



Profiling of Target and Non-target PFAS in Agricultural Soils

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New Jersey Institute of Technology

June 3rd , 2024

Target Analysis

Method 1633, 533,
537 by LC/MS/MS



USEPA

Proposed Maximum
Contaminant Levels
4 ng/L for **PFOA**
4 ng/L for **PFOS**

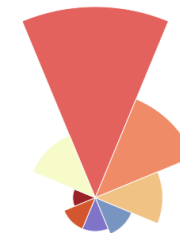


Non-target Analysis

QTOF-MS,
UPLC-HRMS,
Nano-HRMS, etc.

Lack Specific Regulations

Higher Existence



• 6:2 FTSAS • 6:2 FTAB • Thio-8:2 FTCA • 6:2 FTS
• PFOS • 6:2 FTSAS-sulfinyl • TFMS • Others



• PFOS • 6:2 FTSAS • 8:2 FTSAS • 6:2 FTAm • TFMS
• 6:2 FTSAS-sulfinyl • 6:2 FTSAS-sulfinyl7 • Others

Frequently Reported

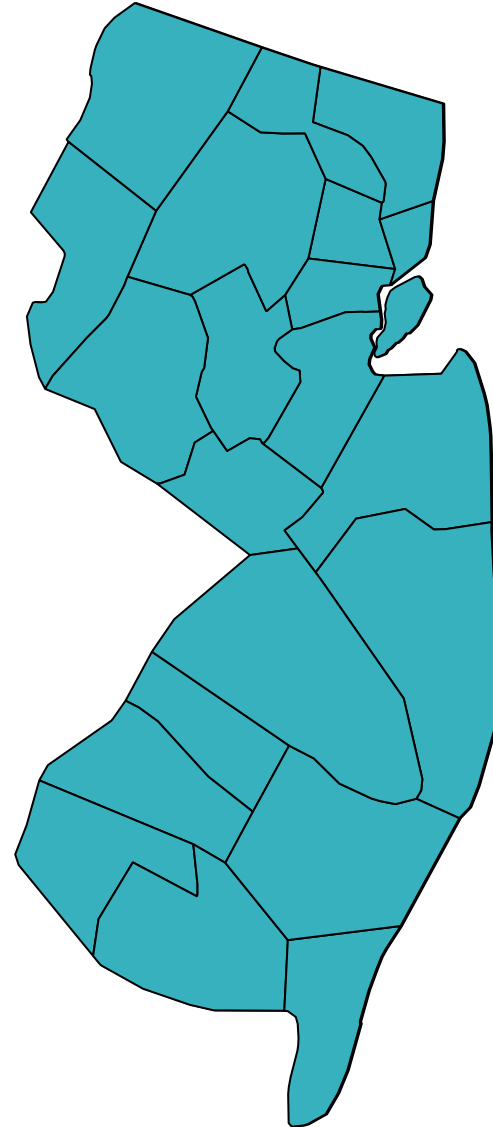
Ringwood Landfill Superfund Site

—
Ford disposed of
wastes, including tons
of paint sludge and
car parts



Native American Tribe

—
Members of the Turtle
Clan of the Ramapough
Lenape Nation lives in
Upper Ringwood





Sampling Site

3

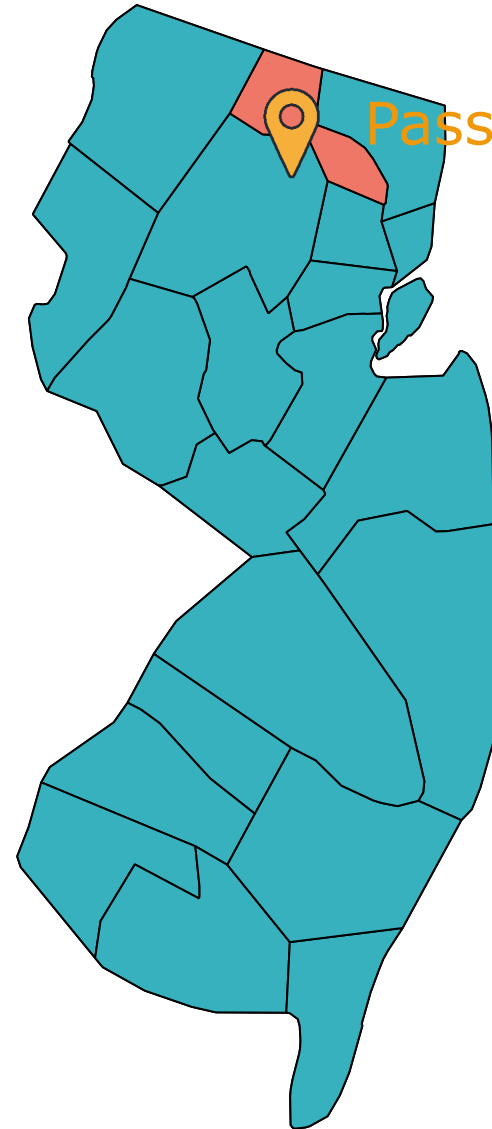
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Ringwood
Passaic Country, NJ

