

## Special Issue

# Machine Learning in Small-Molecule Drug Discovery

### Message from the Guest Editor

Machine learning has evolved as a key technology in small-molecule drug discovery. A rich body of literature documents the capacity of machine learning approaches to design and identify compounds with desired properties, including favorable bioactivity spectra, beneficial ADME properties, low toxicity, synthetic accessibility, and novelty in molecular structure.

On these grounds, this Special Issue seeks original research articles and reviews focusing on all aspects of machine learning relevant to small-molecule drug discovery. Scientists are particularly encouraged to submit contributions on the development and application of machine learning methods for the design of bioactive small molecules with desired chemical and pharmacological properties, the prediction of the macromolecular target(s) of compounds, and the assessment and optimization of ADME properties. Further topics of high interest include automation in drug design, integrated models, machine learning in drug repurposing and natural products research, virtual screening, the performance of methods as a function of the quantity and quality of the training data, concepts of the applicability domain, and benchmarking.

### Guest Editor

Prof. Dr. Johannes Kirchmair

Department of Pharmaceutical Chemistry, University of Vienna,  
Althanstrasse 14, 1090 Vienna, Austria

### Deadline for manuscript submissions

closed (31 March 2021)



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

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### Message from the Editor-in-Chief

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.

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### 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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