



Applying PFAS Forensics to Complex, Multi-Source Sites

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Jacobs

RITS 2026

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Information in this presentation is current as of May 14, 2026.

EXWC: Engineering and Expeditionary Warfare Center
NAVFAC: Naval Facilities Engineering Systems Command

Speaker Introduction



Dora Chiang Ph.D., P.E.



- Ph.D., Environmental Engineering, Georgia Institute of Technology, Atlanta, Georgia, USA
- M.S., Environmental Engineering, Illinois Institute of Technology, Chicago, Illinois, USA
- M.S., Chemistry, Chung Yuan University, ChungLi, Taiwan
- B.S., Chemistry, Chung Yuan University, ChungLi Taiwan
- 25 years in site investigation and remediation
- Practice leader of PFAS and emerging contaminants at multiple engineering consulting firms
- Global principal of PFAS and emerging contaminants at Jacobs since 2024
- Technical director of Jacobs PFAS Forensics Toolset – Pfluorensic
- Principal investigator of PFAS destruction technologies (EO, SCWO, enzyme)
- Co-editor of PFAS Treatment Technologies Book

EO: Electrochemical Oxidation

PFAS: per- and polyfluoroalkyl substances

SCWO: Supercritical Water Oxidation

Past RITS Trainings



- Related Past RITS Presentations
 - FY2025 RITS: [Contextualizing PFAS Detections: Background and Forensics](#) (Jeff Gamlin/GSI Environmental)
 - FY2024 RITS: [Applications of Multivariate Analysis \(MVA\) for Environmental Restoration Sites](#) (Loren Lund/Jacobs)

FY: fiscal year

RITS: Remediation Innovation Technology Seminar

Presentation Overview



- Introduction

- Refresh on Chemistry, Sources, Fate, and Transport
- PFAS in Ambient Environment (Background Study)
- Targeted PFAS Forensics Study Design and Case Study
- DoW-funded PFAS Source Databases
- Key Takeaways

Fingerprinting versus Forensics

- **Fingerprinting**

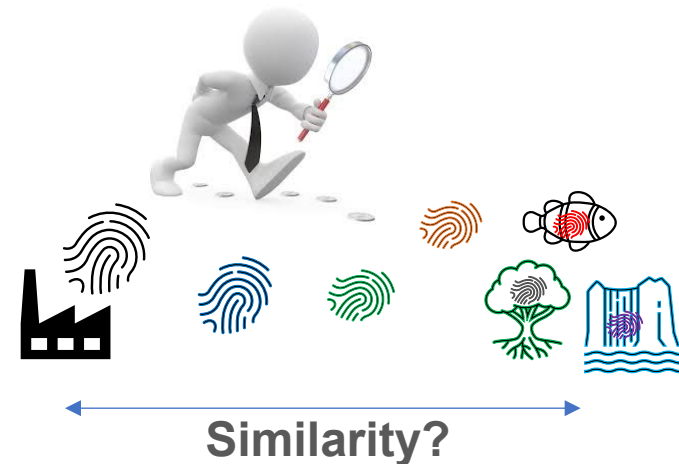
- Primarily used for source identification based on unique chemical signatures
- Useful in verifying identities, linking a chemical to an object, a source, a scene, or eliminate suspects
- Focus solely on fingerprint evidence



CSM: conceptual site model

- **Forensics**

- Used to reconstruct events (e.g., CSM), determine causes or sources, and support legal decisions
- Goals are to find truths, attribution, causation, and evidence validation
- A broader field that can involve chemistry, biology, geology, engineering, data science, toxicology, etc.



Applications of PFAS Forensics



- PFAS forensics may be considered when:
 - Multiple onsite sources are detected, some with unknown nature and source
 - Background study confirms offsite PFAS sources; can help differentiate background vs. onsite sources
 - Characterization of precursors will assist to identify their source, migration pathways, and transformation
- **PFAS forensic study should start with assessing target PFAS data (EPA Method 1633) first**

KEY POINT

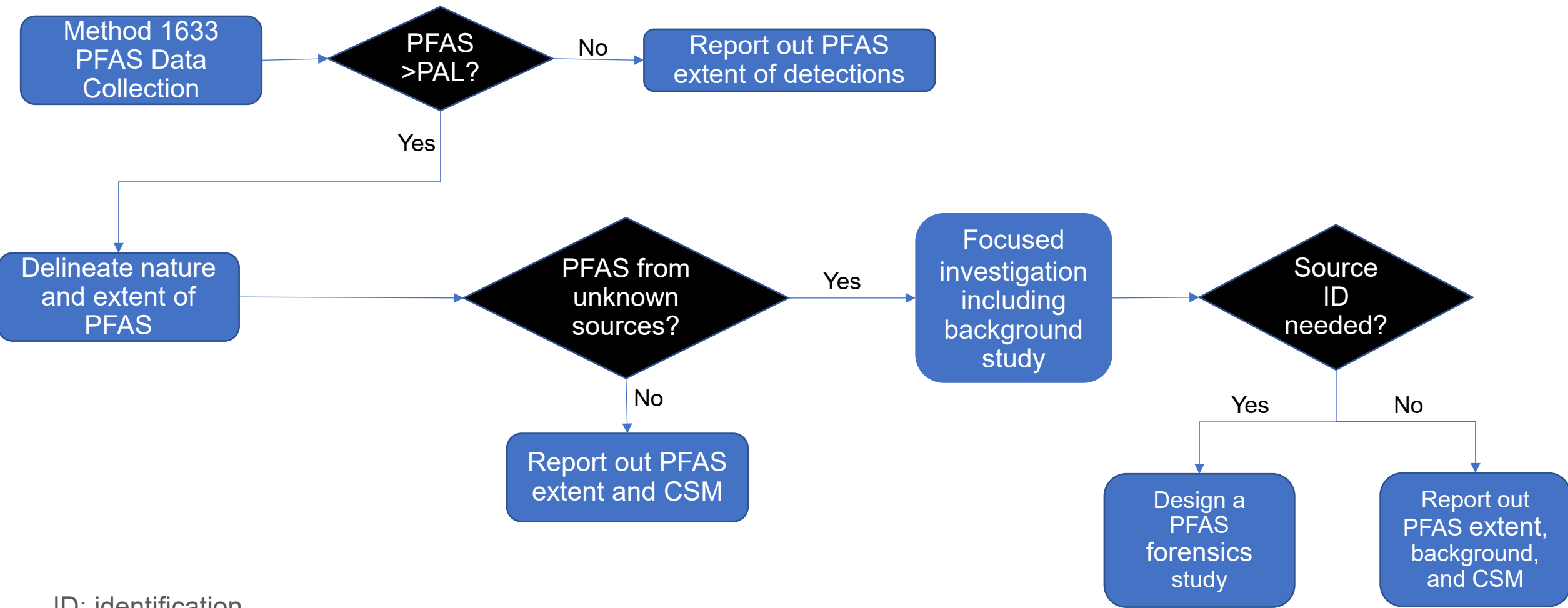
PFAS forensics can be considered in limited site-specific cases. The need must be clearly identified, method selection understood, data quality objectives clearly articulated, and line-of-evidence approach used in accordance with applicable DoW Policy* and in coordination with regulatory partners.

Benefits of PFAS Forensics



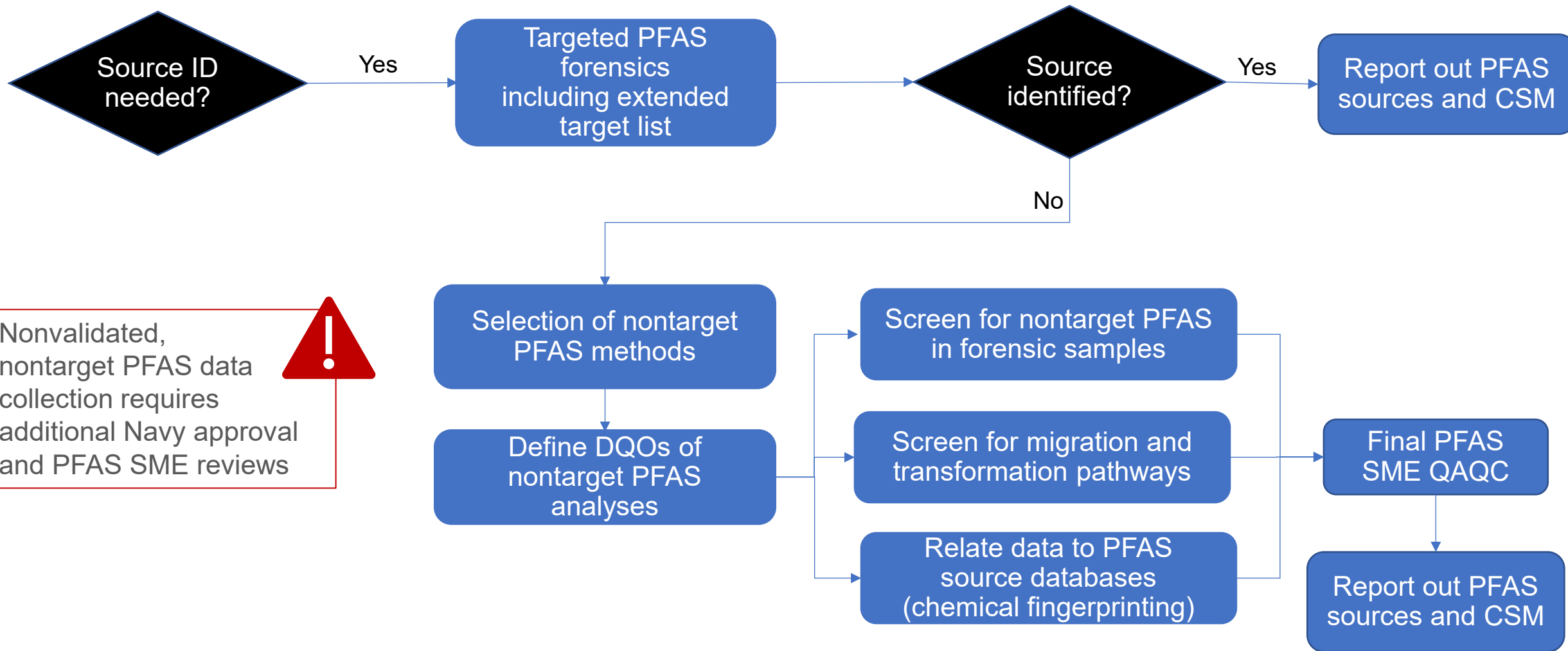
- Refine CSM when the site is impacted by multiple, onsite, and offsite PFAS sources
- Support PFAS background assessment
- Optimize more PFAS management efforts knowing from where the sources originate
- Improve risk assessment and communications
- Better protect human health and reduced exposure pathways

