Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Position dependence of the trigger sequence in the folding and dimerization of a lattice model coiled-coil peptide YUBA BHANDARI, PREM CHAPAGAIN, BERNARD GERSTMAN, Department of Physics, Florida International University — Coiled-coil protein dimerization has been shown to be greatly facilitated by the presence of a trigger segment of amino acids that has a high propensity for forming alpha-helix structure. A three-dimensional lattice model incorporating a Monte Carlo Metropolis Algorithm is used to investigate how the effectiveness of the trigger segment depends on its location in the protein. Heat capacity and free energy were calculated to study the thermodynamics of the folding and dimerization for different positions of the trigger segment. The simulation results show that the dimerization is improved when the trigger segment is located near the middle of the chain as compared to near the ends.

Prem Chapagain
Florida International University

Date submitted: 27 Nov 2009 Electronic form version 1.4