Decoding PFAS Behaviour in soils: Evidence from three PARC case studies

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Walk in the PARC?

PARC = Partnership for the Assessment of Risks from Chemicals

- A public-public **partnership** under Horizon Europe

- Co-fund budget

- Started 1st of May 2022 and has a duration of 7 years

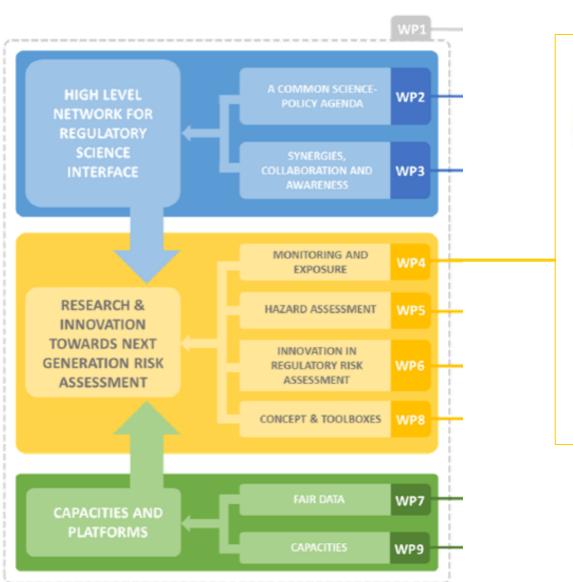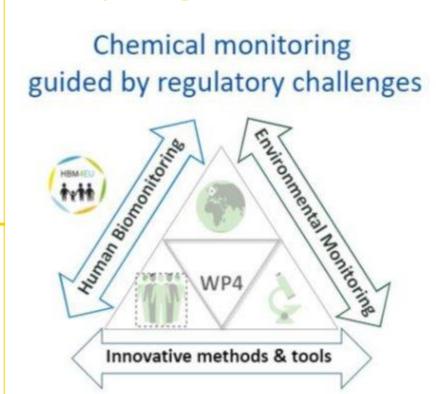- ≈ 200 partners from 29 countries

- Includes 3 European Agencies:

Work packages within PARC

Work package 4:

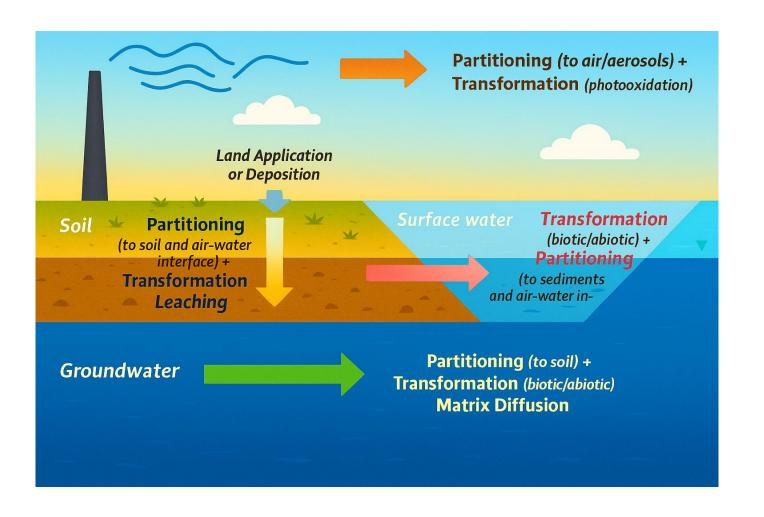Chemical monitoring guided by regulatory challenges

Task 4.2
- EDC campaign
- PFAS case studies
- PFAS baseline
- Prioritisation framework

Aim of PFAS Case Studies

To gain a better understanding of the PFAS fate and pathways from sources to aquatic recipients

PFAS case studies centred around 5 research questions

- What is the role of precursors?

- How far can PFAS precursors be transported?

- How do environmental conditions and PFAS molecular structures influence their transport?

- Can non-target methods contribute to establishing a "PFAS fingerprint", which might improve our understanding of pathways?

- Can fingerprinting be used for source identification and can it be embedded in monitoring?

