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QSAR and Chemoinformatics Tools for Modeling

Guest Editor:

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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.