

Abstract Submitted
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Nonmonotonic Behavior of Nonnative Contacts in Small Proteins: An Exact Study on a Square Lattice CHONG CHEN, PURUSHOTAM GUJRATI — Nonnative contacts are defined as contacts absent in the native state, and can be used to study the process of folding. They are expected to increase with temperature or energy. By *exactly generating* all possible conformations on a square lattice, we have investigated nonnative contacts for proteins in the standard HP model and its modified versions introduced by our group^[1]. This enables us to carry out exact calculation for the nonnative contact density $n_c(e)$ as a function of the energy density e as well as its canonical average $\bar{n}_c(T)$ as a function of temperature of T from which we construct $\bar{n}_c(\bar{e})$ to compare with $n_c(e)$. The sequence dependence of $n_c(e)$ and $\bar{n}_c(T)$ are also investigated. Some new understandings of the role for nonnative contacts play in the protein folding process, as will be discussed during the talk. 1) The density $n_c(e)$ is always monotonically increasing in the standard model. This need not be true for all kinds of interactions. 2) The density $\bar{n}_c(T)$ is usually monotonically increasing. A few violations can be seen. 3) The protein property is sequence dependent, as expected. Reference [1] P. D. Gujrati, B. Lambeth, Jr., A. Corsi, and E. Askanazi, arXiv: 0708.3739 (2007).

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