Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Protein Folding Simulation of Mutant Go Models of the Wild-Type Trp-cage Protein APICHART LINHANANTA, JUNMIN LIU, Department of Physics, Lakehead University — For the past three decades, Go models of protein folding have played important roles in the understanding of how proteins fold from random conformations to their unique native structures. Unfortunately Go models reliance on known NMR or x-ray structures to construct Go interaction potentials severely limit their predictive powers. In this work, we introduce a novel method for constructing Go interaction potentials of mutant proteins based on Go interaction potentials of wild type proteins. As a template we employ the all-atom Go model of the 20-residue Trp-cage protein (A. Linhananta, J. Boer and I. MacKay, J. Chem. Phys., 2005, 122, 114901) as the wild type Go model. Trp-cage mutants are constructed by replacing a Trp-cage residue with a different residue. In particular the Pro-12 residue of the Trp-cage is substituted by Trp-12 to produce the Trp2-cage mutant, whose native structure is not yet known. Monte Carlo simulations, using CHARMM force fields, are performed to determine the ground-state structure mutant. The resulting mutant structures are used to construct the Go interaction potential of the Trp2-cage mutant Go model.

Apichart Linhananta
Department of Physics, Lakehead University

Date submitted: 27 Nov 2007 Electronic form version 1.4