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Ionic salt-bridge dependence of dimerization of the GCN4 Leucine zipper YANXIN LIU, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University, University Park, Miami, FL 33199 — The role that ionic interactions, or salt-bridges, play in protein folding and dimerization is still controversial. We perform computational simulations on the GCN4 leucine zipper to investigate the effect of ionic interactions. A three dimensional lattice model incorporating a Monte Carlo Metropolis Algorithm is employed to simulate the dimeriztion process. Our results show that stronger ionic interactions result in more stable dimers, in agreement with experiments. Our simulations also show that increasing the strength of the ionic interactions does not lead to a monotonic increase in the speed of the dimerization process. We find an optimal intermediate ionic interaction strength at which the dimer is stable and the dimerization process proceeds at the maximum rate. We present quantitative results of dimerization rates, heat capacity, and free energy landscapes as a function of the ionic strength for the GCN4 leucine zipper.

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