

# PFAS 101

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IAWEA Biosolids Conference  
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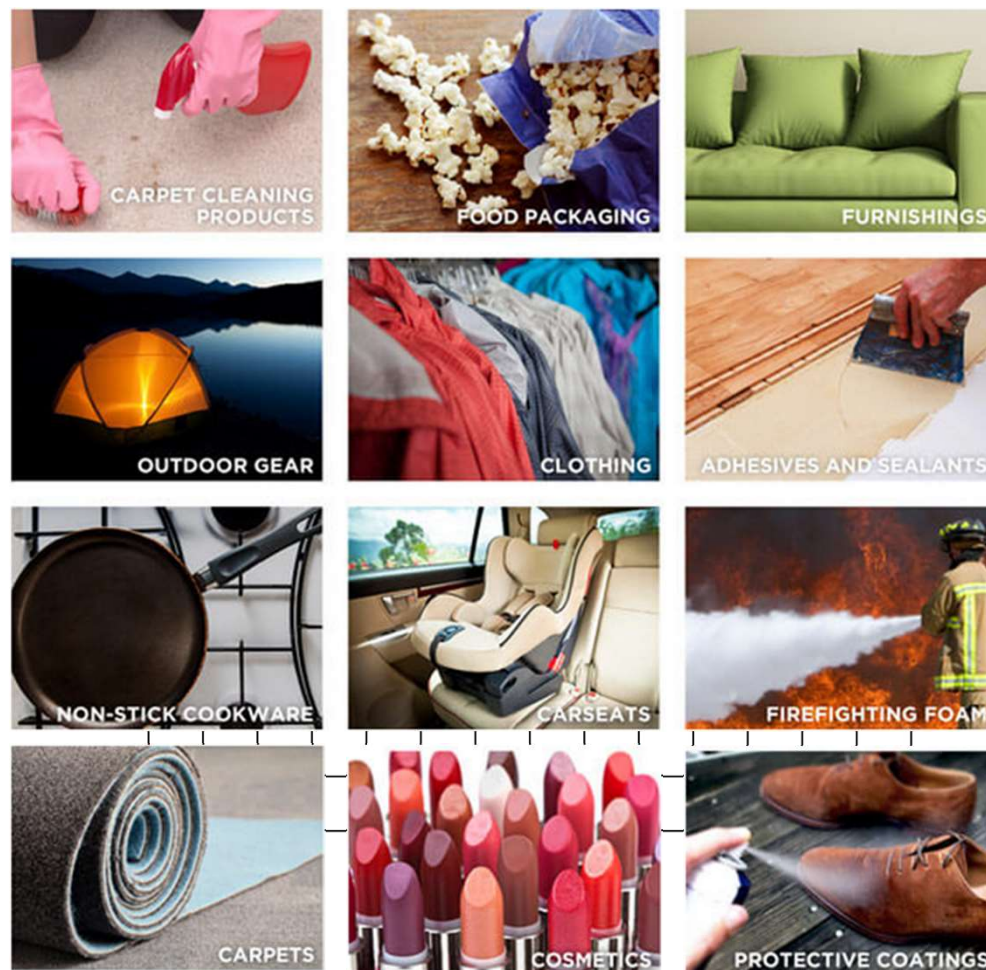


IOWA STATE  
UNIVERSITY



# What are PFAS?

- Per- and polyfluoroalkyl substances
- Class of > 6,000 related chemical compounds
- Contain bonds between carbon and multiple fluorine atoms
  - Very stable: “Forever Chemicals”
  - Hydrophobic and lipophobic
  - Imparts useful properties: oil-, stain-, water-repellent, non-stick

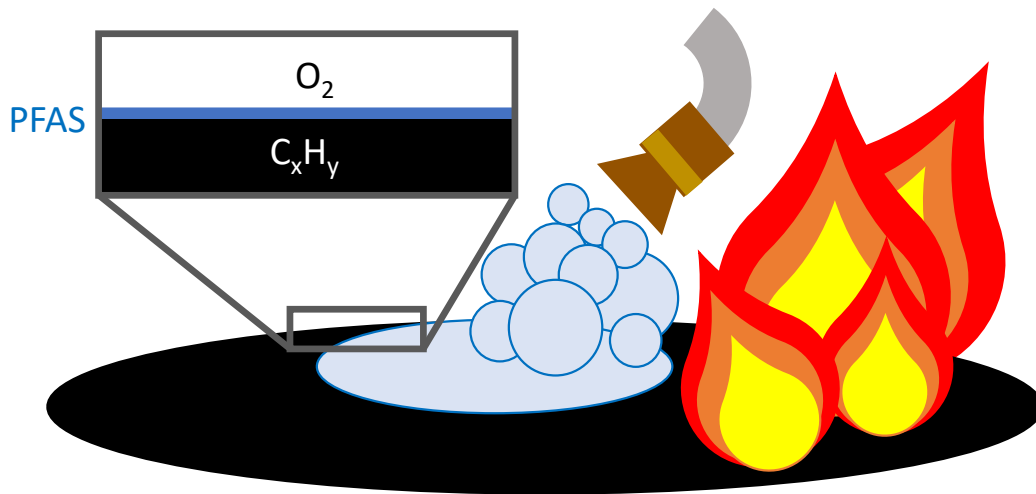


Courtesy: Green Science Policy Institute

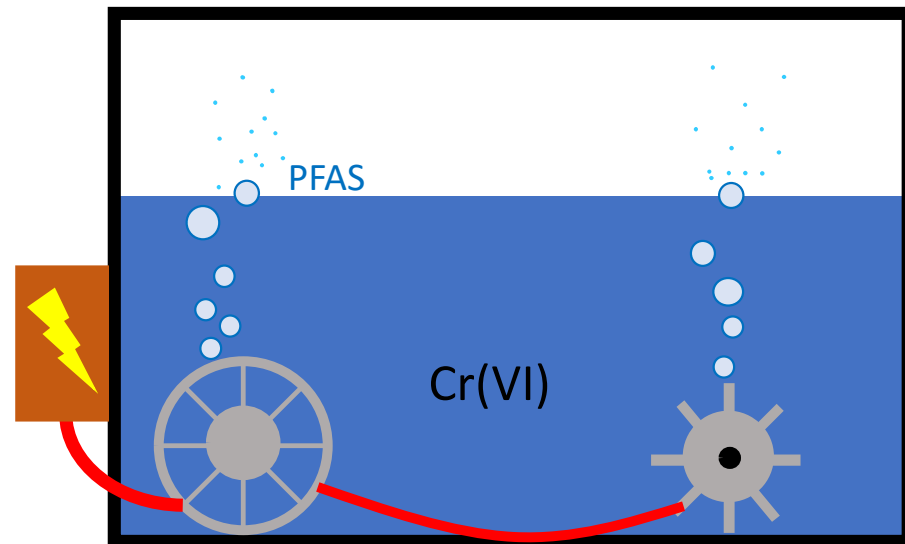
# What are PFAS?

