Special Issue

Advanced In Silico Methods and Digital Platforms for Rational Drug Design and Predictive Toxicology

Message from the Guest Editors

In recent years, the unprecedented advancements in computer-assisted drug discovery and predictive toxicology have allowed powerful and reliable models to be built from large amounts of data. In this respect, pharmaceutical companies and academia have made remarkable investments to generate customizable tools, services, and technologies that are capable of reaching impressive standards. For this Special Issue, we call on medicinal chemists and toxicologists to share their experiences on the design of novel methods and the implementation of digital platforms, in order to provide practical answers to challenging issues related, but not limited to, drug repurposing, target fishing, bioactivity prediction, de novo design, molecular docking, molecular dynamics, homology modeling, virtual screening, QSAR, and alternative methods for the prediction of toxicological endpoints. In light of this, we are delighted to invite international scientists to contribute to this Special Issue with research articles, mini-perspectives, and brief articles describing recent methods and platforms for drug discovery and predictive toxicology.

Guest Editors

Prof. Dr. Orazio Nicolotti

Dr. Daniela Trisciuzzi

Dr. Nicola Gambacorta

Deadline for manuscript submissions

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

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. Maurizio Battino
Department of Odontostomatologic and Specialized Clinical Sciences, Sez-Biochimica, Faculty of Medicine, Università Politecnica delle Marche, Via Ranieri 65, 60100 Ancona, Italy

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