Special Issue

Data and Low-Data Tools for Artificial Intelligence in Medicinal Chemistry

Message from the Guest Editors

In the last few years, the scientific community has witnessed the renaissance of so-called “artificial intelligence” (AI) methods in many scientific domains. This unparalleled emergence of AI can also be observed in medicinal chemistry and toxicology, where machine learning is starting to be routinely applied for several tasks.

In this Special Issue, we welcome original research articles and reviews aimed to improve the current status of data and their usage for AI in medicinal chemistry and related fields. The Special Issue will include, but is not limited to, ligand- and structure-based approaches, molecular design, virtual screening, target identification, drug repurposing as well as bioactivity, safety, and ADMET property prediction. We particularly welcome papers focused on the creation and curation of novel datasets or describing the curation and/or usefulness of well-established databases. We also encourage the submission of papers addressing the development/application of AI approaches in low-data regimes. Papers providing accessible code and data are also particularly welcome.

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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