EPA Superfund Program – RPM Bulletin 2025-02

Environmental Forensic Tools for Understanding PFAS Fate and Transport

June 2025

Purpose

The purpose of this document is to provide an introductory explanation of tools and methods used in per- and poly-fluoroalkyl substances (PFAS) forensic analyses, to assist US EPA project teams with reviewing PFAS forensics analyses. The field of environmental forensics, which evaluates variability in chemical composition, to assess the source apportionment and fate and transport, is not new and has been used for many years to identify sources of PCBs, chlorinated solvents and petroleum mixtures (Erickson, 2020; Morrison, 2000; Wait 2000). Federal agencies are increasingly using forensic techniques for PFAS, in support of source apportionment and remedial decision making under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA). Source apportionment is often done to allocate liability among potentially responsible parties but may also be done to inform the extent of contamination, refine the conceptual site model, or inform the selection of background sample locations.

This Bulletin is designed to assist Remedial Project Managers (RPMs) and Site Assessors who are asked to review data to support forensic analyses. This Bulletin provides an overview of currently available technologies and methods used in forensics analyses and emphasizes the importance of using multiple lines of evidence with a weight-of-evidence approach. If forensic analysis will be used to support background assessments, the approach should be consistent with EPA guidance on background (EPA, 2002; 2018).

Existing Guidance

- Guidance for Comparing Background and Chemical Concentrations in Soil for CERCLA Sites (pdf) EPA 540-R-01-003, OSWER 9285.7-41, September 2002
- Frequently Asked Questions About the Development and Use of Background (pdf) OLEM Directive 9200.2-141 A, March 2018

Background

PFAS forensic analysis, sometimes called fingerprinting, can be used to evaluate multiple sources at an impacted site and improve understanding of PFAS fate and transport (Benotti et al. 2020; Charbonnet et al. 2021). The fingerprinting of targeted PFAS analytical data can support source apportionment by linking offsite detections to potential onsite sources, distinguishing PFAS origins, and identifying historical manufacturing processes that may have contributed to PFAS releases. Forensic methods are not definitive but can provide clues that need to be pieced together. There are many potential confounders, including precursor transformations, differential transport rates and the addition of other sources along the flow paths (Pickard et al., 2024).

Because performing a PFAS forensic analysis is challenging (Benotti et al. 2020; Charbonnet et al. 2021), using multiple lines-of-evidence is favored. Lines of evidence may come from a variety of analytical methods, include complex statistics and modeling, and incorporate site specific hydrogeologic condition and historical operations. The use of multiple lines of evidence is a common strategy to inform decision-making at complex Superfund sites. This bulletin summarizes common methods used to evaluate PFAS sources, fate and transport, and suggests how weight of evidence approaches can be assembled to support decision-making. In addition, the accompanying graphical fact sheet illustrates the concepts in this RPM Bulletin.

Expectations and Considerations

RPMs and project teams should familiarize themselves with the methods that are available and useful to evaluate the distribution of PFAS analytes in the environment to build a weight of evidence approach to forensic analysis using multiple lines of evidence.

1. *Sources and Uses*

PFAS are a large group of multi-functional chemicals that have been and continue to be used in many industrial and commercial processes and products, and in consumer products. Identifying known and potential sources of PFAS releases to the environment is an important first step in any investigation. The distribution of specific PFAS can offer insights into source characteristics. For example, different methods of PFAS synthesis use different precursors and can result in different arrays of PFAS. Specifically, electrochemical fluorination (ECF) can include both branched and linear even and odd chain-length PFAS, whereas PFAAs produced by fluorotelomerization contain mostly even chain-length linear homologs (ITRC 2023). The type of fluorinated carbon chain length may help inform the age of the source. For example, longer-chain PFSA (e.g., C_8) were commonly used in older PFAS-containing aqueous film forming foams (AFFF). Newer formulations were made of shorter chain fluorotelomers (e.g., C_6).

The identity of PFAS sources and uses may be helpful to understanding the type of PFAS that may be present, as well as understanding fate and transport. For example, different combinations of PFAS may be associated with different uses, (e.g., legacy AFFF vs contemporary AFFF, photolithography, chromium plating, etc.) Refer to RPM Bulletin on PFAS Source Areas for suggestions on determining potential sources. Knowing what PFAS assemblages are likely to be present, based on known uses, is key to predicting fate, transport and transformation. Consider also potential non-site-related sources in the vicinity of your site.

PFAS can be polymeric or non-polymeric; most of the concerns are focused on non-polymeric forms. Perfluoroalkyl acids (PFAAs) are generally derived from precursor chemicals, which are PFAS that can break down to form the more persistent PFAAs. Two common subgroups of PFAAs are perfluoroalkyl sulfonic acids (PFSAs) and perfluoroalkyl carboxylic acids (PFCAs), which differ in the type of acid in the head group and vary in the number of carbons in the backbone. There are, however, a very large number of PFAS that we currently know very little about, in terms of identification, fate and transport or toxicity and some that have been more widely studied and can be used in the forensic interpretations. As we learn more about PFAS complex mixtures it is likely that the number of contaminants of interest will continue to expand.

As PFAS move through the environment, transformation into other PFAS compounds is possible, and highly dependent on the hydrogeology and physical, chemical and biological characteristics of the media. As transformation takes place over time and space, this introduces a complexity that is particularly challenging because detected PFAS may differ from those that were part of an initial environmental release. This is further complicated by the current incomplete understanding of all the PFAS degradation products of all PFAS precursors. Using forensics to inform our understanding of what is happening requires that we piece together multiple lines of evidence to form a plausible history.

2. *Conceptual Site Model and Biogeochemistry*

A well-developed Conceptual Site Model (CSM) is essential for effective remedial investigations and decision-making (EPA 2011; 2018; 2020). Hydrogeologic CSMs are particularly important for characterizing PFAS fate, transport, and contamination extent in groundwater, serving as a critical foundation for forensic analysis. A robust CSM will include identification of the presumed historical activities, including timing of releases, which resulted in PFAS distribution in the environment, and a general understanding of subsurface conditions including groundwater flow and site hydrostratigraphy. There are many different site-specific geochemical conditions that can specifically influence fate and transport and PFAS transformation. Assessing site geochemical conditions such as redox potential (oxidation-reduction potential and/or ORP) and pH can also be helpful when conducting PFAS forensic investigations. Biogeochemical conditions can also influence microbial transformation and thus play an important role in the fate and transport of PFAS.

