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Special Issue Reprint

Computational Approaches for Protein Dynamics and Function

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Proteins are fascinating structures that operate at the nanoscale in a complex environment and are involved in an astonishingly wide variety of functions, from ion transport to enzymatic catalysis, metabolism, neurotransmission, and many more functions. Understanding these peculiar functionalities at the single-protein level requires advanced experimental and computational techniques. In the era of high-performance computing, computational methods are particularly well suited to investigating the structure and dynamics of proteins and unravelling how they enable biological functions. Molecular Dynamics (MD), Normal Mode Analysis (NMA), and Elastic Network Models (ENMs) are just a few examples of the computational methodologies that we can use to elucidate protein conformational dynamics, allostery, the impact of mutations, and many other fascinating subjects. This Special Issue comprises eight peer-reviewed papers demonstrating how various computational approaches can be employed to address the ultimate and most crucial question: how do proteins work?

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