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Production of chemical compounds increases over years and their utilizations are diverse, both for industries, agriculture, and domestic purposes. Even if chemicals are useful for many domains, some can have negative impacts on environment, wildlife, or human health. To better estimate the quantity released and the potential impacts on the environment and human health, chemical compounds need to be monitored. However, chemical ingredients in products are often not disclosed and it is thus important to study the chemical composition of environmentally relevant matrices. Early days of chemical monitoring were mainly relying on target analysis, which means that only a set of known compounds was analysed qualitatively and/or quantitatively. During recent years, new methods called nontarget analysis (NTA) were developed to increase the chemical comprehension of environmentally relevant matrices.

The overall aim of this thesis was to optimize a NTA workflow with the purpose of collecting relevant information without prior knowledge of the compositions of four environmentally relevant sample types; fish, dust, aqueous film-forming foams (AFFFs), and gas and soot released during fire emissions. Several sample preparation methods were evaluated for screening of mid- to non-polar compounds in fish, and the performance evaluation of a solid-liquid nontargeted extraction of indoor dust was conducted. Sample preparation tests for both fish and dust samples confirmed the importance to consider matrix effects while conducting comprehensive chemical analysis to not induce bias in reported results. Optimization of the NTA data processing enabled the detection and tentative identification of various classes of compounds such as flame retardants, polyethylene glycols and phthalates in dust, organofluorine and fluorine-free surfactants in AFFFs, and flame retardants and hydrocarbons in fire emissions.

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