

Method development of a HILIC-UHPLC-MS/MS method for the analysis of mobile water contaminations

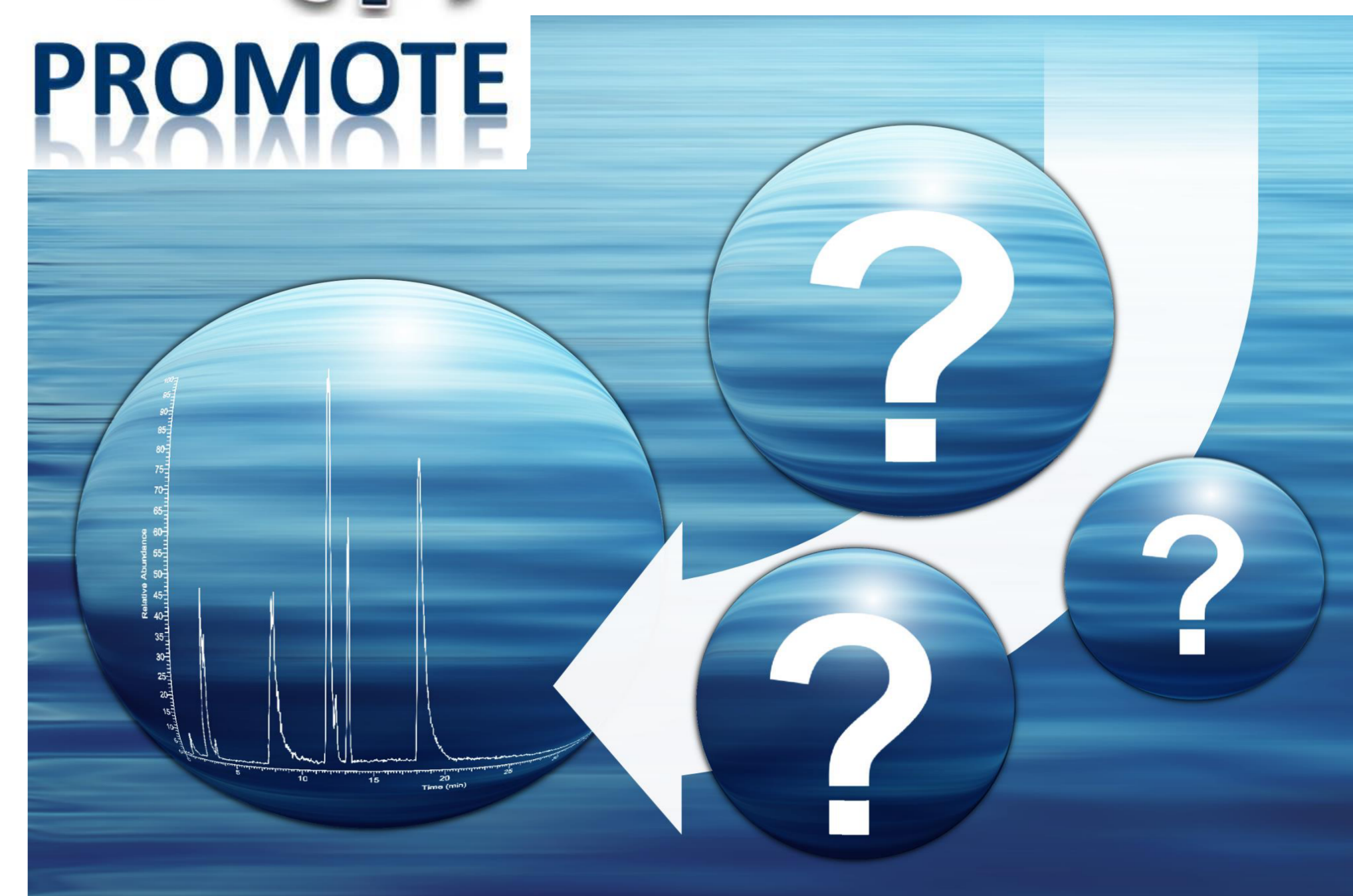
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Introduction

Persistent and mobile organic contaminants (PMOC)¹, such as the recently discovered halogenated methanesulfonic acids², can pass all natural and artificial barriers in the water cycle and thus, may reach raw or even finished drinking water. Since the high polarity of these substances exacerbates their analysis and enrichment from aqueous matrices, only limited data on the presence of PMOC in the water cycle is available.

