Challenges Associated with the Analysis of Consumer Products

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Charles Neslund

Scientific Officer & PFAS Practice Leader

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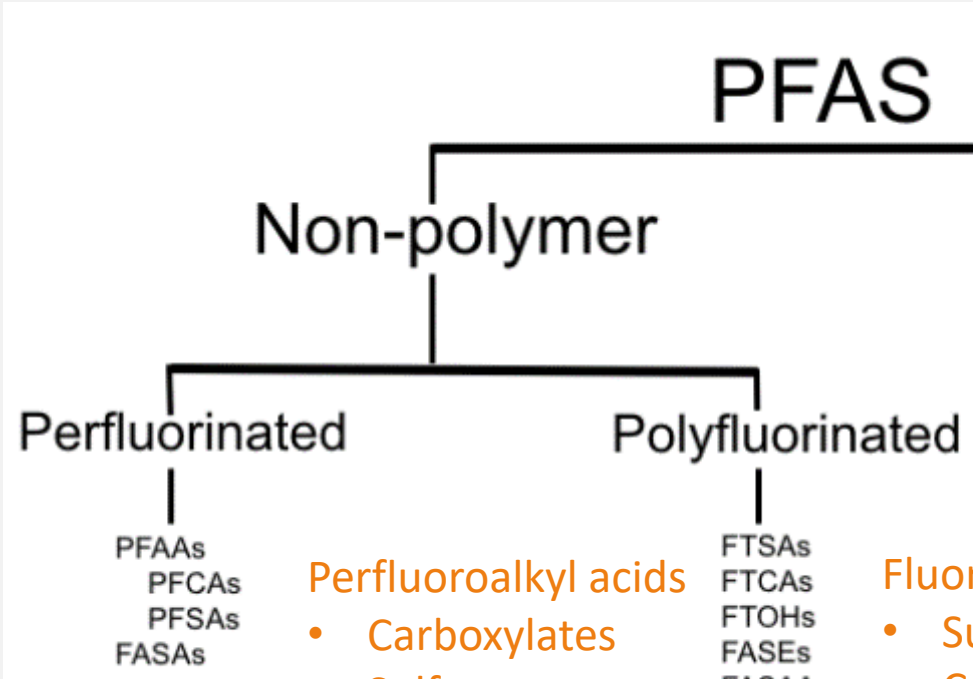
The General Classes of Per- and Polyfluoroalkyl Substances (PFAS)



- Fluoropolymers
- Perfluoropolyethers (PFPE)
- Side-chain fluorinated polymers

Perfluoroalkyl acids
- Carboxylates
- Sulfonates

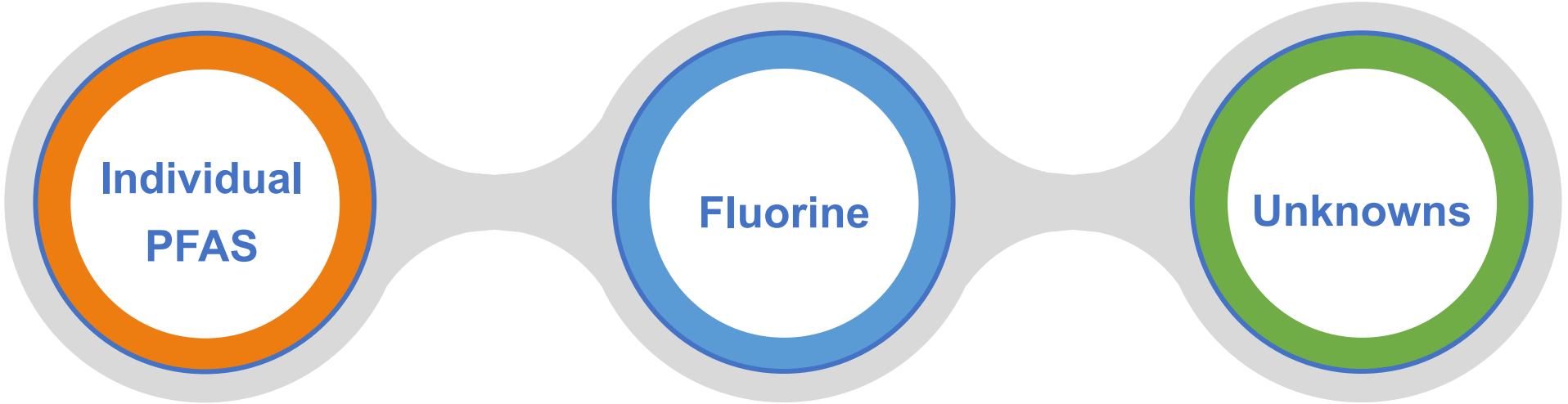
Fluorotelomers:
- Sulfonates
- Carboxylates
- Alcohols

