



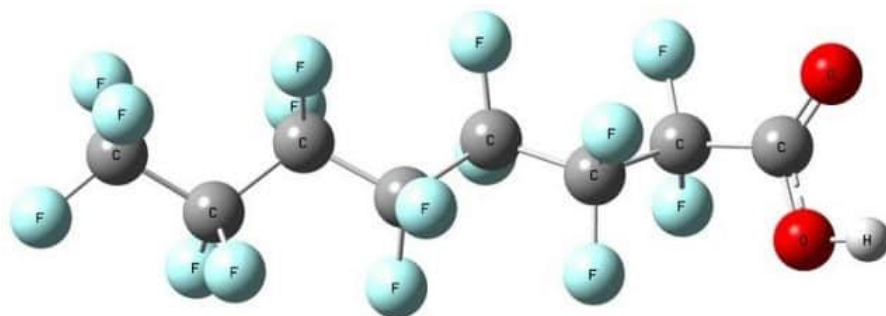
TRI - REGIONAL JETS 2025



Agile PFAS Data Acquisition, Processing and Delivery for PFAS Rookies and SMEs

Dora Chiang, Ph.D., P.E.
Jacobs

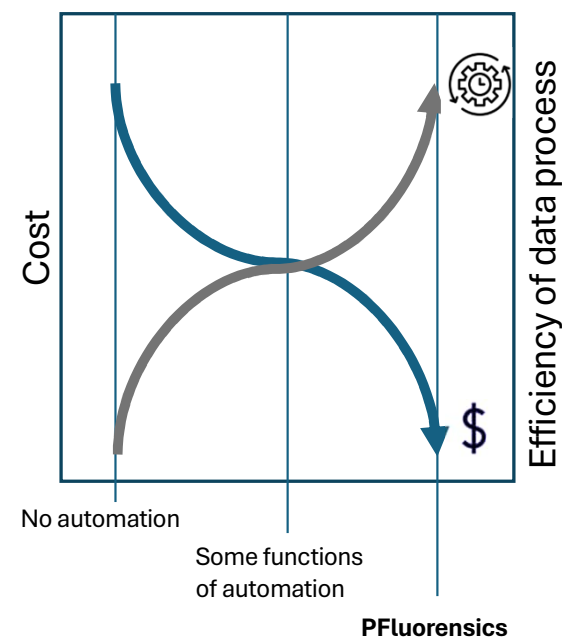
Learning Objectives

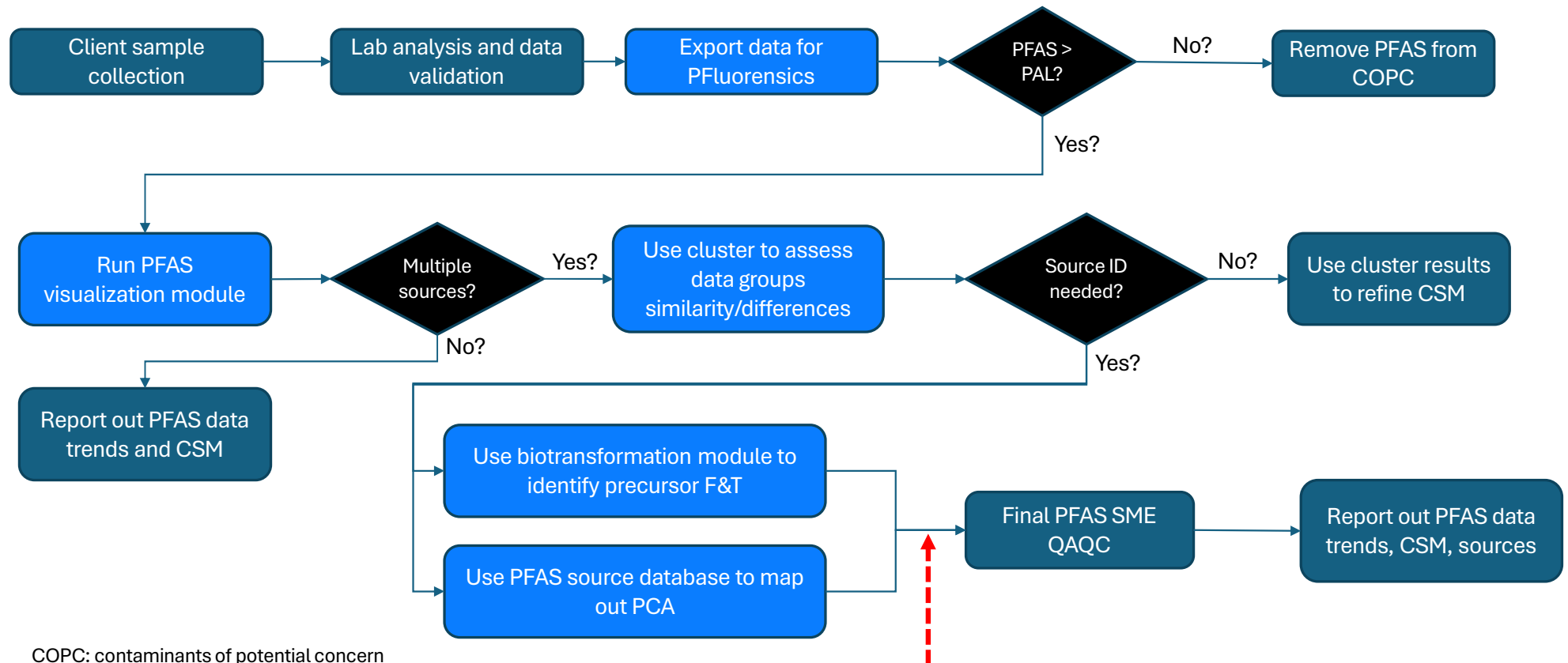


- The need of PFAS data analytic tools
- Phased approach to acquire, process and interpret PFAS data easily and efficiently
- Techniques on PFAS data analysis
- PFAS fingerprinting for PFAS SMEs

Why PFAS Data Evaluation Tools Needed?

- Provides consistent ways to process and visualize PFAS datasets
- Interpret and communicate PFAS data more efficiently
- Reduce human errors, uncertainties
- Provide cost benefits on a complex PFAS project
- Prepare for the expanded PFAS analyte lists





COPC: contaminants of potential concern
CSM: conceptual site model
PAL: project action level
SME: subject matter expert