Chemical properties impart utility:

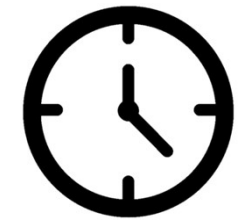
AFFF: Aqueous Fire Fighting Foam  
or  
Aqueous Film-Forming Foam



Metal Plating Mist Suppressant



# Chemical Properties Impart Hazards



## Persistent

- Do not break down into safer substances
- Characteristic life of terminal products ~10,000 years

# Chemical Properties Impart Hazards



## Bioaccumulative

- Most concentrated at the top of food chains
- Partition primarily to proteins (e.g., blood serum)

# Chemical Properties Impart Hazards



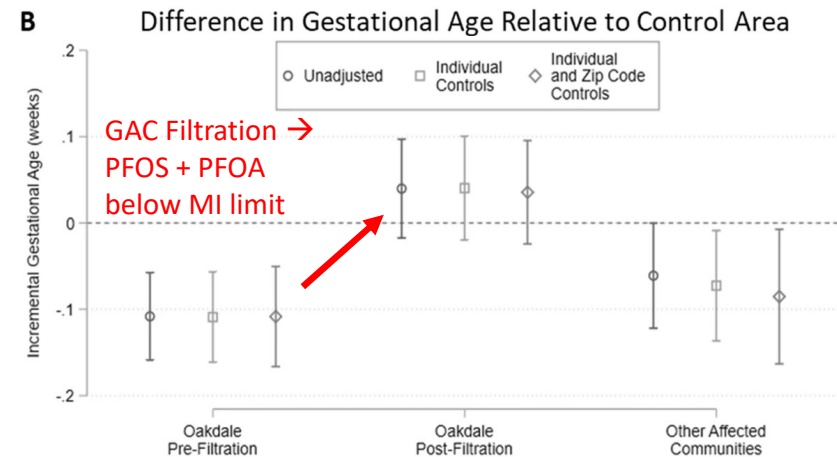
Bioaccumulative



Known association with:

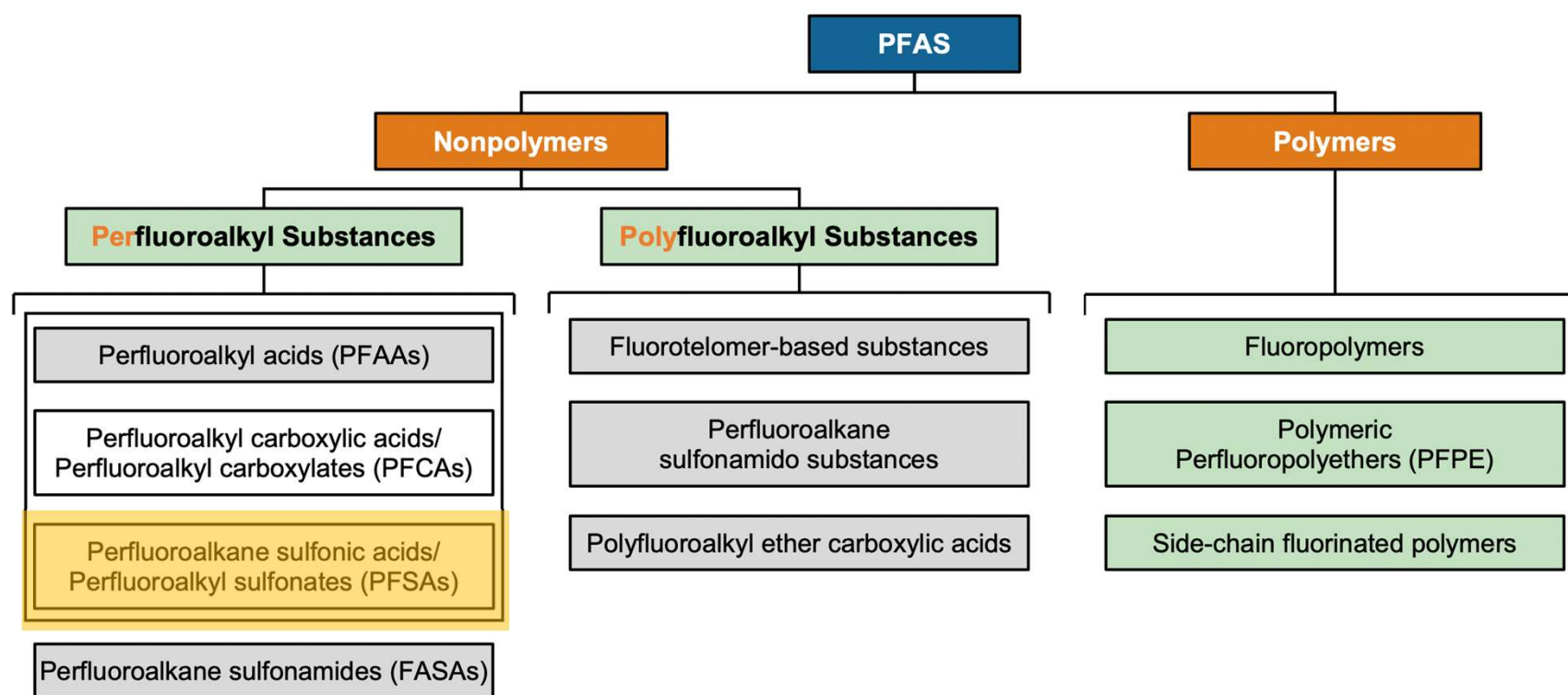
- Liver damage
- High cholesterol
- Obesity
- Cancer
- Thyroid disease
- Immune dysfunction
- Developmental delay
- Infertility and gestational problems

- Most PFAS untested



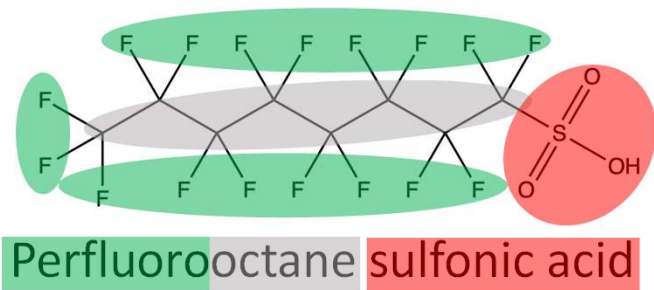
Courtesy: Waterfield et al., *Environ. Health* 2020

# The PFAS Family Tree (and alphabet soup)



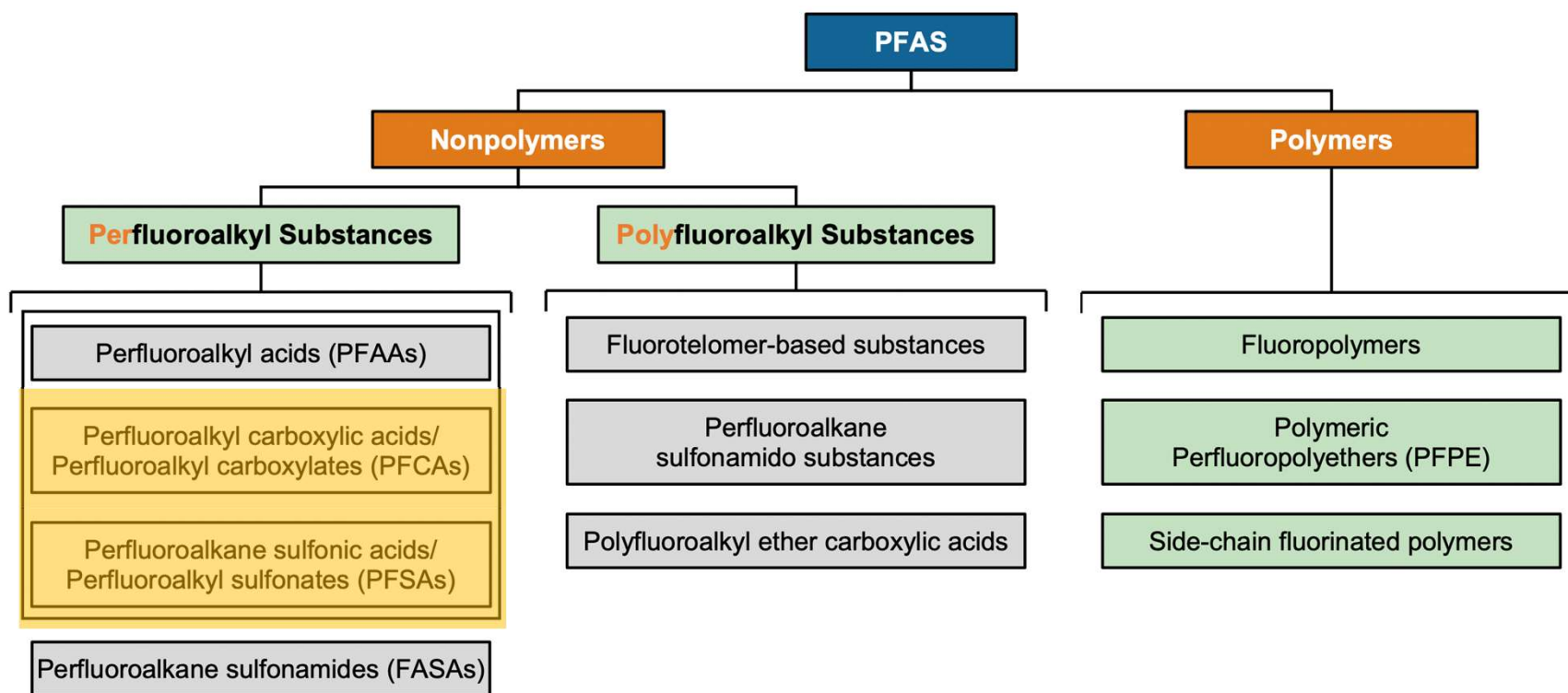
# The PFAS Family Tree (and alphabet soup)