EU PARC – 19 Case studies from 11 countries

PFAS Sources

Environmental matrices

3 case studies from Flanders

1. PFAS mapping at former paper manufacturing site

2. PFAS leaching - Experimental determination of Kd values for PFAS in Flemish soils
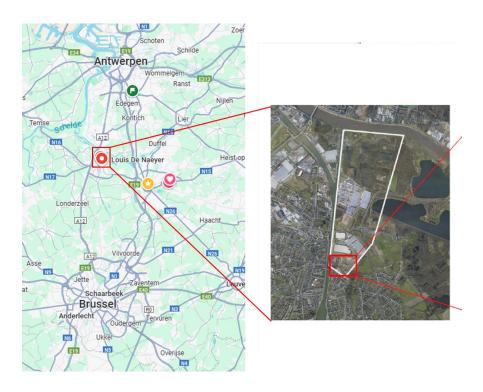
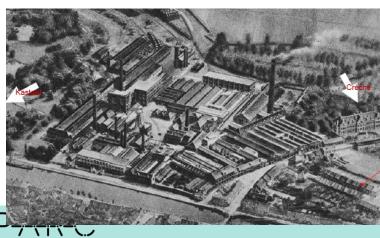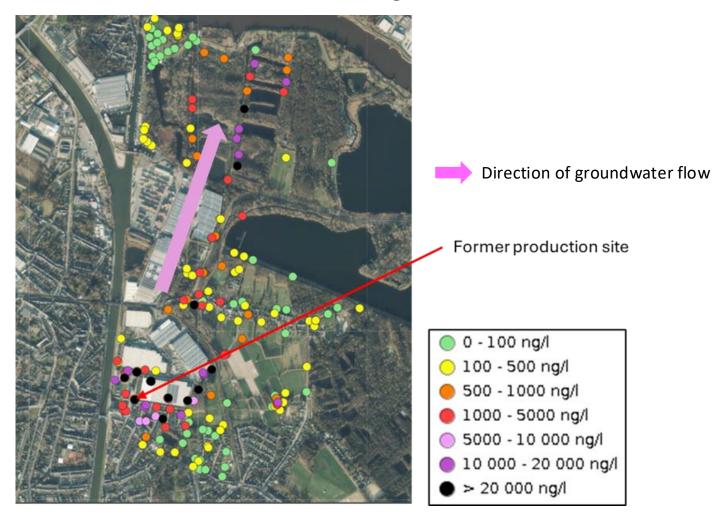3. NTA at PFAS-suspected locations
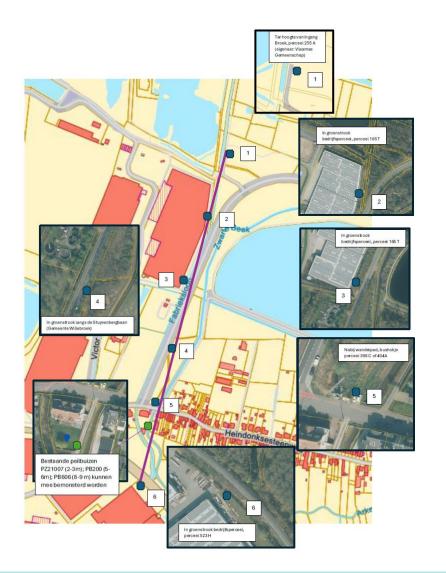
PFAS mapping at former paper manufacturing site

Data available from earlier soil investigations

➡ Direction of groundwater flow

Former production site

🟢	0 - 100 ng/l
🟡	100 - 500 ng/l
🟠	500 - 1000 ng/l
🔴	1000 - 5000 ng/l
🟣	5000 - 10 000 ng/l
🟣	10 000 - 20 000 ng/l
⚫	> 20 000 ng/l

Sample selection to investigate transport

- 6 clusters with increasing distance from former manufacturing site – 150 à 200 m steps

- sampled at 3 depths for soil and groundwater in the presumed groundwater flow direction:
  - Depth 1: 2-3 m
  - Depth 2: 5-6 m
  - Depth 3: 8-10 m

- Target analysis: 42 PFAS of which 6 PFAS linear & total
  - LOQ soil: 0,5 µg/kg
  - LOQ groundwater: 10 ng/L

