



Computer Simulation for Drug Design and Medical Bioengineering

Guest Editors:

Prof. Dr. Catalin Buia

Department of Automatic Control
and Systems Engineering,
Politehnica University of
Bucharest, Splaiul Independentei
313, 060042 Bucharest, Romania

Prof. Dr. Speranta Avram

Department of Anatomy, Animal
Physiology and Biophysics,
Faculty of Biology, University of
Bucharest, Splaiul
Independentei, No 91-95, 050095
Bucharest, Romania

Deadline for manuscript
submissions:

closed (30 June 2023)

Message from the Guest Editors

Dear Colleagues,

The discovery of natural and synthetic chemical compounds as candidates for pharmaceutical drugs is essential scientifically, socially, and economically in medical and bioengineering fields. Improvements in bioinformatics and computational biology have increased the efficiency of many stages of the drug discovery pipeline. Computer-aided tools which are used in drug discovery are critical for many human pathologies. Special attention has been paid to drug design for cancers and brain pathologies and, in the last two years, for SARS-CoV2 infection. Bioinformatics methods such as molecular dynamics, molecular docking, fragment-based screening (FBS), and QSAR, are strategically used when new chemicals being considered for potential drugs. Pharmacological features, represented by pharmacokinetic (ADME), pharmacodynamic (targets discovery), and toxicity profiles are critical for assessing proposed chemical structures for new candidate drugs. Additionally, bioengineering tools being employed to develop in silico tools.

We welcome your submission for our Special Issue in Pharmaceutics, “Computer Simulation for Drug Design and Medical Bioengineering”.





an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Patrick J. Sinko

Department of Pharmaceutics,
Ernest Mario School of
Pharmacy, Rutgers University,
Piscataway, NJ 08854, USA

Message from the Editor-in-Chief

Pharmaceutics (ISSN 1999-4923) is an online open access journal on the science and technology of pharmaceutics and biopharmaceutics. The scientific community, the wider community and the general public have unlimited and free access to the content as soon as a paper is published; this open access to your research ensures your findings are shared with the widest possible audience. Please consider publishing your impressive work in this high quality journal. We would be pleased to welcome you as one of our authors.

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 & Pharmacy*) / CiteScore - Q1 (*Pharmaceutical Science*)

Contact Us

Pharmaceutics Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/pharmaceutics
pharmaceutics@mdpi.com
X@MDPIpharma