International Journal of
Molecular Sciences

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Machine Learning in Small-Molecule Drug Discovery

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)

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.

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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

Message from the Editor-in-Chief

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Journal Rank: JCR - Q1 (*Biochemistry & Molecular Biology*) / CiteScore - Q1 (*Inorganic Chemistry*)

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International Journal of Molecular Sciences Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

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