Special Issue

In Silico Approaches of Drug–Target Interactions

Message from the Guest Editor

In silico approaches are transforming modern pharmaceutics and biopharmaceutics by providing powerful tools for understanding drug–target interactions and optimizing therapeutics. Using computational techniques such as molecular modeling, docking simulations, molecular dynamics, and virtual screening, these methods predict binding affinities and selectivities between drug candidates and biological targets. Recent advances in machine learning and artificial intelligence have further refined these tools, improving drug design precision. Integrating ADME (Absorption, Distribution, Metabolism, and Excretion) predictions also ensures the selection of candidates with favorable pharmacokinetics.

This Special Issue aims to explore the latest advancements in these in silico methods, focusing on their role in enhancing therapeutic efficacy, safety, and efficiency in biomedical science.

We welcome original research and review articles addressing topics such as molecular modeling, machine learning applications, virtual screening, and the optimization of drug safety and efficacy. We look forward to your contributions to this dynamic field of computational pharmaceutics.

Guest Editor

Dr. Stefania Olla

Instituto di Ricerca Genetica e Biomedica, Consiglio Nazionale delle Ricerche, 09042 Monserrato, Italy

Deadline for manuscript submissions

30 November 2025

Pharmaceutics

About the Journal

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.

Editor-in-Chief

Prof. Dr. Patrick J. Sinko
Department of Pharmaceutics, Ernest Mario School of Pharmacy,
Rutgers University, Piscataway, NJ 08854, USA

Author Benefits

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)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 14.9 days after submission; acceptance to publication is undertaken in 3.3 days (median values for papers published in this journal in the first half of 2025).

MDPI