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Microscopic calculation of conformational thermodynamics in bio-macromolecular complexes

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The microscopic basis of connection between protein conformation and function is a fundamental challenge. Recent experiments show the importance of conformational changes in providing stability to protein complexes. The changes in conformational state have both enthalpy and entropic components. It has been possible to quantify the entropy changes due to conformational changes from nuclear magnetic resonance data. Here we show microscopic calculation of both the enthalpy and entropy contribution while protein conformations change from the equilibrium distribution of the dihedral angles of proteins. We have shown that the free-energetically destabilized and entropically disordered residues in each conformation compared to a reference conformation act as binding residues in the given conformation. Here we show that this principle can: 1. ascertain ligand binding of a protein in different conformations, 2. supplement the structure of missing fragments in a protein and 3. serve as a guideline for allosteric changes. All these applications point to tune protein in-silico which would help to design functional materials with protein as building blocks.

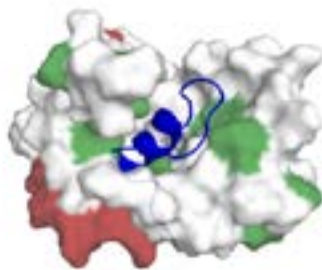


Figure1: Residue wise data from microscopic calculation of conformational entropy (red: disordered; green: ordered)

Biography

Jaydeb Chakrabarti is a Theoretical Physicist trained in condensed matter physics. He considers statics and dynamics of soft matter systems including bio-macromolecules. The theoretical methods used in these studies are: (1) Computer simulations based on Molecular Dynamics, Monte Carlo and Brownian Dynamics, (2) Mean field calculations based on classical density functional theories. The goal of his researches is to relate macroscopic properties to microscopic motions.

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