer to Jell-O. Experiments suggests that, because of this macromolecular crowding effect that confines polymeric dynamics, the kinetics and thermodynamics of protein folding and the association rate constants of protein-protein interactions in a cell (in vivo) are very different from that ina diluted test tube (in vitro). In order to quantitatively understand macromolecular crowding and confinement effects on protein dynamics, we used coarse-grained models that physically captured interactions between crowders and a protein. The folding rates of a model protein nonmonotonically increased with the volume fraction of the crowders. At lower volume fractions, depletion-induced attractions from crowders could be mapped according to the spherical confinement model. A result of spherical confinement was the destabilization of denatured states by disallowing extended configurations that were longer than the pore size. However, at higher volume fractions, conformational fluctuations of a protein were susceptible to the shape of the confining condition. Thus, an approximation of the spherical confinement to mimic crowding effects was no longer effective.

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