Source: ITRC Naming Conventions and Physical Chemical Properties fact sheet

ANALYTICAL METHODS

Analyzing for PFAS in Products

We've got options



Targeted PFAS by LC/MS/MS

"537 Modified" + TOP Assay

Up to 70+ non-polymer PFAS compounds

Oxidizable Precursors

Total or Organic Fluorine by CIC

"TOF-CIC"

Total Fluorine (inorganic + organic)

Total Organic Fluorine (TOF)

(may include polymers)

Non-Target Analysis by LC/QTOF

"NTA"

Unknown non-polymer PFAS present at approximately >10ppb may be detectable and identifiable

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LCMSMS/GCMSMS Analysis

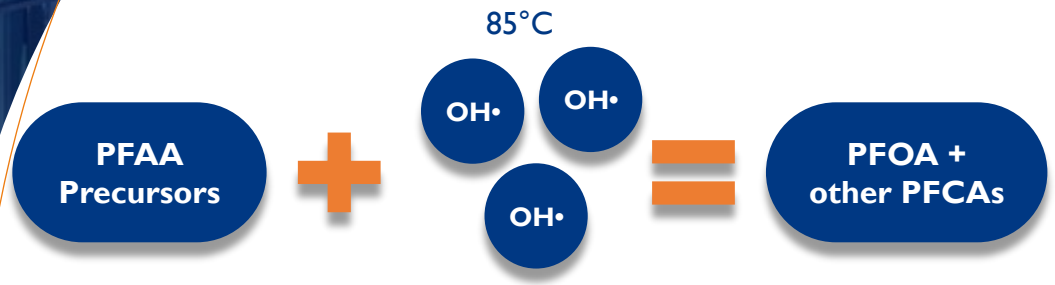
Compounds Included in EPA Draft 1633

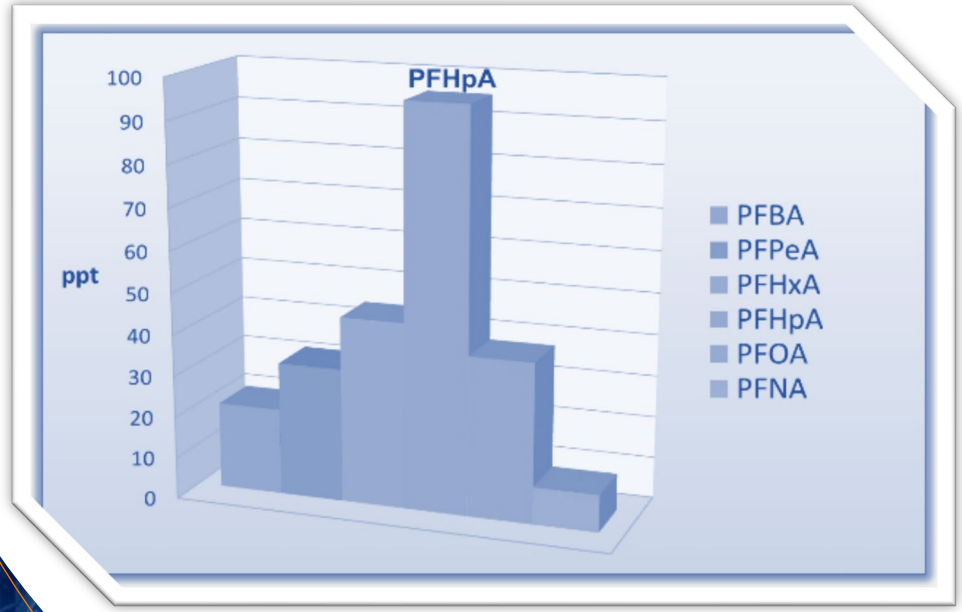
- Perfluorobutanoic acid (PFBA)
- Perfluoropentanoic acid (PFPeA)
- Perfluorohexanoic acid (PFHxA)
- Perfluoroheptanoic acid (PFHpA)
- Perfluorooctanoic acid (PFOA)
- Perfluorononanoic acid (PFNA)
- Perfluorodecanoic acid (PFDA)
- Perfluoroundecanoic acid (PFUnA)
- Perfluorododecanoic acid (PFDoA)
- Perfluorotridecanoic acid (PFTriA)
- Perfluorotetradecanoic acid (PFTeA)
- Perfluorobutanesulfonic acid (PFBS)