Consider non-target analysis

PFAS Matrix

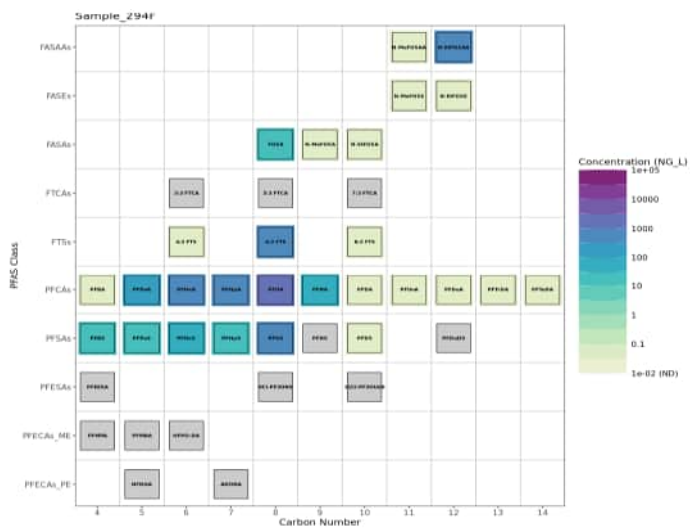
PFAS Class	Carbon Number										
	4	5	6	7	8	9	10	11	12	13	14
FASAA Perfluoroalkyl sulfonamido acetic acids								N-MeFOSAA C ₁₁ H ₂ F ₁₇ NO ₂ S 2355-31-9	N-EtFOSAA C ₁₂ H ₂ F ₁₇ NO ₂ S 2991-50-6		
FASEs Perfluoroalkane sulfonamido ethanols								N-MeFOSE C ₁₁ H ₂ F ₁₇ NO ₂ S 24448-09-7	N-EtFOSE C ₁₂ H ₂ F ₁₇ NO ₂ S 1691-99-2		
FASAs Perfluoroalkyl sulfonamides					FOSA C ₈ H ₂ F ₁₁ NO ₂ S 754-91-6	N-MeFOSA C ₉ H ₂ F ₁₃ NO ₂ S 31506-32-8	N-EtFOSA C ₁₀ H ₂ F ₁₅ NO ₂ S 4151-50-2				
FTCAs Polyfluorinated			3:3 FTCA C ₆ H ₂ F ₁₀ O ₂ 356-02-5		5:3 FTCA C ₈ H ₂ F ₁₁ O ₂ 914637-49-3		7:3 FTCA C ₁₀ H ₂ F ₁₃ O ₂ 812-70-4				
FTSs Polyfluorinated			4:2 FTS C ₆ H ₂ F ₁₀ O ₂ S 757124-72-4		6:2 FTS C ₈ H ₂ F ₁₃ O ₂ S 27619-97-2		8:2 FTS C ₁₀ H ₂ F ₁₅ O ₂ S 39108-34-4				
PFCAs Perfluoroalkylcarboxylic acids	PFBA C ₄ HF ₉ O ₂ 375-22-4	PFPeA C ₅ HF ₁₁ O ₂ 2706-90-3	PFHxA C ₆ HF ₁₃ O ₂ 307-24-4	PFHpA C ₇ HF ₁₅ O ₂ 375-85-9	PFOA C ₈ HF ₁₇ O ₂ 335-67-1	PFNA C ₉ HF ₁₉ O ₂ 375-95-1	PFDA C ₁₀ HF ₂₁ O ₂ 335-76-2	PFUnA C ₁₁ HF ₂₃ O ₂ 2058-94-8	PFDoA C ₁₂ HF ₂₅ O ₂ 307-55-1	PFTxDA C ₁₃ HF ₂₇ O ₂ 72629-94-8	PFTeDA C ₁₄ HF ₂₉ O ₂ 376-06-7
PFSAs Perfluorosulfonic acids	PFBS C ₂ HF ₅ O ₃ S 375-73-5	PFPeS C ₅ HF ₁₁ O ₃ S 2706-91-4	PFHxS C ₆ HF ₁₃ O ₃ S 355-46-4	PFHpS C ₇ HF ₁₅ O ₃ S 375-92-8	PFOS C ₈ HF ₁₇ O ₃ S 1763-73-1	PFNS C ₉ HF ₁₉ O ₃ S 68259-12-1	PFDS C ₁₀ HF ₂₁ O ₃ S 335-77-3		PFDoDS C ₁₂ HF ₂₅ O ₃ S 79780-39-5		
PFESAs Perfluoroalkyl Ether Sulfonic Acids	PFEESA C ₂ HF ₅ O ₃ S 113507-82-7				9Cl-PF3ONS C ₉ HClF ₁₆ O ₃ S 756426-58-1		11Cl-PF3OUDS C ₁₁ HClF ₁₈ O ₃ S 763051-92-9				
PFECAs_ME Perfluoroalkyl Ether Carboxylic Acids Monoether	PFMPA C ₂ HF ₅ O ₄ 377-73-1	PFMBA C ₅ HF ₁₁ O ₄ 863090-89-5	HFPO-DA C ₆ HF ₁₃ O ₄ 13252-13-6								
PFECAs_PE Perfluoroalkyl Ether Carboxylic Acids Polyether		NFDHA C ₅ HF ₁₁ O ₄ 151772-58-6		ADONA C ₇ H ₂ F ₁₅ O ₄ 919005-14-4							

Legend

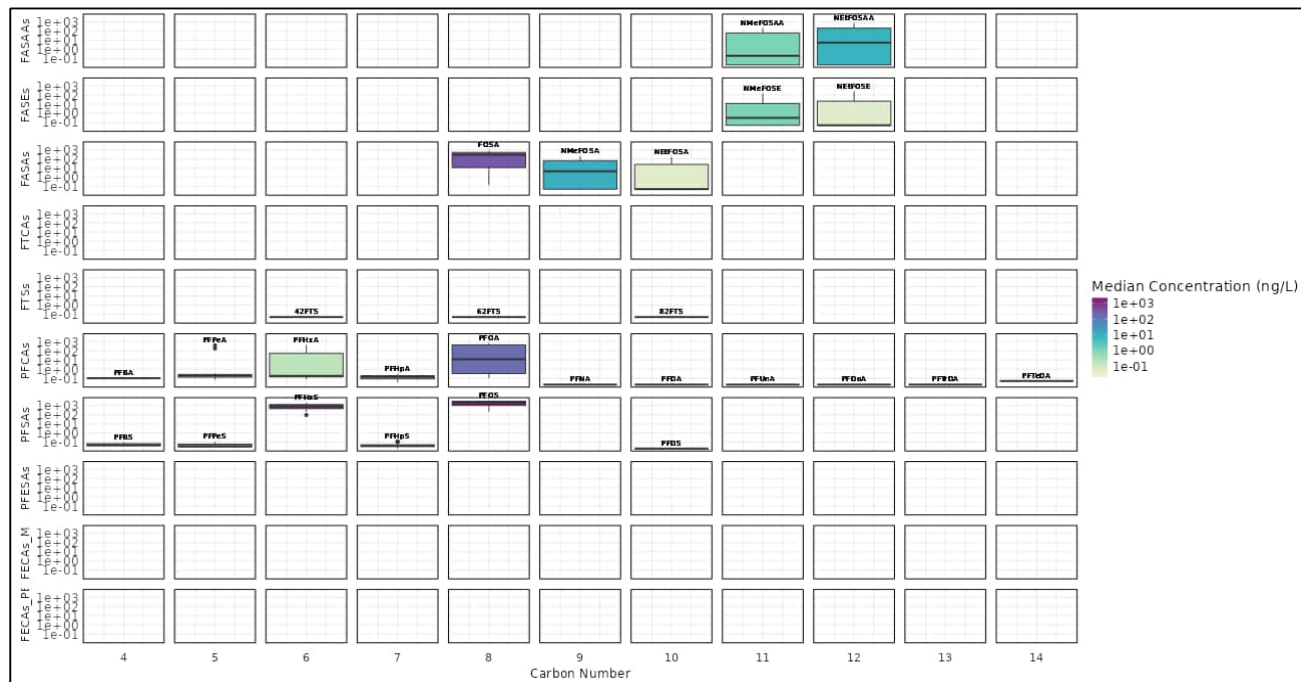
	Electrochemically Fluorinated Precursors
	Fluorotelomer Precursors
	Terminal PFAS
	PFAS Replacements

2D PFAS Matrix

Single dataset

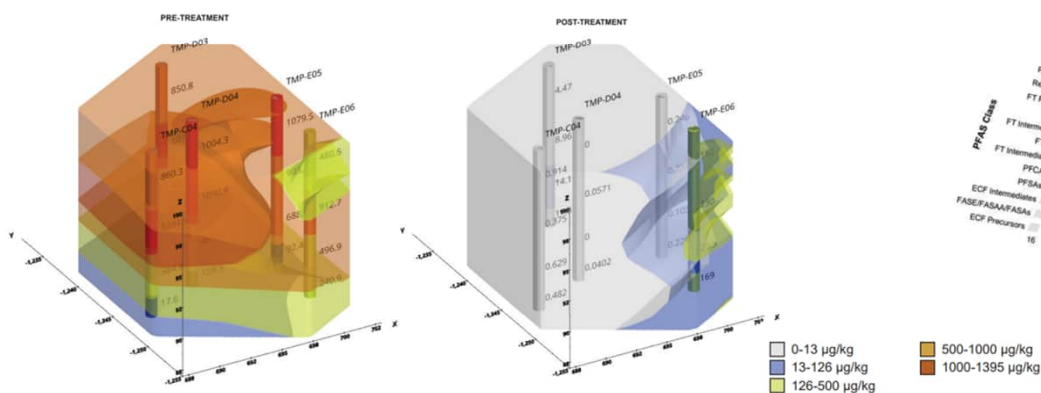
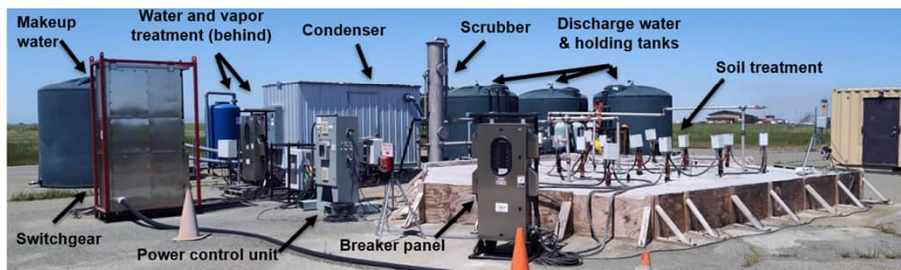


