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Computational Approaches for Protein Dynamics and Function

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Deadline for manuscript submissions:
closed (31 May 2023)

Message from the Guest Editors

Proteins play a pivotal role in almost every biological process. Their biological functionality was found to be strictly related with the three-dimensional structure and modulated by its intrinsic dynamics. This Special Issue is dedicated to the most recent applications of computational methods to the simulation of protein dynamics. Novel research studies, as well as state-of-the-art review papers, related to these and other computational approaches for the understanding of protein dynamics and behavior are welcome.

In this Special Issue we welcome both original research papers and review articles on diverse topics such as:

- protein dynamics
- protein function
- protein flexibility
- molecular dynamics
- normal mode analysis
- elastic network models
- protein conformational change
- protein-ligand interaction
- protein-protein interaction
- multi-scale modeling

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

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