生体分子モデリング&ダイナミクス研究室

蛋白質研究所

Laboratory of Biomolecular Modeling and Dynamics

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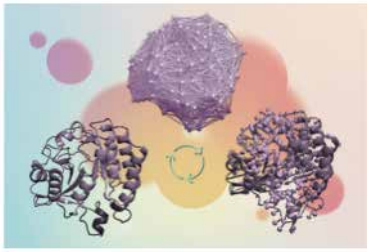
Unlocking the Intricacies of Protein Structures: A Journey into Biologically Relevant Dynamics through Computational Modeling and Simulations

Proteins, the building blocks of life, are not static entities; they possess a dynamic nature, akin to any other object on Earth. At our laboratory, we delve into the fascinating world of proteins, employing structural data gleaned from advanced experimental techniques like X-ray Crystallography, cryo-electron microscopy, and small-angle X-ray scattering. Our mission? To model the myriad conformations these proteins can adopt in solution and, employing the principles of physics, simulate their flexible movements - their dynamics - deciphering the very essence of their functioning.



Our approach is multifaceted, addressing the unique challenges posed by protein structures:

1) **Completing the Puzzle:** Protein structures often present with missing information, requiring us to analyze analogous structures to fill the gaps.

2) **Taming the Data Deluge:** Copious amounts of data can overwhelm, necessitating innovative strategies. We employ techniques such as simplifying their representation through coarse-graining and utilizing methods like elastic network model-based normal mode analysis, which do not demand exhaustive details of their motions.

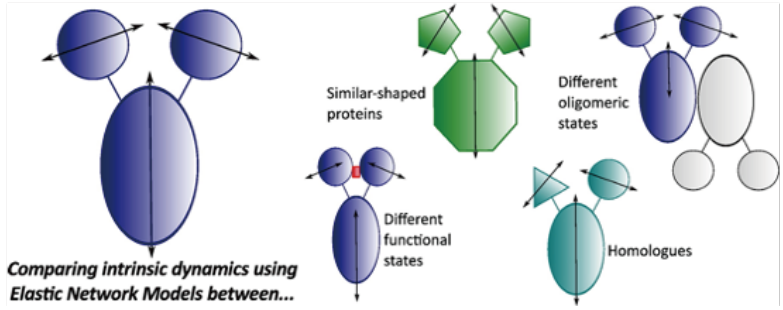
3) **Integrating Insights:** Many experimental methods provide dynamic glimpses but lack molecular resolution. We develop methods that amalgamate information from diverse sources, building a reliable understanding of the system under scrutiny.

Our research spans a wide spectrum of intriguing topics:

- **Protein Allostery:** Unraveling the mysteries of protein regulation.
- **Oligomerization and Biological Complex Assembly:** Investigating the intricate dance of protein interactions.
- **Evolutionary Conservation of Structure and Dynamics:** Exploring the ancient echoes within protein architectures.
- **Proteins of Interest:** Delving deep into proteins like TIM Barrel fold proteins, PyrR, dihydrofolate reductase, leukotriene alpha-4 hydrolase, and more.

Our arsenal of methods includes, but is not confined to:

- **Python Programming:** Harnessing the power of coding for intricate analyses.
- **Statistical Analysis:** Extracting meaningful insights from complex datasets.
- **Bioinformatics Tools:** Employing advanced tools for sequence alignment and structure prediction.
- **Molecular Dynamics Simulations:** Simulating the dynamic dance of proteins at the molecular level.
- **Normal Mode Analysis:** Probing the fundamental modes of protein motion.
- **Deep Learning Approaches:** Leveraging the potential of artificial intelligence for nuanced understanding.
- **Biomolecular Visualization and Animation:** Crafting visual narratives that illuminate the intricate world of proteins.
- **Web-Based Tool Development:** Creating user-friendly interfaces for the broader scientific community.



Join us on this expedition, where we unravel the enigmatic world of proteins, one dynamic movement at a time.

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