



Optimizing nontarget workflows for identification of organic contaminants in various matrices

av

Florian Dubocq

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Opponent: Professor Juliane Hollender
Department of Environmental Chemistry, Eawag
Dübendorf, Switzerland

Örebro universitet
Institutionen för Naturvetenskap och Teknik
701 82 ÖREBRO

Abstract

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Since year 2000, production of chemicals around the world has more than doubled. Chemicals are used in many and diverse applications in our everyday life and even if their properties are useful, some can have a negative impact on environment and humans. It is thus important to monitor these chemicals to better understand their impact on the environment and human health.

In this thesis, nontarget analysis (NTA) was used to detect and identify organic compounds in various environmental and health relevant matrices such as fish, indoor dust, aqueous film-forming foams (AFFFs) and fire emissions. The aim was to optimize the workflow by extracting relevant chemical information from the analysed matrix and mitigate bias in reported results. Tests were thus performed to optimize sample preparation for fish and dust samples as well as processing data from high-resolution mass spectrometry analysis of dust, AFFFs and fire emissions.

Statistical analysis such as analysis of variance (ANOVA) with the help of hierarchical cluster analysis (HCA) enabled the detection of outliers in dust, AFFFs, and gas and soot from fire emissions. Mass defect (MD) plot analysis further enabled the detection of various relevant compounds according to their functional groups and structural properties. The nontarget analysis workflow was supported by target and suspect screening analysis to confirm the efficiency of the optimized overall workflow. Various classes of compounds could be detected and tentatively identified such as flame retardants, liquid crystal monomers or bisphenols in dust samples, organofluorine and fluorine-free surfactants in AFFFs, and flame retardants and hydrocarbons in gas and soot samples. Quality controls were also performed to assess the performance of the optimized workflow.

Keywords: Nontarget analysis, workflow optimization, statistical analysis, mass defect plot, organic contaminants, environmental matrices

Florian Dubocq, School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden, Florian.Dubocq@gmail.com