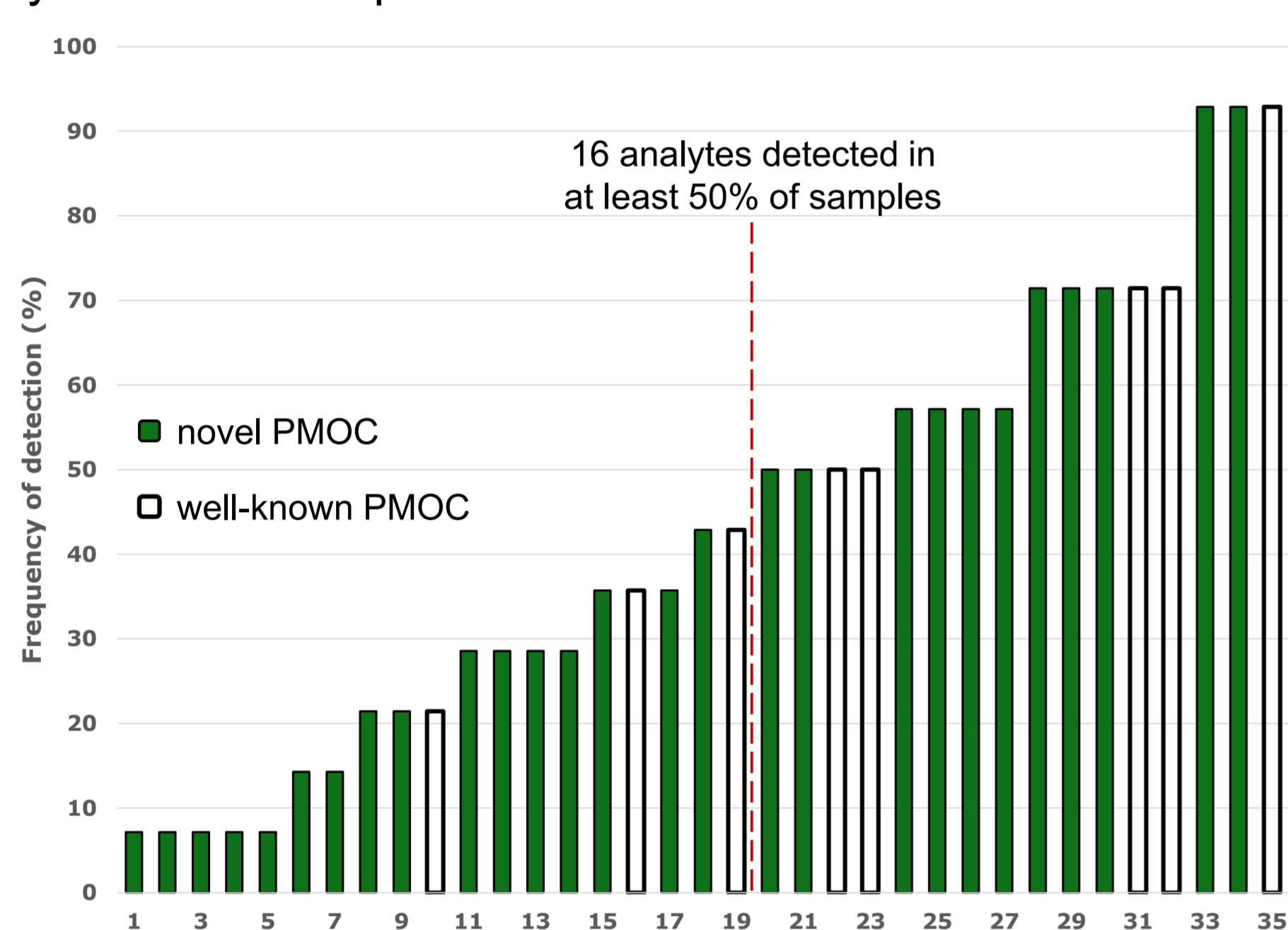
To close this gap in knowledge, a HILIC-UHPLC-sMRM method for a variety of potential PMOC was developed. The investigated substances were selected based on suspect³, non-target², and database^{4,5} screening results and further prioritized by their presence in the environment. After validation, the optimised method⁶ will allow the quantification of a large set of PMOC that have not been analysed before.