Grouped datasets



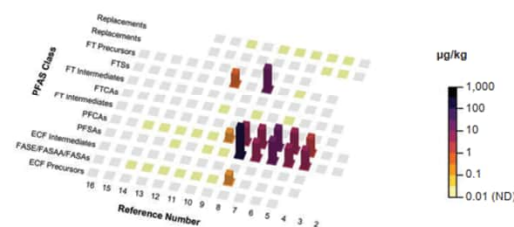
3D Matrix Application

In-situ thermal treatment of PFAS contaminated soil

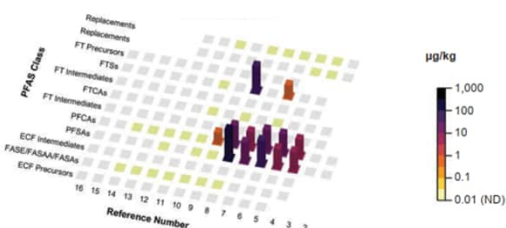


Pre-Treatment

3 – 3.5 ft bgs
Total Detected PFAS: 861 µg/kg

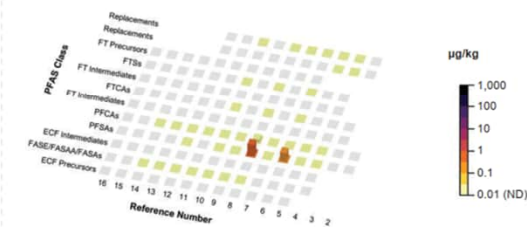


6 – 6.5 ft bgs
Total Detected PFAS: 1,395 µg/kg

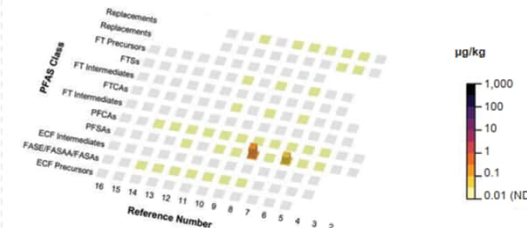


Post-Treatment

3 – 3.5 ft bgs
Total Detected PFAS: 0.913 µg/kg



6 – 6.5 ft bgs
Total Detected PFAS: 0.375 µg/kg



ESTCP Project ER20-D1-5250

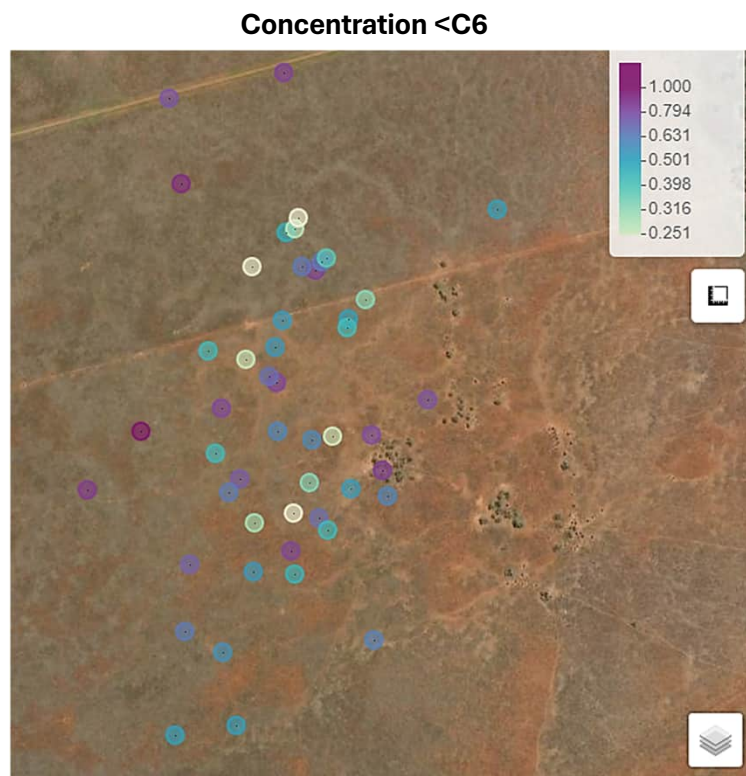
PFAS Concentration Calculations/Conversions

Select Chemical

Concentration <C6

Select All Deselect All

- Perfluorotridecanoic acid (PFTrDA)
- Perfluorooctane sulfonamide (FOSA)
- 4:2 Fluorotelomer sulfonic acid (4:2 FTS)
- Perfluoropropanesulfonic acid (PFPrS)
- Total PFAS
- Total F Calculated
- Total Molar
- ECFs
- PFSAs
- FTs
- PFCAs
- Replacements
- Relative Molar Weight
- Relative Oxidation
- Concentration <C6 ✓
- PFOS/PFHxS
- PFOS/PFOA



Key Metrics:

Total PFAS: Sum of all reported PFAS; indicates total mass burden for screening and reporting.

Total Fluorine Calculated: Estimated total fluorine mass from detected PFAS; fluorine-specific loading for mass balance and source strength.

Total Molar: Sum of PFAS on a molar basis; enables chemically meaningful comparisons for mass balance and transformation potential.

Diagnostic Ratios: Ratios of specific PFAS (e.g., PFOS/PFHxS); evaluate sorption effects, proximity to sources, and relative mobility.

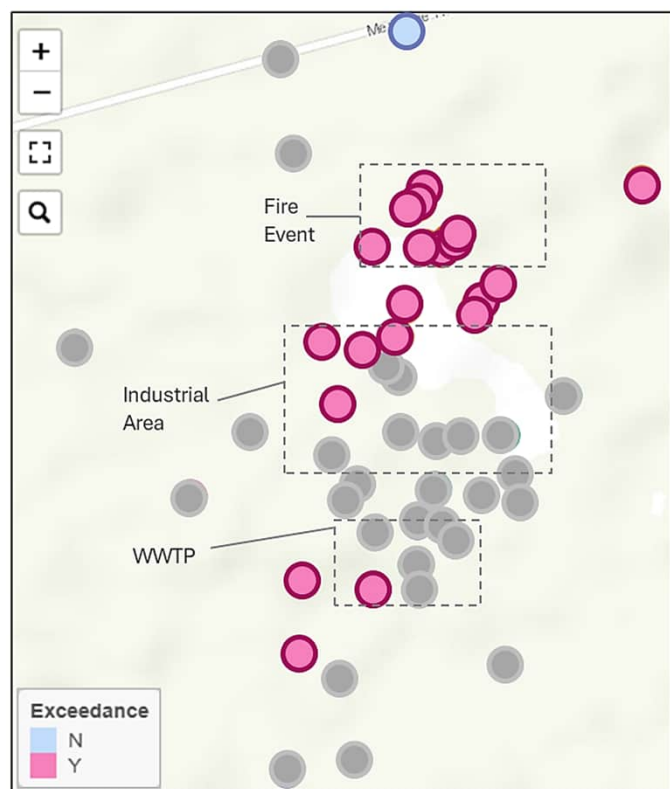
Terminal PFAS: Total molar concentrations for Perfluoroalkyl carboxylates (PFCAs) and sulfonates (PFSAs); used to evaluate PFAS fate, transport behavior, and formation through precursor transformation.

Precursors: Total molar concentrations of ECF- and fluorotelomer-derived precursors; distinguishes source types and estimates transformation potential.

≤C6 Percentage: Proportion of short-chain (≤6 carbon) PFAS; signals modern C6-based foams or long-chain degradation.

Replacement Compounds: Identification and quantification of emerging replacement PFAS; assesses recent releases and shifts in usage.

Exceedances



Geostatistical Analysis

Select Chemical
 Perfluorooctane sulfonic acid (f ▾)

Select Date(s)
 2021-03-08 2021-03-09 2021-03-10 ▾

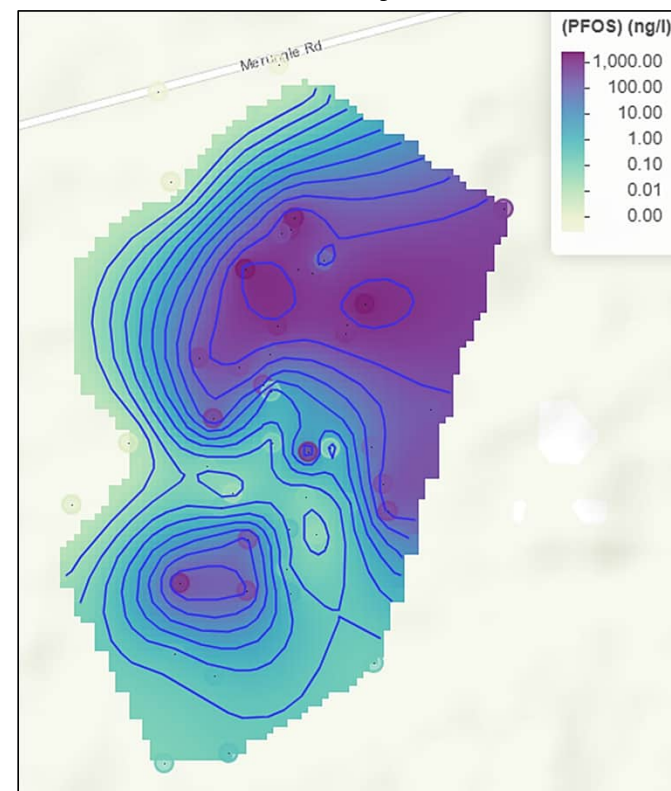
Select plotting locations using dropdown or mapping tools