Location	Quantity
Farmland	17
Playground	3
Church	6
Roadside	6
Upstream	9
Sum	41

Paint Sludge

ENVIRONMENTAL
Science & Technology

pubs.acs.org/est

Article

Paints: A Source of Volatile PFAS in Air—Potential Implications for Inhalation Exposure

Liliana Cabuas, Derek J. Muensterman, Mitchell L. Kim-Fu, Patrick N. Reardon, Ivan A. Titaley, and Jennifer A. Field*

Cite This: Environ. Sci. Technol. 2022, 56, 17070–17079

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ENVIRONMENTAL
Science & Technology **LETTERS**

pubs.acs.org/journal/estlet

Letter

Occurrence of Legacy and Emerging Poly- and Perfluoroalkyl Substances in Fluorocarbon Paint and Their Implications for Emissions in China

Xuan Jia, Hongyan Guan, Zhongbao Guo, Chengjing Qian, Yali Shi,* and Yaqi Cai

Other Contaminants

Paint sludge, car parts, and other pollutants dumped by Ford Motor Co. also provides 1,4-dioxane, benzene, arsenic and lead

Consequences

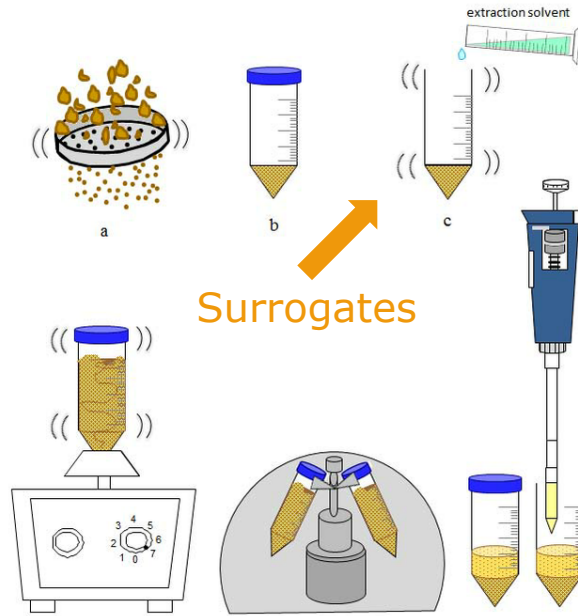


Cancer and other maladies are widespread. Wanaque Reservoir serves more than 3-million people in NJ

Preparation Method

5

Sample Collection,
Preservation, and Storage



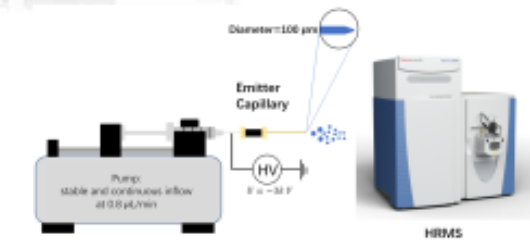
Solid-Phase
Extraction, and
Concentration



