Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Amino Acid Free Energy Decomposition HUI WANG, MICHAEL FAIRCHILD, DENNIS LIVESAY, DONALD JACOBS, University of North Carolina at Charlotte — The Distance Constraint Model (DCM) describes protein thermodynamics at a coarse-grained level based on a Free Energy Decomposition (FED) that assigns energy and entropy contributions to specific molecular interactions. Application of constraint theory accounts for non-additivity in conformational entropy so that the total free energy of a system can be reconstituted from all its molecular parts. In prior work, a minimal DCM utilized a simple FED involving temperature-independent parameters indiscriminately applied to all residues. Here, we describe a residue-specific FED that depends on local conformational states. The FED of an amino acid is constructed by weighting the energy spectrums associated with local energy minimums in configuration space by absolute entropies estimated using a quasi-harmonic approximation. Interesting temperature-dependent behavior is found. Support is from NIH R01 GM073082 and a CRI postdoctoral Duke research fellowship for H. Wang.

Hui Wang
University of North Carolina at Charlotte

Date submitted: 21 Nov 2008 Electronic form version 1.4