

Abstract Submitted  
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**Folding a protein with equal probability of being helix or hairpin<sup>1</sup>**

CHUNG-YU MOU, CHUN-YU LIN, National Tsing Hua University, Taiwan, ROC, NAN-YOW CHEN, National Center for High-Performance Computing, Taiwan, ROC — We explore the possibility for the native state of a protein being inherently a multi-conformation state in an ab initio coarse-grained model. Based on the Wang-Landau algorithm, the complete free energy landscape for the designed sequence 2D4X: INYWLAHAKAGYIVHWTA is constructed. It is shown that 2DX4 possesses two nearly degenerate native states: one has a helix structure, while the other has a hairpin structure and their energy difference is less than 2% of that of local minimums. Furthermore, the hydrogen-bond and dipole-dipole interactions are found to be two major competing mechanisms in transforming one conformation into the other. Our results indicate that degenerate native states are stabilized by subtle balance between different interactions in proteins; furthermore, degeneracy only happens for small proteins of sizes being around 18 amino acids or 40-50 amino acids. These results provide important clues to the study of native structures of proteins.

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