PFAS Investigation – Example Workflow



ID: identification
PAL: project action level

Advanced Forensics (Only Limited Cases Would Apply)



Nonvalidated, nontarget PFAS data collection requires additional Navy approval and PFAS SME reviews



DQO: data quality objective
Navy: Department of the Navy

QAQC: quality assurance quality control
SME: Subject Matter Expert

Presentation Objectives



- Differentiate sources vs. background data
- Design and conduct targeted PFAS forensic study using Method 1633 PFAS data only
- Be familiar with PFAS data analytic techniques (e.g., cluster analysis) for forensic study assessment

Presentation Overview



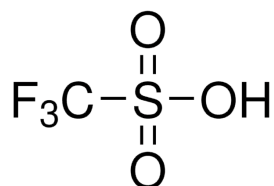
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Complexity of PFAS Chemistry

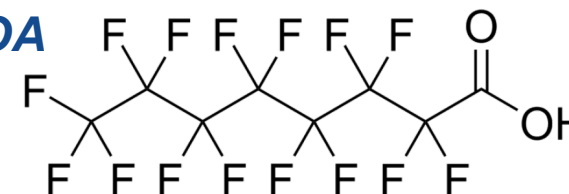


Carbon No.	1	2	3	4	5	6	7	8	9	10	11	12
PFCAs	Ultrashort			Short-Chain				Long-Chain				
			PFPrA	PFBA	PFPeA	PFHxA	PFHpA	PFOA	PFNA	PFDA	PFUnA	PFDoA
PFSAAs	Ultrashort			Short-Chain			Long-Chain					
	TFMS	PFEtS	PFPrS	PFBS	PFPeS	PFHxS	PFHpS	PFOS	PFNS	PFDS	PFUnS	PFDoS

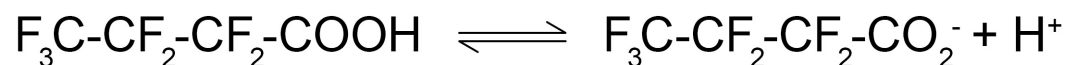
TFMS



PFOA



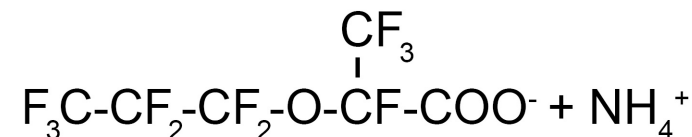
- **PFAS** can contain negative (anionic), positive (cationic), or both charges (zwitterionic)



Perfluorobutanoic acid

Perfluorobutanoate (+ dissociated proton)

- **PFAA replacements** such as GenX chemicals



GenX Ammonium Salt

PFAA: perfluoroalkyl acid

PFOA: perfluorooctanoic acid

PFSA: perfluoroalkyl sulfonic acid

PFCA: perfluoroalkyl carboxylic acid

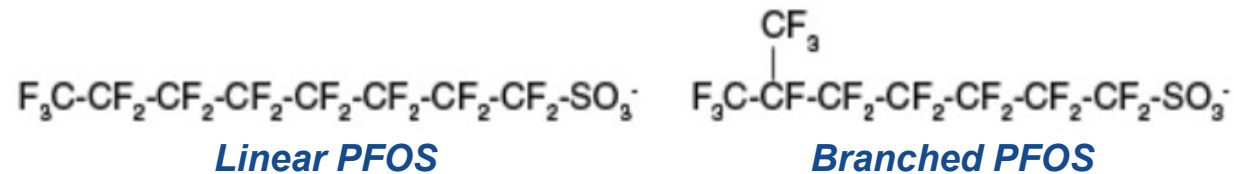
PFOS: perfluorooctanesulfonic acid

TFMS: trifluoromethanesulfonic acid

Complexity of PFAS Chemistry

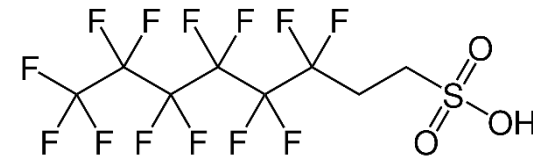
Linear and branched isomers of PFAS

- Example



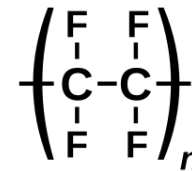
PFAS Precursors

- Example: 6:2 fluorotelomer sulfonic acid



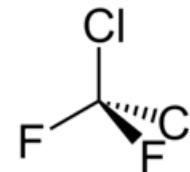
Polymeric PFAS

- Example: Polytetrafluoroethylene (PTFE)



HFCs: Hydrofluorine carbons

- Example: Dichlorodifluoromethane



Considerations of PFAS Detections



- PFAS detection limits are getting sensitive for solids and liquids
- Low concentration detections should be put into perspective with regard to uncertainty interpretation (e.g., false positives, laboratory contamination, etc.)
- When PFAS concentrations are higher, PFAS interpretation for forensics is more certain
- When PFAS concentrations are lower near PQLs, forensic evaluation must keep uncertainty and more scrutiny in mind
- Certain PFAS such as TFA (outside of EPA PFAS definition) can be found in almost any laboratory, and thus low levels should be expected even in laboratory and field blanks; additional considerations are needed for forensic evaluation

PQL: Practical Quantitation Level

TFA: trifluoroacetic acid

Knowledge Check



True or False?

All precursors are considered “poly-fluoroalkyl substances”

True or **False?**

False. PFAS precursors are those PFAS which can be transformed into terminal PFAAs (PFCAs and PFSAAs). Polyfluorinated compounds contain carbons that are not fully fluorinated like FTS, there is great chance that they are precursors. However, not all polyfluorinated compounds are biotically or abiotically transformable. On the other hand, for perfluorinated compounds, although the carbon backbone (the tail) is fully fluorinated, the “head” of PFAS structures can contain functional groups that are transformable.

PFAS Potential Related Sources



Oil and Gas Extraction	Mining	Sewage Treatment Facilities	Textile Mills
Textile Product Mills	Leather and Allied Product Manufacturing	Paper Manufacturing	Printing and Related Support
Petroleum and Coal Products Manufacturing	Chemical Manufacturing	Plastics and Rubber Products Manufacturing	Carpet/Flooring/Building Material Manufacturing
Primary Metal Manufacturing	Fabricated Metal Product Manufacturing	Machinery Manufacturing	Computer and Electronic Product Manufacturing
Electrical Equipment	Appliance and Component Manufacturing	Petroleum and Bulk Terminals	Surgical and Medical Instrument Manufacturing
Airports, Port, and Harbor Operations	Carpet and Upholstery Cleaning	Rail and Truck Transportation	Waste Management
Car Wash, Furniture Repair	Dry Cleaner and Laundry Operators	Fire Protection	National Security

(EPA 2024)

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PFAS Background Study



- RITS 2025: Contextualizing PFAS Detections: Background and Forensics, Jeff Gamlin, GSI Environmental
 - Excerpt from Memorandum on Background PFAS (September 3, 2024)

Long-Term Remedial Actions

CERCLA requires a site-specific risk assessment during the remedial investigation to establish risk-based cleanup levels. This includes considerations of “background” levels of chemicals present at a site, which can be highly variable across the country. Throughout the CERCLA process DoD coordinates with both EPA and state regulators and EPA and DoD jointly select remedies at National Priorities List sites. Accordingly, DoD will work with EPA and state regulators, as appropriate, to evaluate background levels of PFAS on a site-specific basis to determine a final cleanup level.

For remedial actions, the DoD Components will address drinking water down to the MCLs or background, in accordance with CERCLA, once the DoD Component has established levels of PFAS are below the MCLs, then DoD Components will take remedial actions to address PFAS that will meet the MCLs as the final cleanup levels.⁶ If background levels of PFAS are found above an MCL at a site, DoD Components will work collaboratively with regulators and transparently with the public to determine the appropriate remedial goals (i.e., final cleanup levels) at that site.

(DoD 2024)

CERCLA: Comprehensive Environmental Response, Compensation, and Liability Act of 1980

DoD: U.S. Department of Defense

MCL: maximum contaminant level

Statewide PFAS Background Studies



- PFAS background data available for assessment continue to expand
- UCMR data are not included in the tables
- Background samples can be collected by state agencies, consultants, universities and samples were analyzed using different methods for different sets of PFAS analytes

State	Sample Matrix	Analytical Methods or Analytes	Reference
EPA	Water, tissue, air, soil, sediment	Target PFAS	PFAS Analytic Tools (EPA n.d.)
AL	Surface water	17 PFAS	Viticoski et al. 2022
CA	DW, SW	533, 537, 537.1, 1633, AOF	California GeoTracker PFAS Map (SWRCB n.d.)
CO	GW, SW, soil sediment	533, 537.1, 1633	Colorado PFAS Concentration Map (CDPHE 2026)
FL	SW	50 PFAS	Camacho et al. 2024
GA	SW, DW	Target PFAS	Georgia PFAS Story Map (GEPD 2026)
MA	SW, fish	533, 537, 537.1, 1633	ERG 2023

AOF: adsorbable organic fluorine
 DW: drinking water
 GW: groundwater

SW: surface water
 UCMR: Unregulated Contaminant Monitoring Rule

Statewide PFAS Background Studies



State	Sample Matrix	Analytical Methods or Analytes	Reference
ME	GW, DW, SW, WW, biosolids, sludge, soil	533, 537, 537.1, 1633	Maine DEP PFAS Investigation (Maine DEP n.d.)
MI	WWTP, residuals, ambient air,	Target PFAS	EGLE 2025; Woodward et al. 2025
MN	GW, SW, Air, Soil	Target PFAS	MPCA 2025
NC	WWTP, biosolids	537.1 modified for 57 PFAS	NCDEQ 2025
NJ*	Soil, SW	1633	NJDEP 2025; Goodrow et al. 2020
NY	Soil	1633	AECOM 2025
PA	SW	1633	Breitmeyer 2023
VA	SW, fish, sediment	533, 537.1, 1633	VDEQ PFAS Dashboard (2025)
VT	Soil	Target PFAS	Zhu et al. 2022
WA	Biosolids	1633, TOPA, EOF, NTA	Ecology 2025
WI	DW, SW, fish, GW	Target PFAS	WI PFAS Interactive Data Viewer (DNR n.d.); Silver et al. 2023

