Geometry, Symmetry and Protein Folding

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Abstract: We present a simple physical model which demonstrates that the native state folds of proteins can emerge on the basis of considerations of geometry and symmetry. We show that the inherent anisotropy of a chain molecule, the geometrical and energetic constraints placed by the hydrogen bonds and sterics, and hydrophobicity are sufficient to yield a free energy landscape with broad minima even for a homopolymer. These minima correspond to marginally compact structures comprising the menu of folds that proteins choose from to house their native-states in. We show that by introducing a minimal heterogeneity in the hydrophobic interaction one can design hydrophobic-polar sequences that fold into selected structures. Our results lead to an unified framework for understanding protein folding, amyloid formation and it also has implications for natural selection.

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