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Protein Dynamics: New Advanced Computing Methods and Tools

Guest Editor:

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Message from the Guest Editor

Dear Colleagues,

Protein functions are closely associated with internal motions occurring over a wide range of time scales, from atomistic vibrations to global motions, ranging from fs to ms or a longer timescale. Simulation of molecular dynamics is a technique that applies the laws of physics to a protein 3D structure to predict the time-dependent evolution of interacting particle systems.

A route from 3D structure to biofunctions is a connected sequence of different computational stepping-stones—the generation of high-throughput data, post-processing of these data, data analysis, and comprehensive graphical representation.

This Special Issue aims to highlight new methods and/or software tools targeting both the generation of reliable data for highly flexible and large proteins (in particular membrane proteins, intrinsically disordered proteins, etc.) under controlled computational resources, as well as a comprehensive data exploration and rigorous representation of results.

We look forward to your participation!

Kind regards,

Prof. Luba Tchertanov
Guest Editor

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