Topological Invariants in Protein Folding and Their Scaling Properties

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The problem of the three-dimensional structure prediction in terms of the amino acid sequence is still an open question in spite of the progress of the conformational analysis and the molecular dynamics as well as of the more accurate knowledge of the force field. Some years ago we proposed a model which addresses the problem of the general trend of protein folding. Such transconformational process involves entangled movements of the polypeptide chain which are however progressively hampered by the growing importance of long range interactions whence only concerted transconformations can take place. We investigated the topological aspects of such constrained transformations and found that they are characterized by the invariance of the linking number of the polypeptide chain fitting ribbon in order to avoid the overcoming of high conformational energy barriers which would severely repress the kinetics of the process; under such a topological constraint the transconformations become highly cooperative. In order to select the topologically invariant pathways we have identified some significant parameters which characterize all the proteins independently of their tertiary structures. One of these is a topological parameter which quantifies the complexity of folding as the number of chain crossing averaged over all the possible projections of the structure. It is easily calculated and shows interesting and useful fractal properties. Using a folding representation as a complex function of the sequence we are at present trying extending to proteins the model we successfully developed to predict the superstructures of DNA.

Selected references

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