Select Location(s)
 Nothing selected ▾

Contours
Plume boundary shapefile (optional)
 Browse... Select all file extent

Plume Extent Concentration Limit (ng/L)
 30

Run Contours



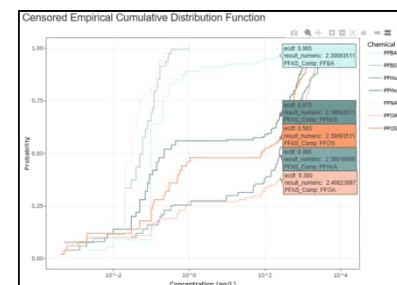
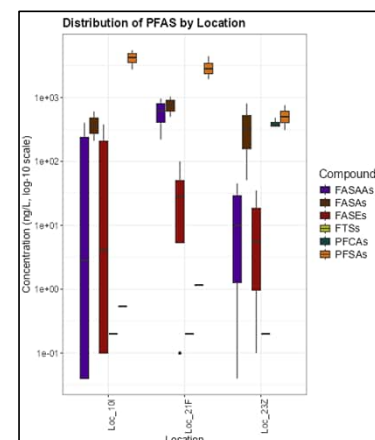
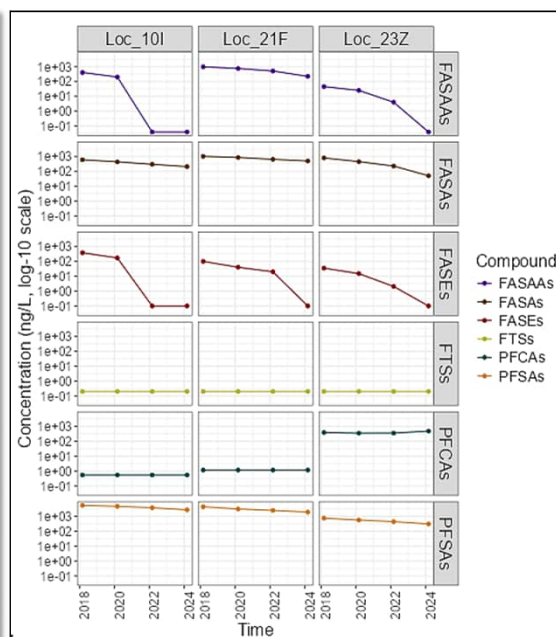
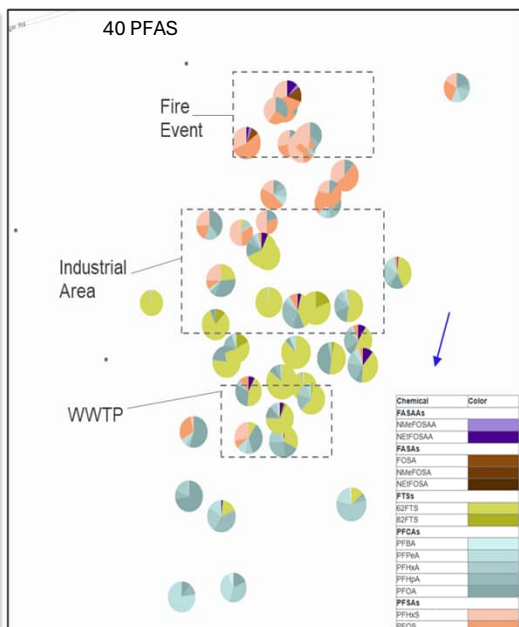
PFAS Class

Fire Event

Industrial Area

WWTP

Class	Color
FTSS	Light Green
FASAs	Dark Green
FASAAAs	Purple
PFASs	Orange
PFCAs	Dark Blue

