

TARGET, SUSPECT AND NON-TARGET SCREENING APPROACHES TO IDENTIFY ORGANIC CONTAMINANT RECORDS IN LAKE SEDIMENTS¹

CHIAIA-HERNANDEZ A.C.^{1,2}, SCHYMANSKI E.L.¹ and HOLLENDER J.^{1,2}

¹ Environmental Chemistry Department, Swiss Federal Institute of Aquatic Science and Technology (Eawag), Überlandstrasse 133, 8600 Dübendorf, Switzerland, ² Institute of Biogeochemistry and Pollutant Dynamics, ETH Zurich, Universitätstrasse 16, 8092 Zurich, Switzerland, E-mail: juliane.hollender@eawag.ch

Lake sediment cores provide a valuable record of historical persistent contamination since they can act as integrators of many inputs within a catchment. In this study a comprehensive screening of medium polar organic contaminants using high resolution mass spectrometry (HRMS) coupled to HPLC was carried out to provide records of historical contamination of previously unreported compounds. A combination of target, suspect and non-target screening using LC-ESI-HRMS/MS was performed on extracts from sediment cores from Lake Greifensee and Lake Lugano located in the north and south of Switzerland, respectively. In the target analysis on average 16 of 200 compounds were detected in both lakes with the most prominent substance classes corresponding to personal care products, pesticides, and biocides. A suspect list was compiled from consumption data of pesticides and pharmaceuticals and refined using the expected method coverage and a combination of automated and manual filters on the resulting measured data. Non-target identification efforts were focused on masses with Cl and Br isotope information available that exhibited mass defects outside the sample matrix, to reduce the effect of analytical interferences. In silico methods combining the software MOLGEN-MS/MS and MetFrag were used for direct elucidation, with additional consideration of retention time/partitioning information and the number of references for a given substance. The combination of all available information resulted in the successful identification of three suspects (the biocide chlorophene, the pharmaceutical flufenamic acid and the pesticide lufenuron) and two nontarget compounds (the bacteriostatic agent hexachlorophene and the mothproofing agent flucofuron), confirmed with reference standards, as well as the tentative identification of two chlorophene congeners (dichlorophene, bromochlorophene) that exhibited similar time trends through the sediment cores. The temporal pattern of the pollution between 1950 and 2010 was reconstructed for all suspect and non-target compounds, revealing different trends. The concentrations of many urban contaminants originating from wastewater correlated with the highest phosphorus input into lake Greifensee as a proxy for treatment efficiency, while concentrations of substances that only came into use more recently or for that the usage increased peaked later.

Keywords: High-resolution mass spectrometry screening, Sediment matrix, Organic Contaminants

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¹ Invited speech