

Searching for Global Minima in Protein Folding

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Abstract

Proteins are complex heterogeneous polymer molecules. Yet proteins fold — often very quickly (in microseconds) — to a unique “native” structure. Described in terms of energy landscapes, a folding protein can find a global minimum of a bumpy landscape very quickly. Using simple exact statistical mechanical models, it has been found that the basis for this speed is that these energy landscapes are funnel-shaped. We have been exploring ways to make use of information about the shapes of protein energy landscapes to find faster conformational search methods for locating the globally optimal states.