Measuring the ORP of a system is a quick and indirect way to assess the geochemical potential for precursor transformation. Sites may have complex oxidizing and reducing (redox) gradients or interfaces that lead to variable PFAS transformation. Under geochemically reducing and anaerobic conditions, aerobic (O_2-dependent) biotransformation of common PFAS precursors would be inhibited. Under geochemically oxidizing and aerobic conditions precursors may be more likely to undergo transformation to PFAAs. Redox conditions can vary significantly between the source area and downgradient and are site specific resulting in differential amounts of terminal PFAAs.

The pH of an aquifer provides insight into transport of PFAS and the kinetics of expected transformations. The pH affects the surrounding media and microbial community, affecting the abiotic and biotic transformation of PFAS (e.g., via hydrolysis). Understanding the pH of the hydrologic system can help elucidate what type of PFAS are expected to be present and what type of PFAS transformations may have occurred.

PFAAs, including carboxylic acids and sulfonic acids, primarily have an anionic charge under environmentally relevant conditions (ITRC 2023). When the pH of an aquifer is acidic, the surface charges of the solid media become more positive. Therefore, under acidic conditions, PFAAs are more likely to sorb electrostatically to solid media. The same is true with cationic precursor compounds and more alkaline pH (i.e., negative surface charges and more electrostatic sorption).

Understanding what PFAS are present downgradient from the source areas and characterizing the biogeochemical conditions of the aquifer can be important lines of evidence in determining PFAS site-specific sources and fate and transport despite the current incomplete understanding of how PFAS transform in the environment.

3. *Targeted Analytical Evaluation*

Targeted PFAS analysis methods primarily focus on measuring a specific subset of PFAAs, with limited inclusion of precursors chemicals. Standard EPA methods, such as 537.1, 533, and 1633, provide critical data on PFAS transport and transformation.

4. *TOP Assay*

The Total Oxidizable Precursors (TOP) assay is a method used to detect unmeasured PFAS that are missed in targeted analysis by converting PFAS precursors via oxidation to readily measured PFAS. To analyze a sample for TOP, two duplicate samples are needed. The first sample is analyzed for a specified list of PFAS through targeted analysis techniques (such as EPA Method 533) (EPA 2022). The second sample undergoes oxidation (Houtz and Sedlak 2012). Ideally, previously undetected PFAS precursors will convert to PFAS end products such as PFCAs or PFSAs through oxidation. The oxidized sample is then analyzed with targeted analysis and compared to the first sample (EPA 2022). The TOP assay is being used in combination with target analytical methods and statistical tools to successfully apportion local contamination (Antell et al. 2023; Balgooyan and Remucal, 2023). If RPMs are reviewing forensics approaches using TOP assay for their sites, they should contact their Superfund Technical Liaison (STLR) for assistance.

5. *Assessment of Linear Versus Branched Isomers*

One of the more accessible and affordable options that can be used to conduct PFAS forensics is to investigate the presence of linear and branched isomers. Different manufacturing processes can produce dominantly linear or linear and branched isomers in specific ratios. Current analytical methods are designed to sum the isomers together to report concentrations as one value. Requesting that data be presented to distinguish between linear and branched isomers as part of targeted analyses can help attribute PFAS impacts to specific manufacturing processes or manufacturers. Linear and branched isomers also have differential transport behaviors that should be considered (Charbonnet et al. 2021; Stults et al. 2022). Note that not all labs have the capacity to distinguish between branched and unbranched isomers.

6. *PFAS Ratio Calculations*

Considering the spatial and/or time-series relationship between target PFAS analytes and source area is one way to perform forensic PFAS analyses to support source contributions, precursor transformation evaluations, evaluating the age of the source, or identifying differential transport. In simple terms, considering the ratios of PFAS homologs, classes, and isomers at a contaminated site can provide a useful line of evidence. In general, these ratios should be considered site-specific and should be selected based on site-specific history and conditions (ITRC 2023). For example, certain sources may be enriched with a single or group of PFAS analytes (so-called sentinel PFAS); or exhibit a distinguishing ratio, such as perfluorohexane sulfonate (PFHxS)/perfluorooctane sulfonic acid (PFOS) (Charbonnet et al. 2021).

Calculating the ratios of select PFAS analytes in the data set may help generate hypotheses regarding sources, transformation, migration and differential transport, or to describe the relationships between PFAS in soils, sediments, surface water, and groundwater. The analysis of PFAS ratios can be accomplished using statistical techniques, such as bootstrapping (Antell et al., 2023).

7. *Nontarget Analyses*

Although the list of target analytes covered by validated EPA methods has expanded over time, the vast majority of PFAS-containing commercial products include substances that are not detected by standard methods, such as EPA Method 1633. Nontarget analysis (NTA) methods based on high-resolution mass spectrometry (HRMS) can be used to identify PFAS that lack commercially available analytical standards, greatly expanding opportunities to identify source-specific patterns, or sentinal PFAS that may be highly differentiating among sources (Charbonnet et al. 2021). patterns, or sentinal PFAS that may be highly differentiating among sources (Charbonnet et al. 2021). Note that a limitation of NTA is that it cannot provide rigorous quantification in the absence of analytical standards, but it can provide semi-quantitative results in some cases.   If RPMs are reviewing forensics approaches using NTA methods for their sites, they should contact their Superfund Technical Liaison (STLR) for assistance.

8. *Total Organic Fluorine Methods*

Some researchers have found that bulk organofluorine measurements can be used to inform the development of PFAS mass balance. Examples of bulk organofluorine methods include Total Organic Fluorine (TOF), Adsorbable Organic Fluorine (AOF) and Extractable Organic Fluorine (EOF). EPA provides a concise summary of bulk organofluorine methods (https://www.epa.gov/cwa-methods/frequent-questions-about-pfas-methods-npdes-permits). Because bulk organofluine methods capture a broader array of chemicals, including pharmaceuticals and pesticides, the information can provide important context for potential diverse sources.

In general, TOF focuses on the difference between total fluorine and inorganic fluorine, and is therefore limited by the concentration of inorganic fluorine present in the sample. AOF and EOF use sorbents. EPA reports that sorbent selectivity may result in poor recoveries for some PFAS. AOF and EOF detection limits are lower than TOF, but detection limits for all organofluorine methods ae much higher than for individual PFAS compounds in tarteted analysis. In 2024, EPA finalzed EPA Method 1621 which measures AOF.

