SOCIÉTÉ CHIMIQUE DE GENÈVE

Digital chemistry: the dual impact of algorithmic and automation illustrated by Swiss Cat+

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Digital chemistry, a field critical for future scientific breakthroughs, relies profoundly on the availability and quality of data. Currently, the chemical data landscape is marked by its sparse, heterogeneous characteristics, and by the slow and costly nature of its production. This situation directly impacts the development of generative algorithms, as their efficacy is contingent upon the caliber of the datasets used for training. The principle "garbage in, garbage out" aptly describes the dependency of output quality on both the algorithm's sophistication and the dataset's robustness.

To address these challenges, automation emerges as a transformative solution for enhancing both the quality and quantity of chemical data. However, implementing automation in chemistry presents significant hurdles, requiring innovative approaches to realize its full potential. One such approach is closed-loop optimization, which holds particular promise in the domain of catalysis. In catalysis, despite the known existence of many significant molecules, there lacks a systematic set of rules for classification and prediction, making the pursuit of rational discovery and design complex.

Recognizing these challenges and opportunities, we have launched the Swiss Cat+ national research infrastructure at EPFL and ETHZ. This initiative aims to harness the powers of automation and closed-loop systems to revolutionize data acquisition, processing, and utilization in digital chemistry, setting a new standard for research and development in the field.

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