EOF: extractable organic fluorine

NTA: non-target analysis

TOPA: Total Oxidizable Precursor Assay

WW: wastewater

WWTP: wastewater treatment plant

*Ambient study

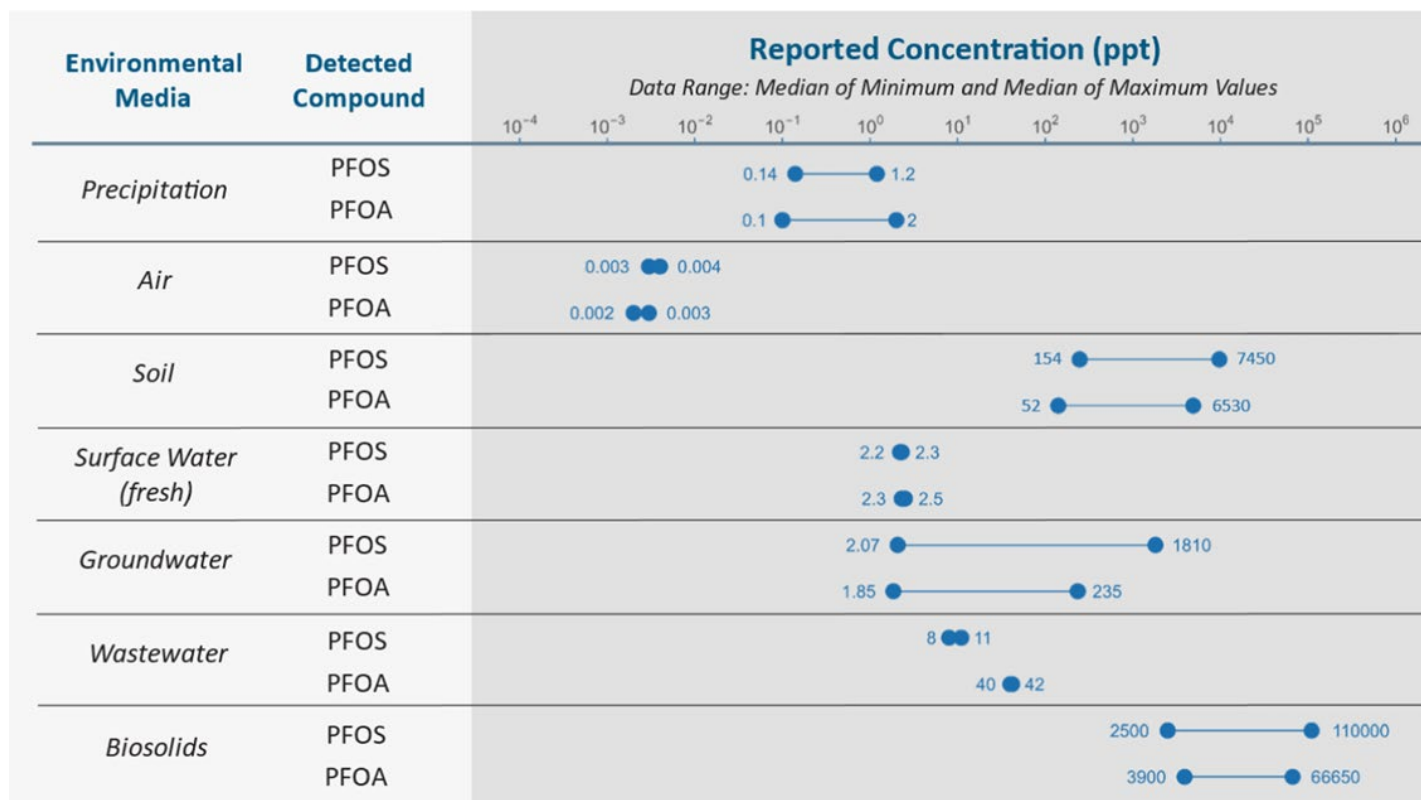
PFAS Background Study – Literature Review



KEY POINT Published background study data quality may vary.

- PFAS background levels have been reported
 - Precipitation
 - Soils
 - Groundwater
 - Wastewater
 - Biosolids
 - Surface water
- Be aware of data quality
 - Data may be collected before EPA Method 1633 is finalized (January 2024)
 - Data may be collected without considering PFAS cross-contamination (e.g., groundwater monitoring well construction)

Comparison of PFAS Occurrence and Concentration Data by Media Based on U.S. Datasets Only



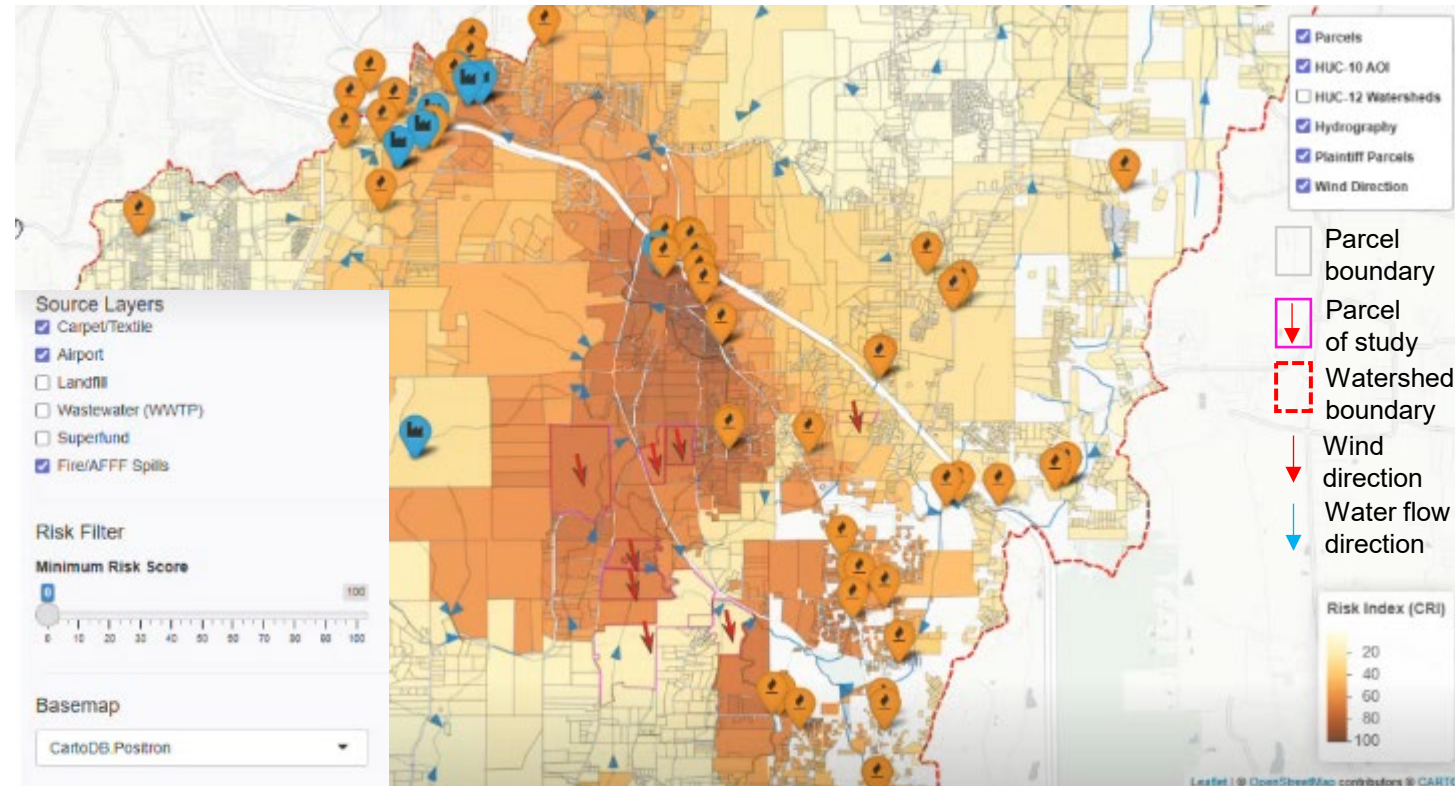
ppt: part(s) per trillion

(Adamson et al. 2026)

Environmental Due Diligence Prior to Background Study

- Environmental due diligence can be conducted prior to background sample collection
- Assess potential PFAS impact in the background study area without PFAS data collection
- Record search
 - Environmental database report
 - Land uses
 - Regional wind and water flow directions
 - State-level compost and biosolid land application records
 - And more

Non-DoW Example of PFAS Risk Mapping to guide selection of background sampling locations



(Conceptual PFAS background risk mapping modeled by Jacobs)

Knowledge Check



True or False? And Why?

PFAS background levels in soil, groundwater, surface water, and biota will change with time

True or False? And Why?

PFAS background levels in soil, groundwater, surface water, and biota will change with time

Yes. Legacy PFAS have been phased out or replaced, but their changes may be slow, complex (e.g., precursor transformation, and media-dependent). Modern PFAS can appear to increase. Site cleanups can help reduce background levels. Even the background level decreased, it does not mean the site cleanup needs to be repeated.

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Ask and Answer These Questions Before Considering PFAS Forensics Study



