NON-TARGET-SCREENING AT AN AFFF*- IMPACTED FIELD SITE

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EAC
Environmental
Analytical Chemistry

PFClean

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* Aqueous Film Forming Foam

HIGHLIGHTS

o **124 PFAS (per- & polyfluoroalkyl substances) identified (42 classes, confidence level 1-3) in soil at an AFFF-contaminated field site in Reilingen, Baden-Württemberg**

o **Examples of highly abundant substances in soil and water samples:**

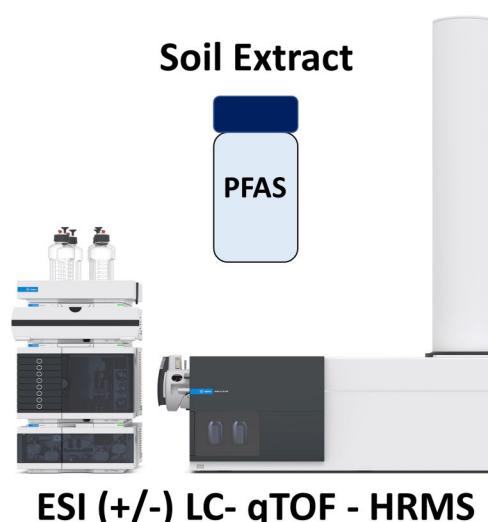PFOS   SF$_5$-PFOS   PFHxSAm-Pr-DiMeAm   6:2 FTSAm-Pr-B ("Capstone B")
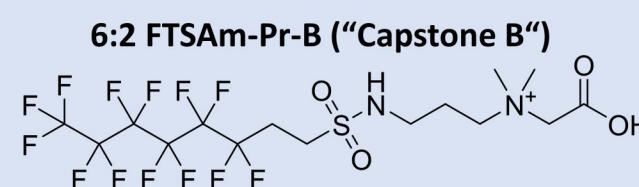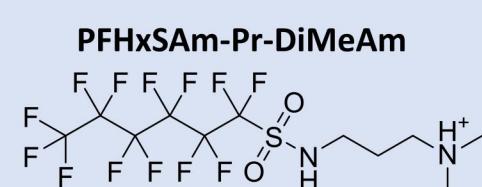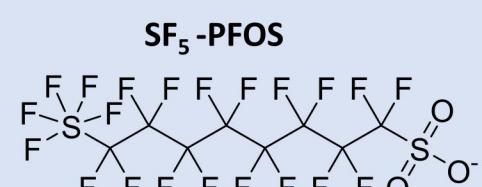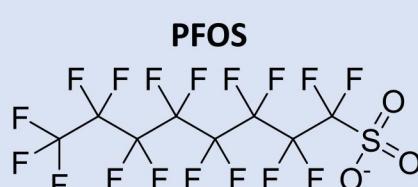
Reilingen

BACKGROUND

o Aqueous film forming foams (AFFF) contain PFAS of anionic, cationic nature as well as zwitterionic substances

o AFFF-contaminated field site in Reilingen, Baden-Württemberg

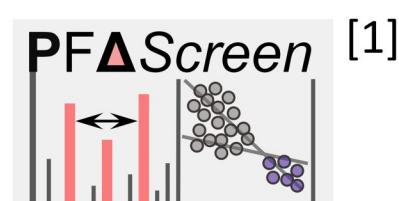o Investigation of soil and groundwater samples via LC-qTOF-HRMS