9. *Principal Component Analysis*

Principal component analysis (PCA) is a multivariate statistical procedure that can be used to identify patterns in PFAS data sets and graphically show the most important features of data that describe similarities and differences (ITRC 2023). PCA can be used to summarize information on individual PFAS concentrations and group them into principal components (PCs) and can be used as another line of evidence.

Changes in PFAS patterns may be associated with fate and transport due to site conditions or to the contribution of additional sources (ITRC 2023). While PCA can be highly useful, its interpretation can be subject to a high degree of variability in interpretation based on pre-processing steps. Small changes in data pre-processing steps can produce major variability in the output results.

Some factors that can create variability include the question to be answered by running PCA, how clean the data set is (e.g., correct qualifiers, consistent units), what normalization technique is used (e.g., a different normalization is needed for data with Gaussian distributions than with other distributions), how PFAS non-detections and qualified data are handled, and if the data are sufficiently non-sparse. These limitations make it imperative that when PCA is used as a line of evidence, all details are explicitly stated to allow an independent party to reproduce the interpretation. PCA is a challenging technique with the potential for misuse, so if it is employed, RPMs should seek technical assistance when reviewing the data and its interpretation.

10. Trends in Targeted and Non-Targeted Analysis

As additional groundwater analytical data are collected, trends in PFAS concentrations between targeted and non-targeted analysis are likely to yield valuable information on transformation and fate and transport and can be further utilized to enhance the forensic analysis.

Actions and Options for EPA Federal Facility Reviews

1. Seek Technical Assistance

Engage your regional chemist, hydrogeologist statistician and/or risk assessor to assist with the review of documents (Quality Assurance Project Plans [QAPPs], sampling and analysis plans [SAPs], draft forensics analyses, etc.). If you cannot access regional technical experts, contact the Federal Facilities Restoration and Reuse Office (FFRRO) for assistance. Depending on your site type and conditions additional technical expertise may be helpful. Contact your regional Superfund technical support liaison to get access to Office of Research and Development (ORD) experts and Environmental Response Team (ERT) assistance. In addition, you can check with your Site-Assessment team to see if that are other potential sources of PFAS releases in the vicinity. Other cleanup programs (RCRA, Removals, Brownfields) may have equities in the area as well.

2. Request Multiple Lines of Evidence Approach

Differentiating PFAS sources calls for a multiple lines-of-evidence approach. It is important to evaluate the chemical analyses within the context of robust CSMs, site history, site geochemistry, groundwater and surface water dynamics, and past and ongoing remedial efforts. The resulting PFAS data acquired via targeted and NTA constitute multiple lines-of-evidence for source allocation, with more confident source identification with more lines-of-evidence.

3. Pay Attention to Data Quality Objectives

Defining investigative data quality objectives (DQOs) is a critical part of beginning a PFAS investigation. Establishing analytical DQOs is important to ensure that the selected analytical tools, sampling rationale, and methods return a reliable level of performance and data of sufficient quality to support decision-making efforts. Investigative DQOs can influence the selection of the analytical tools and methods. The selected analytical tool or method are aligned with the DQOs prior to data being collected to avoid impractical expectations of what is possible with a data set or wasted time and effort on collecting insufficient or inadequate data.

4. *Considerations When Evaluating Data*

While this technical summary discusses powerful analytical tools and methods it also highlights the limitations associated with these components of a PFAS forensic analysis. Therefore, it stands to reason that too much emphasis on any one of these components may lead to unreliable hypotheses or conclusions. ***A balanced and pragmatic approach that relies on multiple lines of evidence is recommended because as multiple components resolve to a common observation/conclusion, the confidence in that observation/conclusion increase.*** The following offers suggestions for questions you may want to ask to substantiate a given hypothesis.

- Were validated EPA methods used for the appropriate environmental matrix?
- Were DQOs clearly defined and met?
- Do the results differentiate between branched and linear PFAS isomers, and are isomer distributions consistent with known manufacturing processes?
- Are multiple potential sources present that could confound source allocation?
- Would NTA or additional forensic techniques strengthen source attribution?
- Are PFAS concentration patterns consistent with the site's CSM and expected fate and transport behavior?

Attachment - Factsheet for EPA PFASs Forensics Technical Summary, April 2025

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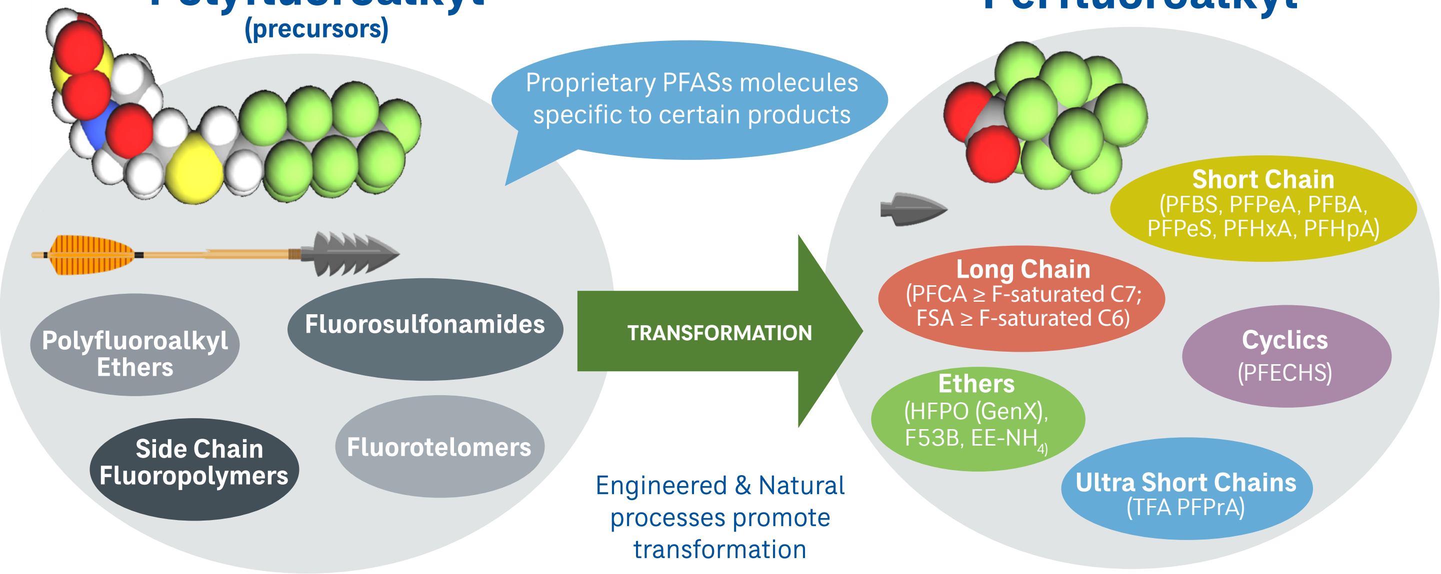
Factsheet for EPA PFASs Forensics Technical Summary

