

## **NATIVE STATES OF PROTEINS AND COMPUTATIONAL MODELING OF THEIR STRUCTURE AND STRUCTURE - FUNCTION RELATIONSHIPS**

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Proteins are main functional units of a living cell. They participate in maintaining cell structure and integrity, reception and transduction of chemical and physical signals from the environment; they function as messengers and catalyze chemical reactions; they are involved in cell reproduction and death processes. In this introductory lecture I will briefly introduce physical and chemical principles of protein structure and function. Properties of globular and membrane proteins will be discussed. Computational and theoretical approaches to protein structure prediction and protein structure-function relations will be introduced. Several examples which illustrate Molecular Modeling methodologies application to protein- ligand interaction, ion channel permeation and conformational transitions in proteins will be presented.