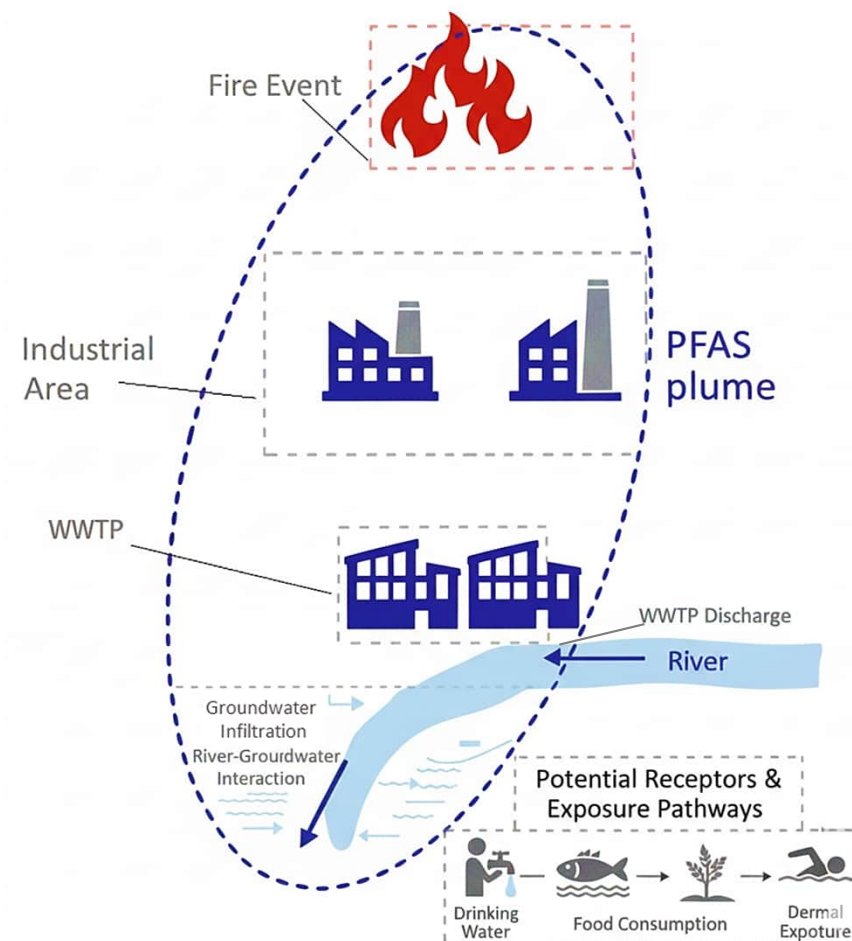


Case Study

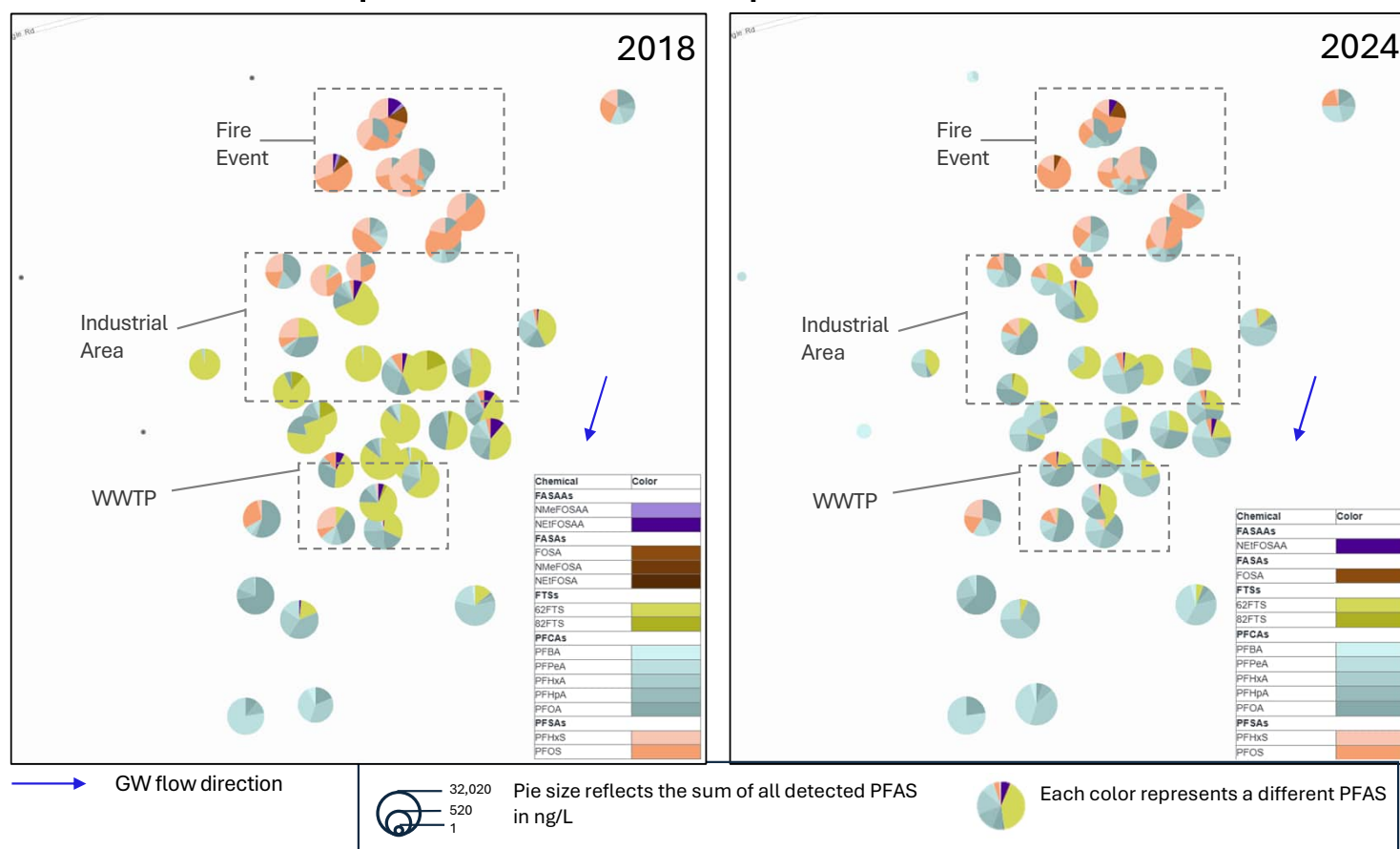


Background

- Pre-1990 Fire Event
 - Large storage facility fire in the late 1980s
 - Firefighting foams used for suppression
 - Site remained inactive for several years afterward
- Industrial Manufacturing Area
 - Textile and paper-coating operations since 1970s
 - Produce treated materials for consumer/commercial use
- Onsite Wastewater Treatment Plant (WWTP)
 - Operating since the 1980s to manage industrial wastewater
 - Continues to treat influent from the facility



The Pies – Spatial and Temporal Distribution



Data Cluster Analysis

Traditional geospatial analysis poses challenges with PFAS complexity

- How similar or different are these PFAS data?
- How many groups can I see?
- What are the relationships between conceptual groups of samples?



K-means Clustering on Multidimensional Scaling (MDS) Analysis

[K-means on MDS Data](#)

Hierarchical Clustering on Multidimensional Scaling (MDS) Analysis

Hierarchical Clustering on MDS Data

Partitioning Around Medoids (PAM) Clustering on MDS Analysis

PAM on MDS Data

K-means Clustering on Distance-Based Redundancy Analysis (dbRDA)

K-means on dbRDA Data

Inferential Statistics

Select Dates

2021-03-15 2021-03-12 2021-03-11 2(▼)

Select Outliers

Nothing selected ▼

Run Preliminary Analysis

Threshold (Value between 0-1):

0.1

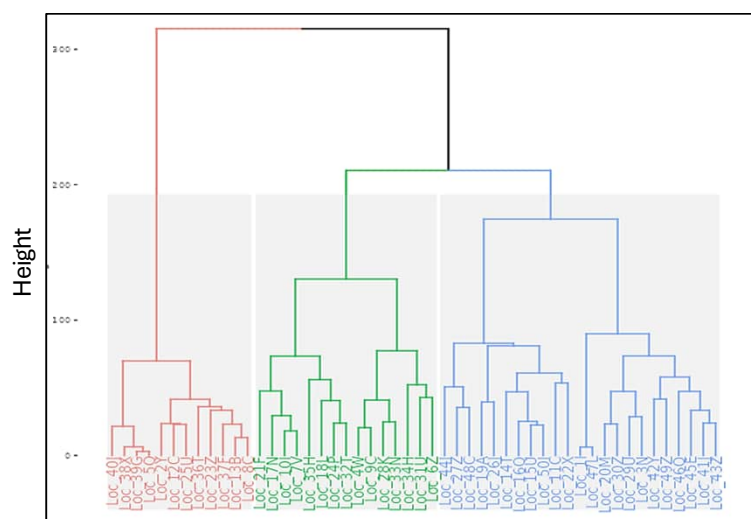
Number of clusters:

3

Run Cluster Analysis

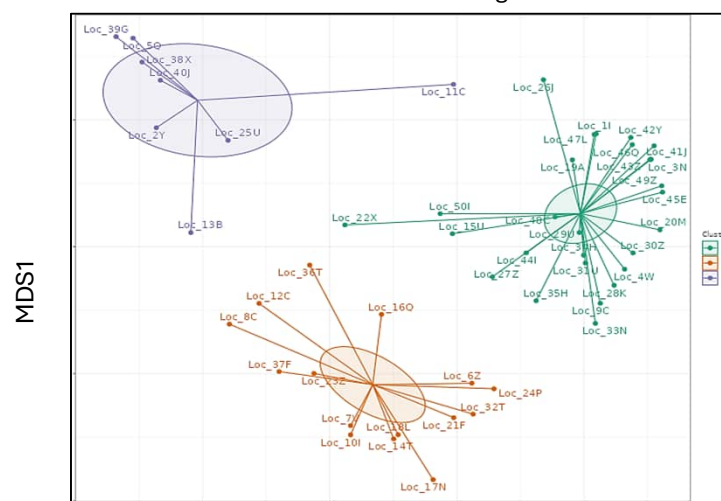
Data Cluster Analysis

Hierarchical Clustering



- Builds nested clusters that reveal relationships among PFAS signatures
- Provides a dendrogram for visualizing similarity and grouping of samples
- Useful for exploratory analysis when the number of clusters is unknown

