Persistent and mobile organic chemicals – An emerging group of ubiquitous water pollutants

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Abstract

The release of persistent and mobile organic chemicals (PMOCs) into the aquatic environment is a risk to the quality of water resources. As a consequence of their aquatic mobility, PMOCs can pass through wastewater treatment plants, natural barriers and drinking water purification processes and are thus of concern for human health (Fig. 1).

The aim of this study was to screen for potential PMOCs of concern in European water samples.

Introduction

1. Selection of Compounds

REACH registered organic chemicals (industrial chemicals) ... with a potential emission into the environment

- that are persistent and mobile in the aquatic environment
- for which analytical standards are available
- that are amenable to analysis by chromatography/mass spectrometry

→ 70 PMOCs were selected according to the above-mentioned criteria

2. Sampling

1x Reversed Osmosis concentrate
1x Reversed Osmosis permeate

3. Extraction

Solid phase extraction
- 1) Graphitized carbon black
- 2) Weak anion exchanger
- 3) Weak cation exchanger
- 4) Moderate cation exchanger
- 5) Hydroxylated polystyrene-divinylbenzene
- 6) Multilayer solid phase extraction

Enrichment factor: 1:20 – 1:500

4. Chromatographic & Detection Methods

a) Reversed Phase Liquid Chromatography – MS/MS (after extraction 1, 2, 4, 5)

Columns:
- Waters HSST3, 2.1x50 mm, 1.8 µm
- Thermo Hypercarb, 2.1x100 mm, 3 µm

Gradient:
- H₂O / MOOH with NH₄HCOO
- H₂O / ACN with diethylamine

b) Supercritical Fluid Chromatography – HRMS (after extraction 1, 2, 4, 5)

Columns:
- Waters UPC² BEH, 3x100 mm, 1.7 µm
- Waters UPC² Torus Diol, 3x100 mm, 1.7 µm

Gradient (both columns):
- CO₂ / MeOH / H₂O with NH₄OH

Make Up Flow:
- MeOH / H₂O with HCOOH

ESI - qTOF-MS:
- Exact mass (mass window: 5 ppm)

Acids

- Acesulfame
- Saccharin
- Guanidines
- Sulfonic Acids

Fig. 6: Examples of detected PMOCs

Screening Results

PMOC No.\(^{a}\)
CAS
PMOC No.\(^{b}\)
CAS

| 1 | 467-16-7 | 24 | 465-58-5 |
| 2 | 7365-45-9 | 25 | 108-80-5 |
| 3 | 6956-55-7 | 26 | 52722-86-8 |
| 4 | 8311-960 | 27 | 140-31-8 |
| 5 | 51410-72-5 | 28 | 1561-92-8 |
| 6 | 52556-40-2 | 29 | 1213764-7-3 |
| 7 | 104-23-4 | 30 | 622-40-2 |
| 8 | 101-77-9 | 31 | 280-57-9 |
| 9 | 134573-75-5 | 32 | 13674-84-5 |
| 10 | 1704-62-7 | 33 | 105-60-2 |
| 11 | 83-04-9 | 34 | 70-55-3 |
| 12 | 5205-93-6 | 35 | 834-12-8 |
| 13 | 2855-11-2 | 36 | 768-94-5 |
| 14 | 288-88-0 | 37 | 1493-13-6 |
| 15 | 81-07-2 | 38 | 25321-41-3 |
| 16 | 80-09-1 | 39 | 19715-19-6 |
| 17 | 23386-52-9 | 40 | 55588-62-3 |
| 18 | 103-83-3 | 41 | 97-39-2 |
| 19 | 542-02-9 | 42 | 5165-97-9 |
| 20 | 56-93-9 | 43 | 104-15-4 |
| 21 | 85-47-2 | 44 | 102-06-7 |
| 22 | 3039-83-6 | 45 | 108-78-1 |
| 23 | 512-42-5 | 46 | |

* Letters a-d indicate the methods for detection of the PMOC

© Some PMOCs were frequently detected in water samples and others rarely (Fig. 5)

© Detection of known water contaminants as well as novel PMOCs (Fig. 4 + 5)

References:


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