

Artificial Intelligence and Analytical Chemistry: How Excited Should We Get

The introduction of advanced chromatography (e.g. GCxGC and LCxLC), advanced mass spectrometry (e.g. qToF and Orbitrap), and their combinations has resulted in wide range of opportunities and challenges. These new analytical tools, with their superior resolving power, provide the possibility of comprehensive chemical characterization of complex samples from environmental to biological matrices. At the same time, these instruments generate a vast amount of complex data to be processed, which require high levels of automation, due to the sheer size of the generated data. Machine Learning (ML) and Artificial Intelligence (AI), as of today, are considered the way forward to handle such complex and large datasets for both pre-processing and mining/interpretation.

In this presentation a selected set of case studies, where ML and AI were highly relevant, will be discussed. These studies cover a wide range application from signal processing to a complete exposomics case study. Through these case studies, the importance of ML and AI for automation of the data processing as well as the further mining of the data will be demonstrated. Finally, future plans for furthering the application of ML and AI in analytical chemistry will be discussed.