Abstract Submitted for the SES05 Meeting of The American Physical Society

Thermodynamically Correct Gō Models: Incorporating Entropic Interactions into Minimalist Models ALEXANDER CHEW, HUGH NYMEYER, Florida State University — Gō-like or "native-centric" protein models have been very successful in describing folding behavior. These models typically treat all atomic interactions as purely enthalpic in origin; however, many interactions, such as the hydrophobic effect at room temperature, are known to be largely entropic. We construct a new Gō-like model that treats atomic interactions as arising from a combination of enthalpic and entropic forces between various hydrophobic and hydrophilic groups. This new model captures the correct temperature dependent behavior of protein contacts, allowing us to observe cold denaturation and derive heat capacity curves that can be compared directly against experimental data.

Hugh Nymeyer Florida State University

Date submitted: 09 Aug 2005

Electronic form version 1.4