Editorial

Artificial Intelligence (AI) is the ability of machines to respond in seemingly intelligent ways, producing outputs in response to new inputs without being expressly programmed to do so. Unlike traditional computer programs, which generate outputs based on explicit sets of instructions, AI systems are designed to make predictions based on data-driven models. As a result, the use of models and data constitutes essential components of this strategy.

AI has the potential to be used for a variety of tasks in the field of chemistry, where complex and often hidden correlations are frequently present in data sets. Because of tremendous expansion in computing power, open-source machine-learning frameworks, and increasing data literacy among chemists, AI is becoming an essential framework for tasks such as molecular property prediction, enablement of laboratory automation, prediction bioactivities of new molecules, optimization of reaction conditions, and recommendation of synthetic pathways to target molecules.

Given its history of emerging medium-large sized chemical companies, Switzerland has served as an incubator since the dawn of the AI revolution. This same journal, CHIMIA, published the first issue on 'Artificial Intelligence in Swiss Chemical Research' in 2019 (*CHIMIA* **2019**, *73*, issue 12). Since then, AI has been at the core of several activities that in the last two years aimed at speeding up the transformation of chemical industries into high-tech businesses. From a community perspective, the year 2021 saw the formation of a global network of digital chemists to collaborate on the research and use of machine learning technologies in chemistry. With the help of the Swiss Chemical Society, this community built the groundwork for a Spring School in Digital Chemistry. The first session, scheduled for April 2023, will focus on digital chemistry technologies for drug discovery.

This is an amazing time to be alive, but where should Swiss Research go in the near future?

We must increase our efforts to develop standards that characterize data, their provenance and uncertainty, as well as the development of technologies to capture and digitalize data more easily. This is not only an academic exercise, since data quality and standardization are crucial for any industrial adoption.

We will need to demonstrate to the rest of society the benefits of adopting AI for real world problems by doubling down the efforts on complex industrial challenges. This is a crucial step for the significant shift towards the digital, machine learning age.

Finally, sustainability should be one of the most critical global concerns for Swiss chemical research. This frequently necessitates taking into account multiple disciplines and their complex interactions, a problem that can be hardly tamed by humans but that is easily facilitated with the capabilities of AI. An example being the recently kicked-off NCCR Catalysis, a significant effort addressing sustainability by putting machine learning and digitalization at the center of research efforts for innovating chemical catalysis.

For this issue of CHIMIA, we selected a collection of Swiss research chemists' contributions and perspectives on AI method development and implementation, ranging from the use of AI/ML for: chemical reaction optimization using a wide range of approaches, chemical reaction prediction, improving water quality, enabling autonomous laboratories, to treasuring the lesson learned from AI/ML in computer science when contextualized with its development in chemistry.

As these new methodologies become more deeply embedded in our discipline, we should learn from lessons learned in other sectors, including the over-reliance on AI or possible societal gaps. Both editors are optimistic in the chemical community's successful, trustworthy, and helpful adoption of AI/ML and that it is driven by the same rigorous considerations that characterized the adoption of past technologies in this field.

We hope you all will enjoy reading!

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SCS Spring School on Digital Chemistry, April 16-20, 2023, www.aisem.scg.ch

The CHIMIA Editorial Board thanks the guest editors, Torsten Luksch and Teodoro Laino, for putting together this very interesting update on Artificial Intelligence in Chemical Research that demonstrates the impressive advances the field has made in a very short time.

Front cover image: The image was created by Teodoro Laino. Image source: created with AI (DALL-E)