KEY POINT

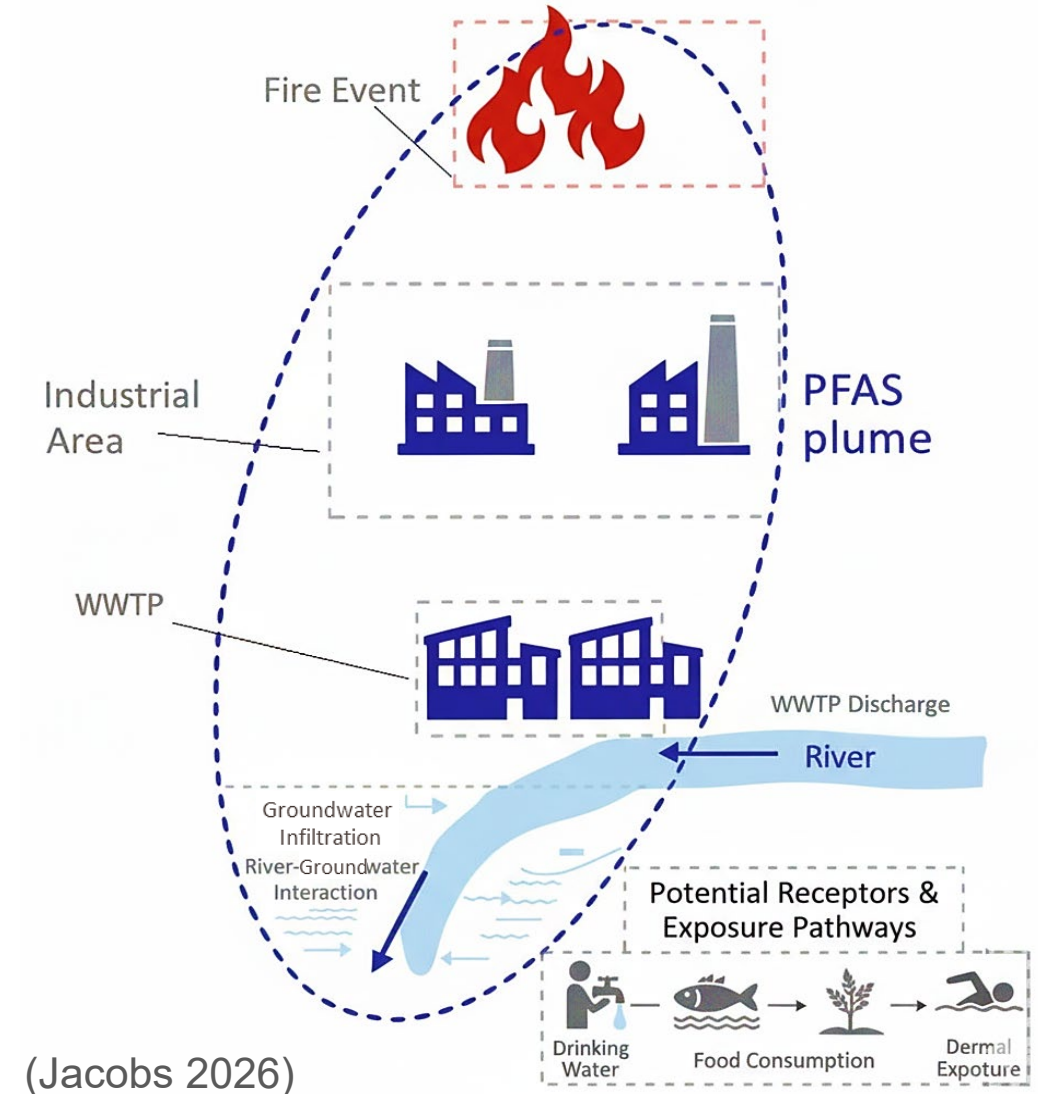
Not all PFAS sites need PFAS forensic study.

Decision Point	Yes/No	Descriptions
PFAS > PALs?	Yes	PALs were exceeded
PFAS are likely from unknown onsite and offsite sources?	Yes	<ul style="list-style-type: none"> • Multiple known and unknown sources onsite • Target precursors detected from sources with potential to transform into regulated PFAAs • Environmental data reports suggested potential offsite sources • Target PFAS detected exceeding PALs from unknown background and onsite locations
Are source identification needed for clarity of CSM and for appropriate remedial goals?	Yes	<ul style="list-style-type: none"> • Suggest to conduct a targeted PFAS forensic study • Navy PFAS SME should be involved for targeted PFAS forensics design and implementation

Targeted PFAS Forensics – Non-DoW Case Study



- Pre-1990 Fire Event
 - Large storage facility fire in 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
- WWTP
 - Operating since 1980s to manage industrial wastewater
 - Continues to treat influent from facility



(Jacobs 2026)

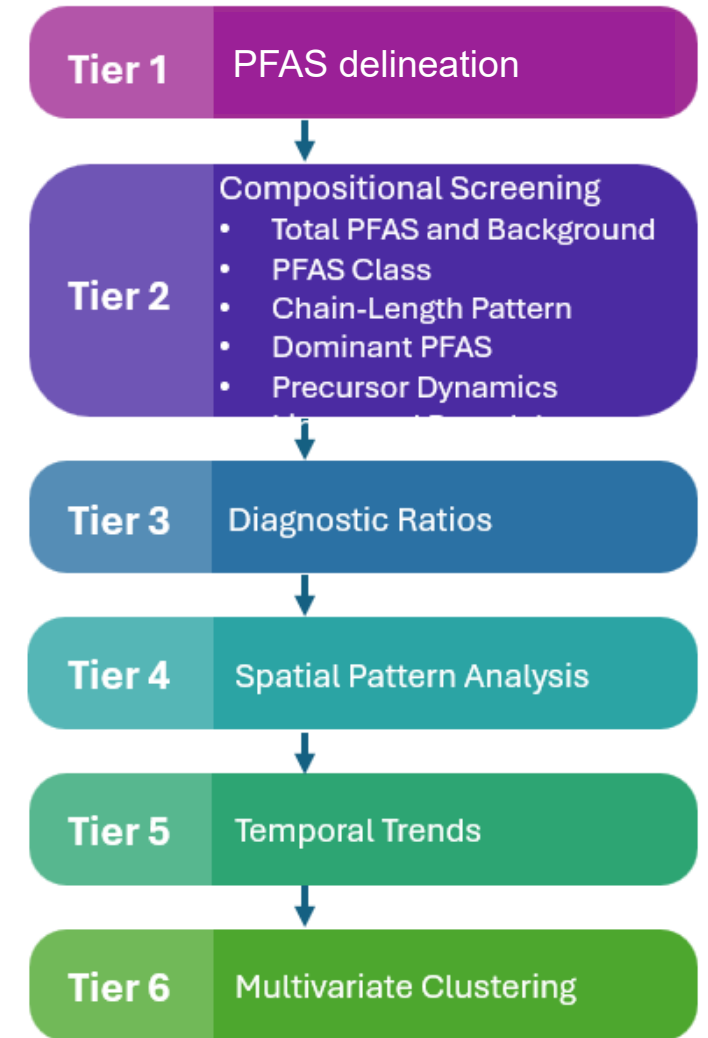
Targeted PFAS Forensics



KEY POINT

PFAS forensics study is site specific. DoW guidance and policy need to be followed for investigating DoW PFAS sites.

- Only target PFAS data are used for targeted PFAS forensics
 - Method 1633
 - Target analytes may vary due to addition of other analytes (e.g., TFSI, PFPrA and additional precursors), extended target analytes can be considered in selected samples assisting in “Targeted PFAS Forensics” when such need is identified on a site-specific basis.
- Analytic techniques used in targeted PFAS forensics should be well documented and are communicated with federal and state agencies



PFPrA: Perfluoropropanoic acid

TFSI: Trifluoromethanesulfonimide

(Zenobio et al. 2026)

PFAS Compositional Screening



- Multiple approaches on PFAS composition evaluation; Pie charts are used in this case study
- Pie sizes
 - Total PFAS concentrations
- Pie slide colors
 - PFAS class-level composition
 - Chain-length composition
- Pie sizes and colors
 - Precursor dynamics



Pie slide color groups: PFAS subclasses
Darker colors: Longer chain PFAS
Lighter colors: Shorter chain PFAS

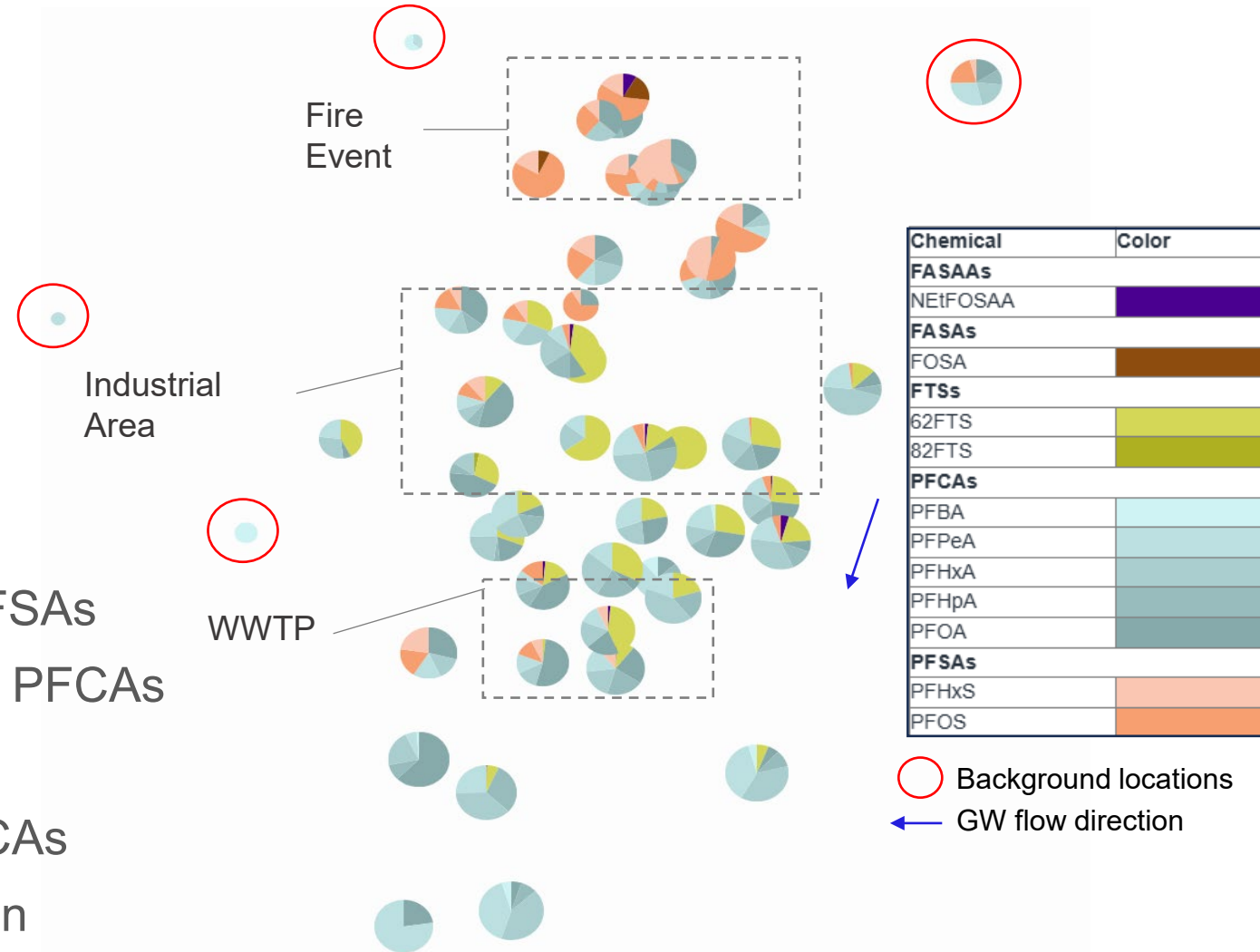
Chemical	Color
FASAAs	
NEtFOSAA	Dark Purple
FASAs	
FOSA	Dark Brown
FTSs	
62FTS	Light Yellow-Green
82FTS	Dark Yellow-Green
PFCAs	
PFBA	Light Cyan
PFPeA	Light Teal
PFHxA	Medium Teal
PFHpA	Dark Teal
PFOA	Very Dark Teal
PFSAs	
PFHxS	Light Orange
PFOS	Dark Orange

