Special Issue

Forces Driving Macromolecular Recognition: Role in Drug Design and Discovery

Message from the Guest Editors

The exquisite machinery in living cells orchestrates an intricate network of macromolecular interactions underpinning vital biological mechanisms and biochemical processes. Recent advances in multidisciplinary approaches incorporating experimental platforms and computational techniques have facilitated the characterization of intrinsic structural and thermodynamic forces driving molecular recognition events. Such biophysical frameworks empower the accurate mapping and quantitative modeling of macromolecular interactions critical to successful drug discovery campaigns. An overarching goal is to design bioactive ligands that selectively bind biomolecular targets and modulate their function. Elucidating the energetic and structural basis of ligand–receptor interactions enables the identification and optimization of lead compounds with enhanced activity, specificity, and bioavailability. This Special Issue welcomes original Research Articles and Reviews that utilize biophysical, computational, and structural methodologies to characterize complex biological processes, underscoring the role of macromolecular recognition as a primary driving force in drug design and discovery.

Guest Editors

Dr. David P. Remeta

Department of Chemistry and Chemical Biology Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA

Dr. Conceição A. Minetti

Department of Chemistry and Chemical Biology Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA

Deadline for manuscript submissions

31 December 2026

Biomolecules

an Open Access Journal by MDPI

Impact Factor 4.8
CiteScore 9.2
Indexed in PubMed

mdpi.com/si/257129

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