AFFF   PFAS
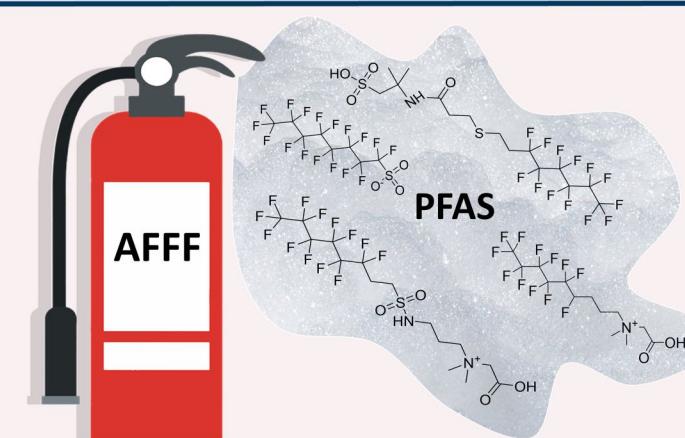
METHODS

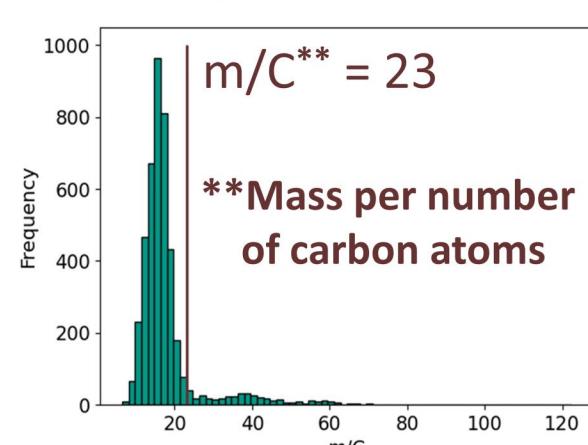### 1. Data Acquisition

Soil Extract

PFAS

ESI (+/-) LC- qTOF - HRMS

2. PFAS adapted NTS

PFΔScreen [1]

o **MS^1: Mass defect, KMD, mD/C-m/C,**
o **MS^2: Fragment differences, diagnostic fragments**
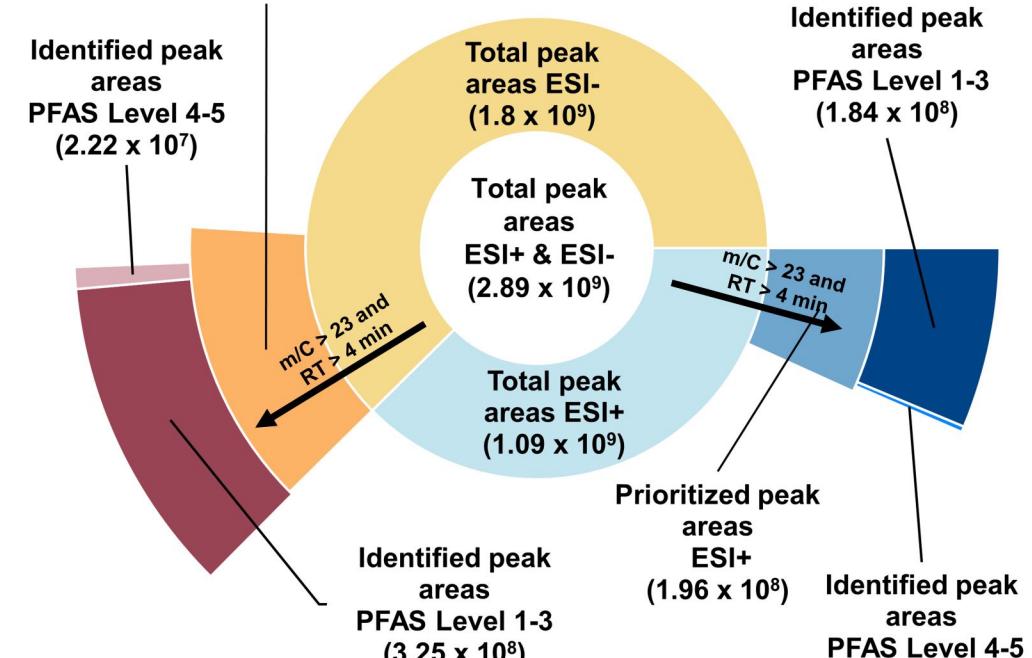o **Suspect screening**

3. Data Reduction

o **The m/C** value is well suited for separation of PFAS from organic sample matrix** [2]
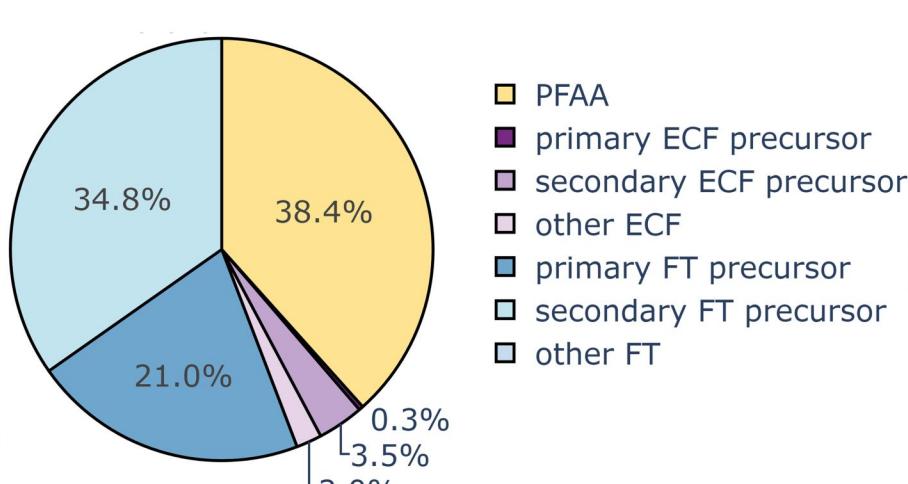o **m/C values of highly fluorinated PFAS: > 23**