Internal
Standards



Chen et al., WR, 2022
Chen et al., WR, 2023



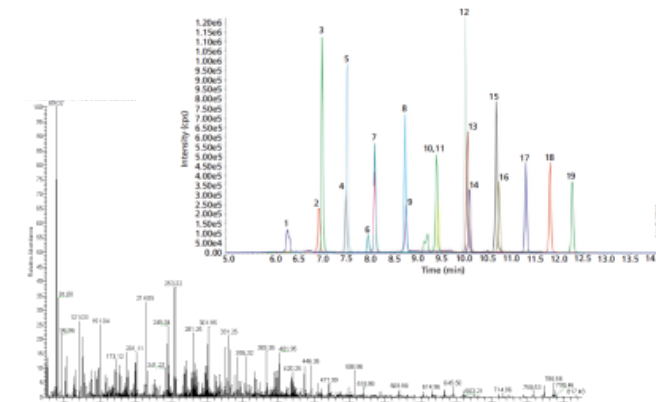
Spectrum
Analysis



Sample
preparation

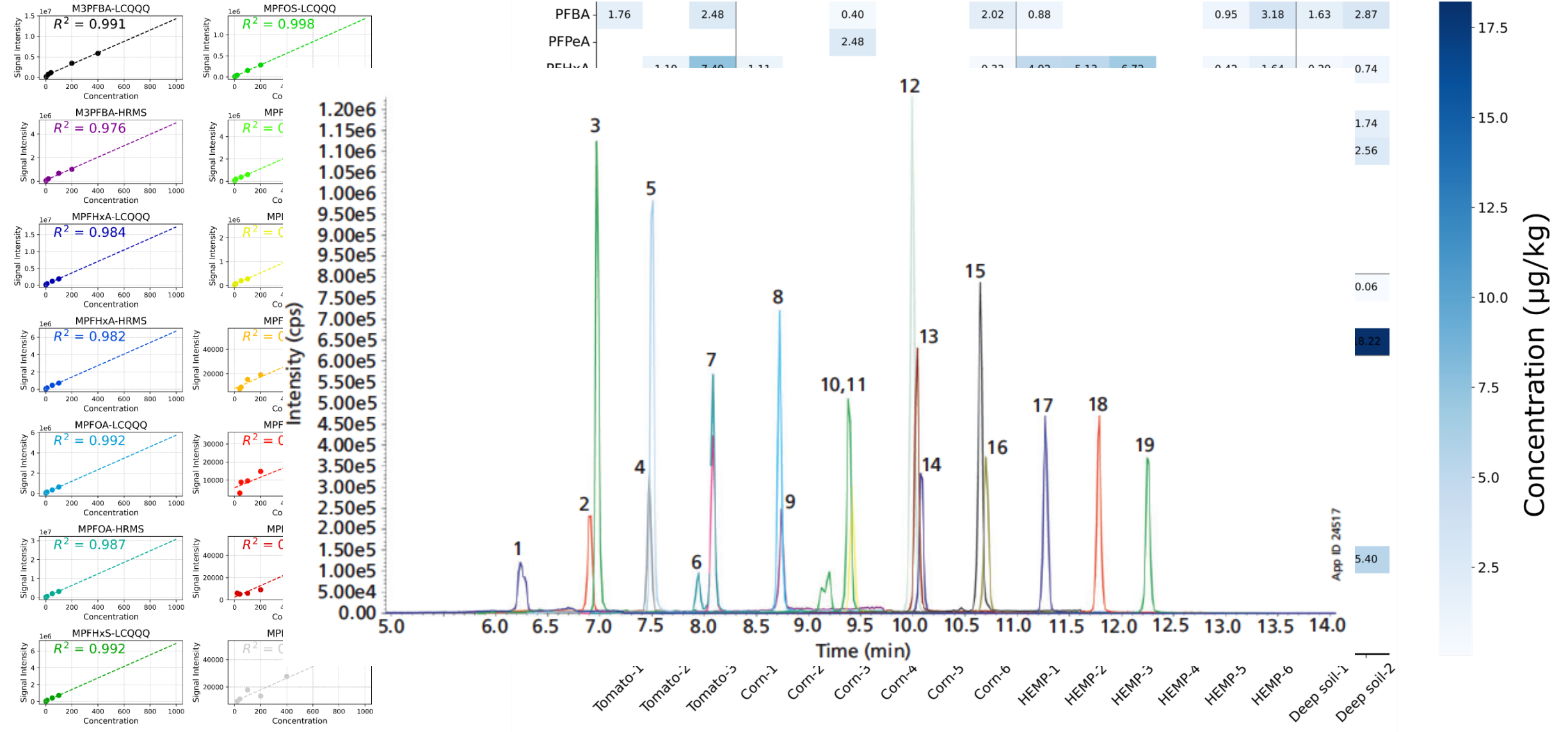


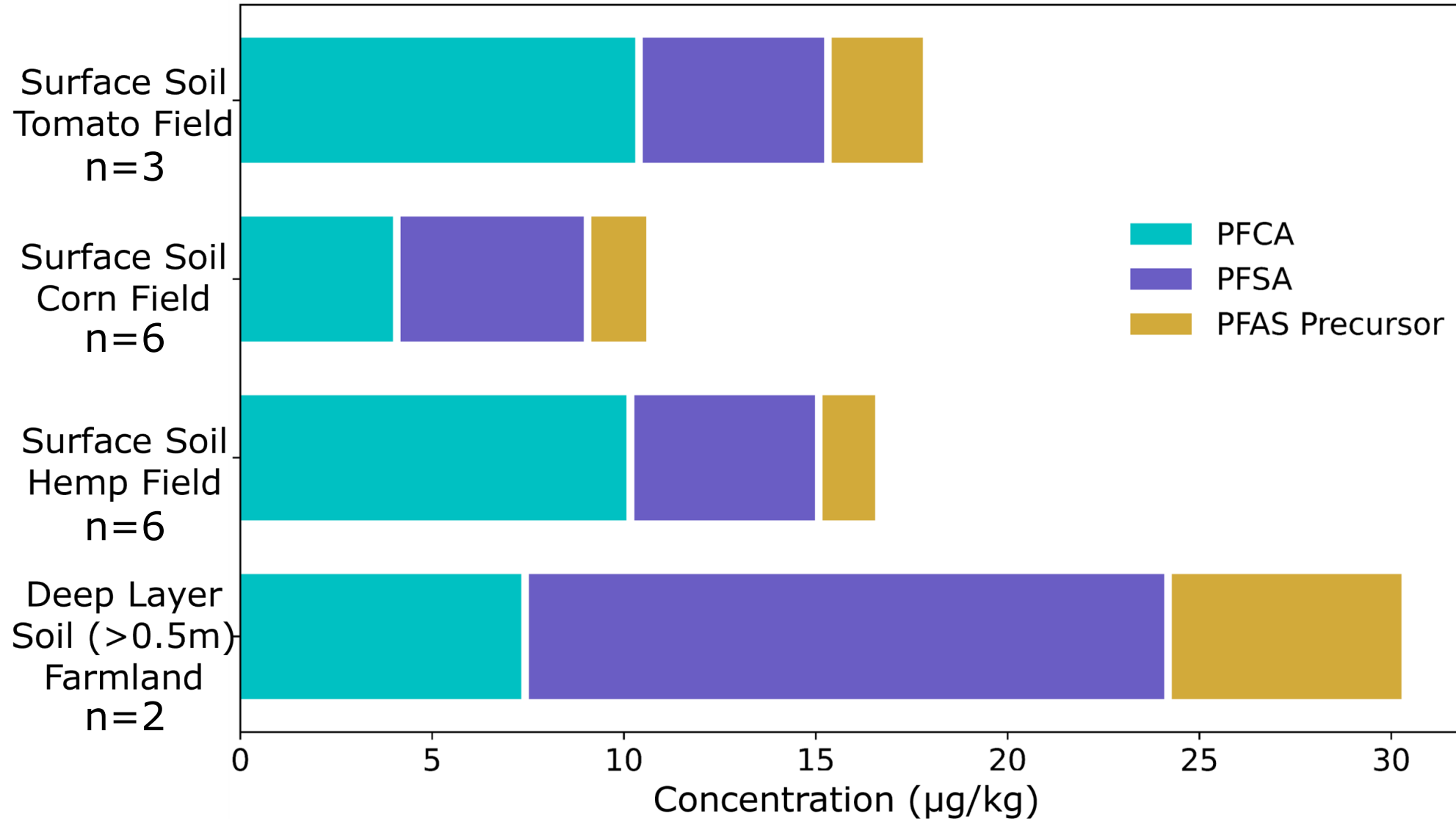