PFOS: One of many PFAS

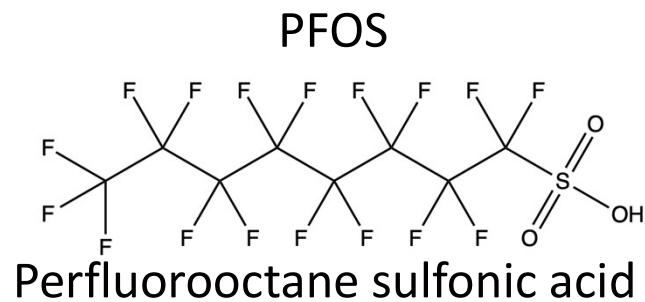




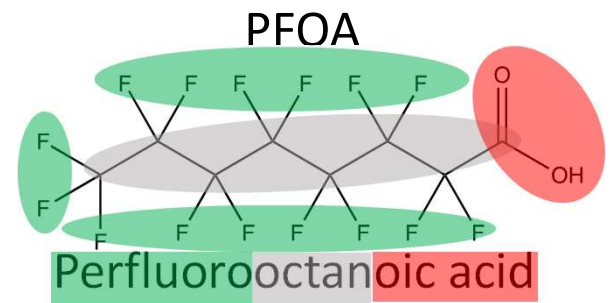
# The PFAS Family Tree (and alphabet soup)



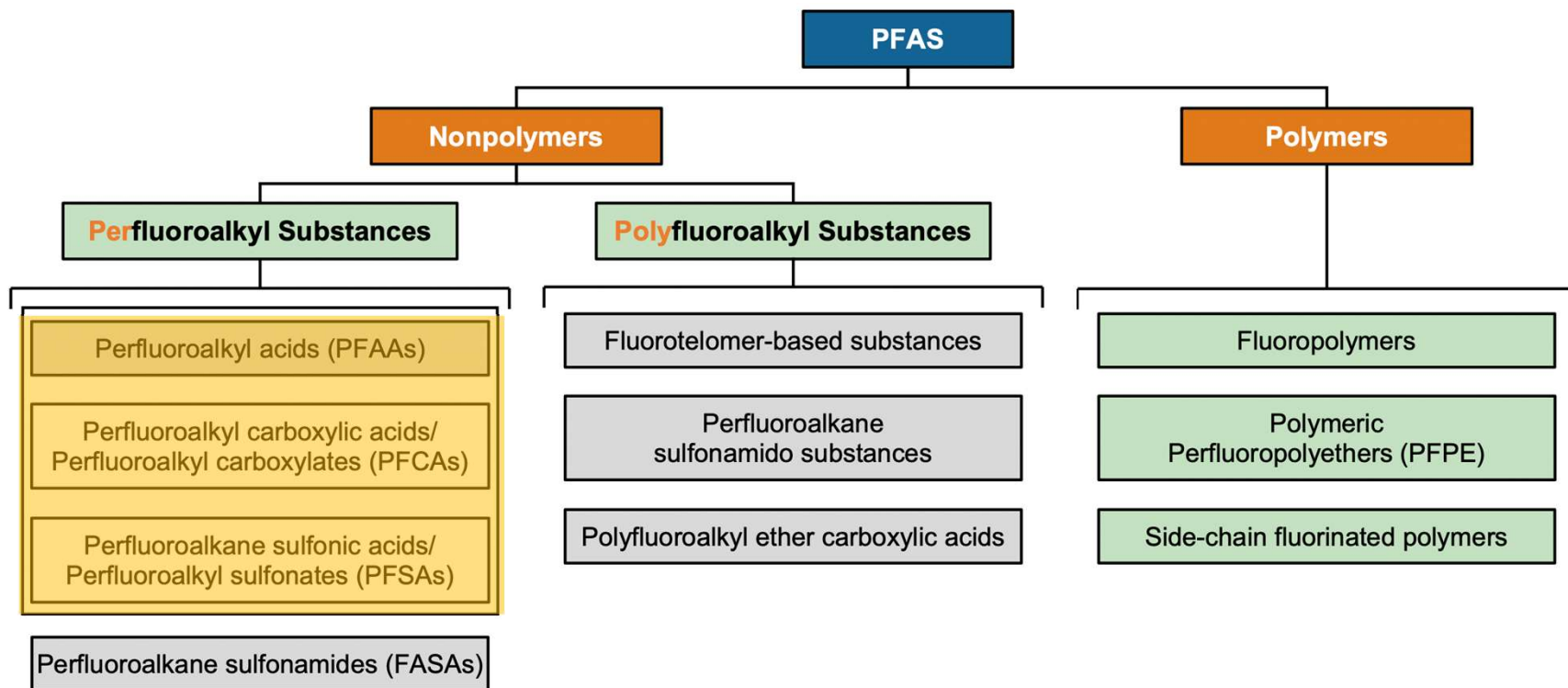
# The PFAS Family Tree (and alphabet soup)



“C8”



# The PFAS Family Tree (and alphabet soup)

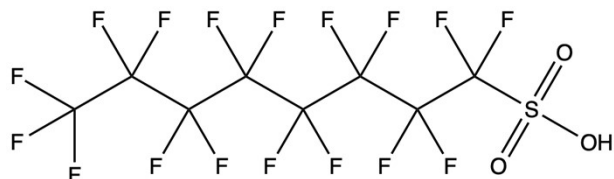


# The PFAS Family Tree (and alphabet soup)

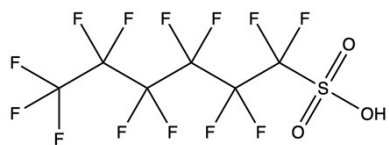
## Perfluoroalkyl Acids (PFAAs)

