Special Issue

Structure, Molecular Dynamics, Assembly, and Evolution of Protein Systems with AI-Enhanced Modeling in Pharmacology and Structural Biology

Message from the Guest Editors

Progress in protein biochemistry, molecular biology, pharmacology, and medicine cannot currently occur without an understanding of the structure, assembly, dynamics, and evolution of protein systems, as well as rational drug design. This Special Issue aims to highlight both experimental and computational advances in the characterization of protein folding, stability, assembly, and interactions — with a particular focus on protein–ligand systems and drug-target mechanisms. We welcome submissions on molecular dynamics simulations, protein evolution, structural bioinformatics, or ligand docking. Of particular interest are studies that integrate machine learning (ML) techniques with deep learning (DL) and Neural Networks (NNs) with cheminformatics to elucidate structure–function relationships, discover novel bioactive compounds, or model receptor-binding processes, including those for challenging protein classes. Appropriate experimental validation is essential for studies mainly relying on computational methods.

Guest Editors

Dr. Michal Blazej Ponczek

Department of General Biochemistry, Faculty of Biology and Environmental Protection, University of Lodz, Pomorska 141/143, 90-236 Łódź, Poland

Prof. Dr. Mohamed Ragab AbdelGawwad

Genetics & Bioengineering Program, Faculty of Engineering and Natural Sciences, International University of Sarajevo, Hrasnička Cesta br. 15, Ilidža, 71210 Sarajevo, Bosnia and Herzegovina

Deadline for manuscript submissions

31 March 2026

Biomolecules

an Open Access Journal by MDPI

Impact Factor 4.8
CiteScore 9.2
Indexed in PubMed

mdpi.com/si/253465

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