- Non-targeted analysis: DART + NTA

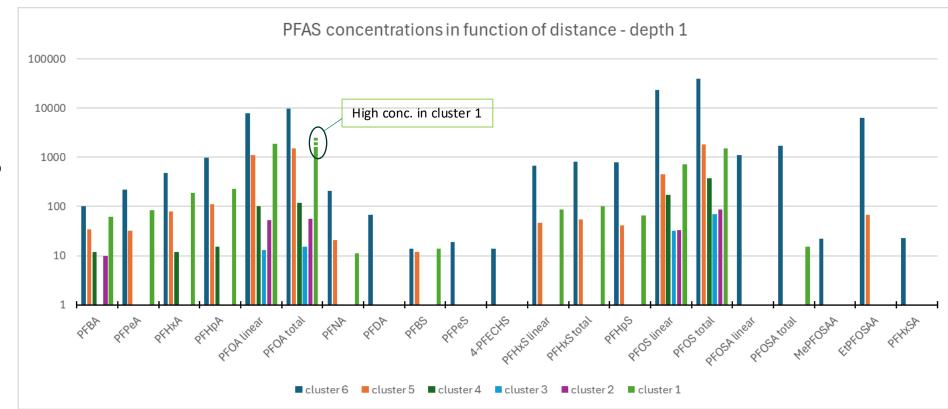# How do PFAS molecular structures influence transport?

HORIZONTAL

- Soil:
  - FoQ: PFOA, PFOS and 4:2 FTS have been detected at sampling depth 1.
  - In deeper layers no PFAS detected (LOQ soil: 0,5 µg/kg)

- Groundwater:
  - 22 out of 42 PFAS detected.
  - PFBA, PFOA, PFOS and PFHxA in > 75% of the samples
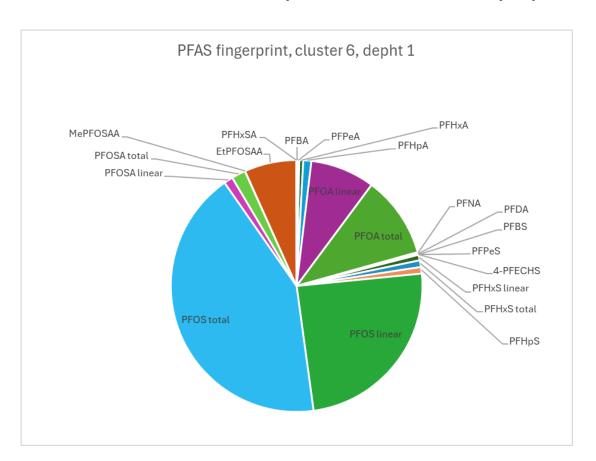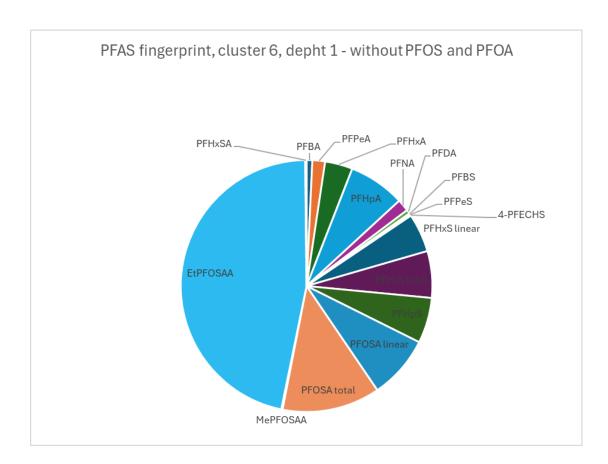 - Horizontal distribution – changes with distances from source

PFAS concentrations in function of distance - depth 1

High conc. in cluster 1

How do PFAS molecular structures influence transport?