Persistent and mobile organic contaminants may impact drinking water

Analysis of 16 water samples from different compartments of the water cycle and 4 European countries

35 potential PMOC detected in environment

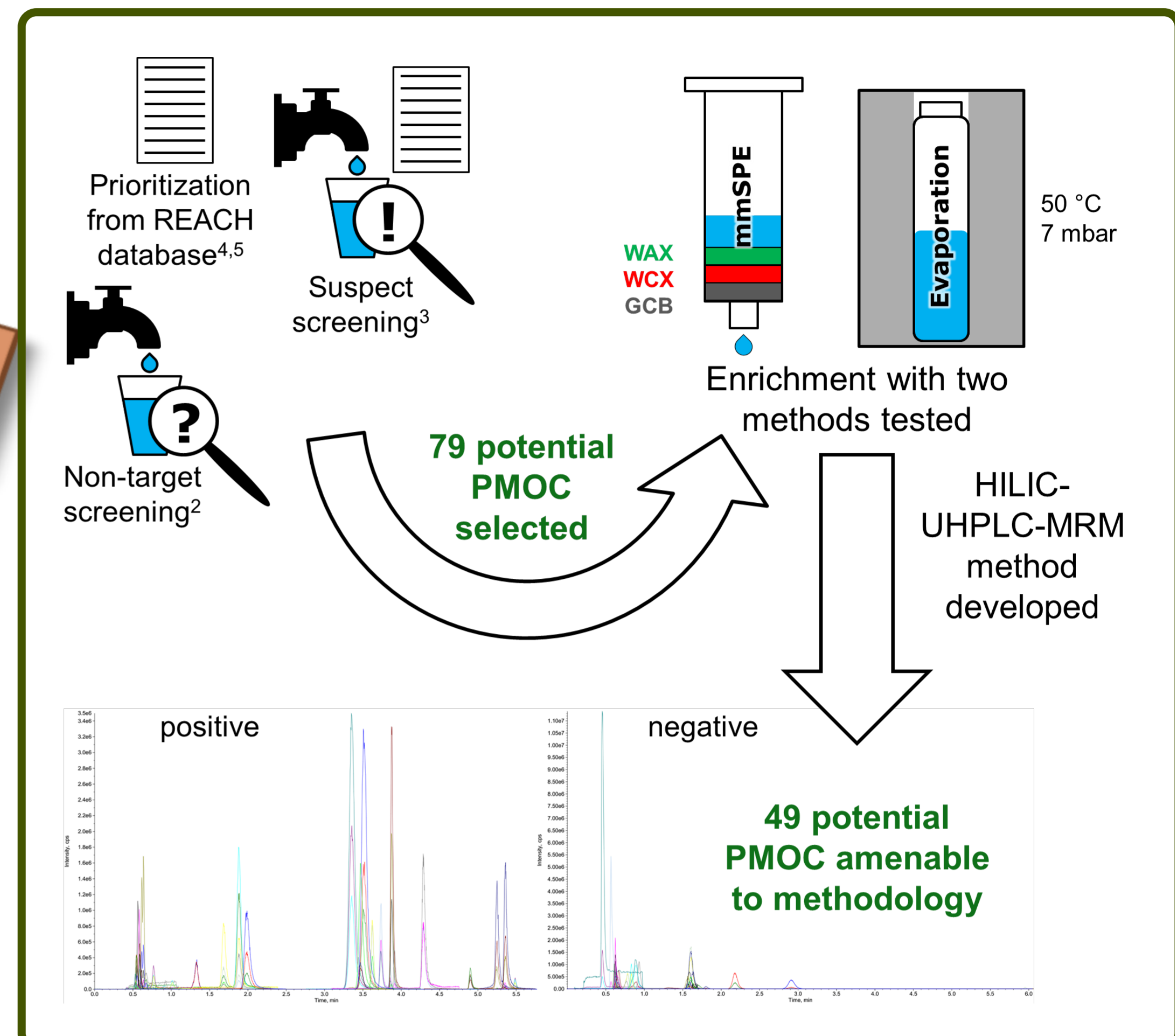


CAS numbers of detected analytes

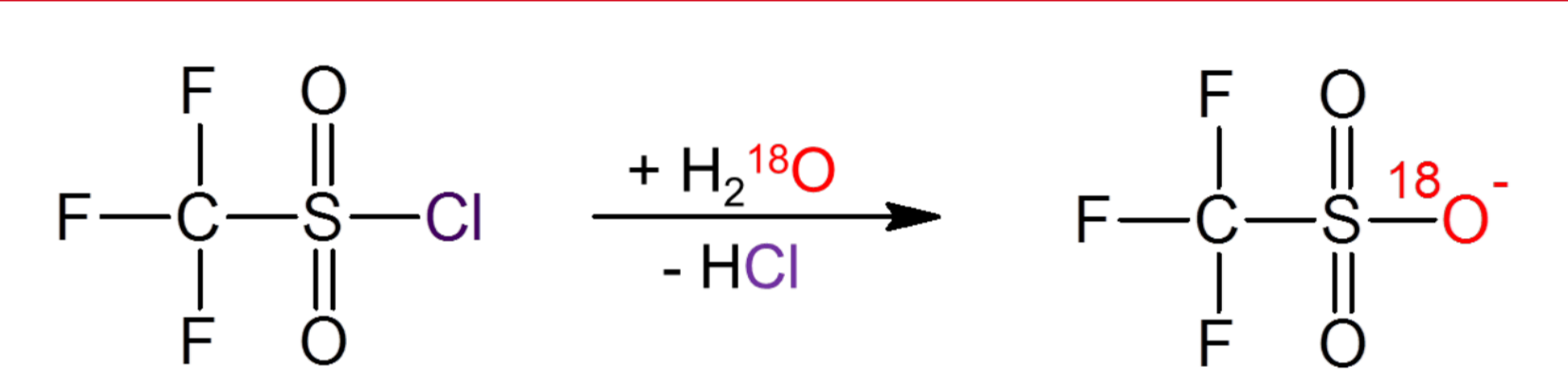
Substance #	CAS number	Substance #	CAS number
1	51410-72-1	19	108-80-5
2	5205-93-6	20	140-31-8
3	497-18-7	21	5165-97-9 + 15214-89-8
4	52556-42-0	22	121-47-1 + 121-57-3
5	6331-96-0	23	108-78-1
6	512-42-5	24	52722-86-8
7	91-76-9	25	1493-13-6
8	1704-62-7	26	3039-83-6
9	100-97-0	27	461-58-5
10	81-07-2	28	1561-92-8
11	2855-13-2	29	622-40-2
12	104-15-4	30	768-94-5
13	102-06-7	31	1300-72-7 + 25321-41-9
14	105-60-2	32	13674-84-5
15	103-83-3	33	19715-19-6
16	542-02-9	34	834-12-8
17	288-88-0	35	55589-62-3
18	280-57-9		

