

Machine Learning for Bioactivity Prediction from Chromatographic and Mass Spectrometric Data

Background

Assessing the safety of complex chemical mixtures, such as those present in recycled food contact materials, is a huge challenge with many open knowledge gaps. One main issue is the observed genotoxicity of recycled polyolefins. An interdisciplinary approach between microbiology, analytical chemistry and machine learning tries to investigate the reasons. Previous work demonstrated the link between bioassays and instrumentally detected compounds. However, it remains unclear whether risk identification can be automated using data-driven approaches and machine learning techniques.

Objective

Can machine learning predict genotoxicity from chromatographic and mass spectrometric fingerprints of complex chemical mixtures? Within a collaboration between the **Institute of Analytical Chemistry and Food Chemistry (ACFC)** and the **Signal Processing and Speech Communication Laboratory (SPSC)** at TU Graz, this master thesis project aims to investigate the potential of machine learning for the interpretation of analytical chemistry data and the prediction of bioactivity.

Candidate Profile

We are looking for a highly motivated student with an interest in interdisciplinary research at the interface of analytical chemistry and data science. In particular,

- Students in Chemistry with a strong background in analytical chemistry, chromatography and/or mass spectrometry and a keen interest in machine learning, statistics and data analysis.
- Students in Computer Science, Data Science, with expertise in machine learning, artificial intelligence, statistics and signal processing and an interest in applying these methods to real-world analytical chemistry challenges.

What We Offer

- An interdisciplinary research project at the interface of analytical chemistry and artificial intelligence with joint supervision by two research groups at TU Graz.
- Access to state-of-the-art analytical instrumentation and real-world datasets.
- Opportunities to contribute to scientific publications and follow-up research projects.
- Paid position as student project assistant for 6 months.

Starting Date: As soon as possible.

Contacts

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