

Protein Structure and Modeling

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Preface

Structure of proteins, nucleic acids, polysaccharides, and lipids is very important for our understanding of biological processes and life functions. Biological macromolecules are very complex objects to study. Proteins represent the largest and most extensively studied group of biopolymers. Comprising thousands of atoms, they exhibit several levels of organization, multiple isoforms, dynamic behavior, and diverse functions. With advancements in sequencing, complete genomes of many organisms are being decoded. We are able to compare healthy and diseased organisms and observe changes during development. These rapid methods bring new data on the basic building blocks of living organisms and allow their thorough comparison and elucidation of principles of organization. X-ray crystallography, NMR, electron microscopy, and other methods reveal structure of macromolecules at atomic resolution which contributes to significant progress in many areas of biomedical research, medicine, biotechnology, and design of new drugs. With growing amount of data, new approaches in biochemistry, mathematics, biophysics, structural biology, and other areas lead to development and refinement of theoretical models. Increase in accuracy and number of experimental and theoretical models helps better understand and even design new living organisms.

Proteins are remarkably regular objects in spite of being very heterogeneous and irregular at some levels. They perform functions that require precise organization. We explain their precise organization and performance by structural principles. As molecular machines they function according to concerted work of their constituent parts with each atom at precise location at precise time. We admire their work. Perhaps the same way we see the ocean wave and admire its beauty. Its motion is governed by laws of nature.

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