Project title: The influence of enviro-chemical characteristics on ecosystem exposure to ionizable organic compounds.
Level: Master and/or Bachelor
Start: a.s.a.p.
Project duration: 12 weeks (BSc)/ 24 weeks (MSc)
Project form: Literature study, database analysis, modelling
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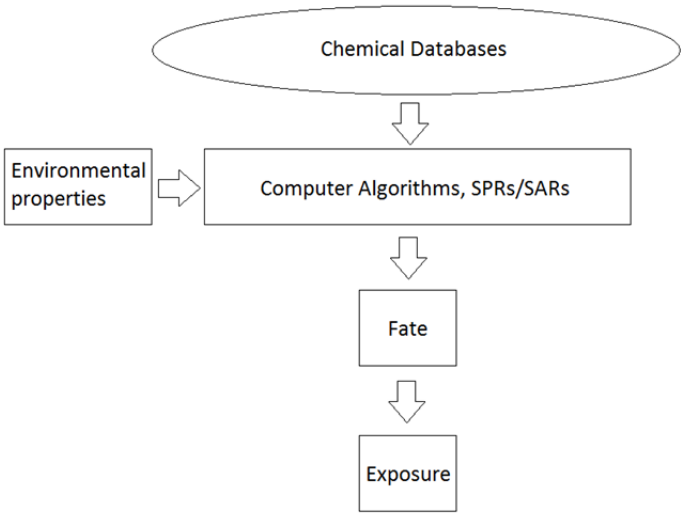
Description of the project:
More and more data show that pharmaceuticals, i.e., ionizable organic molecules, enter the environment. They have for example been detected in surface water and crops. Organisms exposed may suffer adverse effects, such as reproductive disorders from hormone disrupting substances (e.g., estradiol) or death of vultures due to diclofenac exposure (India/Pakistan). Though regulation and monitoring is increasing, the sheer number of compounds and exposure pathways calls for prioritization and intelligent testing.

Commonly, environmental concentrations are determined by partitioning and compartment-specific degradation kinetics. These processes are dictated by the complex interplay between enviro-chemical properties, the compound's bioavailability and the physiology, behavior, and metabolism of the biota. Pharmaceuticals form a special case because their varying ionization, complexation and adsorption capacity make partitioning and chemo-, photo- and bio- degradation highly variable.

In this internship, you will explore the current structure-property (SP) structure-activity (SA) modelling tools that predict degradation and partitioning based on molecular properties. You will perform a sensitivity analysis of the models as function of enviro-chemical characteristics, e.g. pH, hardness, DOC content, turbidity. This may be achieved by evaluating different environmental concentrations reported in literature by implementing specific biophysicochemical characteristics in the reviewed modelling tools. Characteristics may be implemented following the interests of the student representing e.g. different environmental media or sewage treatment plants. Ultimately, you will use the models to identify leading enviro-chemical fate parameters and develop mechanistic/empirical relationships predicting the environmental concentrations of ionizable organic molecules.



Literature:

Monteiro SC, Boxall ABA. **2010**. Occurrence and Fate of Human Pharmaceuticals in the Environment. *Reviews of Environmental Contamination and Toxicology* 202:53-154.

Lei H, Snyder SA. **2007**. 3D QSPR models for the removal of trace organic contaminants by ozone and free chlorine. *Water Research* 41:3271-3280.