• Groundwater – depth 1, closest to paper manufacturing site:

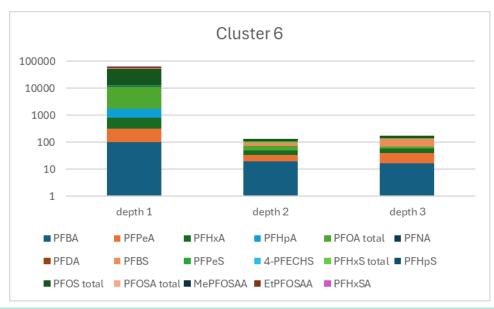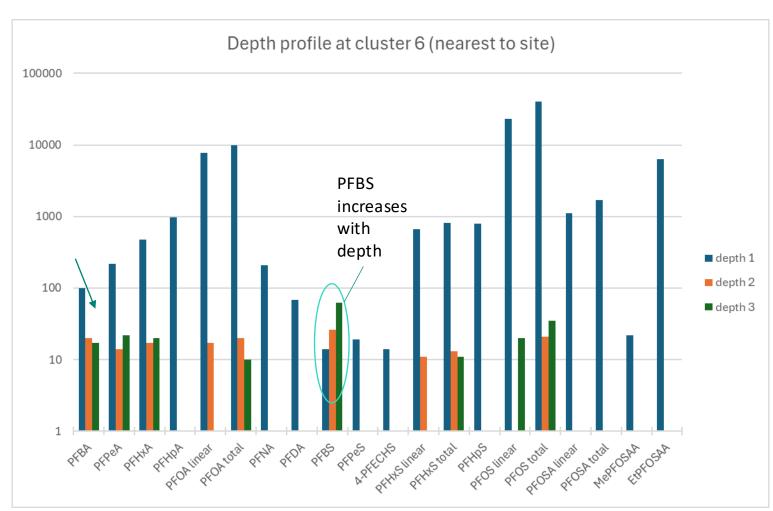# How do PFAS molecular structures influence transport?

- Groundwater:
  - Highest concentrations in upper layers, except for PFBS
  - In general: Longer chain – less observed in deeper layers

Cluster 6

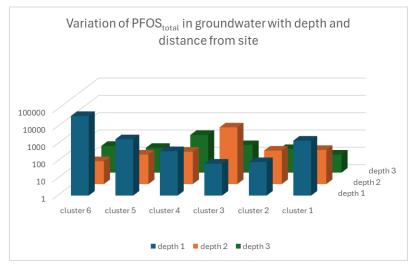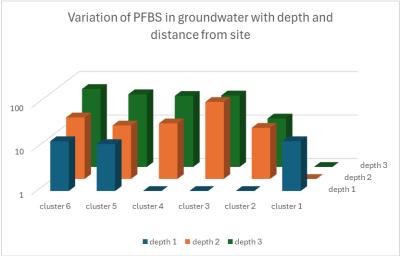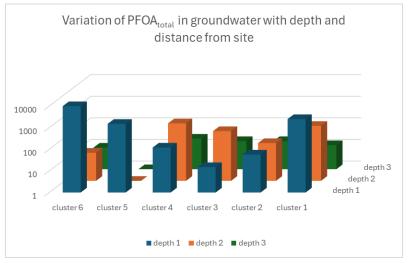Depth profile at cluster 6 (nearest to site)

PFBS increases with depth
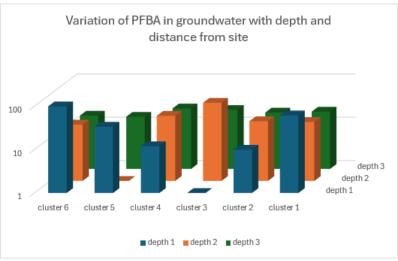
Groundwater in 3D

