biomolecules

IMPACT FACTOR 5.5

Indexed in: PubMed

CITESCORE 8.3

an Open Access Journal by MDPI

Machine Learning for Molecular Modelling in Drug Design

Guest Editor:

Dr. Pedro J. Ballester
Cancer Research Center of Marseille, INSERM U1068, F-13009 Marseille, France

Deadline for manuscript submissions:
closed (25 September 2018)

Message from the Guest Editor

Machine Learning (ML) has become a crucial component of early drug discovery. This research area has been fuelled by two main factors. The first one is the fast-growing availability of bioactivities between molecules of known chemical structure and non-molecular and molecular targets. This trend has been catalysed by the development of community resources (e.g., ChEMBL, PubChem or PDB) that facilitate re-using these data sets for predictive modelling. The second factor is the easy access to high-quality implementations in R or Python of a range of ML algorithms, along with the continuous introduction of new advances (e.g., XGBoost, deep learning or conformal prediction). As a result, an increasing number of data-driven ML models are being proposed and found advantageous in some way to identify new starting points for the drug discovery process.

We invite scientists working on this area to submit their original research or review articles for publication in this Special Issue. Topics of interest include (but are not limited to) docking, QSAR, target prediction, virtual screening or lead optimization. Both application and methodology research studies are welcome.

biomolecules

IMPACT FACTOR 5.5
Indexed in: PubMed
CITESCORE 8.3

an Open Access Journal by MDPI

Editors-in-Chief

Prof. Dr. Peter E. Nielsen
Department of Cellular and Molecular Medicine, Faculty of Health and Medical Sciences, University of Copenhagen, Blegdamsvej 3C, DK-2200 Copenhagen, Denmark

Prof. Dr. Lukasz Kurgan
Department of Computer Science, Virginia Commonwealth University, Richmond, VA 23284, USA

Message from the Editorial Board

Biomolecules is a multidisciplinary open-access journal that reports on all aspects of research related to biogenic substances, from small molecules to complex polymers. We invite manuscripts of high scientific quality that pertain to the diverse aspects relevant to organic molecules, irrespective of the biological question or methodology. We aim for a competent, fair peer review and rapid publication. Please look at some of the exciting work that has been published in *Biomolecules* so far. We would be delighted to welcome you as one of our authors.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.
High Visibility: indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Embase, CAPlus / SciFinder, and other databases.
Journal Rank: JCR - Q1 (*Biochemistry & Molecular Biology*) / CiteScore - Q1 (*Biochemistry*)

Contact Us

Biomolecules Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/biomolecules
biomolecules@mdpi.com
𝕏@Biomol_MDPI