

Evaluation of sample preparation methods for highly polar organic contaminants from aqueous matrices

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Introduction

Highly polar organic contaminants are mobile (MOCs) in the water cycle because they are able to pass natural and artificial barriers. If they are **persistent (PMOCs)**, dilution is the only way of concentration reduction, and thus these substances may reach raw and drinking waters in significant concentrations^[1]. When PMOCs are present in high concentrations or toxic^[2], their presence in the water cycle may have adverse effects on aquatic organisms or on human health.

The analysis of MOCs is exacerbated by the same physicochemical properties that facilitate their mobility (e.g. low molecular mass and high polarity). The lack of suitable enrichment methods for MOCs from aqueous samples is a major problem in their trace analysis, and thus two independent methods, a multimodal solid phase extraction (mmSPE) method^[3] and an evaporation method, were developed to facilitate the analysis of MOCs.





mmSPE method neutral positive negative 120 **%** 100 recovery mSPE 50%

- In total, **17 analytes** were determined with the mmSPE method and 19 analytes for the evaporation method
- Neutral analytes were most problematic for the mmSPE method
- **Mean recovery** was 50% for the mmSPE and 58% for the evaporation method

Evaporation method





- A combination of both methods is able to enrich 84% of the model substances by a threshold of 30% For the **mmSPE method**, matrix effects seem to correlate well with matrix **TOC/DOC**
- For the evaporation method, the salt concentration appears to have a significant influence on matrix effects
- **Matrix effects** for the evaporation method increase ි significantly if the enrichment factor is increased from 10 to 20 (data not shown)

- Significance of matrix
 - effects for the **mmSPE** method
- Significance of matrix effects for the \longrightarrow





Method comparison





• 10⁷ - 10⁸ • 10⁶ - 10⁷ Signal intensity: • $10^5 - 10^6$ >10⁸

- **Tap water** was enriched with a **generic HLB** (hydrophilic and lipophilic balanced) SPE material method and the **mmSPE** method
- The mmSPE method shows higher recoveries (mean mmSPE: 52%; HLB: 21%) for the enrichment of MOCs
- Non-target screening of ground water sample enriched with all three enrichment methods
- Analysis with HILIC-HRMS allows rough estimation of analyte hydrophilicity with retention time

References:

Number of detected ions was highest for HLB

- Mean and median retention time, and thus capability to enrich hydrophilic compounds increases in order HLB, Evaporation, and mmSPE
- The highest number of high intensity ions $(>10^7)$ were detected after enrichment with mmSPE

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