Special Issue

QSAR and Chemoinformatics Tools for Modeling

Message from the Guest Editor

In the past decade, quantitative structure–activity relationships (QSARs) have become a well-established field of scientific research, a field where many different mathematical tools are applied to detect predictive relationships between molecular structure and pharmacological activities, toxicological/ecotoxicological properties, and adverse effects of molecules on human health.

In the proposed Special Issue, the main idea is not only to present QSAR results on new datasets/modelling campaigns, but also to compare different chemometric and chemoinformatic tools on benchmark data sets, especially including (together with the classical regression and classification methods) read-across approaches, ranking models, machine learning, and deep learning methods.

Authors are also invited to pay attention to the concept of the applicability domain of the models, their prediction ability, and models obtained by data fusion and consensus approaches.

Molecular applications aimed to model endocrine disruptors effects, carcinogenicity, and mutagenicity as well as studies on *omics* data will be particularly appreciated.

Guest Editor

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Deadline for manuscript submissions

closed (31 October 2019)

International Journal of Molecular Sciences

an Open Access Journal by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed

mdpi.com/si/21709

International Journal of Molecular Sciences
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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.

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