Abstract Submitted for the MAR17 Meeting of The American Physical Society

Thermodynamic Properties of Protein Folding Process VATTIKA SIVISED, THEJA DE SILVA, Augusta University — Proteins are one of the fundamental building blocks of life and they are present in almost all biological and cellular processes. Proteins consist of amino acids held together in a long chain by peptide bonds. When proteins function in biological processes, they fold in to three-dimensional structures by curling the chain. The folding of a peptide chain into a three dimensional structure is a thermodynamically driven process such that the chain naturally evolves to form domains of similar amino acids. The formation of this domain occurs by curling the one dimensional amino acid sequence by moving similar amino acids proximity to each other. We model this formation of domains or ordering of amino acids using q-state Potts model and study the thermodynamic Properties using a statistical mechanics approach. Converting the interacting amino acids into an effectively non-interacting model using a mean-field theory, we calculate the Helmholtz free energy (HFE). Then by investigating the HFE, we qualitatively study the properties of protein folding transition. We find that the protein folding phase transition is strongly *first* order and the specific heat shows the experimental signatures of this phase transition.

> Theja De Silva Augusta University

Date submitted: 08 Nov 2016

Electronic form version 1.4