

Special Issue

Computational (In Silico) Approaches for Drug Target Discovery and Disposition

Message from the Guest Editors

Computational approaches have revolutionized drug discovery by enabling the more efficient and accurate identification of potential therapeutic targets. This Special Issue aims to showcase the latest advancements in and practical application of computational (in silico) tools throughout the process of drug development. We seek to foster cross-disciplinary collaborations among computational chemists, pharmacologists, biologists, and data scientists, thus driving innovation in predictive pharmacology and drug modeling. By featuring studies that integrate PBPK, PBBM, machine learning, and simulation, we hope to accelerate the design of safer and more effective therapeutics. We welcome contributions that explore emerging computational techniques for drug disposition. We welcome articles that detail the development, validation, or application of computational tools to drug–target interactions, ADME/Tox properties, and translational research. We also encourage the submission of studies that highlight clinical relevance and collaborative efforts between experimental and computational disciplines.

Guest Editors

Dr. Frederico Severino Martins

1. Faculty of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, São Paulo 14040-900, Brazil
2. Simulations Plus, Lancaster, CA, USA

Dr. Leonardo Luiz Borges

Central Campus, State University of Goiás, Anápolis, Goiás, Brazil

Deadline for manuscript submissions

20 August 2025



Pharmaceuticals

an Open Access Journal
by MDPI

Impact Factor 4.8
CiteScore 7.7
Indexed in PubMed



mdpi.com/si/231591

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

[mdpi.com/journal/
pharmaceuticals](https://mdpi.com/journal/pharmaceuticals)





Pharmaceuticals

an Open Access Journal
by MDPI

Impact Factor 4.8
CiteScore 7.7
Indexed in PubMed



[mdpi.com/journal/
pharmaceuticals](https://mdpi.com/journal/pharmaceuticals)



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

Departamento de Química e Bioquímica (DQB) e Centro de Química Estrutural (CQE), Institute of Molecular Sciences, Faculdade de Ciências, Universidade de Lisboa, Lisboa, Portugal

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, PMC, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Pharmacology and Pharmacy) / CiteScore - Q1 (Pharmaceutical Science)