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Exploring the landscape for protein folding: from function to molecular machines[1]

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Globally the energy landscape of a folding protein resembles a partially rough funnel with reduced energetic frustration. A consequence of minimizing energetic frustration is that the topology of the native fold also plays a major role in the folding mechanism. Some folding motifs are easier to design than others suggesting the possibility that evolution not only selected sequences with sufficiently small energetic frustration but also selected more easily designable native structures. The overall structures of the on-route and off-route (traps) intermediates for the folding of more complex proteins are also strongly influenced by topology. Going beyond folding, the power of reduced models to study the physics of protein assembly, protein binding and recognition, and larger biomolecular machines has also proven impressive. Since energetic frustration is sufficiently small, native structure-based models, which correspond to perfectly unfrustrated energy landscapes, have shown to be a powerful approach to explore larger proteins and protein complexes, not only folding but also function associated to large conformational motions. A discussion of how global motions control the mechanistic processes in the ribosome and molecular motors will be presented. For example, this conceptual framework is allowing us to envisage the dynamics of molecular motors and the ribosome from the structural perspective and it provides the means to make quantitative predictions that can be tested by experiments.

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