Special Issue

New Horizons in Enzyme Inhibitor Discovery: Targets, Design and Evaluation

Message from the Guest Editors

Researchers are showcasing innovative strategies related to the design and development of new enzyme inhibitors, with significant achievements in potentialtarget validation and new drug discovery. Emerging research methods and paradigms, such as Artificial Intelligence-Driven Drug Discovery (AIDD), open science, and ultra-high-throughput screening, are poised to significantly enhance the discovery of the next generation of enzyme inhibitors. To highlight the latest research and cutting-edge developments in enzyme inhibitor discovery, we are inaugurating this Special Issue. It will feature advancements in various aspects of the field, including but not limited to the design, screening, synthesis, and biological evaluation of novel enzyme inhibitors; pharmacokinetic studies; innovative methodologies; structure-activity and structureproperty relationship studies; and the application of structural biology and computational studies for SAR analysis. Contributions to all of the areas outlined above and beyond are welcome. Please ensure that submissions adhere to the current Author Guidelines of Biomedicines.

Guest Editors

Dr. Chenzhou Hao

Dr. Jing Guo

Dr. Yin Sun

Dr. Tongchao Liu

Deadline for manuscript submissions

31 March 2026



an Open Access Journal by MDPI

Impact Factor 3.9 CiteScore 6.8 Indexed in PubMed



mdpi.com/si/214058

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

mdpi.com/journal/biomedicines





an Open Access Journal by MDPI

Impact Factor 3.9 CiteScore 6.8 Indexed in PubMed





About the Journal

Message from the Editor-in-Chief

Biomedicines (ISSN 2227-9059) is an open access iournal devoted to all aspects of research on human health and disease, the discovery and characterization of new therapeutic targets, therapeutic strategies, and research of naturally driven biomedicines, pharmaceuticals, and biopharmaceutical products. Topics include pathogenesis mechanisms of diseases, translational medical research, biomaterial in biomedical research, natural bioactive molecules, biologics, vaccines, gene therapies, cell-based therapies, targeted specific antibodies, recombinant therapeutic proteins, nanobiotechnology driven products, targeted therapy, bioimaging, biosensors, biomarkers, and biosimilars. The journal is open for publication of studies conducted at the basic science and preclinical research levels. We invite you to consider submitting your work to Biomedicines, be it original research, review articles, or developing Special Issues of current key topics.

Editor-in-Chief

Prof. Dr. Felipe Fregni

- Neuromodulation Center and Center for Clinical Research Learning, Spaulding Rehabilitation Hospital and Massachusetts General Hospital, Harvard Medical School, Boston, MA 02114, USA
- 2. Department of Epidemiology, Harvard T.H. Chan School of Public Health, Boston, MA 02115, USA

Author Benefits

High Visibility:

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

Journal Rank:

JCR - Q1 (Pharmacology and Pharmacy) / CiteScore - Q1 (Medicine (miscellaneous))

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 17 days after submission; acceptance to publication is undertaken in 2.9 days (median values for papers published in this journal in the first half of 2025).