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Quantifying Energy, Entropy and Free-Energy in Protein Folding Funnels[1] BERNARD GERSTMAN, PREM CHAPAGAIN, Department of Physics, Florida International University — The folding of proteins is a self-organizing process in which a long chain heteropolymer in a disorganized configuration spontaneously changes its shape to a highly organized structure. Several different forces work together to organize the structure while random thermal motion tends to cause disorganization. In order for folding to occur in a biologically relevant time, the Levinthal Paradox shows that folding cannot occur by a process that samples all of configuration space by randomly jumping from one microstate to another. Instead, folding pathways allow the organizing forces to incrementally direct the chain to ever-shrinking regions of configuration space in a funneling process. In order to understand how these self-organizing forces direct folding, we have quantified the narrowing of the folding funnel for a model two helix bundle. We have calculated the dependence of entropy and free-energy as a function of average energy by determining the statistical mechanical canonical probability for the chain to occupy each possible configuration as a function of average energy.

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