Special Issue

Molecular Dynamics Simulations in Structural Biology: From Proteins to Complex Biomolecular Systems

Message from the Guest Editor

This Special Issue The purpose of this is to gain insights into the atomic structures and the temporal evolution of proteins, including experimental techniques, as well as mathematical and computational modeling approaches for the comprehension of biological function. There is also interest in molecular interactions involved in the protein function and molecular docking. It is known that the role biological of new proteins is usually very complicated to determine.For this reason, dynamic simulations are extraordinary tool for predicting the behavior in the binding side. Therefore, the objective of this Special Issue is to publish high-quality articles, including original research, reviews, short communications, and clinical reports on diagnosis, investigation, and treatment, where the proteins and their biocomplexes are participants at the molecular level.

Guest Editor

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Message from the Editor-in-Chief

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