Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods (Series in Computational Biophysics)

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The Latest Developments on the Role of Dynamics in Protein Functions

Computational Approaches to Protein Dynamics: From Quantum to Coarse-Grained Methods presents modern biomolecular computational techniques that address protein flexibility/dynamics at all levels of theory. An international contingent of leading researchers in chemistry, physics, and biology show how these advanced methods provide insights into dynamic aspects of biochemical processes. A particular focus is on intrinsically disordered proteins (IDPs), which lack a well-defined three-dimensional structure and function as dynamic ensembles.

The book covers a wide spectrum of dynamics, from electronic structure-based to coarse-grained techniques via multiscaling at different levels. After an introduction to dynamics and historical overview of basic methodologies, the book addresses the following issues:

- *Is there a quantitative relationship between enzymatic catalysis and protein dynamics?*
- *Which are the functionally relevant motions of proteins?*
- *How can structural properties and partner recognition mechanisms of IDPs be simulated?*
- *How can we speed up molecular dynamics?*
- *How can we describe conformational ensembles by the synergistic effort of computations and experiments?*

While dynamics is now considered essential for interpreting protein action, it is not yet an integral component in establishing structure–function relationships of proteins. Helping to reshape this classical view in biochemistry, this groundbreaking book explores advances in computational methodology and contributes to the new, ensemble way of studying proteins.

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