Poly- & Perfluoroalkyl Substances (PFASs) are a large class of **Xenobiotics**



Polyfluoroalkyl

(precursors)

Polyfluoroalkyl Ethers

Fluorosulfonamides

Side Chain Fluoropolymers

Fluorotelomers

Proprietary PFASs molecules specific to certain products

TRANSFORMATION

Engineered & Natural processes promote transformation

Perfluoroalkyl

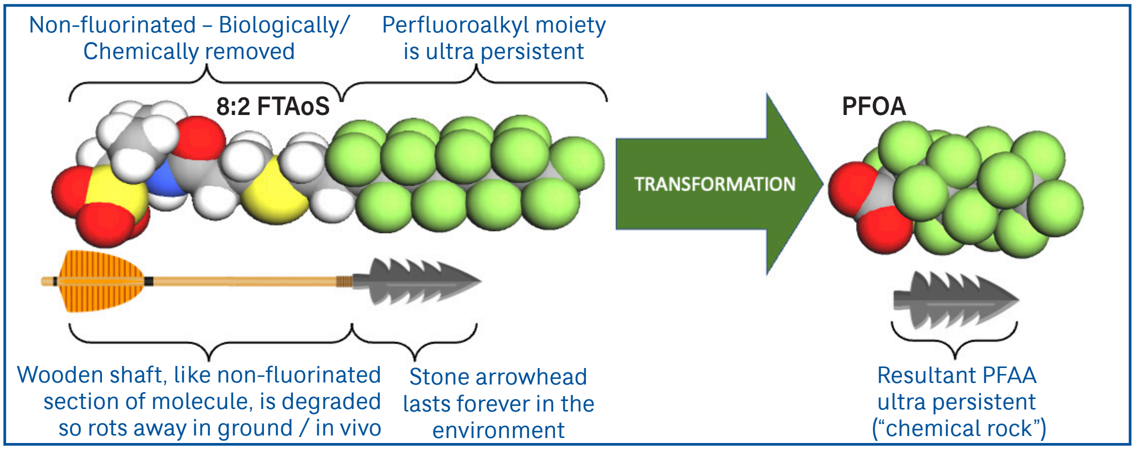
Short Chain (PFBS, PFPeA, PFBA, PFPeS, PFHxA, PFHpA)

Long Chain (PFCA ≥ F-saturated C7; FSA ≥ F-saturated C6)

Cyclics (PFECHS)

Ethers (HFPO (GenX), F53B, EE-NH_4)

Ultra Short Chains (TFA PFPrA)



Non-fluorinated – Biologically/ Chemically removed

Perfluoroalkyl moiety is ultra persistent

8:2 FTAoS

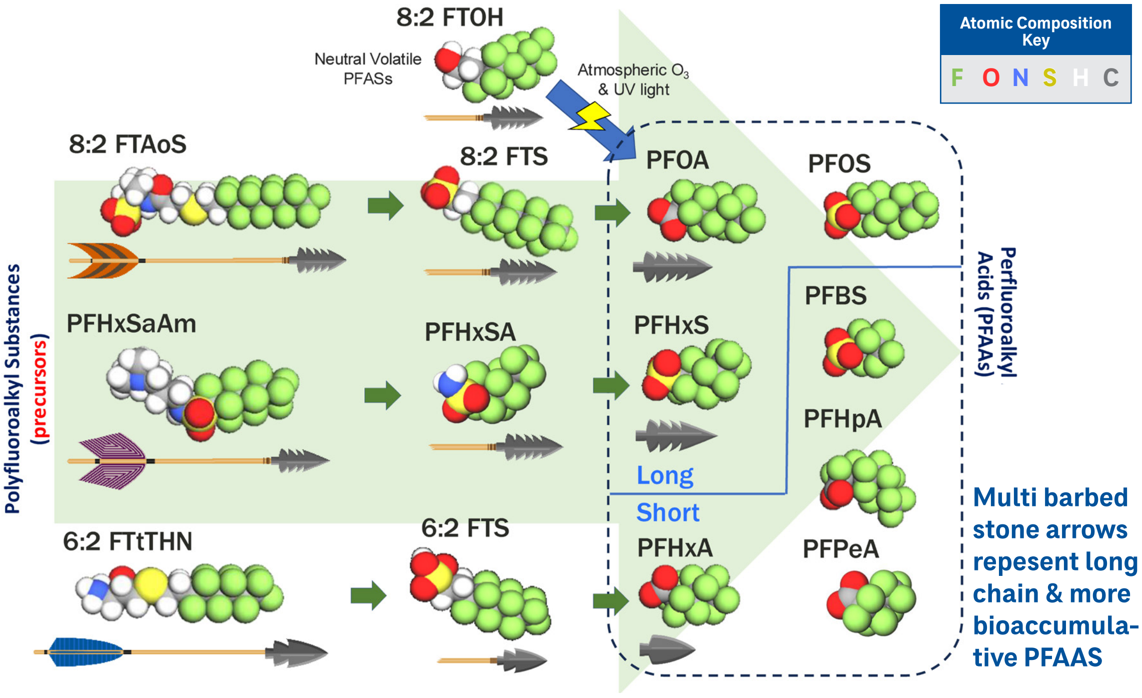
TRANSFORMATION

PFOA

Wooden shaft, like non-fluorinated section of molecule, is degraded so rots away in ground / in vivo

Stone arrowhead lasts forever in the environment

Resultant PFAA ultra persistent (“chemical rock”)



