Special Issue

Computational Predictions of Molecules with Potential Therapeutic Effects: 2nd Edition

Message from the Guest Editor

We invite submissions of original research, reviews, short communications, and perspectives on biophysics, medicinal chemistry, novel therapeutic agents, drug delivery systems, and computer-aided drug design (CADD) for our special issue. This issue also aims to highlight the latest advancements and innovative research driving the convergence of these fields, covering topics such as structural and functional studies of biomolecules, e.g., the identification of new proteins or protein targets, and integration of artificial intelligence (AI) & machine learning (ML) into the design and optimization of therapeutic agents, innovative drug delivery systems, and structure-activity relationships. We seek to disseminate cutting-edge research, promote interdisciplinary collaborations, and showcase practical applications in biomedical research, with a particular emphasis on advancing drug discovery and development. Our goal is to highlight studies that not only contribute to the fundamental understanding of biological processes but also offer tangible solutions to current challenges in medicine. Submission should contains validation studies. We look forward to your pioneering contributions.

Guest Editor

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Deadline for manuscript submissions

30 April 2026

About the Journal

Message from the Editor-in-Chief

Because of your expertise in the field of drug sciences, I kindly invite you to consider publishing your current work, in the form of a research article or a review, in the open access electronic journal *Pharmaceuticals*. *Pharmaceuticals* is characterized by an active editorial board and a dynamic editorial staff. Manuscripts are peer-reviewed and a final decision is provided to authors within 4–6 weeks after submission. Papers are published on the web immediately after acceptance. For details on the submission process or any other matter, please do not hesitate to contact us.
We hope to handle your contribution to *Pharmaceuticals* soon.

Editor-in-Chief

Prof. Dr. Amélia Pilar Rauter
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