### Perfluoroalkane sulfonic acids (PFSA)

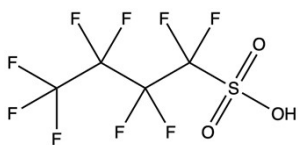
PFOS



Perfluorooctane sulfonic acid



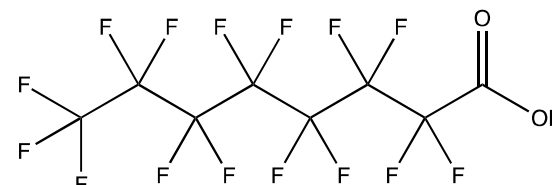
PFHxS



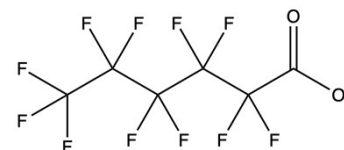
PFBS

### Perfluoroalkane carboxylic acids (PFCA)

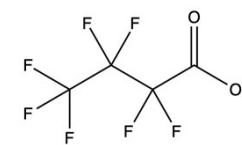
PFOA



Perfluorooctanoic acid



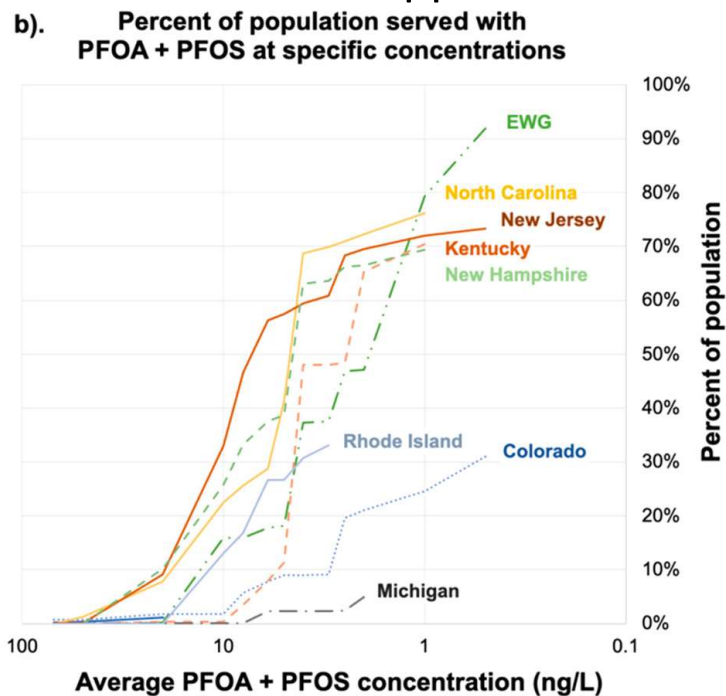
PFHxA



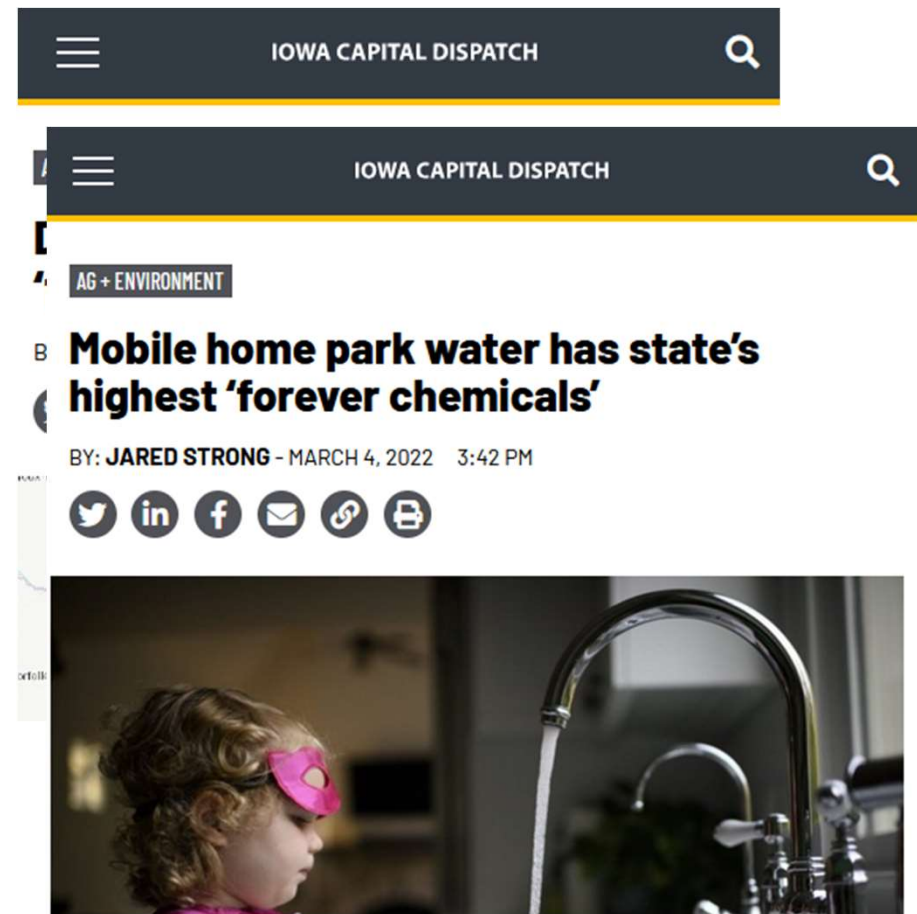
PFBA

# PFAS Impacts: Drinking Water

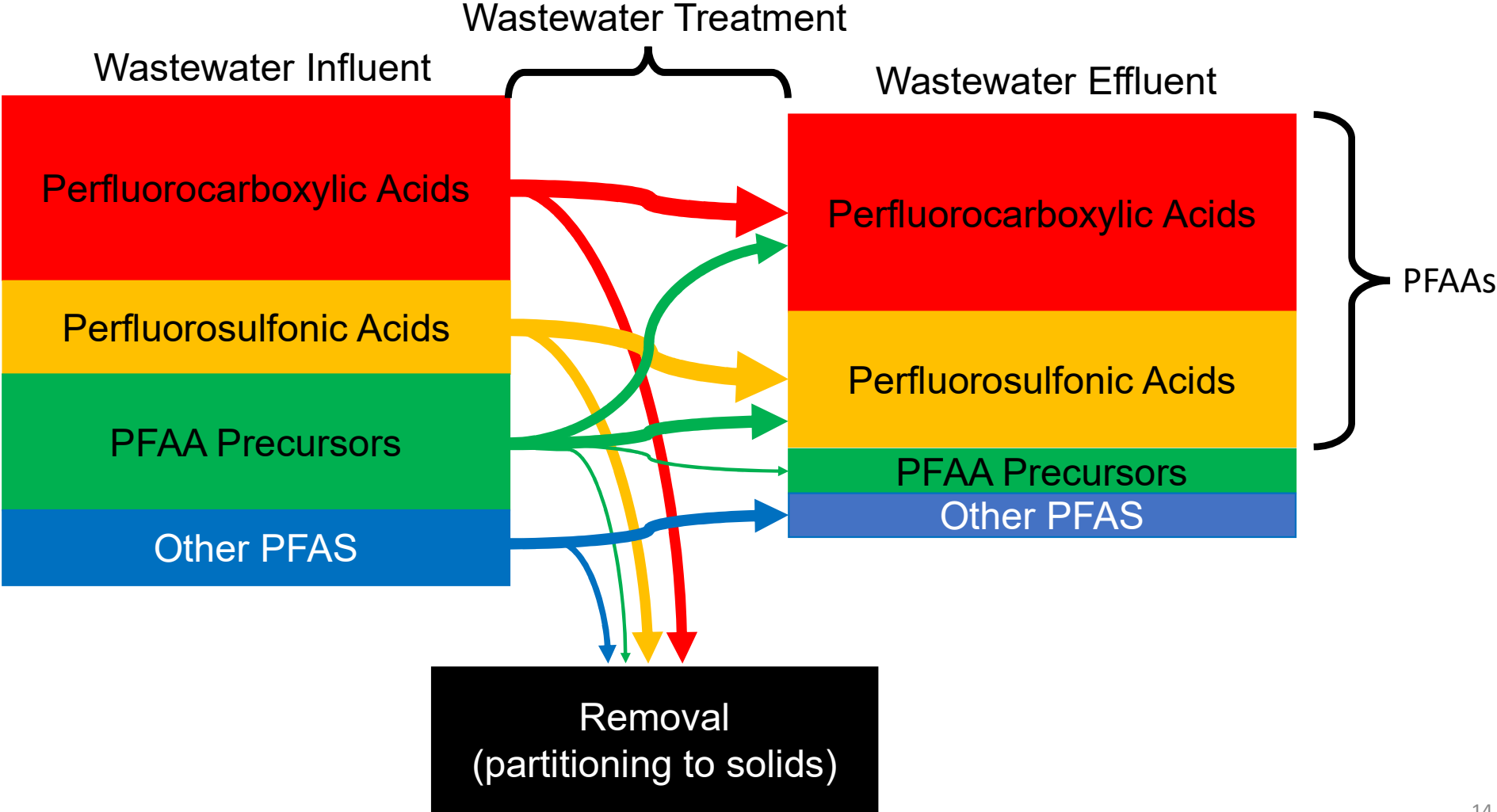
- Yesterday: Proposed MCL for 6 PFAS released
  - PFOA & PFOS: 4 ppt each
- Drinking water supplies for 18-80 million Americans exceed 10 ppt PFOA + PFOA