Multi barbed stone arrows repesent long chain & more bioaccumulative PFAAS

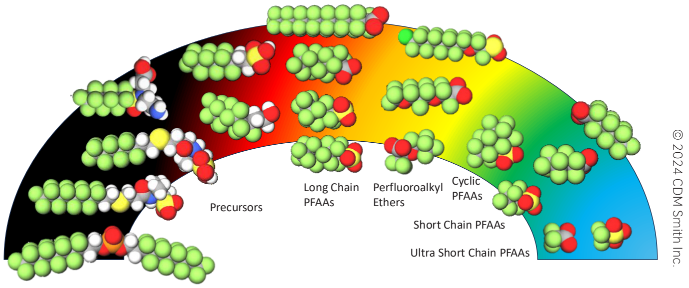
Identifying PFAA-precursors, by applying forensic chemical analytical tools, can determine the source of PFASs and whether they constitute ‘background’.

Factsheet for EPA PFASs Forensics Technical Summary

Key Elements of PFASs Forensics

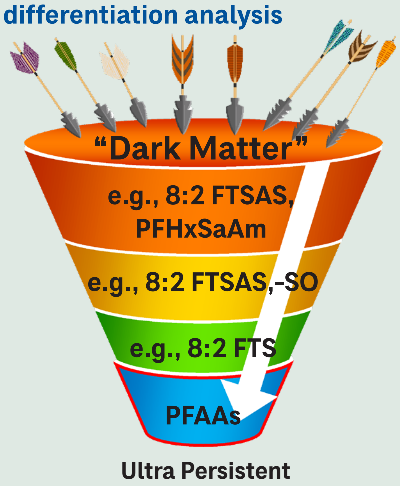
PFASs Forensics enables:

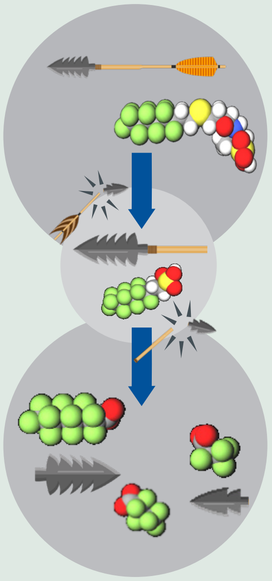
- Connection of offsite PFASs & onsite sources
- Reasonable approximate contribution from background concentrations
- Differentiation of PFASs sources and transformation mechanisms
- Identification of potential historical manufacturing origin



Transformation Pathways (Biotic/Abiotic)

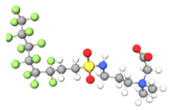
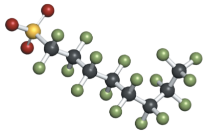
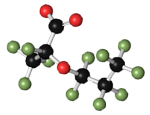
Most PFASs are PFAA-precursors, undetected by targeted analysis, which transform into PFAAs supporting PFASs sources differentiation analysis





Uses & Manufacturing Processes

PFASs are identified by their manufacturing process, through patents, and through specific uses

Linear	**Fluorotelomerization** (FT; DuPont patent)	
Linear and Branched	**Electrochemical Fluorination** (ECF; 3M patent)	
Perfluoroalkyl Ethers	**Oligomerization**	

PFASs Forensics

Applicability of Multiple Chemical Analytical Tools

Appropriate chemical analysis is tied to project objectives; multiple techniques are complementary but expensive

10s-100s of PFASs
Regulated PFASs
Established methods

Targeted Analysis

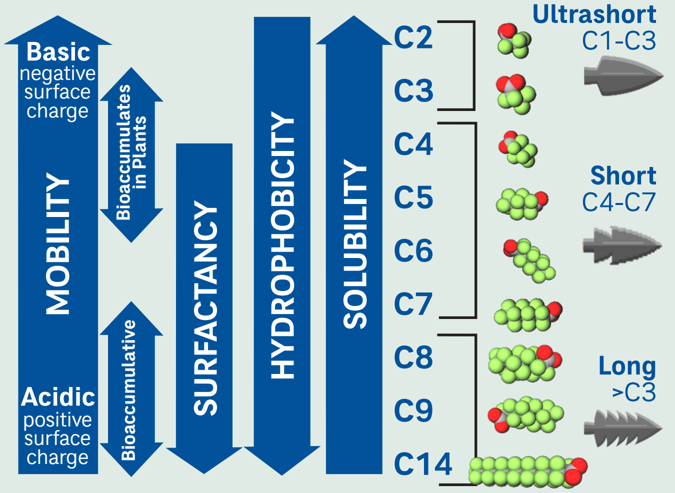
Non-targeted Analysis

TOP Assay
AOF/EOF
HRMS
^{19}F NMR

Precursor quantification
Molecular structure elucidation

Fate & Transport

Transport is influenced by physico-chemical properties which vary by chain length and the presence of charged functional groups (such as carboxylic or sulfonic acid)



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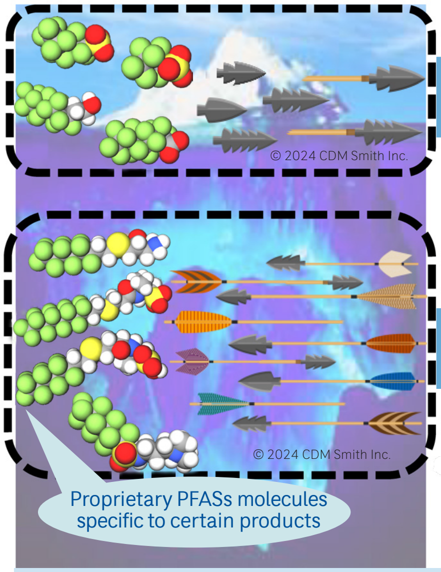
Forensic Tools: Targeted and Non-Targeted Analysis

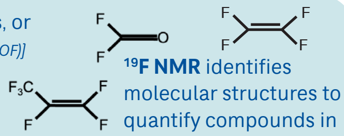


TARGETED
(EPA Method 537.1, 533, 1633)

~130 PFASs detectable with standard Liquid Chromatography & Tandem Mass Spectroscopy (isotope dilution & solid phase extraction improve quality)

