Special Issue

Drug Discovery: New Concepts Based on Machine Learning

Message from the Guest Editors

The ML/Al-based methodology era enables and opens new avenues that can boost the growth of new methods and their increasing importance. The computational-aided drug design exposes the impacts on drug discovery (new targets, the targeting of small molecules, targeted protein–protein interactions, SAR generation using data-driven experimental databases and integrated platforms, drug delivery pathways, etc.). The Special Issue will cover the following topics: targeting small molecules;

protein-protein interactions;

protein dynamics;

docking studies:

logP and pKa computational methods;

solvation-free energy;

QSPR/QSAR studies;

fragment-based drug discovery (FBDD). We also welcome papers dedicated to computational and machine learning for drug discovery. The new ML approach for drug design and CADD was developed and designed for de novo drug design methods to generate a space for novel chemical compounds with desirable properties in a cost-efficient manner. We are happy to welcome papers dedicated to fragment-based drug discovery (FBDD) as a powerful tool to recognize and classify a new compound as the initial point for drug development.

Guest Editors

Dr. Miroslava Nedyalkova

Department of Chemistry, University of Fribourg, Chemin du Musée 9, 1700 Fribourg, Switzerland

Dr. Andrew S. Paluch

Department of Chemical, Paper, and Biomedical Engineering, Miami University, 64 Engineering Building 650 E High Street, Oxford, OH 45056, USA

Deadline for manuscript submissions

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

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Editor-in-Chief

Prof. Dr. Patrick J. Sinko

Ernest Mario School of Pharmacy, Rutgers, The State University of New Jersey, William Levine Hall, Room 225C, 160 Frelinghuysen Road, Piscataway, NJ 08854-8020, USA

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