- Perfluoropentanesulfonic acid (PFPeS)
- Perfluorohexanesulfonic acid (PFHxS)
- Perfluoroheptanesulfonic Acid (PFHpS)
- Perfluorooctanesulfonic acid (PFOS)
- Perfluorononanesulfonic acid (PFNS)
- Perfluorodecanesulfonic acid (PFDS)
- Perfluorododecanesulfonic acid (PFDoS)
- Perfluorooctanesulfonamide (FOSA)
- NEtFOSA
- NMeFOSA
- NMeFOSAA
- NEtFOSAA
- NMeFOSE
- NEtFOSE
- 4:2 FTS
- 6:2 FTS
- 8:2 FTS
- 9Cl-PF3ONS
- 11Cl-PF3OUdS
- DONA
- HFPO-DA (GenX)
- 3:3 FTCA
- 5:3 FTCA
- 7:3 FTCA
- NFDHA
- PFMBA
- PFMPA
- PFEESA

Target Compounds Not Part of EPA Draft 1633

- 10:2 FTS
- 6:2 FTCA
- 8:2 FTCA
- 10:2 FTCA
- 6:2 FTUCA
- 8:2 FTUCA
- 10:2 FTUCA
- PFECHS
- PFPrS
- PFPrA
- PFMOAA
- PFECAG
- PFO4DA
- PFO3OA
- PFO2HxA
- R-EVE
- NVHOS
- Hydro-EVE Acid
- Perfluoro-n-octadecanoic acid (PFODA)
- Perfluoro-n-hexadecanoic acid (PFHxDA)
- EVE Acid
- PFO5DA
- PMPA
- PEPA
- MTP
- PS Acid
- Hydro-PS Acid
- R-PSDA
- Hydrolyzed PSDA
- R-PSDCA
- 6:2 diPAP
- 8:2 diPAP
- 6:2/8:2 diPAP
- 10:2 diPAP
- 10:2 FTOH (RL= 20 ng/L)
- 8:2 FTOH (RL= 20 ng/L)
- 7:2 FTOH (RL= 20 ng/L)
- 6:2 FTOH (RL= 20 ng/L)
- 4:2 FTOH (RL= 20 ng/L)