Instrumental
Measurement

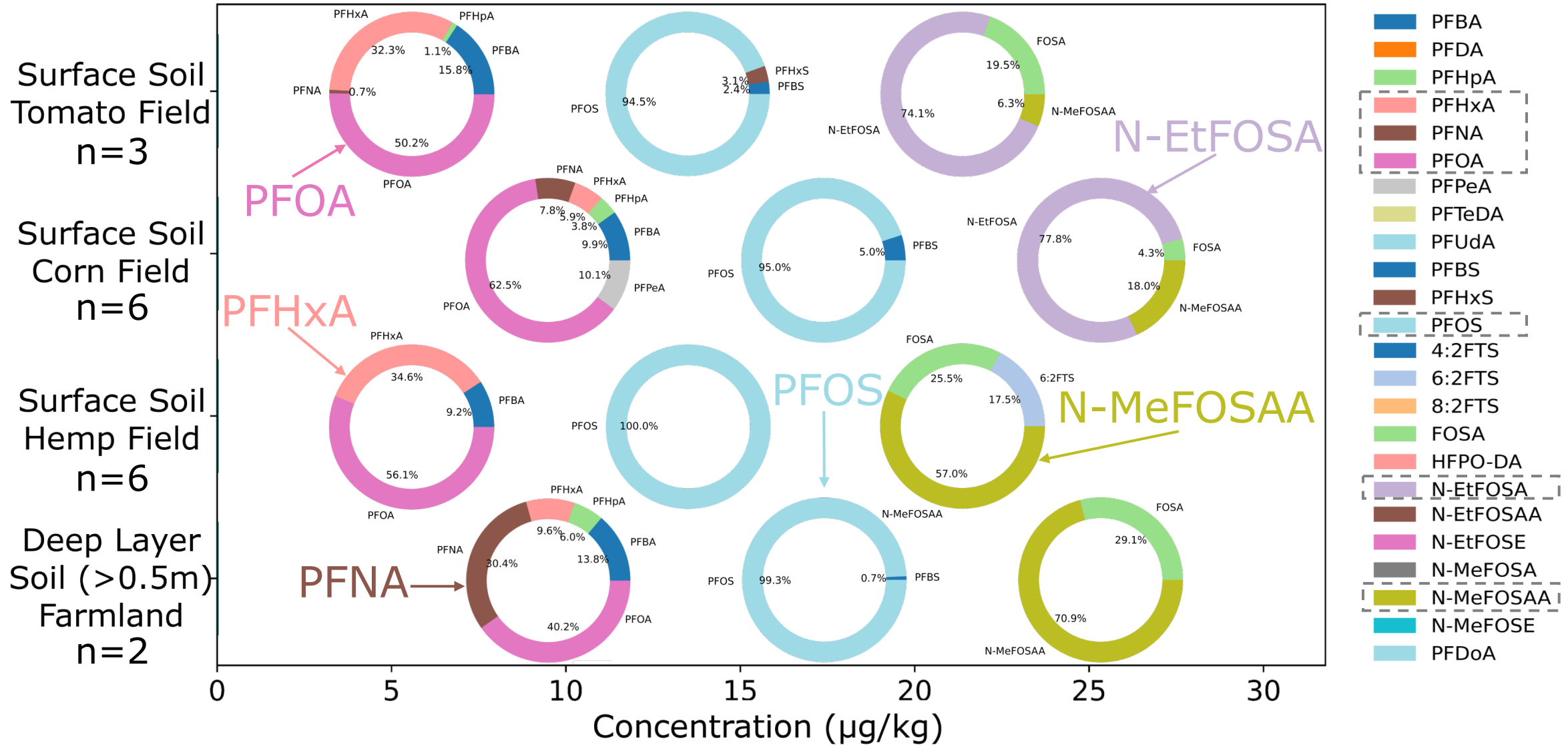


Result-Target Analysis

6





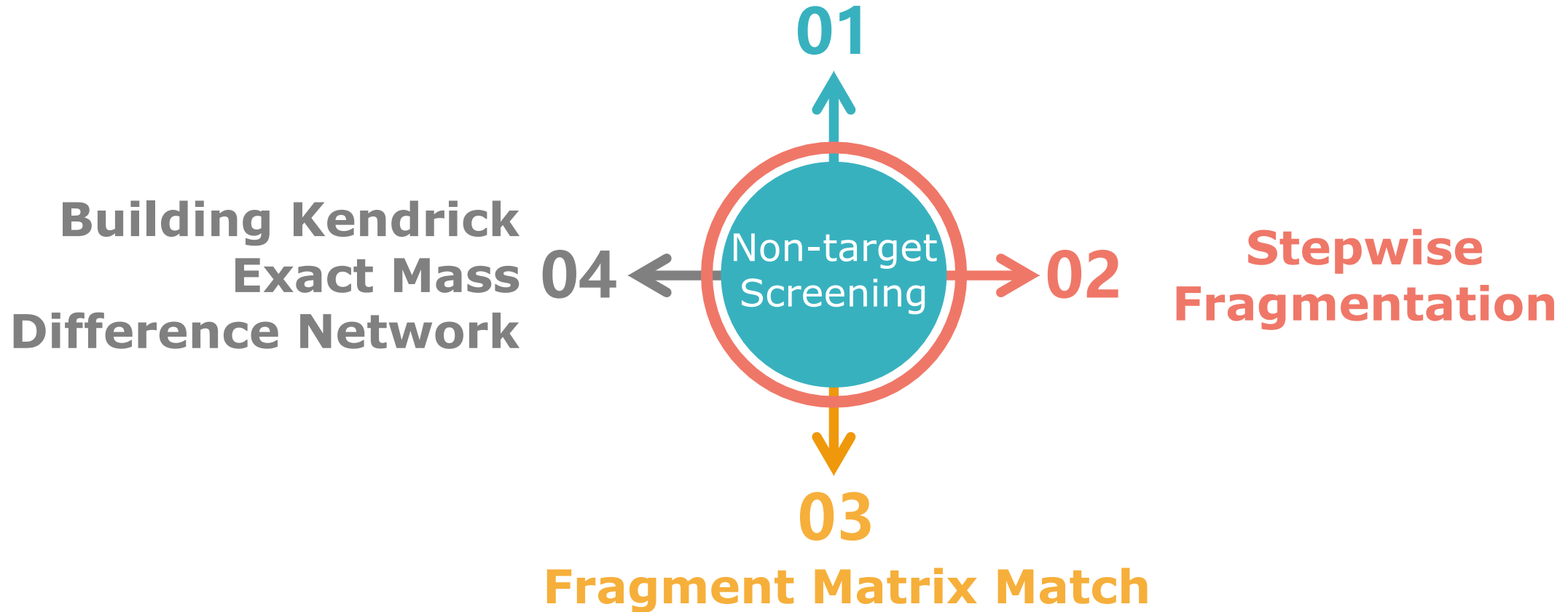