K-Means Clustering

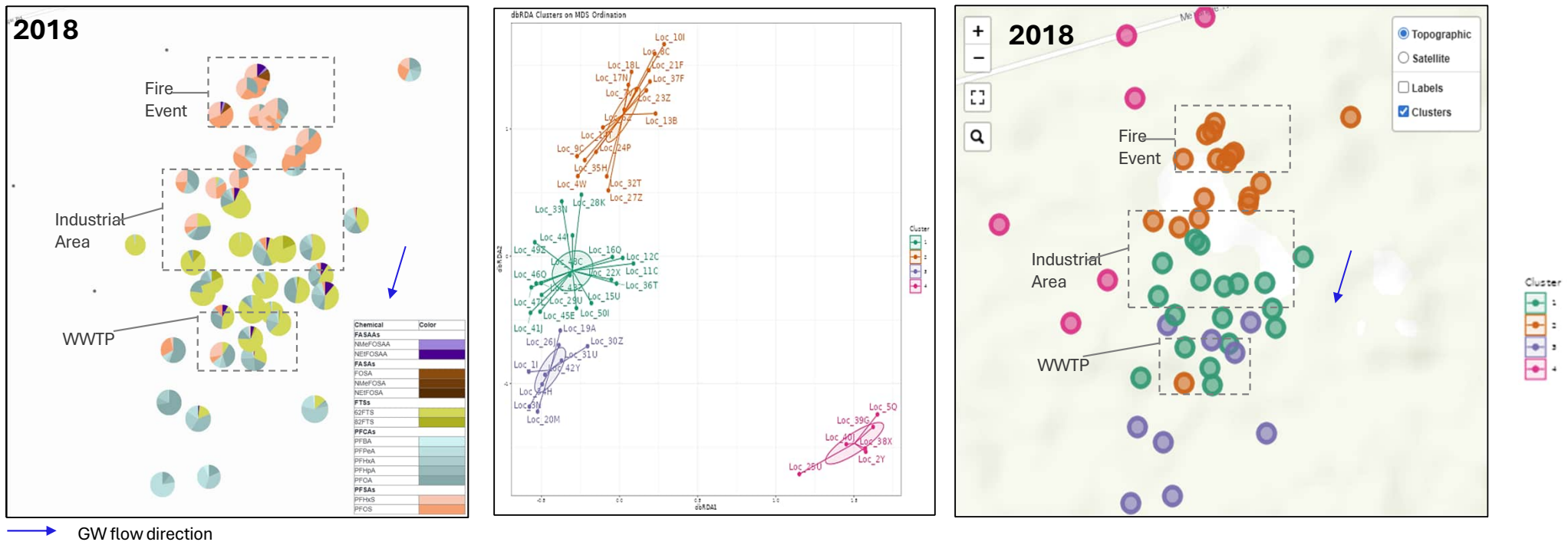


MDS1

MDS2

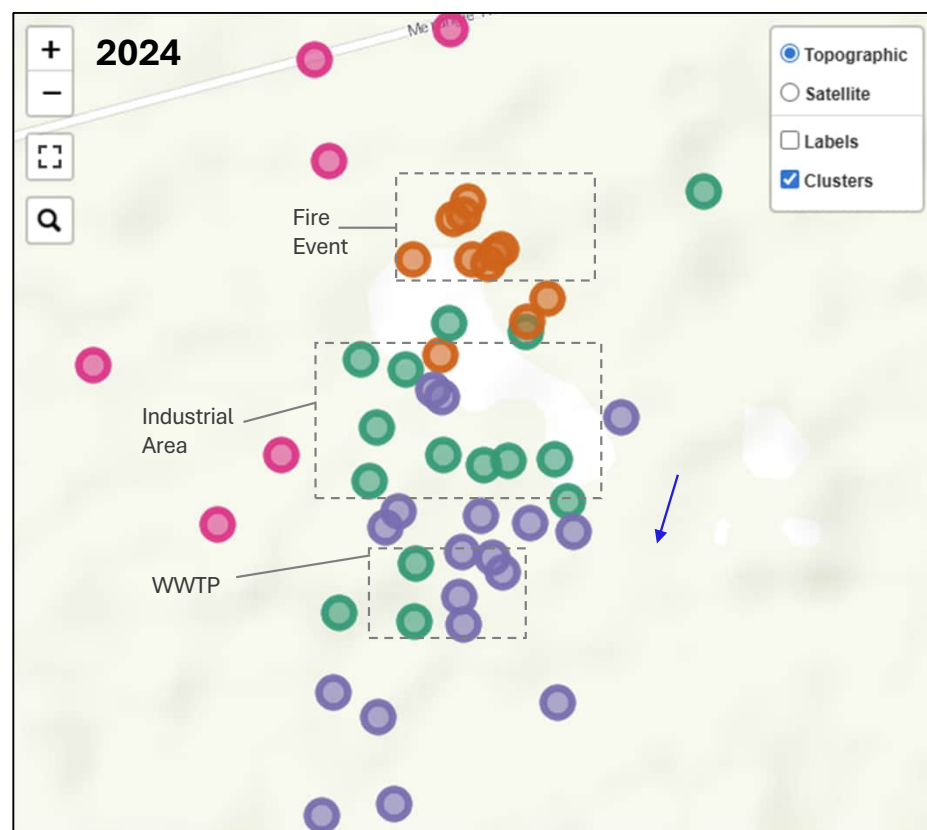
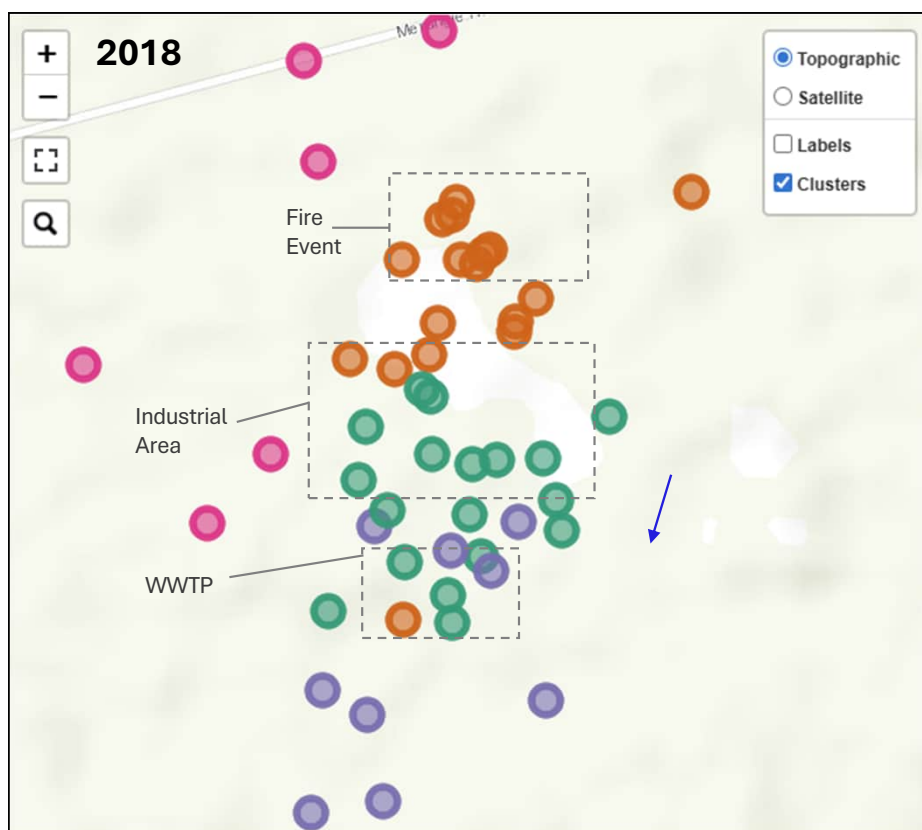
- Groups samples into clusters based on PFAS composition and concentration magnitude
- Recognizing broad patterns of contamination sources or site-wide concentration gradients
- Computationally efficient, making it practical for large monitoring datasets

Clustering and the Conceptual Site Model



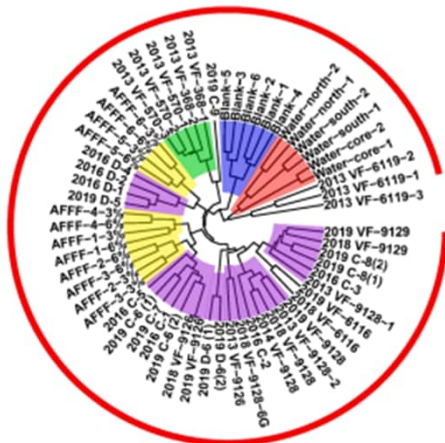
Cluster analysis shows agreement with compositional differences observed in the pie plot visualization

Temporal Changes

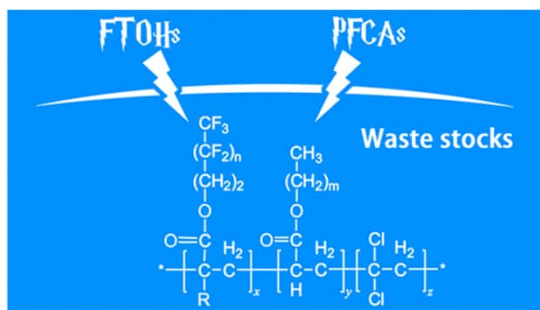


Chemical Fingerprinting

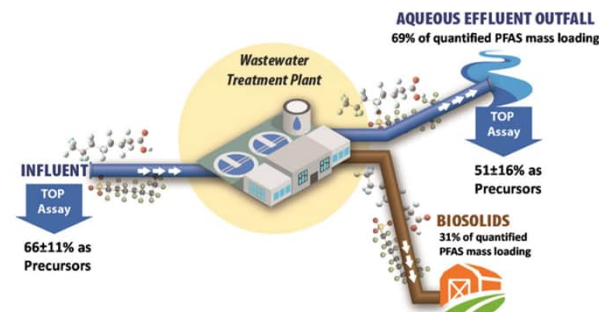
Characteristics	AFFF	Textile	WWTP
Manufacturing process	ECF vs FT, dictate specific non-polymeric PFAS present	Use side-chain fluorotelomer polymers (SCFP) which can be based on different carbon chains	None
Primary PFAS	Legacy C8 and modern foams with C6 and their precursors	Includes both polymeric and non-polymeric PFAS. SCFP can break down to FT precursors and form different PFCAs	Vary widely depending on the source of PFAS entering WWTP



<https://doi.org/10.1016/j.envint.2022.107398>
Abundant references on AFFF signature identification and comparison



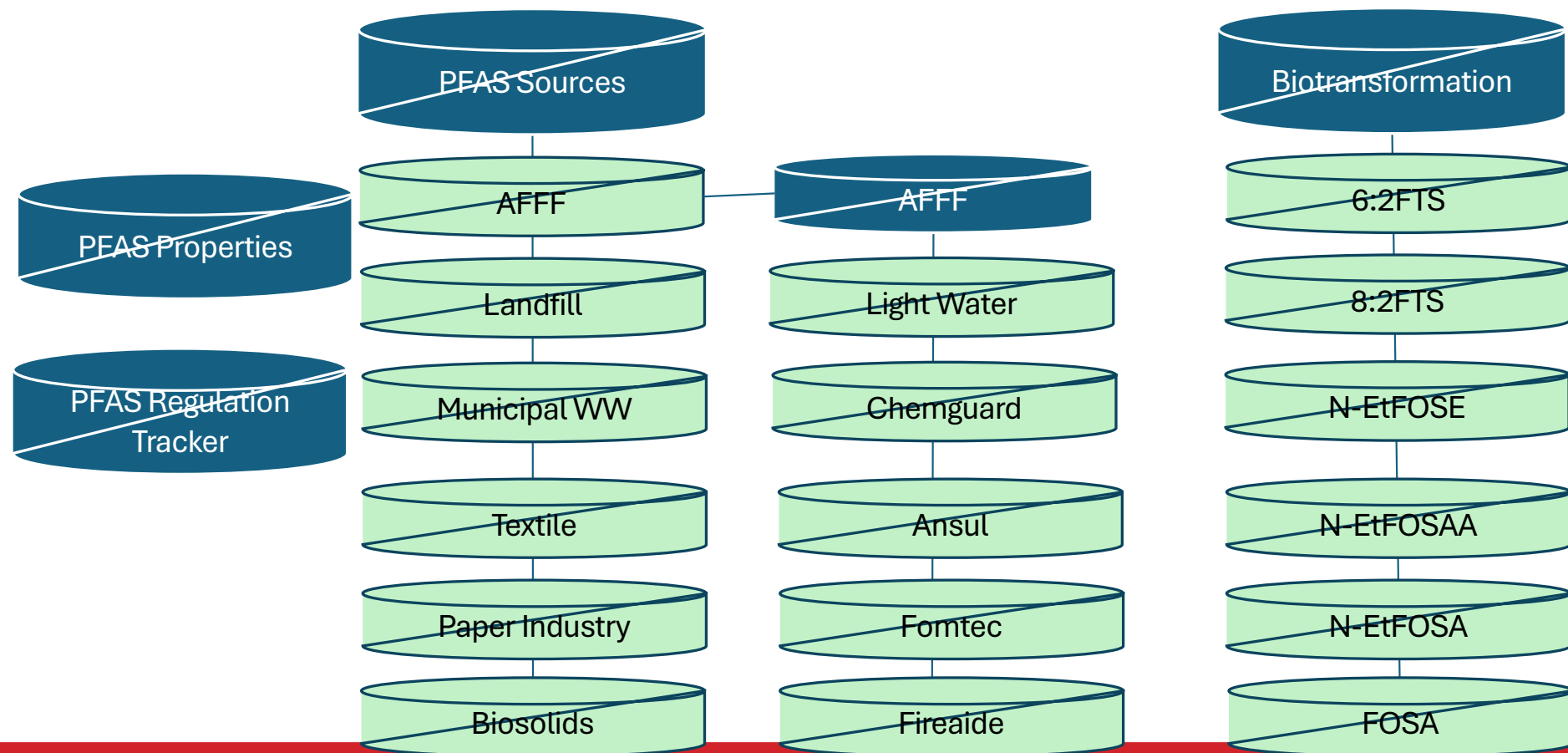
SCFP and other PFAS used in textile are less documented for source tracking



