Universität Zürich[UZH]

Department of Chemistry

MSc Thesis in Environmental Chemistry

Title of Thesis: Transformation products of pharmaceuticals – reading across environmental compartments in regulatory tests to assess biotransformation

Description / Project:

Pharmaceuticals are ubiquitously found in surface freshwater bodies because they are not completely removed during conventional wastewater treatment. Once in the environment, pharmaceuticals undergo degradation processes that form transformation products (TPs), which could be linked to specific biotic and abiotic reactions. Standard tests to assess biotransformation of pharmaceuticals in the environment use batch experiments of the compound in different media (sediment, water and/or soil). Biotransformation tests using activated sludge from wastewater treatment plants are more time and cost efficient than regulatory simulation tests. However, it is important to assess if biotransformation reactions in activated sludge are representative of those in environmental compartments. Therefore, a systematic comparison between TPs of pharmaceuticals formed in short biotransformation tests in activated sludge and TPs in standard simulation tests with sediment, water and/or soil is needed.

In this project, we aim to screen and identify TPs of a selected group of known pharmaceuticals in high-resolution mass spectrometry data from batch experiments performed in activated sludge. Samples from the batch experiments are measured by liquid chromatography- high-resolution tandem mass spectrometer (LC-HRMS/MS). Mass spectra are acquired by full-scan positive mode and MS2 is aquired in data dependent Top5. A suspect list of TPs will be obtained from standard biotransformation tests (i.e. OECD 307, 308 and 309) in the literature and regulatory risk assessment brochures. Non-target screening of additional TPs in the batch experiments might also be included.

Methods:

LC-HRMS/MS (QExactive Plus, Thermo Scientific) data analysis, target, suspect or non-target screening, use of Compound Discoverer / TraceFinder or similar software

What we expect from you:

Interest in biotransformation processes, suspect and non-target screening of chemicals, analysis of large datasets and interpretation of mass spectra (MS2) data.

Starting date: Spring / Summer / Autumn

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