(Jacobs 2026)

PFAS Compositional Screening



- Most PFAS detections exceeded PALs
- Background locations exhibit low PFAS concentrations and dominant by PFCA only, except one exhibits PFAS composition similar to fire event area
- Multiple onsite sources:
 - High FTS and PFCA compositions in the industrial area
 - FTS and PFCA also dominant in the WWTP area with some locations with PFSA
 - Downgradient locations are dominant by PFCAs
- Data gaps
 - FTS biotransformation potential into PFCAs
 - Statistical similarities/differences between background vs. source areas

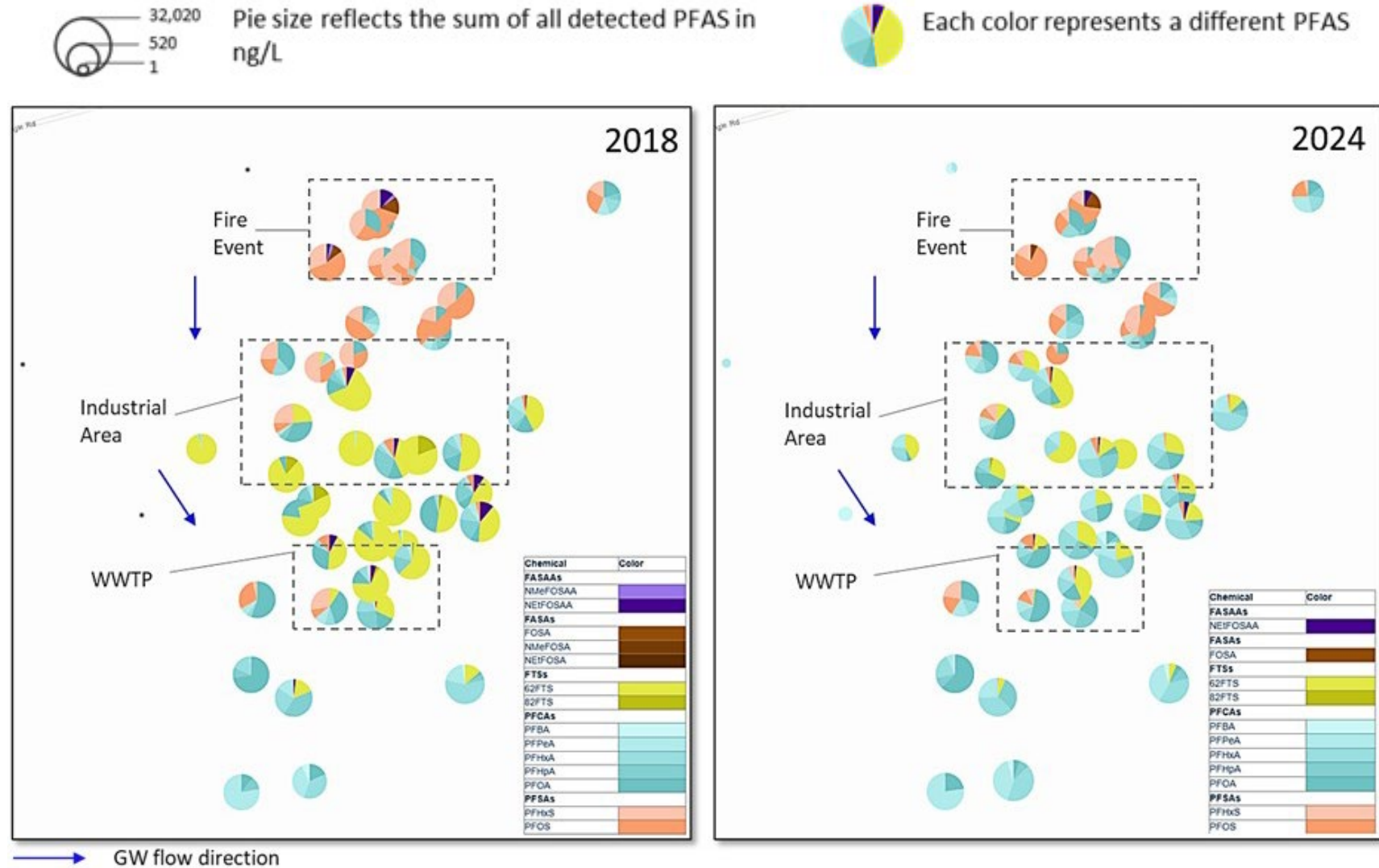


(Jacobs 2026)

Temporal Trends



- Notable PFAS composition changes from 2018 to 2024 in the industrial and WWTP areas
 - FTS conversion into PFCAs
- No significant changes on total PFAS concentrations
- Total PFAS in some background wells have increased

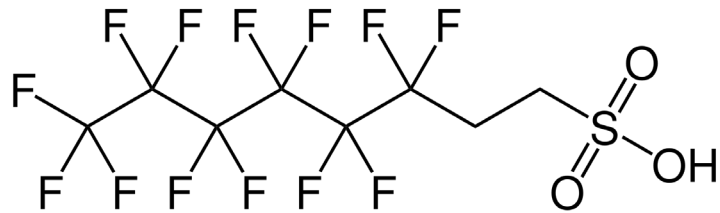


ng/L: nanogram(s) per liter

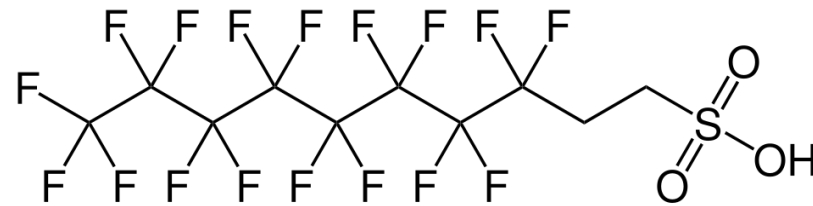
(Jacobs 2026)

Precursor Transformation Dynamics

- Multiple precursors were detected
- Dominant precursors were 6:2 FTS and 8:2 FTS



6:2 FTS

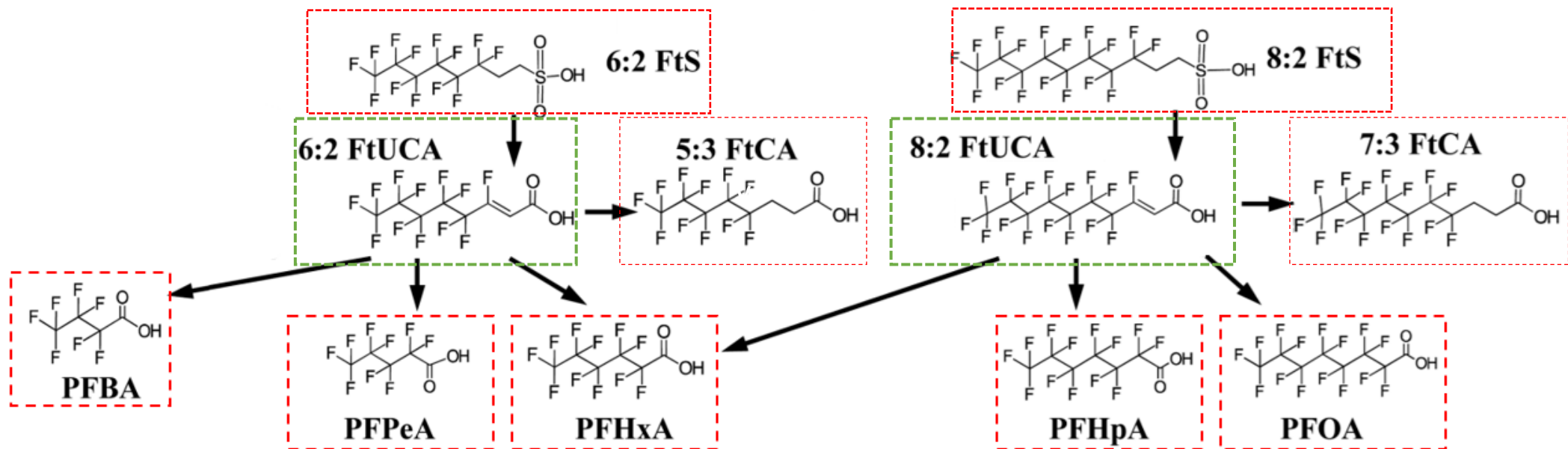


8:2 FTS

- Apparent precursor transformation patterns in industrial and WWTP areas were observed
- Without temporal datasets, forensics and source differentiation can be misleading

Precursor Dynamics

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



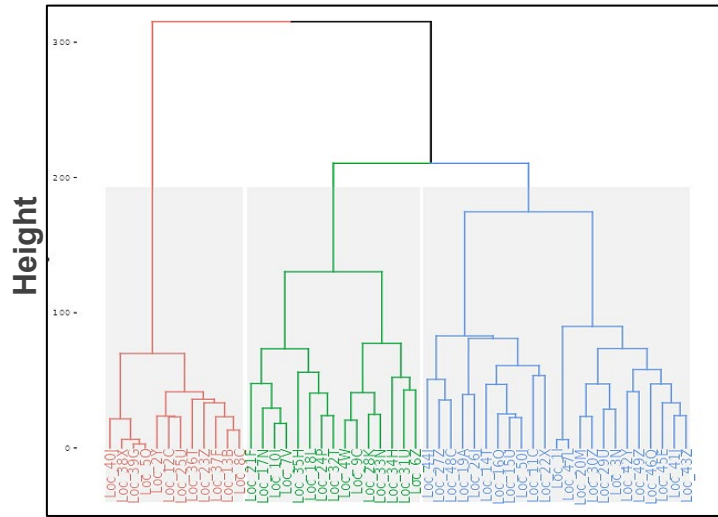
Rate of transformation 



- EPA Method 1633
- Extended target PFAS analyte list

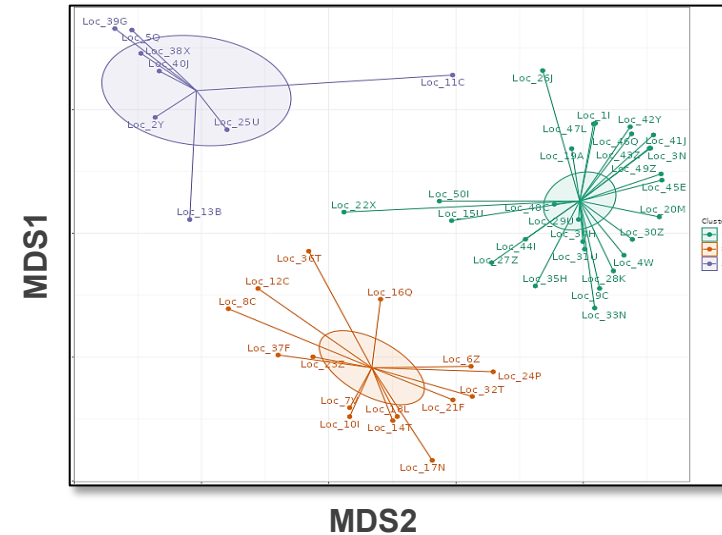
Clustering Analysis

Hierarchical Clustering



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

K-Means Clustering



- Groups samples into clusters based on PFAS composition and concentration magnitude
- Recognizes broad patterns of contamination sources or sitewide concentration gradients
- Computationally efficient; makes it practical for large monitoring datasets