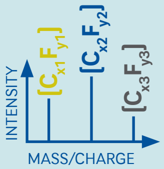
NON-TARGETED

EOF/AOF combusts either samples, sorbents, or extract to measure F- via IC *[EPA Method 1621 (AOF)]*



^{19}**F NMR** identifies molecular structures to quantify compounds in complex mixtures

HRMS determines highly precise mass, enabling structural formula & identification of suspect PFASs



TOP Assay oxidizes precursors (arrows–wooden shafts burn) to reveal PFAAs (arrow heads remain)

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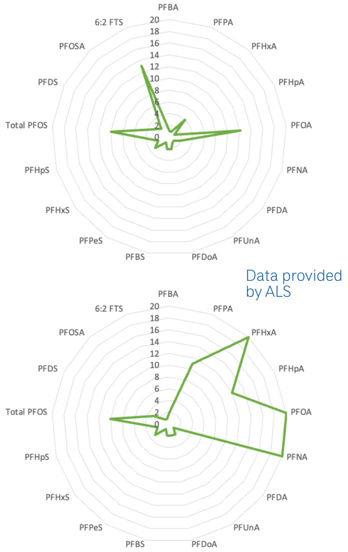
Staged approach to forensics balancing cost and objectives that begins with targeted analysis and incrementally adds more analytical complexity is advisable.

Forensic Tools: Data Visualization & Interpretation

Pre-Oxidation Analysis

TOP Assay (Oxidation)

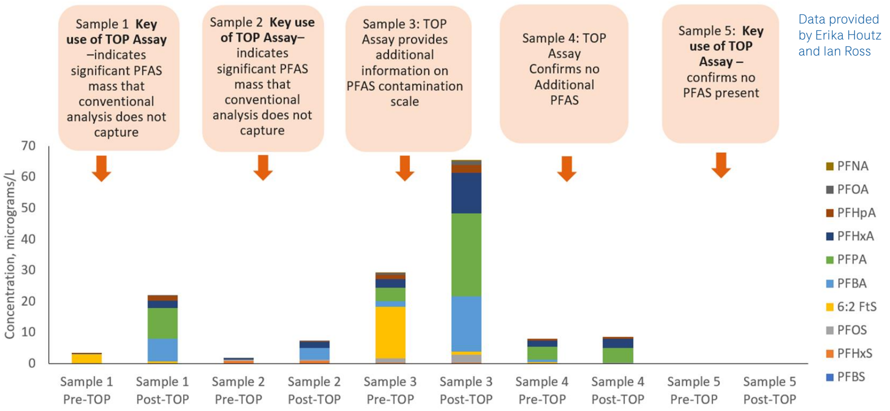
Post-Oxidation Analysis



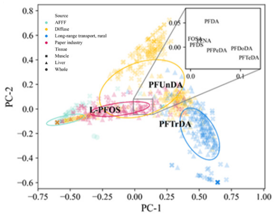
Data provided by ALS

There are more PFASs than can be detected using targeted analysis. Source allocation can be supported using non-targeted analysis. Patterns within targeted analysis are limited and further non-targeted analysis is necessary (i.e., TOP assay).

Side-by-side pre- and post-oxidation data from TOP assay is applicable to multiple observations



Data provided by Erika Houtz and Ian Ross



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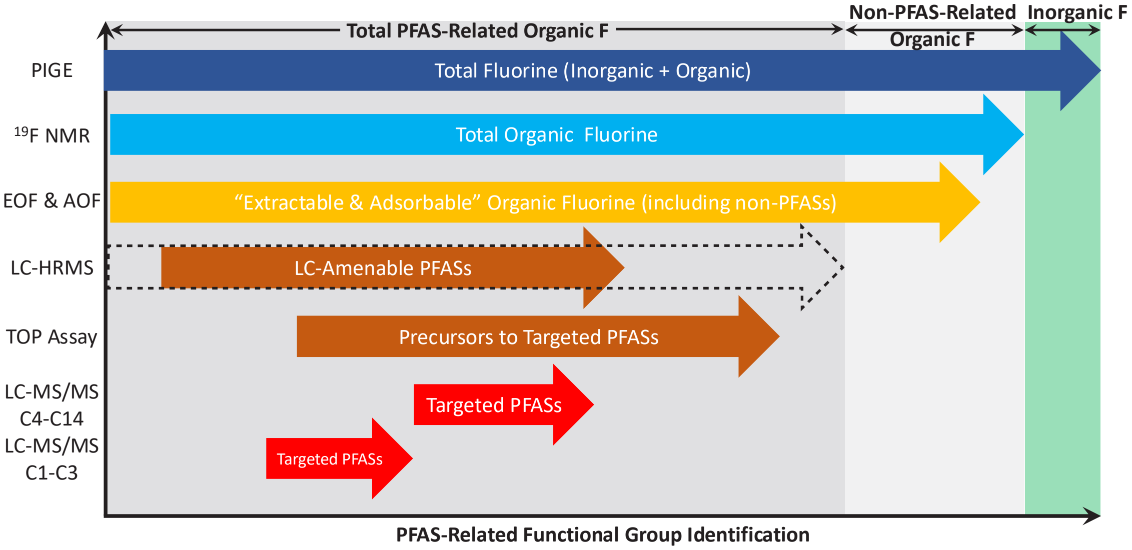
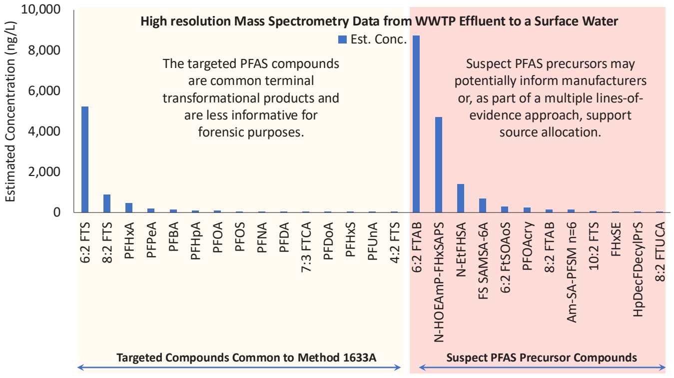
There are also multivariate statistical tools (PCA & linear regression) to identify relationships in data

Polyfluoroalkyl substances represent the majority of PFASs in most commercial products, and few are detected using conventional targeted analysis. There are multiple analytical techniques to assess PFASs comprehensively, and selection of the most appropriate techniques is a balance of cost and project objectives.