Courtesy: Andrews and Naidenko, *ES&T Letters* 2020



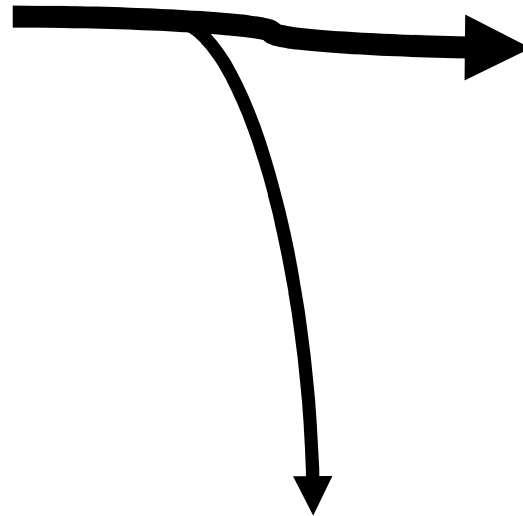
# PFAS Impacts: Wastewater



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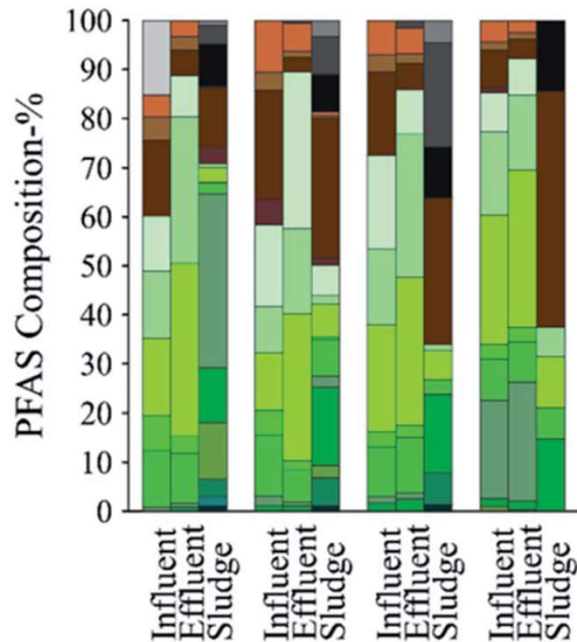
## Wastewater Influent:

- Total PFAS concentration typically ~30-300 ppt
  - Only 16 - 33% directly measured PFAAs



## Wastewater Influent:

- Total PFAS concentration typically ~30-200 ppt
  - 33 - 100% directly measured PFAAs



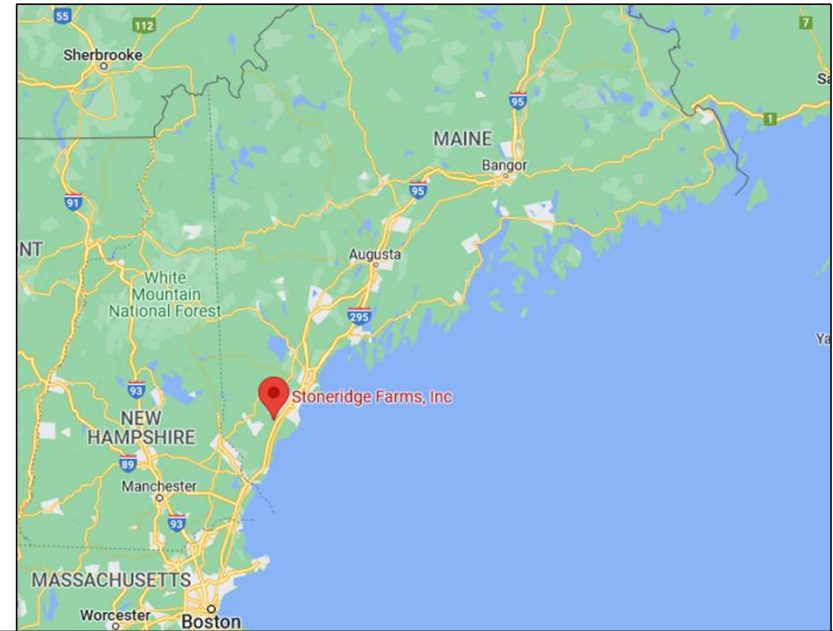
Courtesy: Tavasoli et al., *ES:PI* 2021

## Sludge & Biosolids:

- 300-750 times higher concentrations in sludge than water
- Enriched in long-chain PFAS

# PFAS Impacts: Wastewater

- 2016: Drinking water monitoring near Maine farm finds 8,000 ppt PFAS.
  - Follow-up soil testing finds 475 **ppb** PFAS.
  - High PFAS levels found in milk, cows: Herd culled.
  - Biosolids from pulp and paper mills implicated.
- 2019: Maine requires PFAS testing in all biosolids land application programs
  - State investigates 700 farm soils
- 2022: Maine bans land application of wastewater biosolids