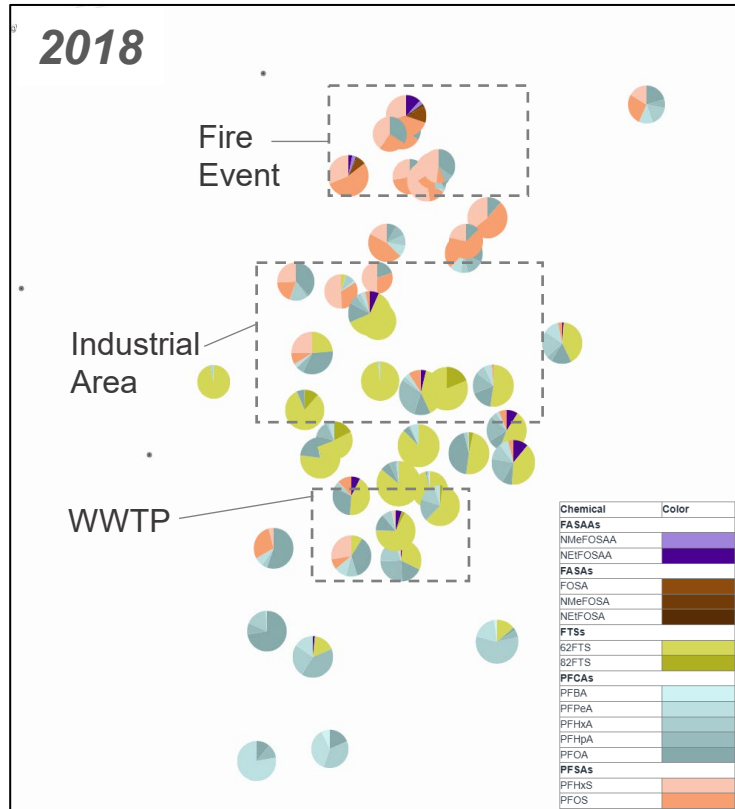
KEY POINT

The cluster analysis may not be appropriate for dilute plumes where PFAS used to differentiate sources are not detected.

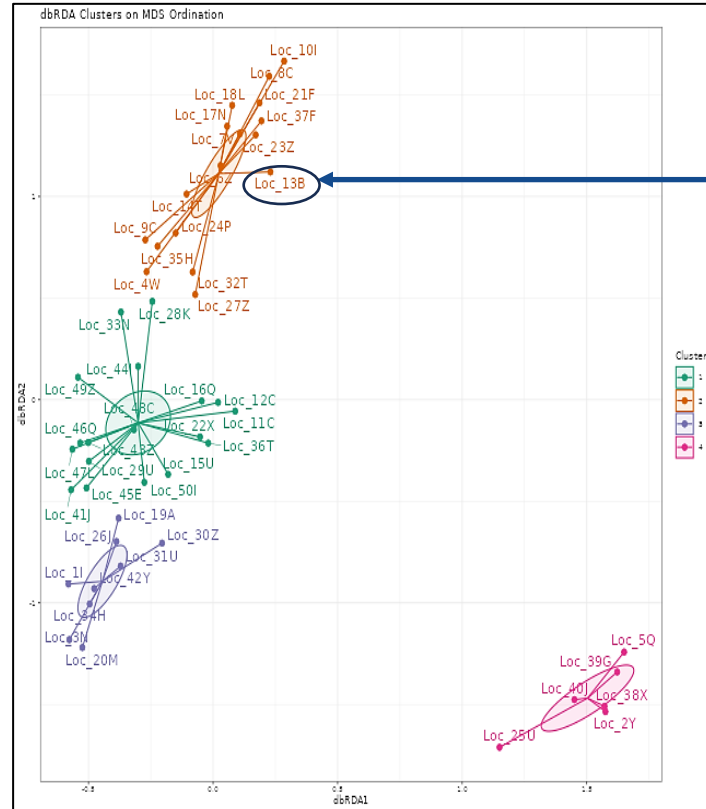
Clustering Analysis



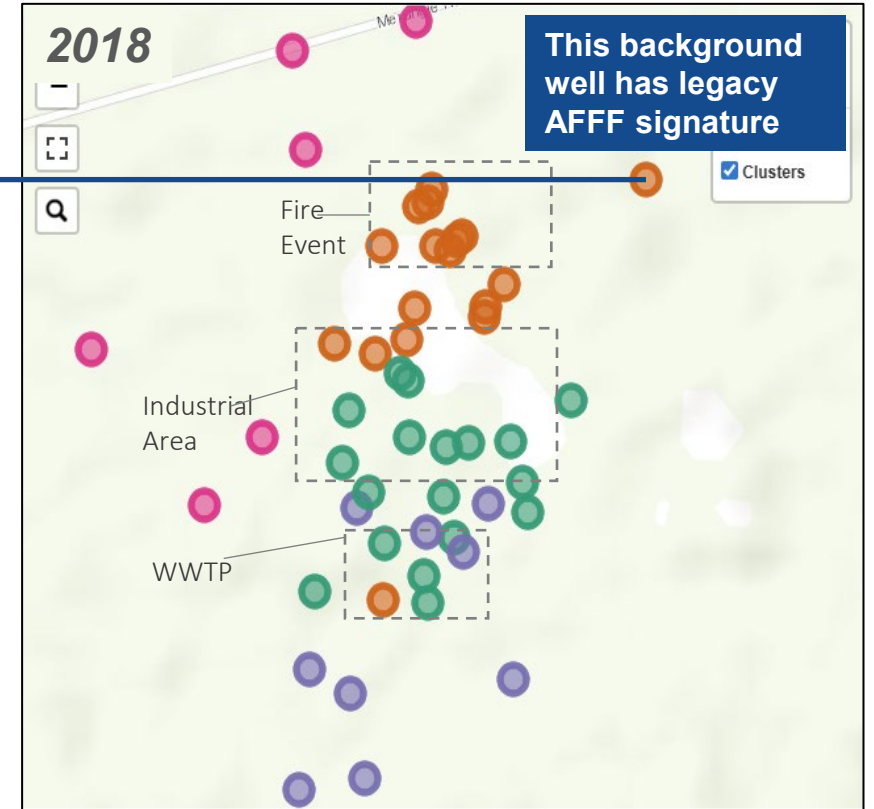
Cluster analysis shows agreement with compositional differences observed in the pie plots



PFAS composition and extent



K-mean clustering analysis (K=4)



Locations of 4 clusters

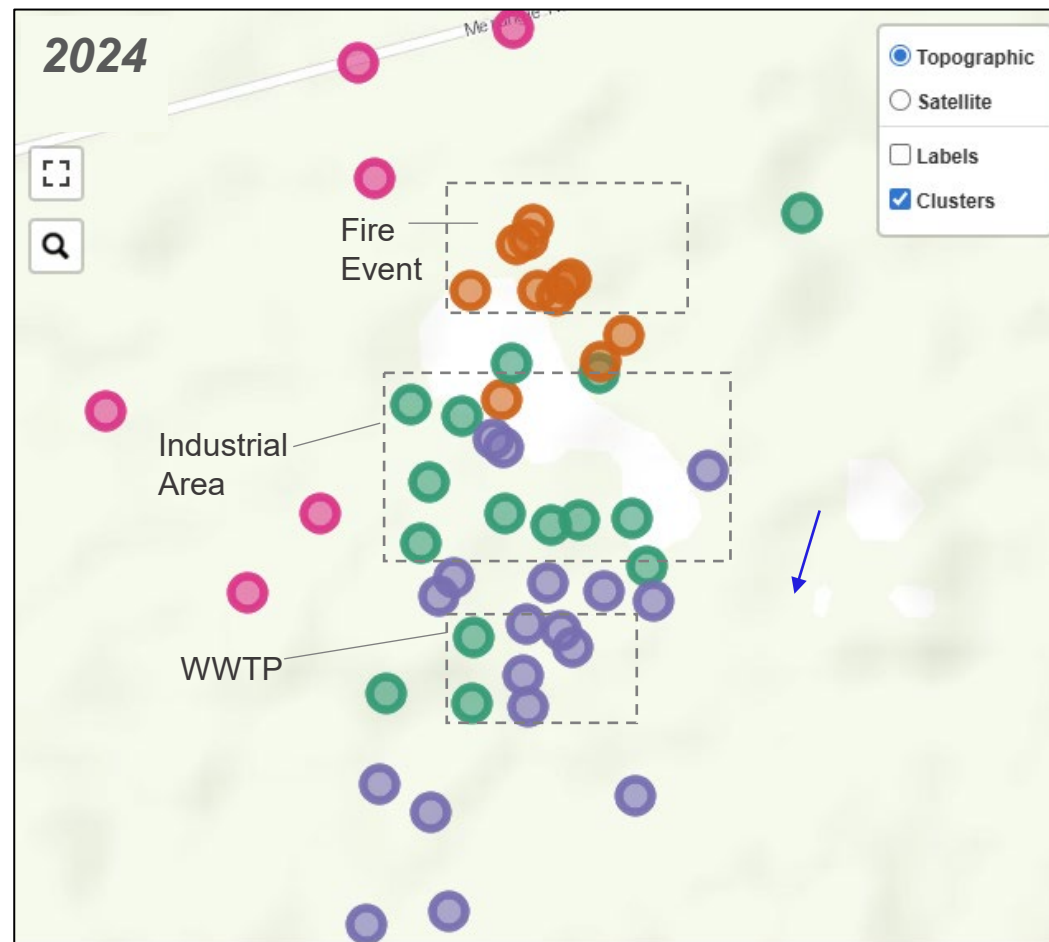
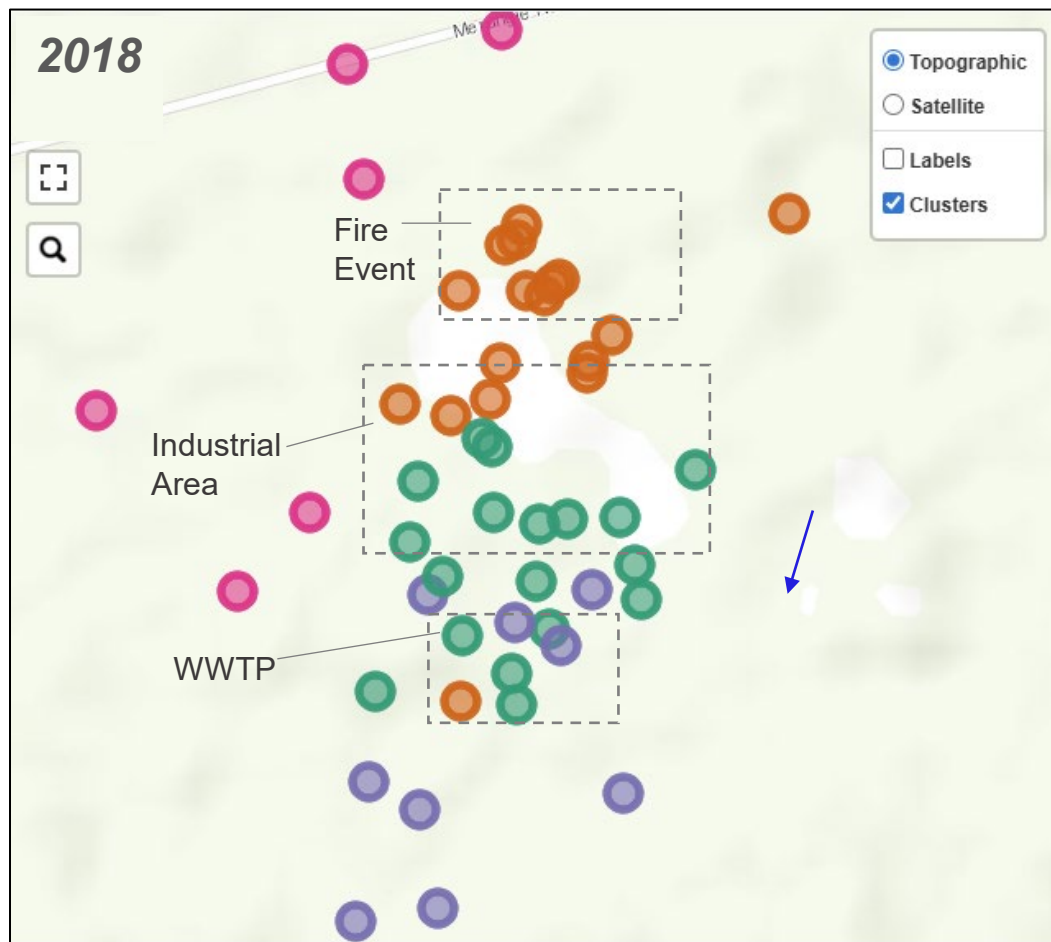
AFFF: aqueous film-forming foam