m/C** = 23

Mass per number of carbon atoms

(y-axis: Frequency; x-axis: m/C)

RESULTS

Prioritized peak areas ESI-
(3.86 x 10^8)

Identified peak areas PFAS Level 4-5 (2.22 x 10^7)

Total peak areas ESI- (1.8 x 10^9)

Identified peak areas PFAS Level 1-3 (1.84 x 10^8)

Total peak areas ESI+ & ESI- (2.89 x 10^9)

m/C > 23 and RT > 4 min

Total peak areas ESI+ (1.09 x 10^9)

m/C > 23 and RT > 4 min

Identified peak areas PFAS Level 1-3 (3.25 x 10^8)

Prioritized peak areas ESI+ (1.96 x 10^8)
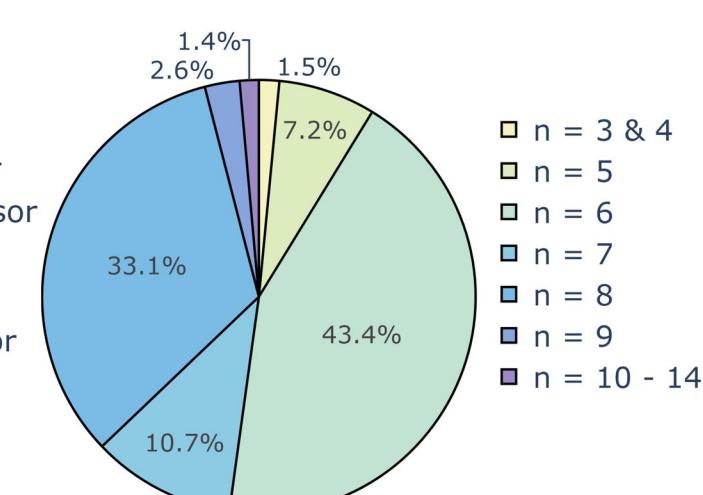
Identified peak areas PFAS Level 4-5 (5.92 x 10^6)

o Efficient reduction of peak areas

o Identification of 92% of total prioritized peak areas in ESI- and 94% in ESI+ (confidence level 1-3)

(a) Primary/secondary precursor/PFAA

- 38.4% PFAA
- 34.8%
- 21.0%
- 0.3%
- 3.5%
- 2.0%

Legend:
- ☐ PFAA
- ☐ primary ECF precursor
- ☐ secondary ECF precursor
- ☐ other ECF
- ☐ primary FT precursor
- ☐ secondary FT precursor
- ☐ other FT

(b) Fluorinated chain length

- 1.4%
- 2.6%
- 1.5%
- 7.2%
- 33.1%
- 43.4%
- 10.7%

Legend:
- ☐ n = 3 & 4
- ☐ n = 5
- ☐ n = 6
- ☐ n = 7
- ☐ n = 8
- ☐ n = 9
- ☐ n = 10 - 14

o **9** PFAS classes were identified in soil for the first time

o **14** out of 42 substance classes were also found in ground-water samples

o **2** completely new substances were identified

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GEFÖRDERT VOM
Bundesministerium
für Bildung
und Forschung

[1] Zweigle J, Bugsel B, Zwiener C (2022) FindPFΔS: Non-Target Screening for PFAS–Comprehensive Data Mining for MS2 Fragment Mass Differences. Analytical Chemistry 94 (30):10788-10796. doi:10.1021/acs.analchem.2c01521

[2] Zweigle J, Bugsel B, Zwiener C (2023) Efficient PFAS prioritization in non-target HRMS data: systematic evaluation of the novel MD/C-m/C approach. Anal Bioanal Chem 415:1791–1801. doi:10.1007/s00216-023-04601-1