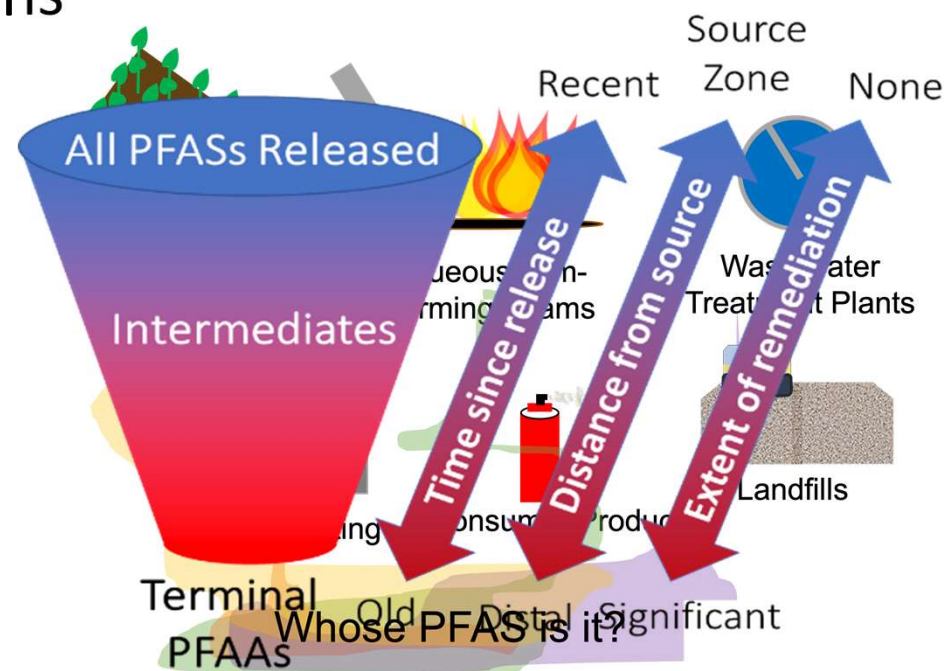




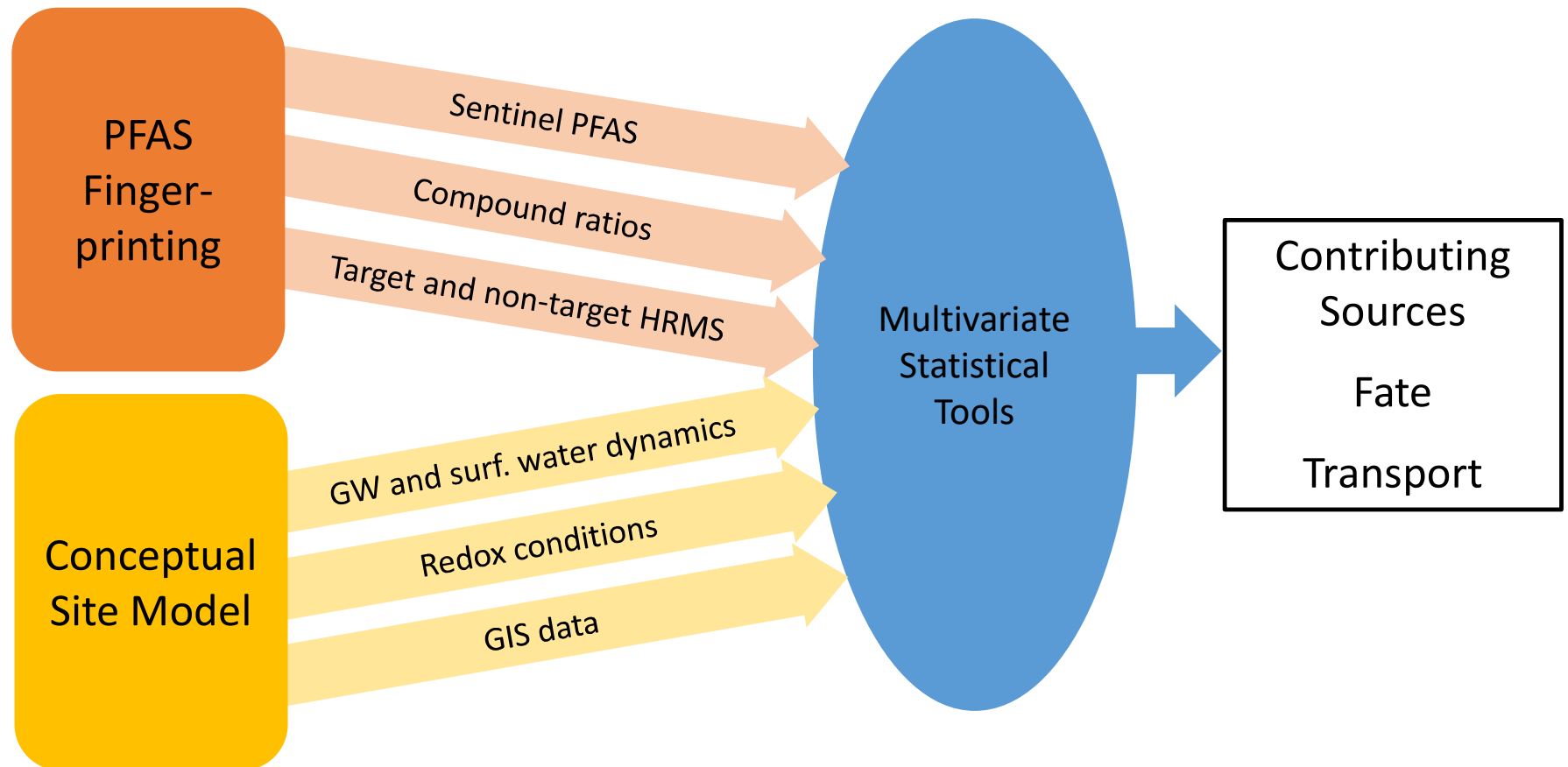
# The Challenge of PFAS Forensics

## Unknown PFAS sources or contributions

- Use in many industries
- Persistent & mobile
- “Funnel Effect”



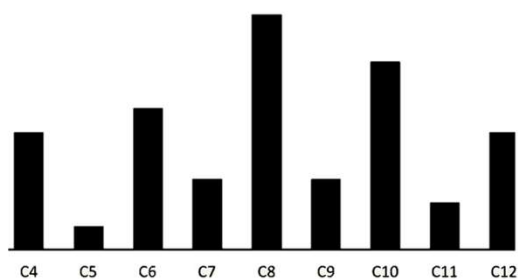
# PFAS Source Tracking



# PFAS Fingerprints

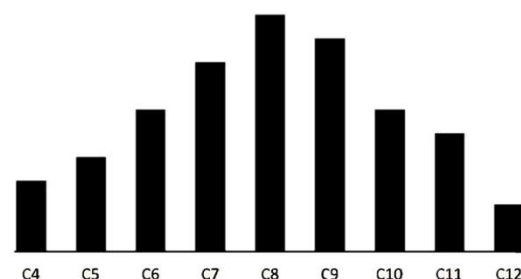
Mixture *compositions* vary based on synthesis:

## Fluorotelomerization



Bias towards odd- or even-length chains

## Electrochemical Fluorination

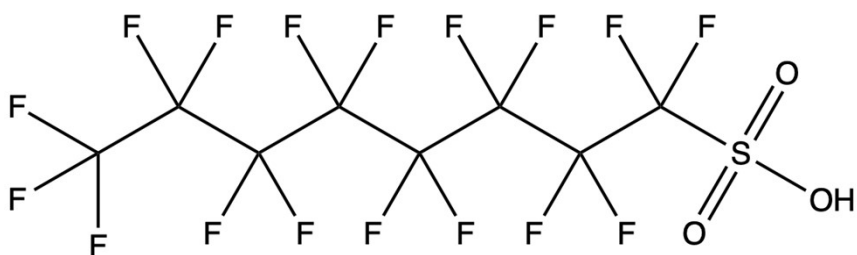


Even-length chains  $\approx$  odd-length chains

# PFAS Fingerprints

Mixture *compositions* vary based on synthesis:

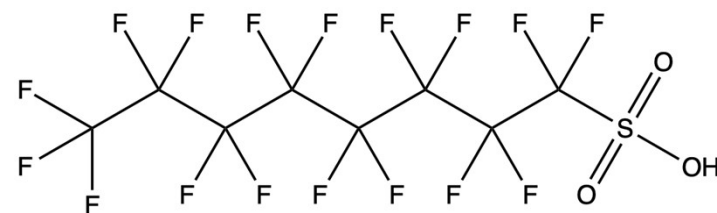
## Fluorotelomerization



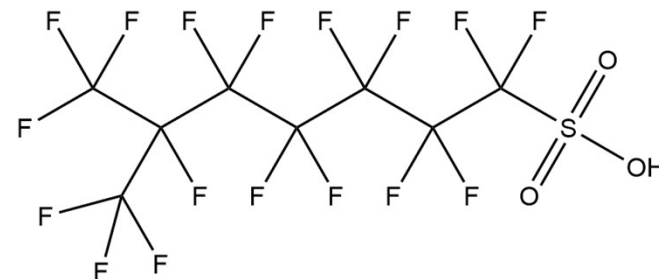
Virtually all linear isomers

## Electrochemical Fluorination

~75-67%  
linear isomers



~25-33%  
branched isomers

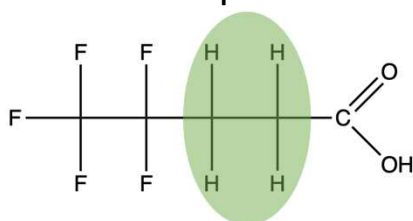


# PFAS Fingerprints

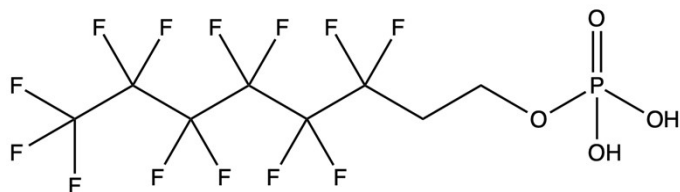
Mixture *components* vary based on synthesis:

## Fluorotelomerization

Un-fluorinated portion of “tail”

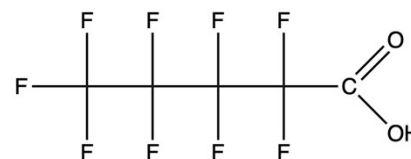


6:2 fluorotelomer phosphate monoester: (Food) paper coating

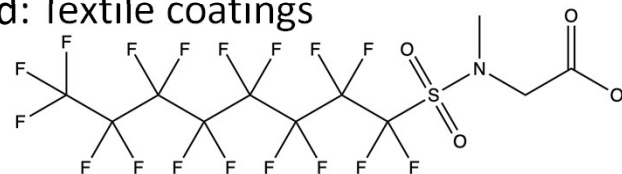


## Electrochemical Fluorination

Fully-fluorinated “tail”