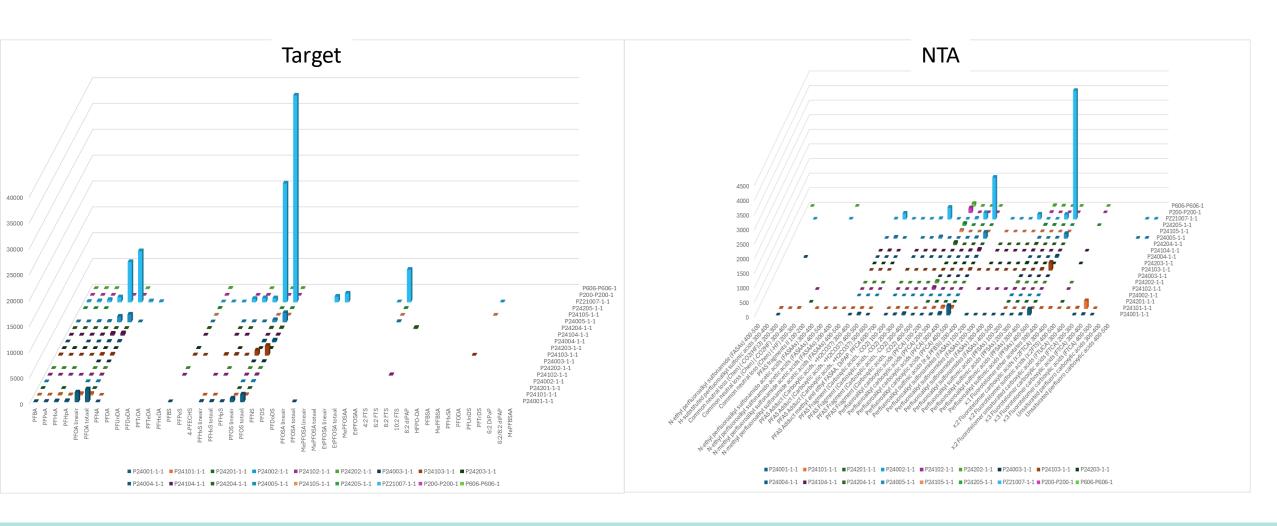- Groundwater – evolution with depth and distance
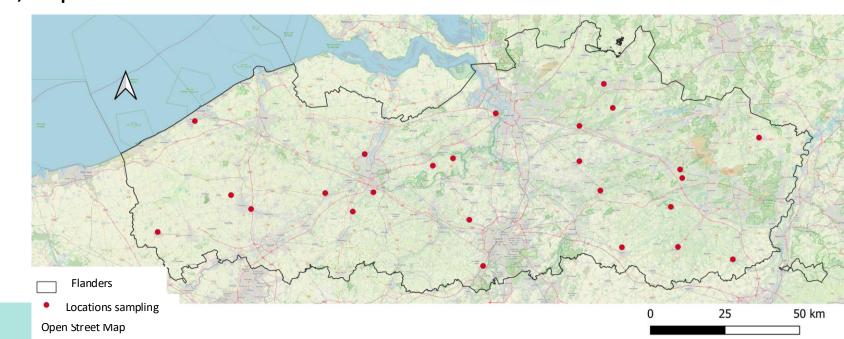
Fingerprinting with NTA

- Good match!

Experimental determination of Kd values for PFAS

- Datasets of PFAS Koc-values are available in scientific literature, but:

  Large variation in obtained results (soil types, climatic zones, …)
  Variety of techniques to determine Kd-values (modelling, lab experiments, …)

- Goal: determine Kd/Koc-values for PFAS for Flemish soils, including ultrashort chain PFAS.

- 26 soil samples from 25 sites, representative for PFAS in Flanders

Flanders

Locations sampling

Open Street Map

Lab analysis

- Multiple soil samples at each sampling site

- Limited sampling depth (max. 4 meters below ground surface)

- Subselection of most "promising" sample based on DART-MS screening

- 24h leaching test (shaking) with 0.01M $CaCl_2$ and an L/S of 10

- Target PFAS analysis on the soil, and both the eluate and solid residue after the shaking test
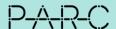
Calculation of Kd-values

- 48 target parameters analysed (42 PFAS with 6 PFAS linear & total)

- 7 additional ultrashort chain PFAS analysed in soil and eluate: TFA, 2,3,3,3-TeFPA, 2,2,3,3-TeFPA, PFPrA, TFMS, PFEtS, PFPrS

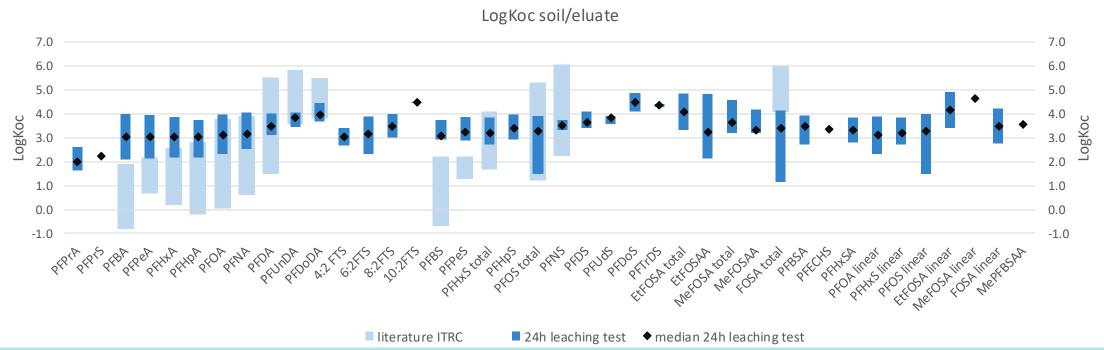- Only Kd-values if both the soil/residue and eluate concentrations are above the LOQ