Water Research Volume 233 April 15 2023, 119724

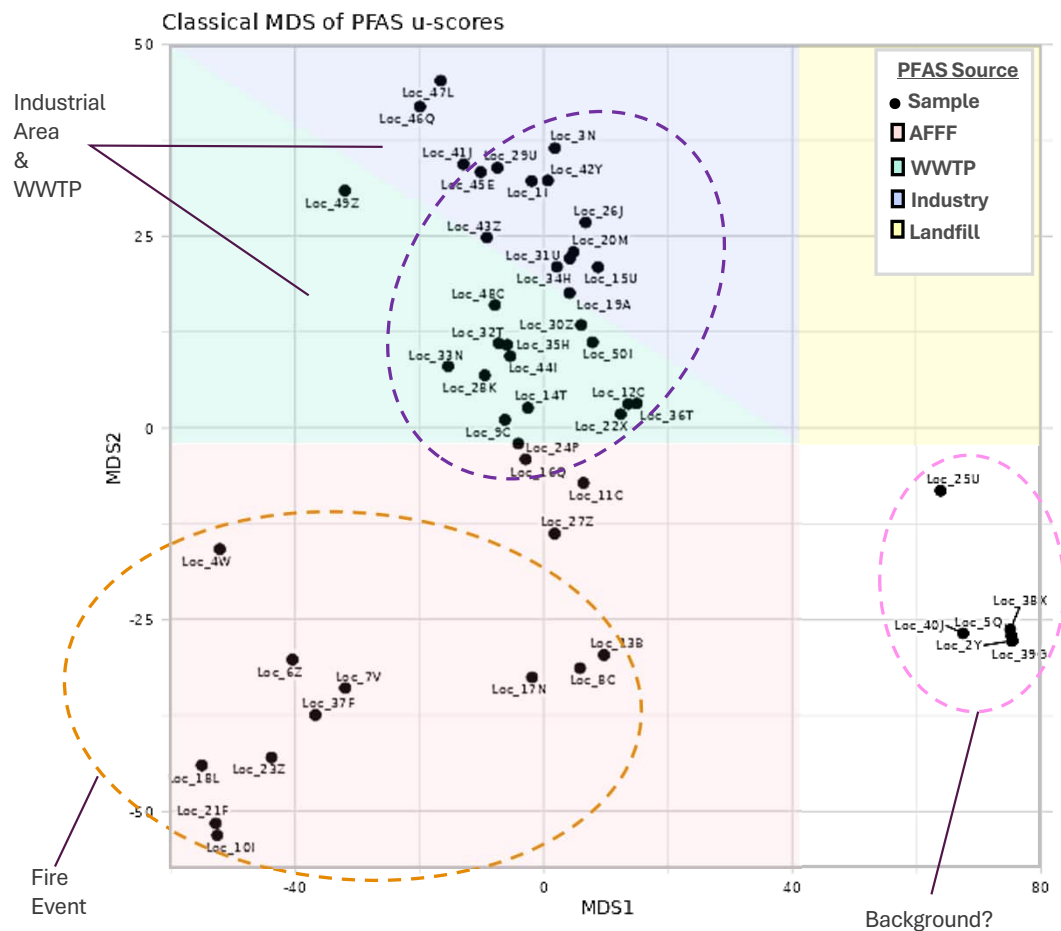
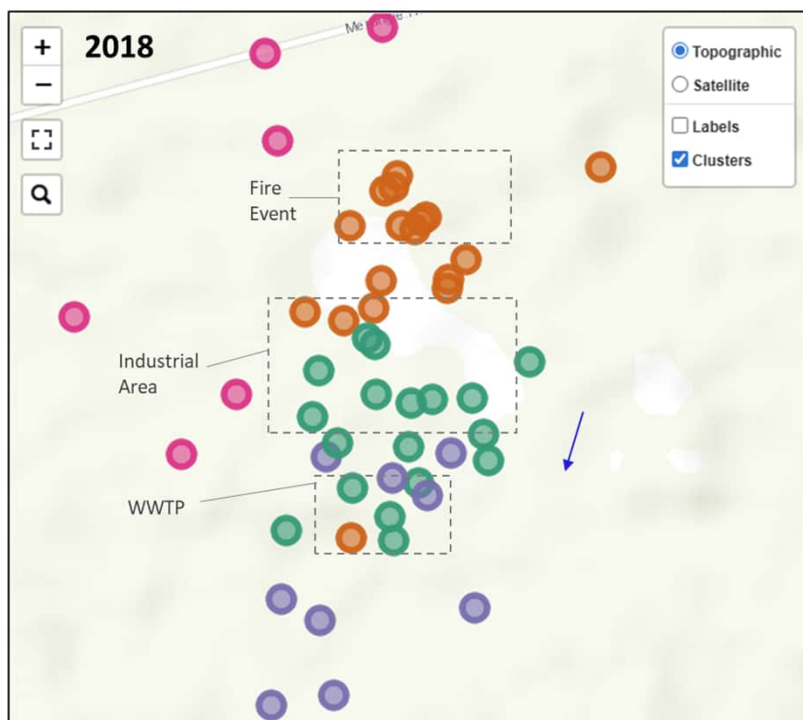
High precursor loading can be possible to WWTP, however, source tracking cannot point to specific PFAS manufacturing processes