Identification Capabilities of Various PFASs-Related Analyses

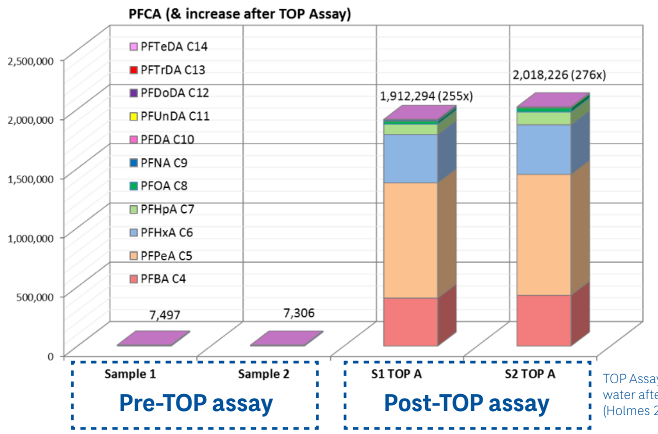


Example: High Resolution Mass Spectrometry (HRMS)

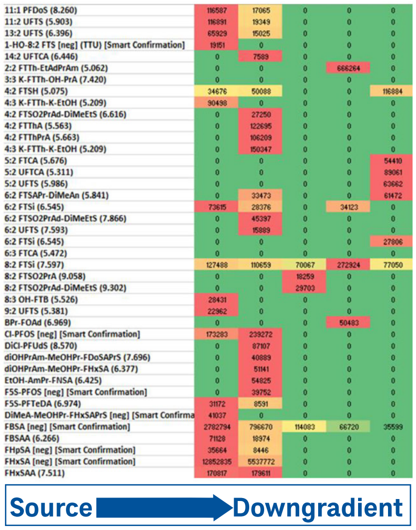


Adapted from data provided by Thermo Fisher and ALS

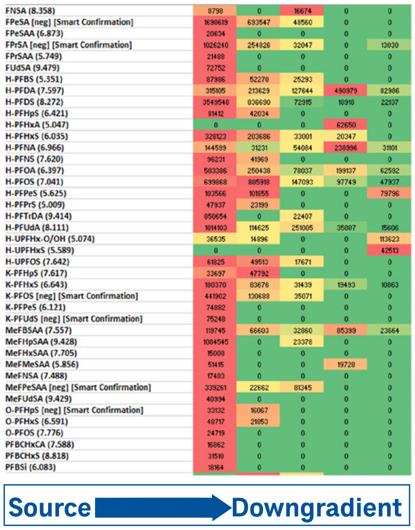
Example: TOP Assay



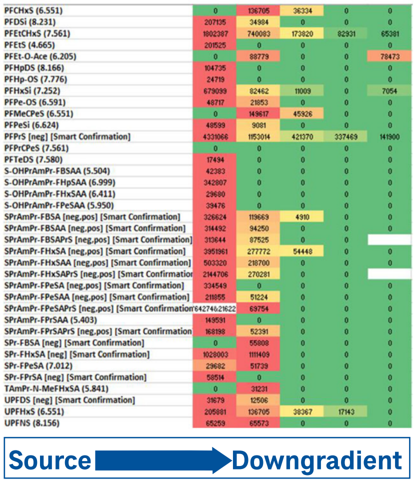
TOP Assay on surface water after an AFFF release (Holmes 2017)



11:1 PFDoS (8.260)	116587	17065	0	0	0
11:2 UFTS (5.903)	116891	19349	0	0	0
13:2 UFTS (6.396)	65929	15025	0	0	0
1-HO-8:2 FTS [neg] (TTU) [Smart Confirmation]	19151	0	0	0	0
14:2 UFTCA (6.446)	0	7589	0	0	0
2:2 FTTh-EtAdPrAm (5.062)	0	0	0	666264	0
3:3 K-FTTh-OH-PrA (7.420)	0	0	0	0	0
4:2 FTSH (5.075)	34676	50088	0	0	116884
4:3 K-FTTh-K-EtOH (5.209)	90498	0	0	0	0
4:2 FTSO2PrAd-DiMeEtS (6.616)	0	27250	0	0	0
4:2 FTThA (5.563)	0	122695	0	0	0
4:2 FTThPrA (5.663)	0	106209	0	0	0
4:3 K-FTTh-K-EtOH (5.209)	0	150347	0	0	0
5:2 FTCA (5.676)	0	0	0	0	54410
5:2 UFTCA (5.311)	0	0	0	0	89061
5:2 UFTS (5.986)	0	0	0	0	63662
6:2 FTSAPr-DiMeAn (5.841)	0	33473	0	0	61472
6:2 FTSi (6.545)	73615	28376	0	34123	0
6:2 FTSO2PrAd-DiMeEtS (7.866)	0	45397	0	0	0
6:2 UFTS (7.593)	0	15889	0	0	0
6:2 FTSi (6.545)	0	0	0	0	27806
6:3 FTCA (5.472)	0	0	0	0	0
8:2 FTSi (7.597)	127488	110659	70067	272924	77050
8:2 FTSO2PrA (9.058)	0	0	18259	0	0
8:2 FTSO2PrAd-DiMeEtS (9.302)	0	0	29703	0	0
8:3 OH-FTB (5.526)	28431	0	0	0	0
9:2 UFTS (5.381)	22962	0	0	0	0
BPr-FOAd (6.969)	0	0	0	50483	0
Cl-PFOS [neg] [Smart Confirmation]	173283	239272	0	0	0
DiCl-PFUdS (8.570)	0	87107	0	0	0
diOHPrAm-MeOHPr-FDoSAPrS (7.696)	0	40889	0	0	0
diOHPrAm-MeOHPr-FHxSA (6.377)	0	51141	0	0	0
EtOH-AmPr-FNSA (6.425)	0	54825	0	0	0
F5S-PFOS [neg] [Smart Confirmation]	0	39752	0	0	0
F5S-PFTeDA (6.974)	31172	8591	0	0	0
DiMeA-MeOHPr-FHxSAPrS [neg] [Smart Confirma	41037	0	0	0	0
FBSA [neg] [Smart Confirmation]	2782794	796670	114083	66720	35599
FBSAA (6.266)	71128	18974	0	0	0
FHpSA [neg] [Smart Confirmation]	35664	8446	0	0	0
FHxSA [neg] [Smart Confirmation]	12852835	5537772	0	0	0
FHxSAA (7.511)	170817	179611	0	0	0



