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How important is the sample preparation step for non-target screening of micropollutants in urban waters?

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Introduction
Non-target screening (NTS) has gained interest in recent years for environmental monitoring purposes because it enables the analysis of a large number of pollutants without predefined lists of molecules. However, sample preparation methods are diverse, and few have been systematically compared in terms of amount and relevance of the information obtained by subsequent NTS analysis.

Objectives
• Testing different natures of phases for solid phases extraction (SPE) to retain a large range of micropollutants on real samples
• Developing a strategy based on different types of relevant indicators to compare the results in NTS
• Applying the developed strategy on urban water samples

Methods
Panel of 9 commercially available (HLB, C18, X-AW, X-CW, SDBL, ENV+, C18/ENV+, X-A, X-C) stationary phases + 1 home-made multilayer cartridge
C18 chromatography and ESI + with m/z [100-1000]

Results
Evaluation of the retention ability
Based on EEM spectra, regions II and IV were well retained by X-AW and Multilayer (≥80%). Those regions can be associated with simpler, more polar and nitrogenous compounds (Zhang et al., 2008). These chromatograms seem to be the most efficient to retain hydrophobic materials as well as smaller and more polar compounds for a global screening of the molecules present in the sample.

X-AW exhibits high retention of fluorescent materials but few features in HRMS which is the total opposite of HLB. This can be associated with a higher retention of dissolved organic matter which could contribute to a competition with the retention of organic compounds.

However, Multilayer does not seem to suffer such matrix effects, retaining both high content of fluorophores and organic compounds. Moreover, Multilayer retains molecules with a wider range of molecular weight, making it interesting for the screening of a large range of micropollutants.

Discrimination based on HRMS features
Multilayer is the cartridge with the highest number of specific features (323 features only found in this cartridge), but also the one with the highest number of intersected features (20 intersections with features found on other tested cartridges for a total of 212 features intersected), making it the most interesting cartridge for non-target studies by retaining the most extensive set of features (i.e., with diverse properties).

Conclusions
The Multilayer cartridge (HLB, ENV+, X-AW, X-CW):
• is the most effective at retaining a large range of HRMS features
• is less affected by the adsorption of dissolved organic matter
• takes advantage of the four phases in terms of diversity of compounds
Ongoing investigation: better characterize the chemical space (log Kow, pKa, chemical functions...) covered by each cartridge. This could help determining the relevance of each type of cartridge towards specific purposes (e.g., focus on more polar compounds).

Acknowledgment: