



MSc Thesis in Environmental Chemistry

Title of Thesis: Building machine learning models to predict biotransformation half-lives of micropollutants in activated sludge

Description / Project:

The abundance of micropollutants in the environment is a threat to the integrity of water and soil ecosystems. For many chemicals such as pharmaceuticals and pesticides, biodegradation is the main route of elimination and is harnessed by biological wastewater treatment to reduce the environmental load of chemical pollution. In activated sludge, microorganisms catalyse biotransformation reactions that break down the micropollutants into transformation products. The biodegradability of compound in activated sludge is therefore an important indicator of its environmental persistence.

Predicting biodegradation half-lives of chemicals is not only important to assess their potential environmental risk, but it can also be used in the design of new pharmaceuticals to eliminate highly persistent compounds at an early stage in drug development. However, predicting half-lives from molecular structure is an open challenge, which is mainly due to the scarcity of suitable and standardized data.

In this project, we will use data analysis tools to analyse and curate an in-house database containing biodegradation data for 91 micropollutants in activated sludge. We will then use the curated to build machine-learning models that can predict biotransformation half-lives in sludge and evaluate the new models against existing tools.

Methods:

Data curation and analysis, cheminformatics, machine learning, scripting in Python

What we expect from you:

Ideally, some experience in scripting with R and/or Python or at least an avid interest to learn it.

Starting date: Any time, preferentially before September 2022

Responsible IfC professor: Prof. Kathrin Fenner (Universität Zürich und Eawag)

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