**Early identification of organic contaminants by a multimedia fate model and high resolution mass spectrometry**

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There are several tens of thousands of organic chemicals on the market and it is an important, but challenging task to identify those causing a potential long-term environmental contamination. Analytical campaigns and monitoring programs can cover only a selection of chemicals, therefore strategies for identifying priority chemicals for analytical measurements are needed. In this study we aim to identify relevant chemicals starting from an extensive computer-based screening from the Swiss customs statistics and other databases indicating a present or previous use in Switzerland, followed by a complementary monitoring campaign of representative soils and sediments, two environmental matrices that can act as integrators of many inputs within a catchment and until now not well explored.

The first step in the study was to developed a phase partitioning multimedia environmental fate model with dimensions of Switzerland to identify chemicals with a presence of 90% or more in soil or sediment. The results show that 2550 out of 9187 chemicals have high affinity to soil or sediment with many of these chemicals containing fluorinated, chlorinated and brominated aromatic and aliphatic substances often with highly branched substituents, ether and tertiary amine groups, trifluoromethyl groups, and phosphate ester groups. As a first approach, a subgroup of only halogenated chemicals (520 chemiclas) were prioritized to facilitate the analytical analysis due to their characteristic isotopic pattern and often with mass defects outside the sample matrix which can reduce the effect of analytical interferences.

Furthermore, 14 sites from the Swiss National Soil Monitoring Network (NABO) were chosen according to land use and vicinity to industrial and urban areas, as well as previously measured soils with persistent organic chemicals such as polychlorinated biphenyls. Sediment cores were obtained from Lake Greifensee, located in a semi-urban area in the north of Switzerland. Temporal characterization (up to 80 years) was conducted at different location points to obtain a coarse survey of the contamination of the lake and different patterns of organic contaminants with time due to wastewater treatment plants effluents and agricultural runoff.

Soils and sediments were extracted by means of pressurized liquid extraction and analyzed by liquid chromatography followed by electrospray ionization (ESI) coupled to high resolution mass spectrometry (HRMS/MS). The list of selected chemicals was further filtered by eliminating compounds that were not likely to be ionized by ESI using rules like the presence or absence of functional groups. The complete list of “suspect candidates” that were estimated to fall in the domain of the analytical method (367 suspects) were then screened in the chromatograms using their exact mass of the expected ions [M+H]+ or [M−H]−and other important adducts (e.g., NH4+, Na+, HCO2−,and H3C2O2-).

Identification was performed with the aid of *in silico* methods (MOLGEN-MS/MS and MetFrag), a public repository of mass spectral data (MassBank) and retention time/partitioning information. Preliminary results show that the combination of the developed multimedia fate model and HR-MS analysis resulted in the successful identification of different antibacterial substances such as hexachlorophene, triclocarban, triclosan and diferent fungicides like propiconazole, as well as the tentative identification of further chlorinated, brominated and quaternary ammonium compounds.