

Special Issue

Artificial Intelligence and Machine Learning in Drug Development

Message from the Guest Editor

Human biological complexity and genomic variability lead to different responses to therapeutic approaches at both the individual and population levels. Molecular profiling is now able to stratify diseases into their distinct molecular subtypes for matching with appropriate drugs, thus beginning to shape a translational systems medicine for better tailored predictive and pharmacotherapeutic guidance. This new research paradigm, powered by state-of-the-art artificial intelligence (AI)/machine learning (ML)-based prediction algorithms, presents great challenges and opportunities for researchers in the field.

This Special Issue welcomes original research, short communications, and review papers. Potential topics include, but are not limited to, the application of AI/ML to: target identification and characterization; protein networks/pathways prediction; mechanism of disease; drug–target complex formation and characterization; drug identification; drug repurposing; generation of novel drug candidates; drug efficacy metrics; and toxicology, biopharmaceutical properties prediction, etc. Wet-lab and clinical-data-based submissions with biomolecular experiments are welcomed.

Guest Editor

Dr. Irina Moreira

1. Department of Life Sciences, University of Coimbra, Calçada Martim de Freitas, 3000-456 Coimbra, Portugal
2. Center for Innovative Biomedicine and Biotechnology, University of Coimbra, 3004-535 Coimbra, Portugal

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Prof. Dr. José L. Quiles
Department of Physiology, Institute of Nutrition and Food Technology
"Jose Mataix", Biomedical Research Center, University of Granada,
Avda. Conocimiento s/n, 18100 Armilla, Granada, Spain

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