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EDITORIAL

Advanced Editorial to announce a JCAMD Special Issue on Artificial Intelligence and Machine Learning

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The application of Machine Learning and Artificial Intelligence methods to molecular design is an area of sustained but dramatically increasing current interest. The collision of these two different domains of knowledge often leads both to synergies and advances, but also to the re-discovery of known challenges when domain knowledge and experience are not properly transferred. To support the effective cross-fertilisation in a time of increasing productivity, JCAMD will be publishing a special edition on the application of AI methods to molecular design problems, with original peer-reviewed papers from leading groups in the field. Complementing other timely discussions of specific flavors of "AI for drug discovery", this special issue will focus on providing a comprehensive overview of the contributions that current machine learning expertise and technology has on distinct, classical challenges of cheminformatics and automated molecular design.

Specifically, a major focus will be on the role of data—highlighting issues of data set curation, size, and the assessment of domain coverage. Furthermore, we will cover the topic of de novo generative chemistry; how to make it efficient and the output relevant to the problem at hand. We will discuss the tension between exploration and exploitation as well as between novelty and synthetic feasibility. Consequently, the advances in retrosynthesis tools will be addressed, examining our ability to rigorously and effectively apply retrosynthetic analysis to a molecule or even a library of structures. This is one factor in the assessment of machine learning tools. The effect of different multiparametric optimisation schema on the fitness landscape is key to our understanding of the metaparameter used to create models. Even though models are quick to use, they still take time and care to set up. This also relates to the next topic of particular importance: validation. How do we know when an AI method has done significantly better than current state-of-the-art workflows? How should we set up suitable standards for control experiments? What standards are needed for publication and what can be considered relevant progress in the field?

The Special Issue on AI in Molecular Design will publish innovative studies that discuss and tackle these questions to contextualize the recent hype of artificial intelligence surrounding the established field of computer-guided molecular design and provoke further debate and sustained research.

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