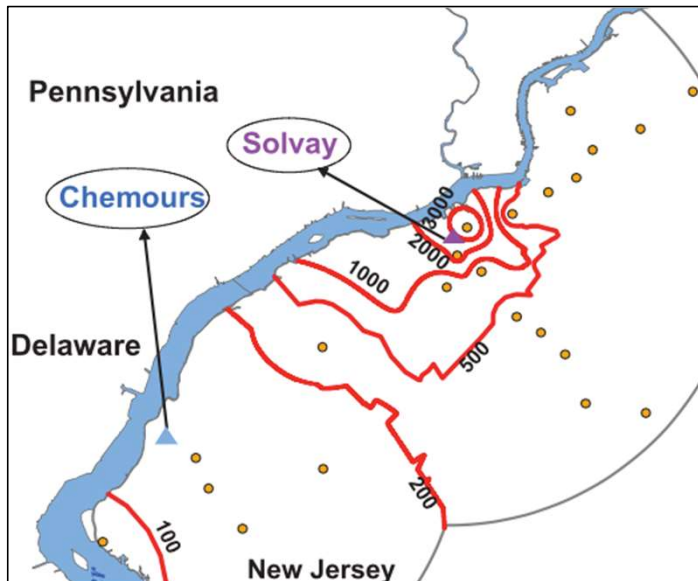


Methyl-perfluorooctane sulfonamido acetic acid: Textile coatings



# Conceptual Site Model

Baseline understanding of how contaminants migrate



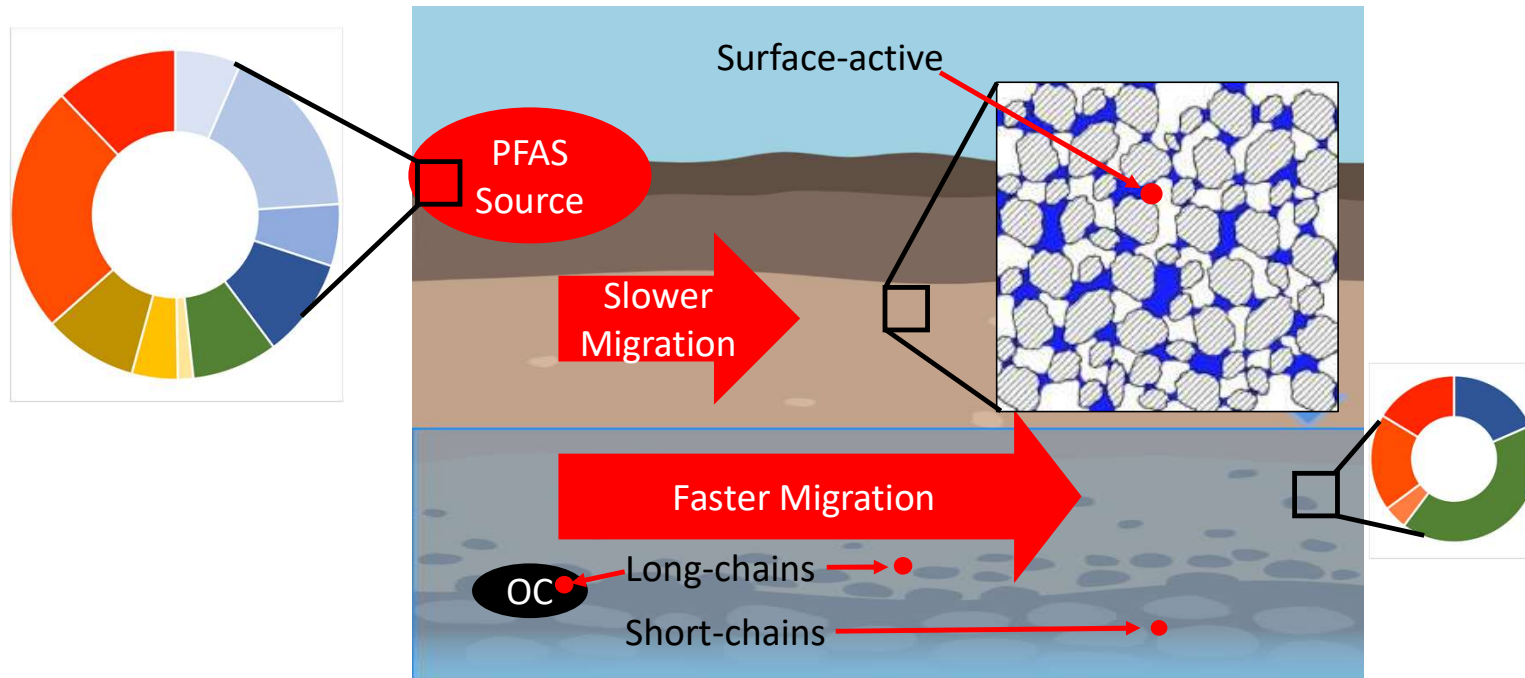
GIS data can relate potential sources to observed contamination.

## Site data:

- Groundwater and surface water features
- Soil composition/hydrogeology
- Chemical redox conditions
- Co-contaminant distribution
- Point source discharges/industry