Analyte prioritisation

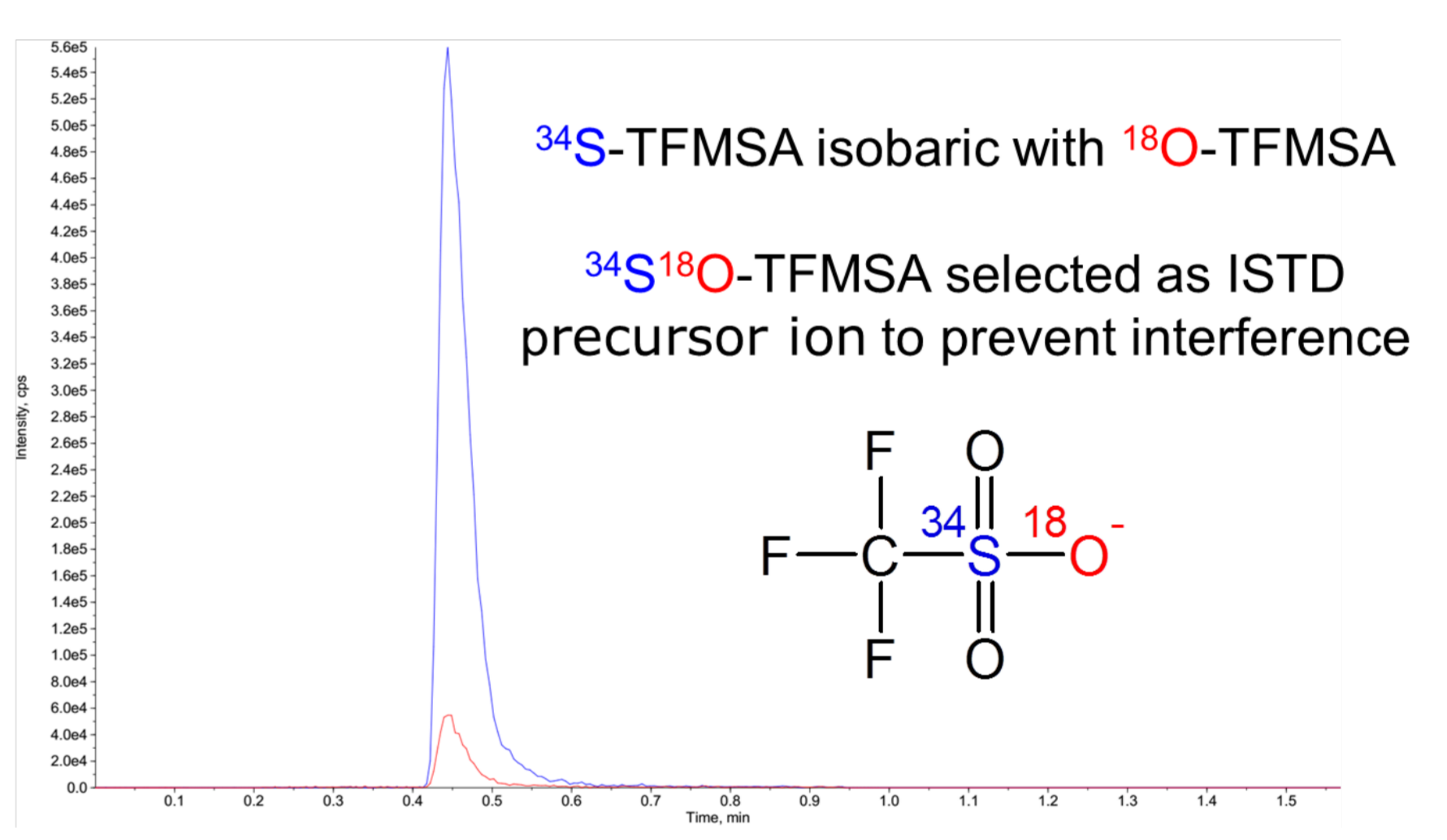
Method development



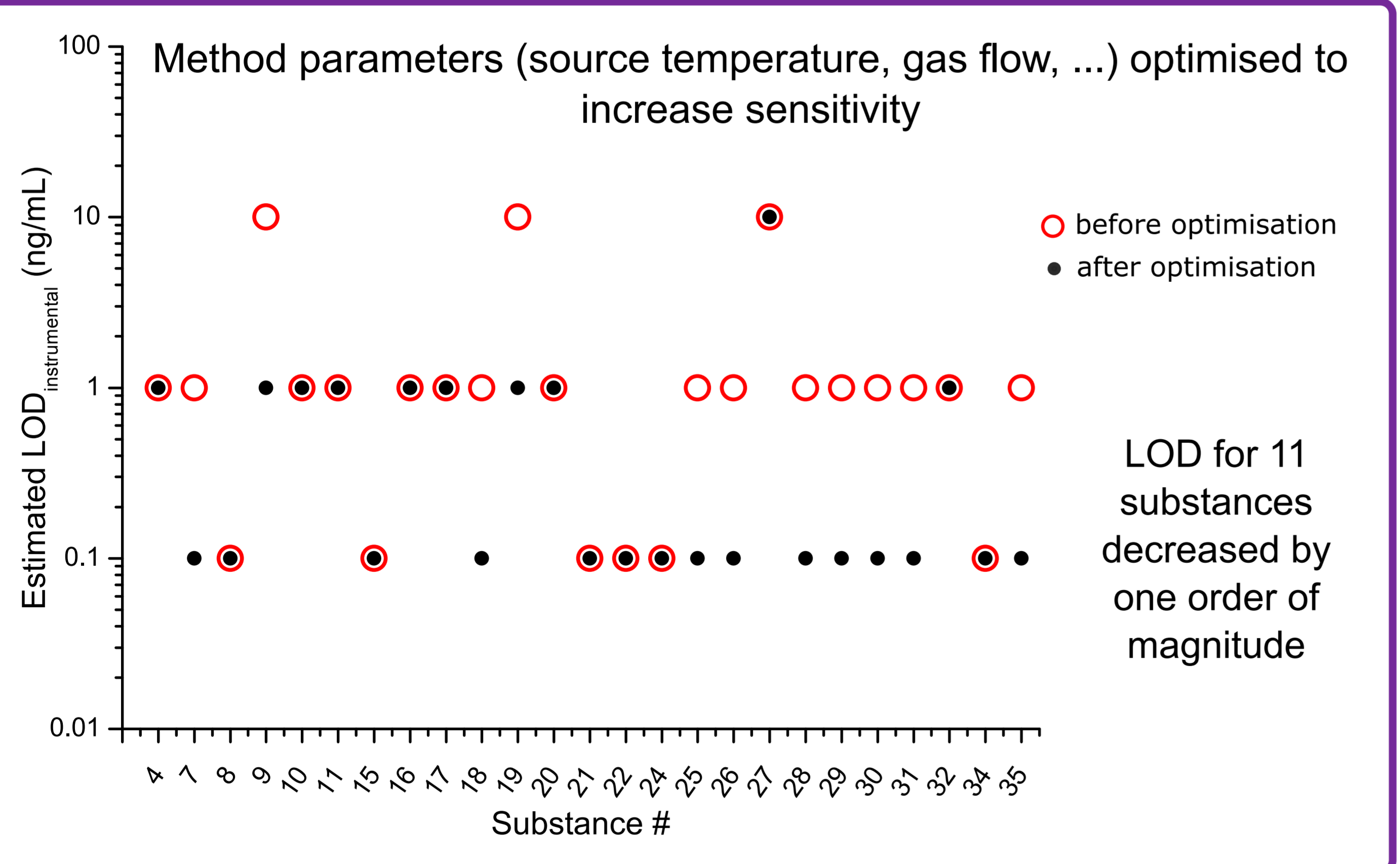
Synthesis of ISTD



Synthesis of ISTD by hydrolysis in H₂¹⁸O and subsequent purification with SPE (WAX)



Method optimisation



Method validation

- Matrix effects
- Linearity
- Recovery
- LOD
- LOQ
- ...

HILIC-UHPLC-sMRM method to monitor PMOC

- HILIC-UHPLC-sMRM was successfully developed and optimised
- First data suggests presence of many investigated PMOC in the environment
- Isotope-labelled TFMSA was synthesised as ISTD
- After successful validation, the method will be deployed to quantify PMOC in environment and during drinking water production

References:
 [1] Reemtsma, T., et al. *Environmental Science & Technology* **2016**, 50, 10308-10315.
 [2] Zahn, D., et al. *Water Research* **2016**, 101, 292-299.
 [3] Montes, R. et al. *Environmental Science & Technology* **2017**, accepted manuscript
 [4] Arp, H. P. et al. *Environ. Sci. Process Impacts*, under revision
 [5] Schulze, S. et al. in preparation
 [6] Zahn, D. et al. in preparation

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