(Jacobs 2026)

Temporal Trends + Clustering Analysis

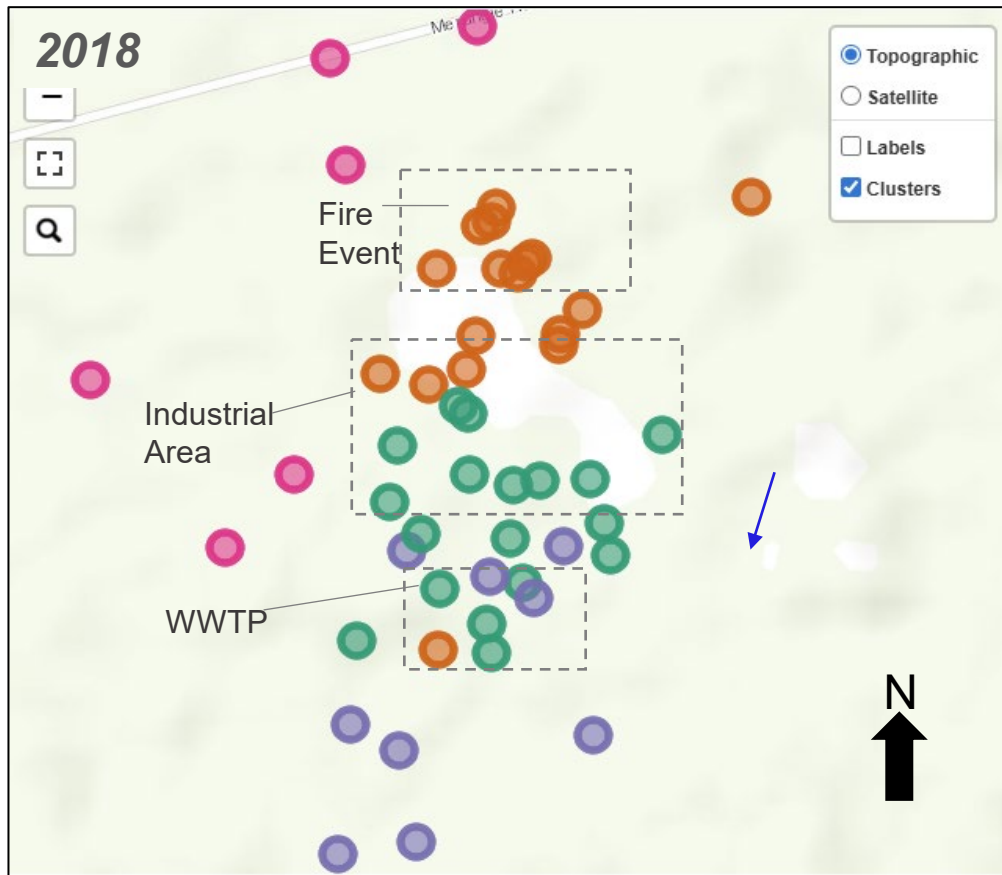


Temporal clustering analysis shows compositional shifts due to precursor transformation



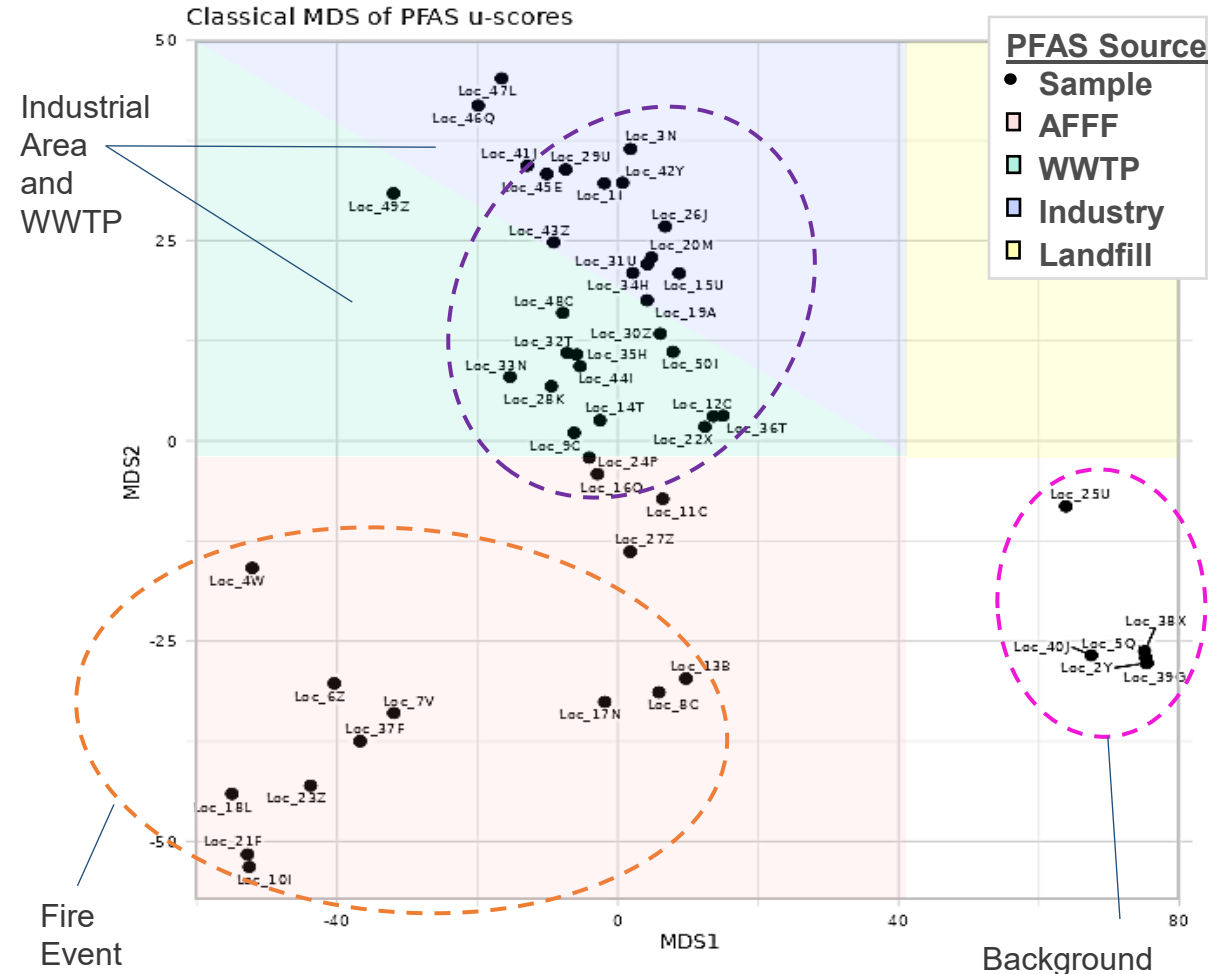
Matching Target PFAS Data with Specific Chemical Fingerprints

Spatial distribution of PFAS clusters



(Jacobs 2026)

Multidimensional scaling (MDS) technique to visualize similarity PFAS source



Knowledge Check



True or False

Spatial and temporal data are equally important on source identifications

Knowledge Check



True or False

Spatial and temporal data are equally important on source identifications

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Source Databases



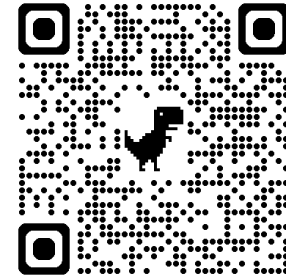
- Introduce DoW-R&D funded PFAS source databases
 - AFFF chemical fingerprinting database
 - PFAS biotransformation pathway database
- Discuss how applications of these databases for source identifications can be potentially used