Databases Available in PFAS Toolset

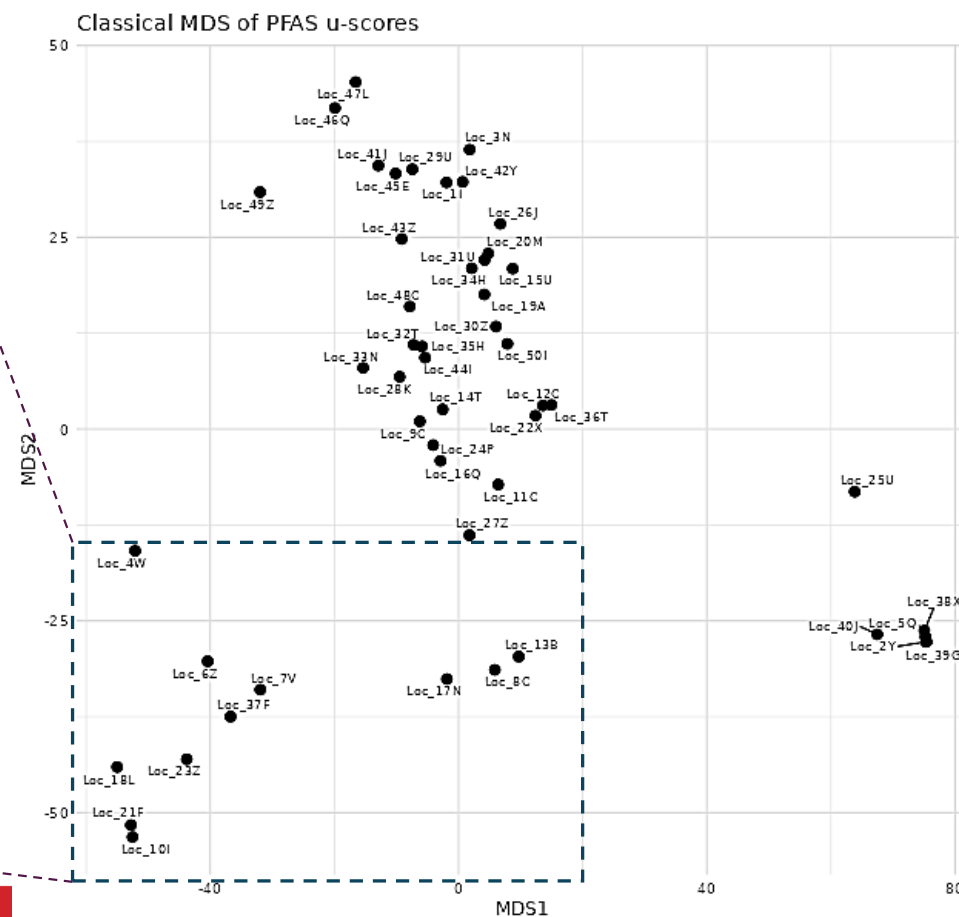
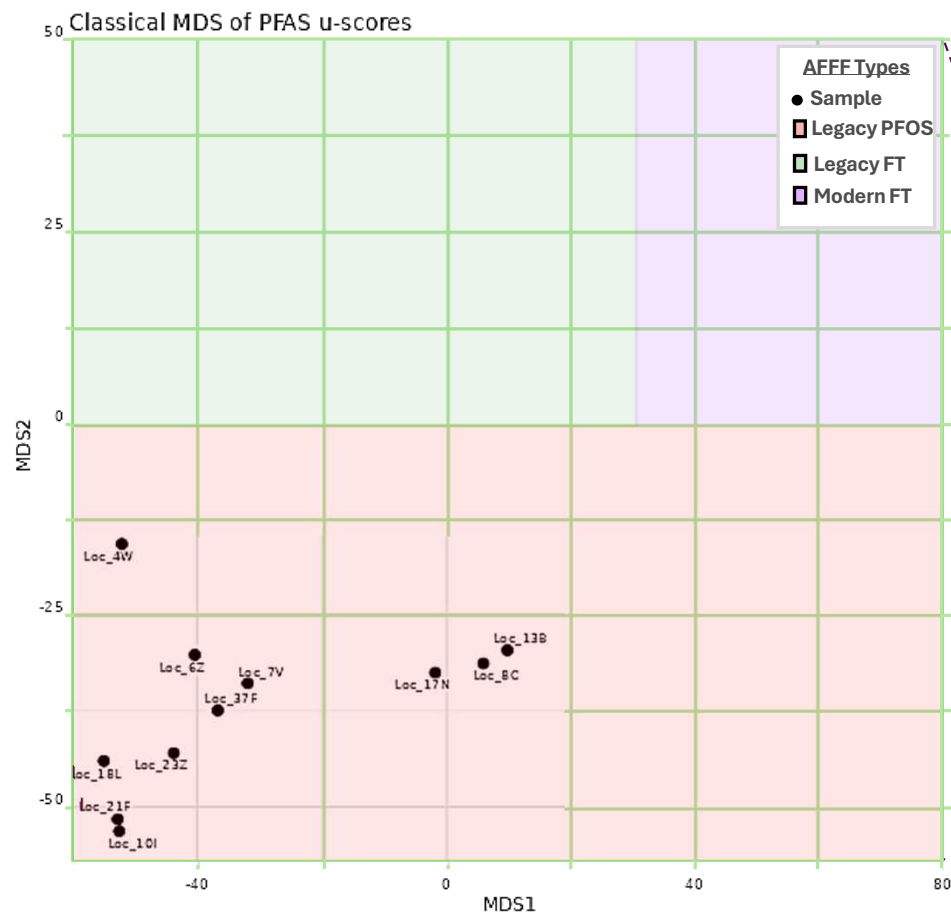


Source Categories

Source PFAS library used to run MDS, a distance-based ordination technique, for profile matching



AFFF Fingerprints



Biotransformation

Biotransformation can alter the PFAS profile

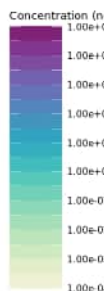
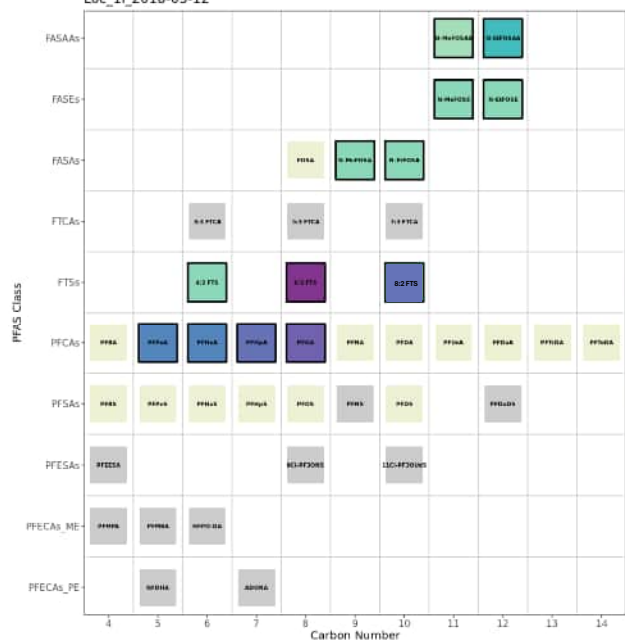
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Biotransformation
Database

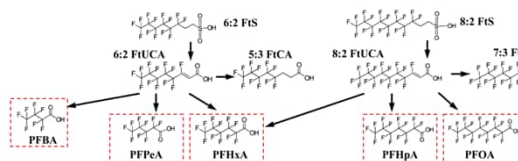
Look for
Biotransformation
products of 6:2 FTS
and 8:2 FTS

2018

Loc_11_2018-03-12

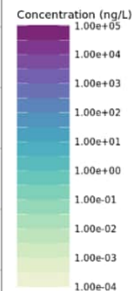
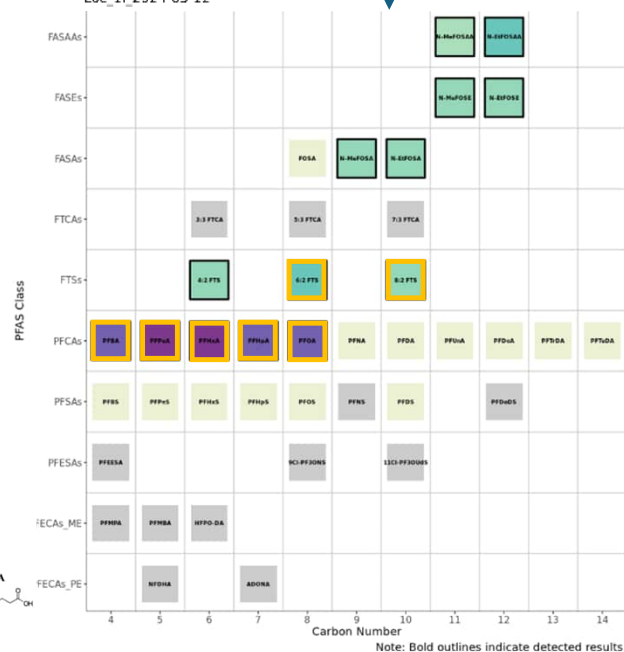


Pathway identified for 6:2 FTS and 8:2 FTS using the biotransformation library



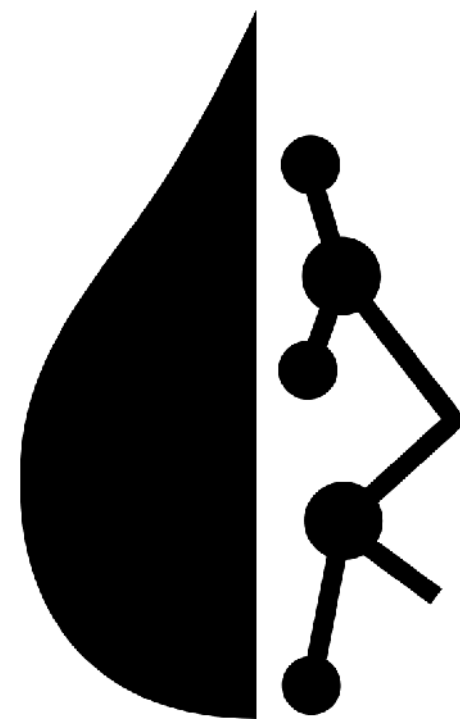
2024

Loc_11_2024-03-12



Benefits of PFAS Digital Tool

- Allows for:
 - Automated Visualization
 - PFAS Fingerprinting
 - Understanding of Biotransformation
- Helps reduce costs and schedule when evaluating PFAS impacts on projects.
- Allows PFAS SMEs to focus on interpretation of data and technical evaluation instead of data management and manipulation
- Expedites CSM development and reaching conclusions.





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