Special Issue

Protein Dynamics: New Advanced Computing Methods and Tools

Message from the Guest Editor

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,

Guest Editor

Prof. Luba Tchertanov

ENS Paris-Saclay, Université Paris-Saclay, CNRS, Centre Borelli, 4 av. des Sciences, F-91190 Gif-sur-Yvette, France

Deadline for manuscript submissions

closed (31 December 2021)

Biomolecules

an Open Access Journal by MDPI

Impact Factor 4.8
CiteScore 9.2
Indexed in PubMed

mdpi.com/si/68528

Biomolecules
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
biomolecules@mdpi.com

mdpi.com/journal/biomolecules

Biomolecules

an Open Access Journal by MDPI

Impact Factor 4.8
CiteScore 9.2
Indexed in PubMed

mdpi.com/journal/biomolecules

About the Journal

Message from the Editorial Board

Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

Editors-in-Chief

Prof. Dr. Peter E. Nielsen
Department of Cellular and Molecular Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Blegdamsvej 3C, DK-2200 Copenhagen, Denmark

Prof. Dr. Lukasz Kurgan
Department of Computer Science, Virginia Commonwealth University, Richmond, VA 23284, USA

Author Benefits

Open Access

— free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Biochemistry)

MDPI