International Journal of Computational Biology and Drug Design

OA Special Issue on: "Computational Insights in Biomedical Discovery: From Biology to Drug Design"

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Introduction

Computational biology and drug design have emerged as powerful tools in the quest for novel therapeutics and insights into biological systems. This special issue aims to showcase the latest advancements, challenges, and applications in computational biology and drug design. The intersection of biology and computational science has led to the development of innovative tools that can model complex biological interactions, predict drug efficacy, and analyse vast datasets from genomic, proteomic, and metabolomic studies. This special issue seeks to highlight cutting-edge research that bridges the gap between computational models and practical biomedical applications, fostering a deeper understanding of biological phenomena and accelerating drug discovery.

Objective

The primary objective of this special issue is to showcase the latest advancements in computational approaches that are driving breakthroughs in biomedical research and drug design. We seek to bring together contributions from interdisciplinary fields to address critical challenges in modern biomedical research, promoting collaborations between computational scientists and experimental biologists. The goal is to provide readers with novel methodologies and insights that can be applied to enhance drug discovery pipelines and improve therapeutic outcomes.

Readership

This special issue is intended for a broad audience of researchers, professionals, and students working at the intersection of computational science and biomedical research. The target readership includes:

- Computational biologists and bio-informaticians
- Pharmaceutical researchers involved in drug design and development
- Machine learning experts focusing on biomedical applications
- Biotechnologists and systems biologists
- Academic researchers and postgraduates in biology, chemistry, and computational sciences
- Healthcare professionals interested in the applications of computational techniques in drug development

Subject Coverage

Suitable topics include, but are not limited, to the following:

- Computational modelling of biomolecular structures
- Molecular dynamics simulations
- Protein-Ligand docking and virtual screening
- Pharmacophore modelling and QSAR/QSPR studies
- High-throughput screening data analysis
- Systems biology and network pharmacology
- Drug repurposing and polypharmacology
- Computational toxicology and ADMET prediction
- Machine learning and artificial intelligence in drug discovery
- Structural bioinformatics and genomics
- Molecular evolution and phylogenetics
- Personalised medicine and precision drug design
- Computational approaches to antibiotic resistance
- Multi-omics data integration and analysis
- Drug delivery systems and nanomedicine

Notes for Prospective Authors

Submitted papers should not have been previously published nor be currently under consideration for publication elsewhere. (N.B. Conference papers may only be submitted if the paper has been completely re-written and if appropriate written permissions have been obtained from any copyright holders of the original paper).

All papers are refereed through a peer review process.

All papers must be submitted online. To submit a paper, please read our Submitting articles page.

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Important Dates

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Notification to authors: *30 June, 2025*

Final versions due by: *31 August, 2025*