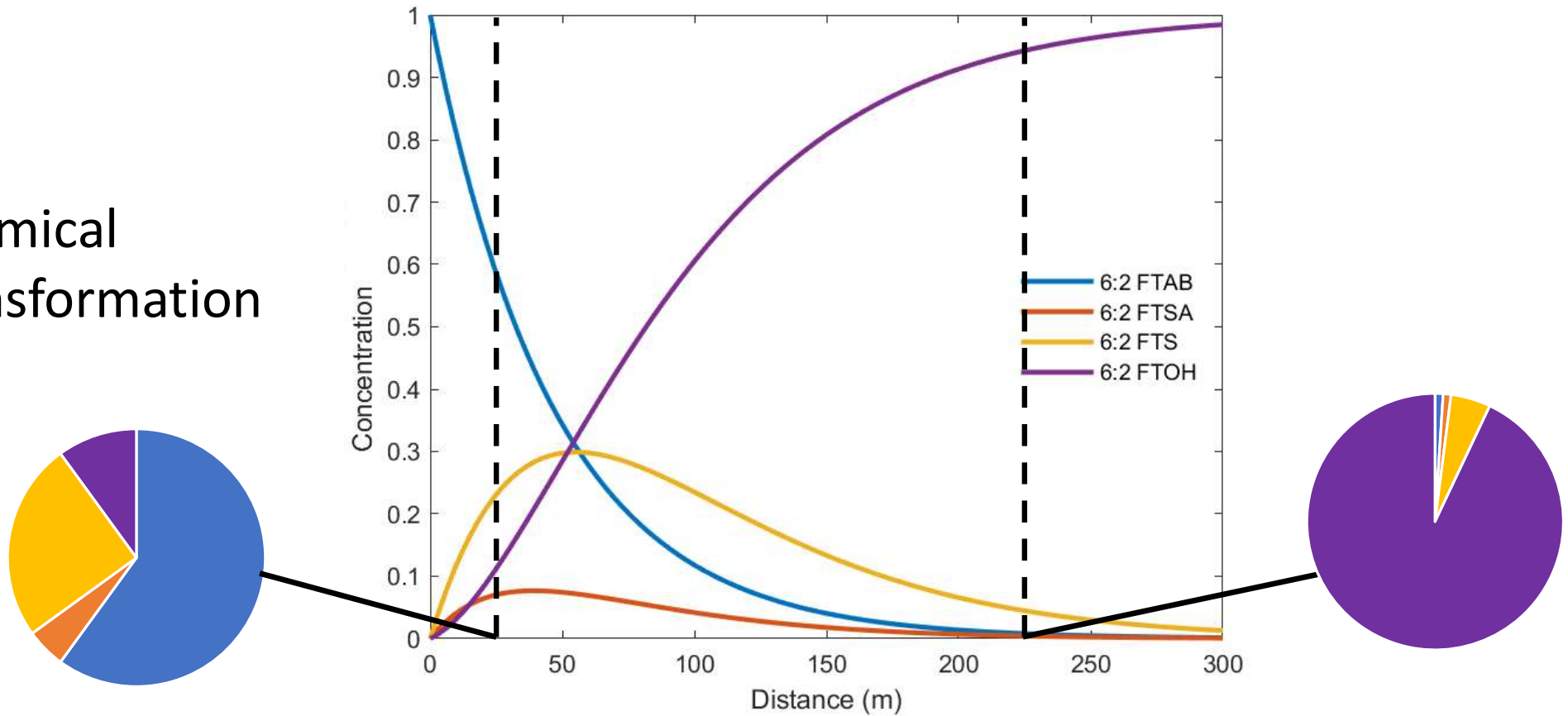
# Conceptual Site Model

## Chemical Partitioning



# Conceptual Site Model

Chemical Transformation





# Multivariate Statistical Analyses

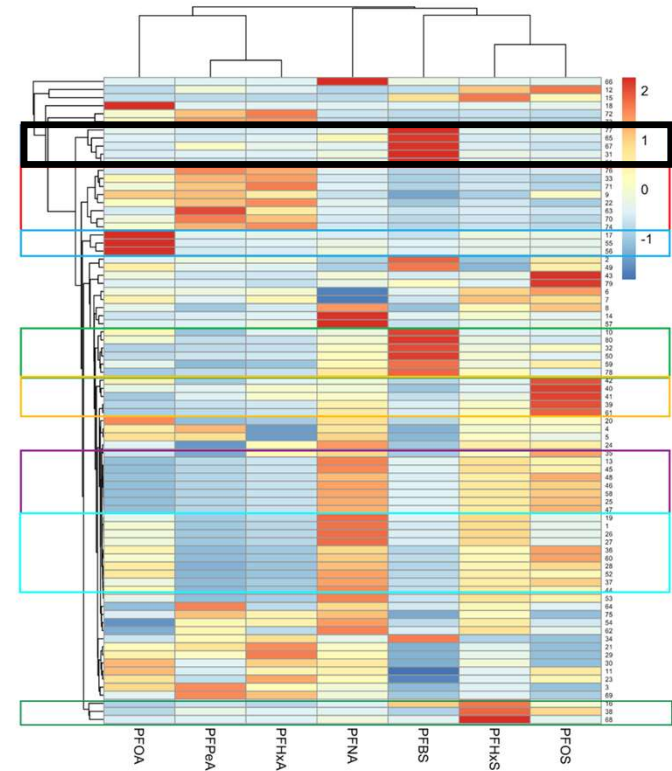
Methods to classify, group, and rank PFAS of similar origin

## Supervised techniques

- Classification
- Regression

## Unsupervised techniques

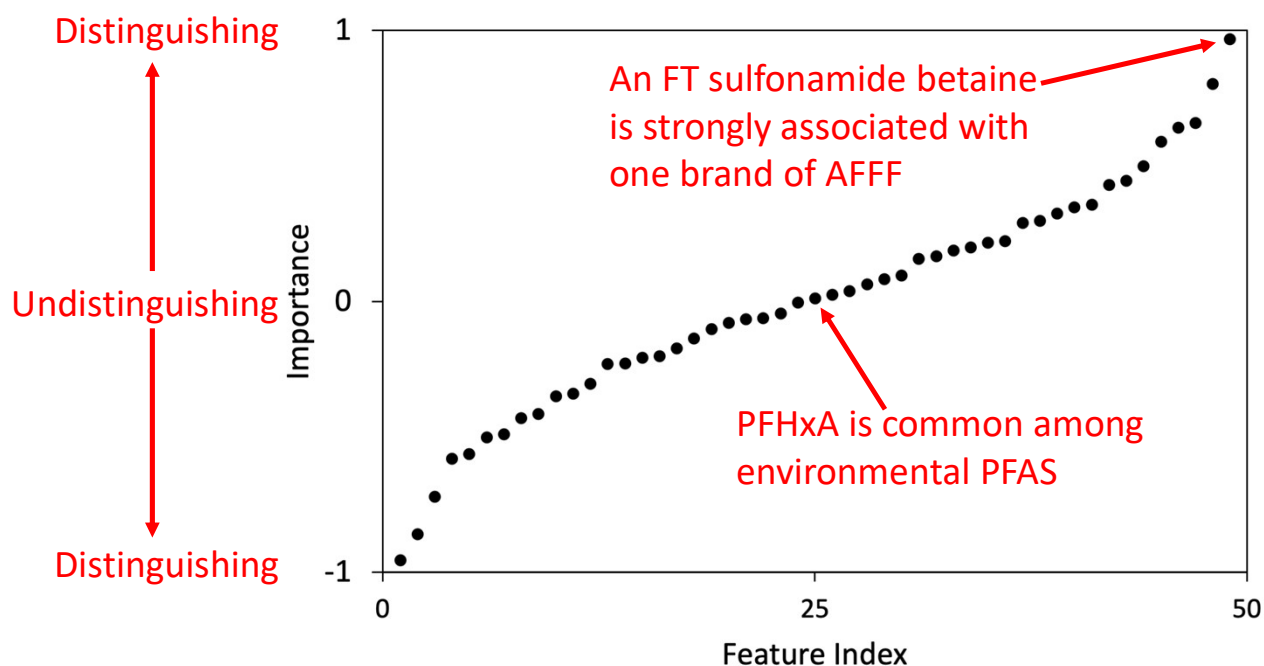
- Hierarchical Clustering Analysis
- Principal Component Analysis



HCA clusters PFAS and groundwater sites. 5 sites with high concentrations of PFBS and relatively low concentrations of other PFAS.

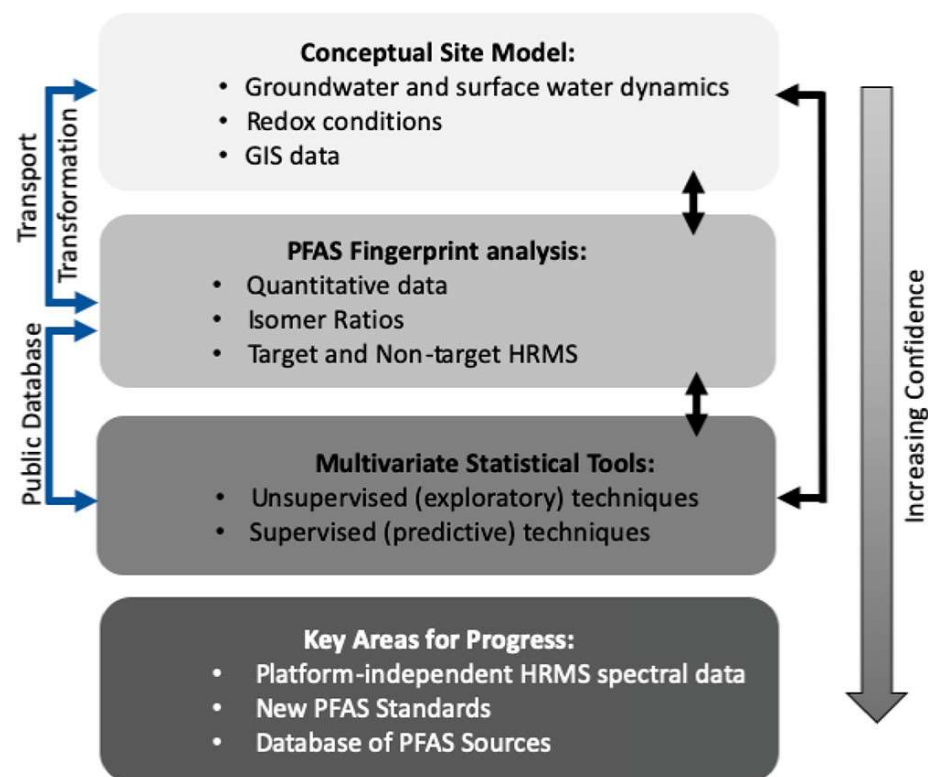
# Multivariate Statistical Analyses

Model ranks how distinguishing chemical features are



# Advancing Source Tracking

- Detailed PFAS fingerprints
  - Identify ratios of key compounds
  - Target consistent analytes with standards
- Publicly accessible data
  - Platform-independent
- Supervised and unsupervised learning
- Iterate



# Acknowledgements

## Co-Authors

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# Questions