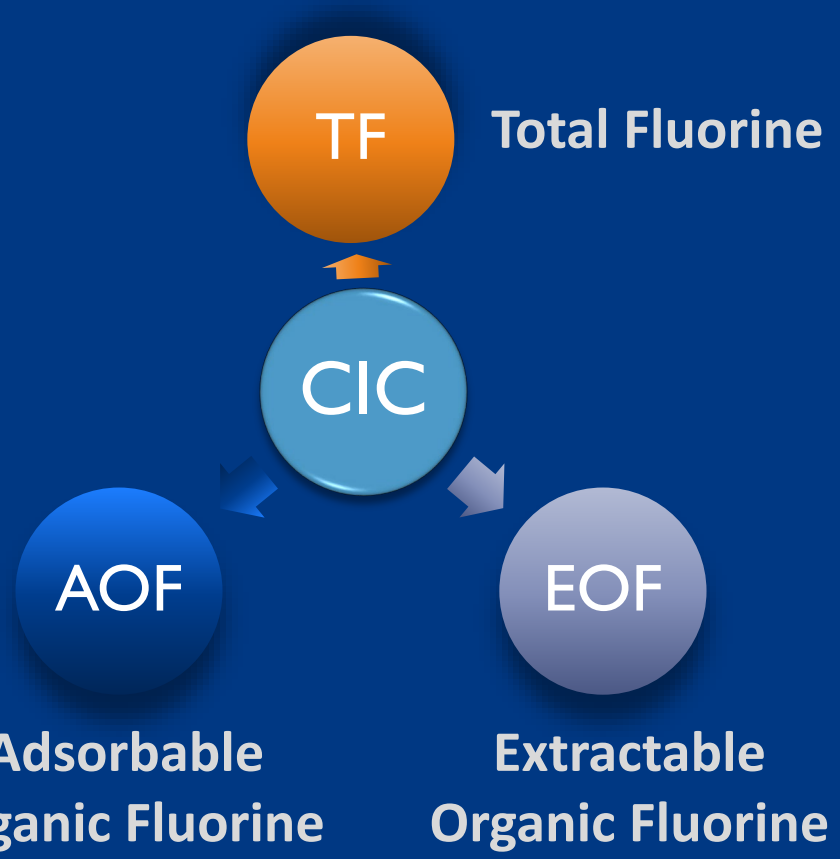
TOP Assay





Compound	Pre-Ox	Post-Ox	Difference
PFBA	ND	98 ng/l	98 ng/l
PFPeA	ND	87 ng/l	87 ng/l
PFHxA	5 ng/l	61 ng/l	56 ng/l
6:2 FTS	100 ng/l	ND	- 100 ng/l
PFHpA	11 ng/l	32 ng/l	21 ng/l
PFOA	7 ng/l	26 ng/l	19 ng/l
PFOS	56 ng/l	52 ng/l	- 4 ng/l
8:2 FTS	26 ng/l	ND	- 26 ng/l
PFNA	ND	5 ng/l	5 ng/l

Total Fluorine Analysis by Combustion Ion Chromatography (CIC)



Strengths & Utility

~ Proxy for entire class of PFAS
~300ppb – 1ppm reporting limit

Weaknesses

~ Doesn't quite close the mass balance
~ Subject to certain interferences

Non-Target Analysis

LC-QToF-MS

Liquid Chromatography
Quadrupole Time of Flight
Mass Spectrometry

Targeted Analysis

Suspect Screening Analysis

Non-Targeted Analysis

REPORTING LIMITS

Detectable Limits in Textiles

Targeted PFAS

Minimum RL = 0.2ppb

Matrix dependent range = 0.2ppb – 1ppm

Total Fluorine (TF)

Minimum RL = 200ppb

Matrix dependent range = 200ppb – 10ppm

Total Organic Fluorine (TOF)

Minimum RL = 200ppb

Matrix dependent range = 200ppb – 10ppm

Targeted PFAS

Up to ~80 PFAS Analytes

Strengths: Selectivity

Sensitivity at ~1-5ppb

Can be used for risk assessment

Weaknesses: Limited list of compounds

Total Fluorine

Organic & Inorganic Fluorine

Strengths: Captures polymers and non-polymers

Weaknesses: Sensitivity at 500ppb

Potential high bias from inorganic fluorine

Not specific

Non-Target Analysis

Unknown PFAS Analytes

Strengths: Ability to identify ‘unknowns’ with specificity

Weaknesses: Limited to libraries

Limited quantitation

Limited sensitivity ~10ppb

Total Organic Fluorine

Organic Fluorine

Strengths: Closest proxy for Total PFAS

Weaknesses: Sensitivity at 1ppm

Potential bias from adsorption or extraction prep

Potential low bias for polymers

Not specific

https://www.epa.gov/water-research/pfas-analytical-methods-development-and-sampling-research

THANK YOU

Charles.Neslund@ET.EurofinsUS.com
717-799-0439

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