- Two variants of Kd-values calculated:
  - Soil / eluate concentrations
  - Solid residue / eluate concentrations

Comparison with literature based on log(Koc)

- Koc-values based on the measured organic carbon content

- $Koc = \frac{(K_d * 100)}{\%OC}$

- Kd and Koc values for 37/48 target PFAS and 2/7 USC PFAS

LogKoc soil/eluate

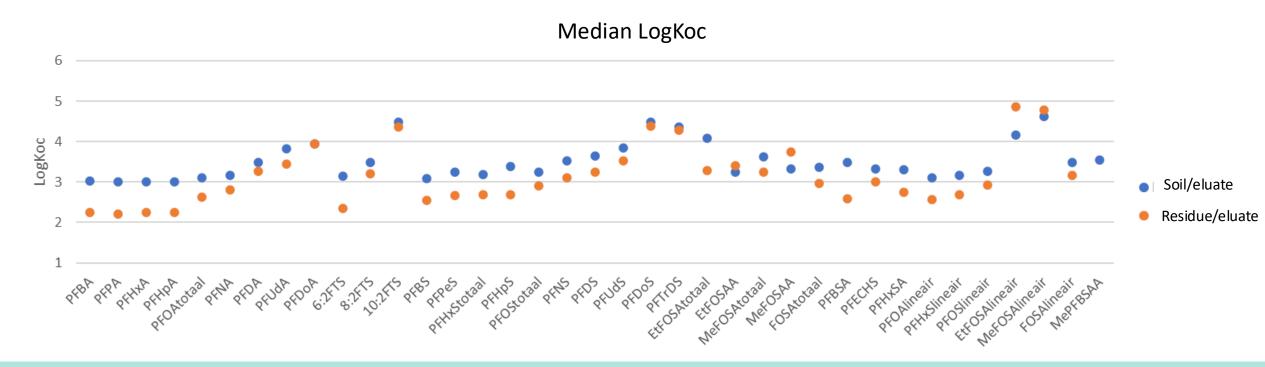# Comparison of soil/eluate & residue/eluate results

- General trend: Koc of soil/eluate is higher (up to one order of magnitude)

- This effect is most significant at shorter chain lengths, due to more leaching

Median LogKoc

NTA (non-targeted analysis) at PFAS-suspected locations

- What does the PFAS fingerprint look like at different sites and how does this correspond to the PFAS source?

- Selection of PFAS contaminated sites (33 sites):
  - Textile industry (3 sites)
  - Firefighting and fire-related contamination (21 sites)
  - Paper manufacturing (2 sites)
  - Metal plating (e.g. chromating) (4 sites)
  - Waste recycling (2 sites)
  - PFAS production (1 site)

