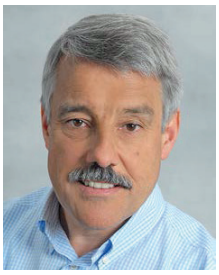
Editorial

Torsten Luksch



Hans Peter Lüthi

Artificial Intelligence: New Opportunities for Chemical Research?

Artificial Intelligence (AI), *i.e.* intelligence demonstrated by machines, became an academic discipline already in the mid-fifties, at a time when modern computers were still in their infancy. The vision that one day computers would mimic cognitive functions and be able to solve problems based on their own learning, was already present in the heads of the early computer scientists.

After several waves of optimism, followed by waves of frustration, AI has claimed its spot in science and technology. It has reached our daily life: Applications such as near-human-level speech or object recognition, handwriting transcription and machine translation mark the increasingly strong presence of AI.

Now that AI is established in many fields, there is the question of the status and potential of the discipline for chemical research. Chemistry always had an eye on these emerging opportunities: Automated spectra interpretation or computer-aided synthesis planning are two examples of intense activity of early adopters in chemistry.

Having access to huge data-storage facilities, unprecedented compute power and extensive software libraries, the development and use of machine learning tools is no longer as demanding as it was in the past. Programming a neural network, for instance, does not require writing countless of lines of code any more (such as in ref. [1]), but simply comes down to making a few library calls. Basic knowledge of a programming language such as Python will do.[2]

However, a key requirement for the development of successful AI applications is the availability of large and high quality datasets. As pointed out by various authors in this thematic issue of CHIMIA, the pre-processing of data still accounts for most of the effort involved in the development of an application. To train a machine, there is not only the need for large data volumes but also for 'negative information', *i.e.* information on reactions or other processes that will *not* work under the given conditions. Our community has a culture of communicating positive results. To leverage the new technologies, we will need to focus on at least two data-related aspects: can we put in place an efficient mechanism to publish negative data and can we establish best practice in data provision to journals to support open data sharing?

Having pizza and beer one evening in 2017, the Basel Modelers, an informal group of computational chemists and cheminformaticians from industry and academia, decided to look at the AI developments in chemistry more closely. They invited leaders in the area of AI from industry and academia to a symposium entitled 'Artificial Intelligence in Chemical Research (AICR)' hosted by Syngenta in Stein (AG). The goal of the symposium was to have an answer to the question "what is in it for chemical research?"[3]

The response of the community to this symposium was overwhelming: The available 200 seats for participants were filled in no time. Not only researchers, but also managers and decision makers, most of them from industry, were present. The event was a very positive experience, if not an eye-opener for most participants. We decided to maintain the momentum created by this event and to make an effort to build a Swiss community of researchers using or developing AI methods.

This issue of CHIMIA showcases contributions of Swiss research chemists to AI method development and application. The exploration of the chemical space, quantum chemistry and molecular dynamics based on machine learning methods, data-driven chemical reaction prediction all the way to an emerging discipline such as pharmacoepidemiology, form the scope of the subject matter addressed in this issue of CHIMIA. Given the wealth of expertise of the Swiss AICR community, there are plenty of opportunities for collaboration, including collaboration in the pre-competitive space of industry research.

Enjoy reading!

Torsten Luksch
Syngenta

Hans Peter Lüthi
ETH Zurich

[1] T. H. Fischer, W. P. Petersen, H. P. Lüthi, 'A new optimization technique for neural networks used in prediction of force constants of large molecules', *J. Comp. Chem.* **1995**, *16*, 923
[2] F. Chollet, 'Deep Learning with Python', Manning, Shelter Island (NY), **2018**.
[3] *https://ai18.chemistrycongresses.ch/en/*

The Editorial Board of CHIMIA expresses its thanks to the coordinating guest editors Torsten Luksch and Hans Peter Lüthi for their efforts in realizing this issue on Artificial Intelligence in Swiss Chemical Research, providing an excellent overview to an area of great future potential to chemistry.