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Perspective

Structural and Kinetic Properties of Protein Folding

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DESCRIPTION

Proteins are the most important functional elements in living cells. DNA contains genetic information. To make this information available, DNA must be transcribed into MRNA, which is then translated into protein. The codes for DNA are four bases and protein is twenty amino acids. In the 1950s, the genetic code was discovered, with each amino acid coded by three consecutive nucleotides. The amino acid sequence, however, is only the fundamental structure of proteins. To be functional, proteins must bend into the tertiary structure, which is the ideal composition of secondary structures, particularly alpha-helix and beta-sheet. In some circumstances, the tertiary structures of many proteins or subunits must combine to generate a quaternary structure. The "protein folding" problem is primarily concerned with the exact physical transition process from primary to tertiary structure.

The protein folding mechanism consists of two major issues: kinetics and thermodynamics. Thermodynamically, the native state is the dominant and most stable state for proteins. Kinetically, however, there are various routes for nascent proteins to reach the native state Experiment evidence is required to prove or invalidate any theory. Several approaches have been developed or applied to the protein folding problem. First, the structure of the examined protein must be determined using X-ray crystallography or nuclear magnetic resonance (NMR). It is preferable to have a high-resolution X-ray structure.

However, because many of the model proteins are unable to be crystallized, only NMR structures are accessible. Circular dichroism is a well-known technique for studying protein folding. The CD spectrum can represent the proportion of secondary structures. The changes in the CD spectrum to temperature or denaturant concentration can be utilized to calculate the melting temperature or unfolding free energy. However, CD alone is insufficient for studying the folding process of DNA. Ultrafast mixing, laser temperature leap, and other time-resolved techniques are examples. Natural or engineered fluorescence probes, in addition to CD, can be employed to monitor the folding process. Because of the artificial folding environment, the "actual" folding process may not be accurately mirrored in these folding studies. Proteins are generated on the ribosome one residue at a time in living cells, and the final products exist in a crowded physiological situation. However, in the folding experiments, proteins remain in free artificial solution and are subjected to various perturbations such as denaturation. Furthermore, the spectroscopic signal of individual probes cannot be read simply as global protein folding; rather, it only reflects the distance between two selected residues.

Proteins are produced in cells or in vitro as unstructured polypeptide chains that self-assemble into functionally active three-dimensional forms in most situations. This process, known as protein folding, occurs over a wide variety of durations, from microseconds to seconds and beyond. From a purely physical-chemical standpoint, it should be able to define the folding mechanism of a given protein at atomic precision and rebuild its free-energy landscape using molecular dynamics simulations based on simple physical principles.

CONCLUSION

Fast-folding protein discovery and design greatly reduced the timing gap between simulations and experiments, making such simulations viable, at least for the fastest-folding proteins.Protein folding demonstrates how long-timescale molecular dynamics simulations can provide direct access to a wide range of thermodynamic and kinetic folding properties. Most computed observables correlate reasonably well with tests, with the main differences being that the calculated heat capacity for folding is lower than in the experiments and folding speeds are three times slower.

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