PFAS Source Databases

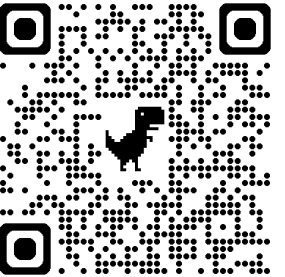


- DoW SERDP/ESTCP Projects
 - ER20-1375 and ER20-1121: Developed "forensic library" (e.g., landfill leachate, AFFF, municipal wastewater effluent, and chromium plating facilities)
 - ER20-1056: Store and manage PFAS mass spectral information and metadata ([complete](#))
 - ER20-1205: Machine learning to search for patterns in samples, aiming to assign probabilities that originate from specific sources ([complete](#))
 - ER20-1265: Apply ultra-high-resolution mass spectrometry to identify unique marker compounds in different AFFF formulations and other sources ([complete](#))

ER20-1375



ER20-1205



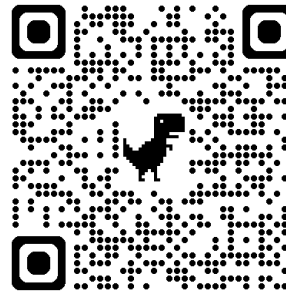
ER20-1121



ER20-1265



ER20-1056



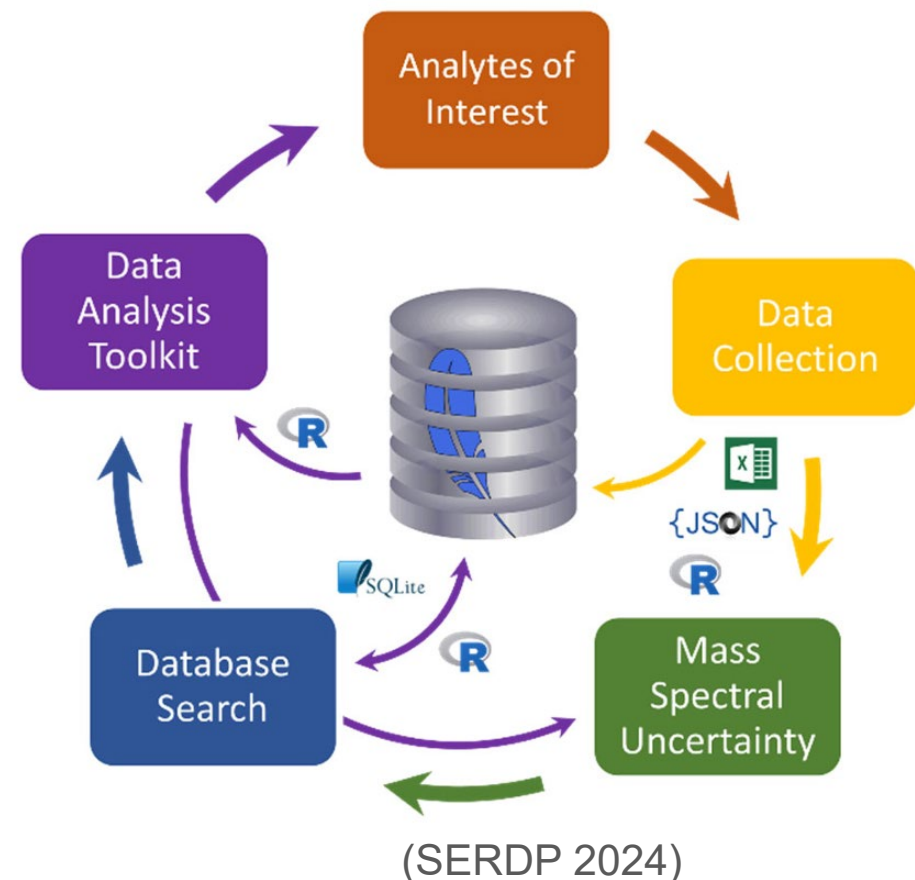
*Also see
references
for links*

SERDP: Strategic Environmental Research and Development Program
ESTCP: Environmental Security Technology Certification Program

ER20-1056 NIST Library and NTA Data Comparability



- Created and curated a NIST PFAS suspect list containing nearly 5,000 PFAS structures, providing a comprehensive chemical universe of suspect screening and discovery workflow
- Generated and quality-assured 351 consensus reference mass spectra covering 132 PFAS addressing a critical gap in high-quality reference data for PFAS NTA
- Built an integrated toolkit to support standardized data reporting, quality control, and spectral matching for PFAS identification
- Established a world-class quality assurance and training framework ensuring database remains freely available, expandable, and capable of supporting future PFAS research, forensics source attribution, and regulatory needs
- **Conducted a large interlaboratory study with 34 laboratories demonstrating wide variability in PFAS identification performance**



NIST: National Institute of Standards and Technology

SERDP: Department of Defense Strategic Environmental Research and Development Program

- Open-source Biotransformation data package (access login required)
- A collection of literature-reported biotransformation pathways for PFAS, last updated Jan 7, 2026

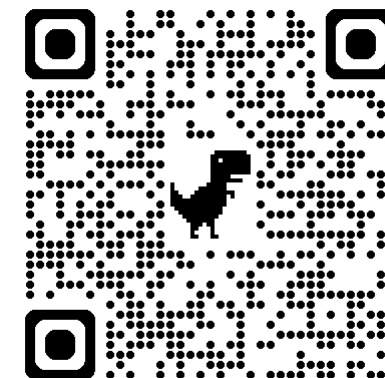
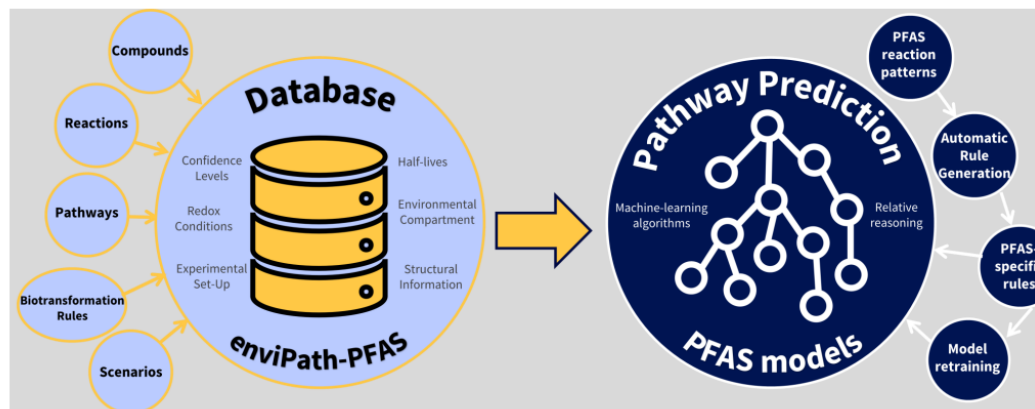


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aquatic research

Outlook for the enviPath-PFAS package

1. We need more data!
2. New pathway prediction models will be trained with PFAS biotransformation data
3. There are likely new PFAS-specific biotransformation rules that need to be implemented into prediction models



<https://legacy.envipath.org/package/d2cfb5af-4ea0-4375-9a48-f2e776e44636>

<https://community.envipath.org/t/pfas-resources-in-envipath/122>

Presentation Overview

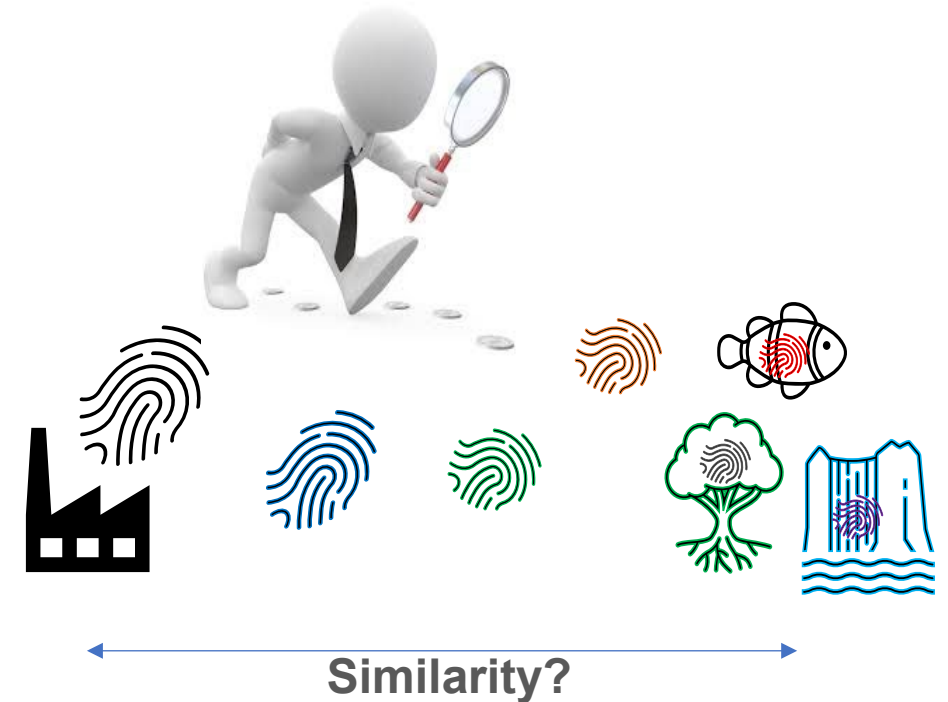


- Introduction
- Refresh on Chemistry, Sources, Fate, and Transport
- PFAS in Ambient Environment (Background Study)
- Targeted PFAS Forensics Study Design and Case Study
- DoW-funded PFAS Source Databases
- **Key Takeaways**

PFAS Forensics Techniques Summary



- PFAS RI and background study data can help determine if PFAS forensics may be helpful
- PFAS forensic study should start with target PFAS data only
- While PFAS forensic study could be used with appropriate approvals, projects need to ensure compliance with applicable DoW requirements for decision-making



RI: Remedial Investigation

PFAS Forensics Techniques Summary



- When targeted PFAS forensics is not sufficient to identify PFAS sources that are critical to site management considerations:
 - Nontarget data collection may be applied, but to limited cases with management/SME support, and based on budget availability
 - Nontargeted forensic study plan should identify/define DQO with clear and transparent justifications for completion
 - There should be awareness of the potential cost impacts to an RI project when nontargeted forensic study is proposed
- Each PFAS forensics technique has its pros, cons, and limitations
 - Analytical techniques
 - Data analytic techniques
- There could be data and knowledge gaps

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