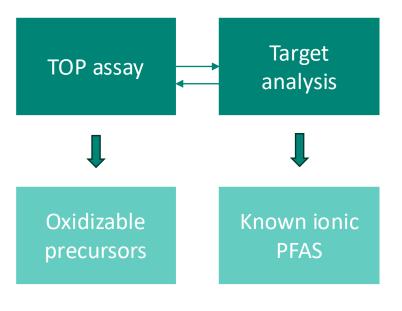# Analytical approach

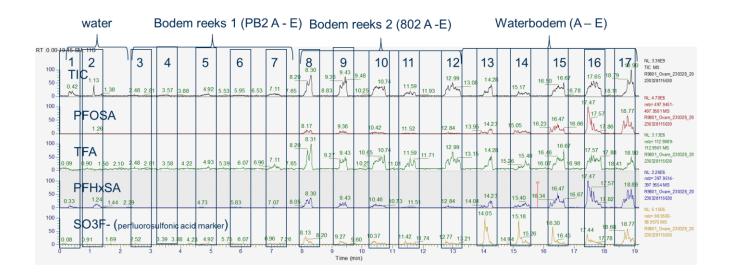# Selection of most promising samples: DART-MS
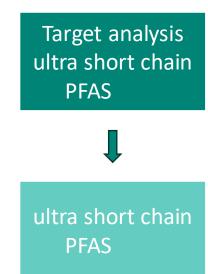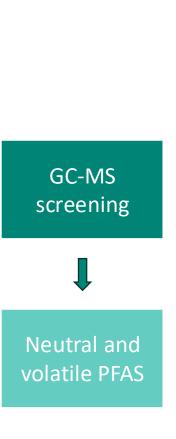
- DART-MS can be used to
  - Select samples out of multiple repeats
  - Select samples based on the estimated amount of PFAS
  - Select samples for NTA or only target analysis
  - Show depth and horizontal profiles
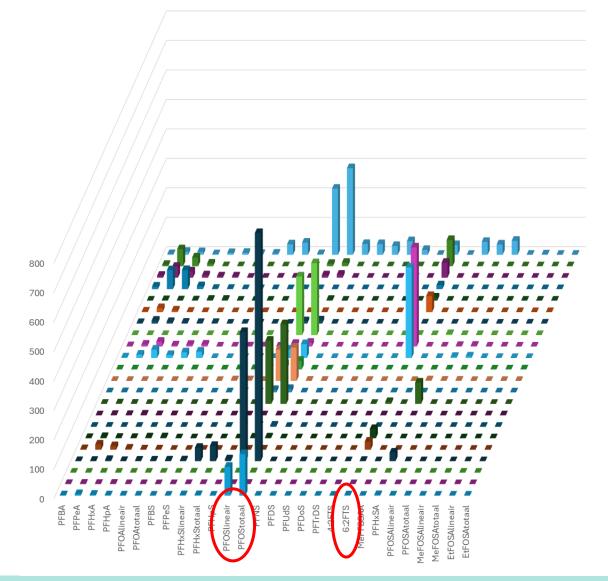
Similar source of contamination shows different fingerprints

We can't generalise that each PFAS pressure has its typical fingerprint.

For example: different fingerprints observed for fire-related contamination
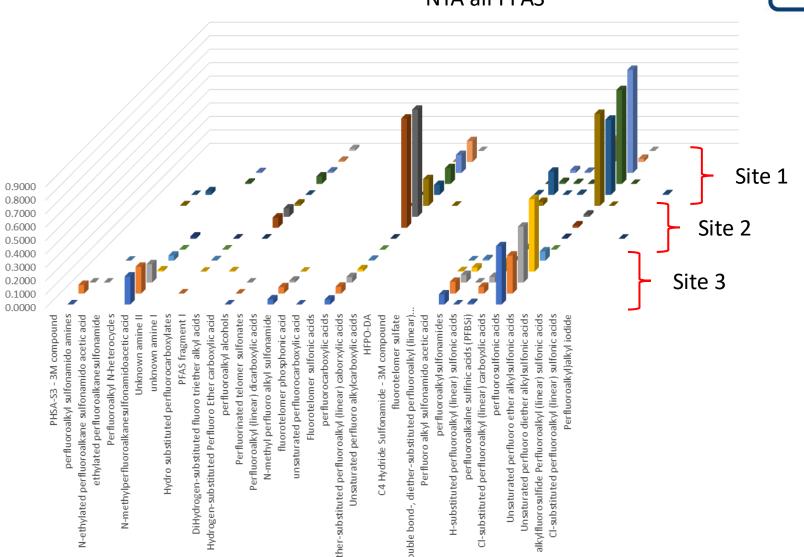

Fingerprinting fire-related sites

Use of fingerprints to determine contamination source

NTA all PFAS

At one location and with a known source, fingerprints can be used to link pollution to the site of origin

Site 1

Site 2

Site 3

Other remarks

Added value of TOPA could not be demonstrated for soil: technical developments needed?

DART <-> LC (target/NTA) correlation seems to be better than correlation between LC and TOPA or EOF/AOF

DART is not universal yet, but provides added value

Many thanks

PARC