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Enhanced protein folding by removal of kinetic traps YANXIN LIU, PREM CHAPAGAIN, JOSE PARRA, BERNARD GERSTMAN, Department of Physics, Florida International University, Miami, FL 33199 — The presence of non-native kinetic traps along the free energy landscape of a protein may significantly lengthen the overall folding time so that the folding process becomes unreliable. We used a computational 3-D lattice model to investigate the free energy landscape of a model alpha helical hairpin peptide. We used two slightly different sequences and show that strategic substitutions of only a few amino acid residues greatly enhance the folding process. These strategic substitutions prevent the formation of long-lived misfolded configurations which not only lengthen the folding time but also may cause unwanted aggregation. Detailed kinetic and thermodynamic analysis was carried out for the folding of these two sequences and the results are consistent with the experimental and molecular dynamics simulations of small helical bundle proteins.

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