FNSA (8.358)	8798	0	16674	0	0
FPeSA [neg] [Smart Confirmation]	1690619	693547	48560	0	0
FPeSAA (6.873)	20634	0	0	0	0
FPrSA [neg] [Smart Confirmation]	1026240	254826	32047	0	13030
FPrSAA (5.749)	21488	0	0	0	0
FUdSA (9.479)	72752	0	0	0	0
H-PFBS (5.351)	87986	52270	25293	0	0
H-PFDA (7.597)	315105	213629	127644	490979	82986
H-PFDS (8.272)	3549548	836690	72915	18918	22137
H-PFHpS (6.421)	81412	42034	0	0	0
H-PFHxA (5.047)	0	0	0	62650	0
H-PFHxS (6.035)	328123	203686	33001	20347	0
H-PFNA (6.966)	144599	31231	54084	238996	31101
H-PFNS (7.620)	96231	41969	0	0	0
H-PFOA (6.397)	503386	250438	78037	199137	62592
H-PFOS (7.041)	699868	805918	147093	97749	47937
H-PFPeS (5.625)	103566	101855	0	0	79796
H-PFPrS (5.009)	47937	23199	0	0	0
H-PFTrDA (9.414)	850654	0	22407	0	0
H-PFUdA (8.111)	1014103	114625	251005	35807	15606
H-UPFHx-O/OH (5.074)	36535	14896	0	0	113623
H-UPFHxS (5.589)	0	0	0	0	42513
H-UPFOS (7.642)	61825	49513	17671	0	0
K-PFHpS (7.617)	33697	47792	0	0	0
K-PFHxS (6.643)	180370	83676	31439	19493	10863
K-PFOS [neg] [Smart Confirmation]	441902	130688	35071	0	0
K-PFPeS (6.121)	74882	0	0	0	0
K-PFUdS [neg] [Smart Confirmation]	75248	0	0	0	0
MeFBSAA (7.557)	119745	66603	32860	85399	23664
MeFHpSAA (9.428)	1084545	0	23378	0	0
MeFHxSAA (7.705)	15008	0	0	0	0
MeFMeSAA (5.856)	51415	0	0	19728	0
MeFNSA (7.488)	17483	0	0	0	0
MeFPeSAA [neg] [Smart Confirmation]	339261	22662	81345	0	0
MeFUdSA (9.429)	40934	0	0	0	0
O-PFHpS [neg] [Smart Confirmation]	33132	16067	0	0	0
O-PFHxS (6.591)	48717	21853	0	0	0
O-PFOS (7.776)	24719	0	0	0	0
PFBCHxCA (7.588)	16862	0	0	0	0
PFBCHxS (8.818)	31510	0	0	0	0
PFBSi (6.083)	18164	0	0	0	0



PFCHxS (6.551)	0	136705	36334	0	0
PFDSi (8.231)	207135	34984	0	0	0
PFEtCHxS (7.561)	1802387	740083	173820	82931	65381
PFEtS (4.665)	201525	0	0	0	0
PFEt-O-Ace (6.205)	0	88779	0	0	78473
PFHpDS (8.166)	104735	0	0	0	0
PFHp-OS (7.776)	24719	0	0	0	0
PFHxSi (7.252)	679099	82462	11009	0	7054
PFPe-OS (6.591)	48717	21853	0	0	0
PFMeCPeS (6.551)	0	149617	45926	0	0
PFPeSi (6.624)	48599	9081	0	0	0
PFPrS [neg] [Smart Confirmation]	4331066	1153014	421370	337469	141900
PFPrCPeS (7.561)	0	0	0	0	0
PFTeDS (7.580)	17494	0	0	0	0
S-OHPrAmPr-FBSAA (5.504)	42383	0	0	0	0
S-OHPrAmPr-FHpSAA (6.999)	342807	0	0	0	0
S-OHPrAmPr-FHxSAA (6.411)	29680	0	0	0	0
S-OHPrAmPr-FPeSAA (5.950)	39476	0	0	0	0
SPrAmPr-FBSA [neg,pos] [Smart Confirmation]	326624	119669	4910	0	0
SPrAmPr-FBSAA [neg,pos] [Smart Confirmation]	314492	94250	0	0	0
SPrAmPr-FBSAPrS [neg,pos] [Smart Confirmation]	313644	87525	0	0	
SPrAmPr-FHxSA [neg,pos] [Smart Confirmation]	3951961	277772	54448	0	0
SPrAmPr-FHxSAA [neg,pos] [Smart Confirmation]	503320	218700	0	0	0
SPrAmPr-FHxSAPrS [neg,pos] [Smart Confirmatio	2144706	270281	0	0	
SPrAmPr-FPeSA [neg,pos] [Smart Confirmation]	334549	0	0	0	0
SPrAmPr-FPeSAA [neg,pos] [Smart Confirmation]	211855	51224	0	0	0
SPrAmPr-FPeSAPrS [neg,pos] [Smart Confirmation	64274&21622	69754	0	0	0
SPrAmPr-FPrSAA (5.403)	149591	0	0	0	0
SPrAmPr-FPrSAPrS [neg,pos] [Smart Confirmation	168198	52391	0	0	0
SPr-FBSA [neg] [Smart Confirmation]	0	55808	0	0	0
SPr-FHxSA [neg] [Smart Confirmation]	1028003	1111409	0	0	0
SPr-FPeSA (7.012)	29682	51739	0	0	0
SPr-FPrSA [neg] [Smart Confirmation]	58514	0	0	0	0
TAmPr-N-MeFHxSA (5.841)	0	31231	0	0	0
UPFDS [neg] [Smart Confirmation]	31679	12506	0	0	0
UPFHxS (6.551)	205881	136705	38367	17143	0
UPFNS (8.156)	65259	65573	0	0	0

Non-targeted PFASs screening vs. distance from a source can indicate considerable PFAA precursor source mass & support source allocation.

- 🟥 High abundance of specific PFAS
- 🟩 Low abundance of specific PFAS

Forensic tools can differentiate PFASs background and assist with apportioning liabilities between responsible parties.