Non-Target Analysis Method

8

Peak Selection Process



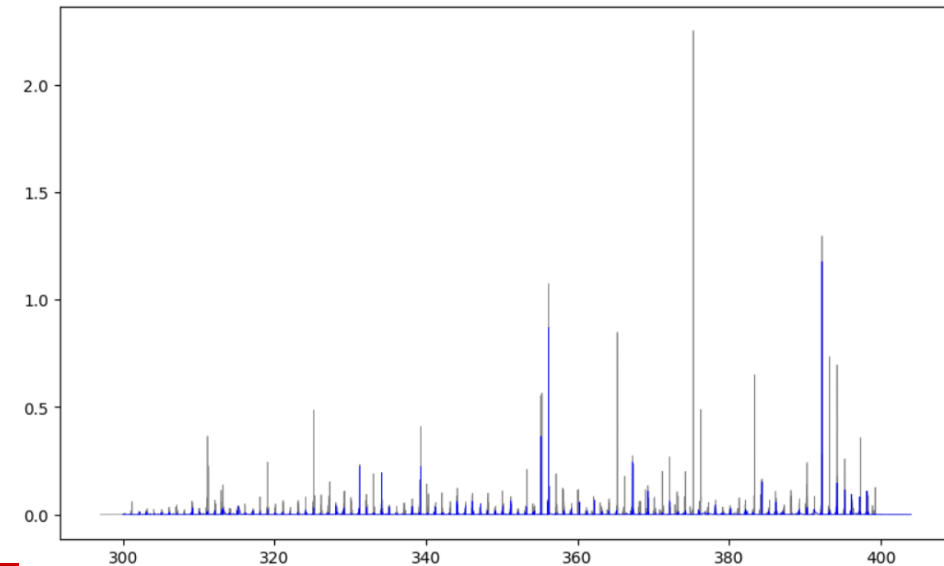
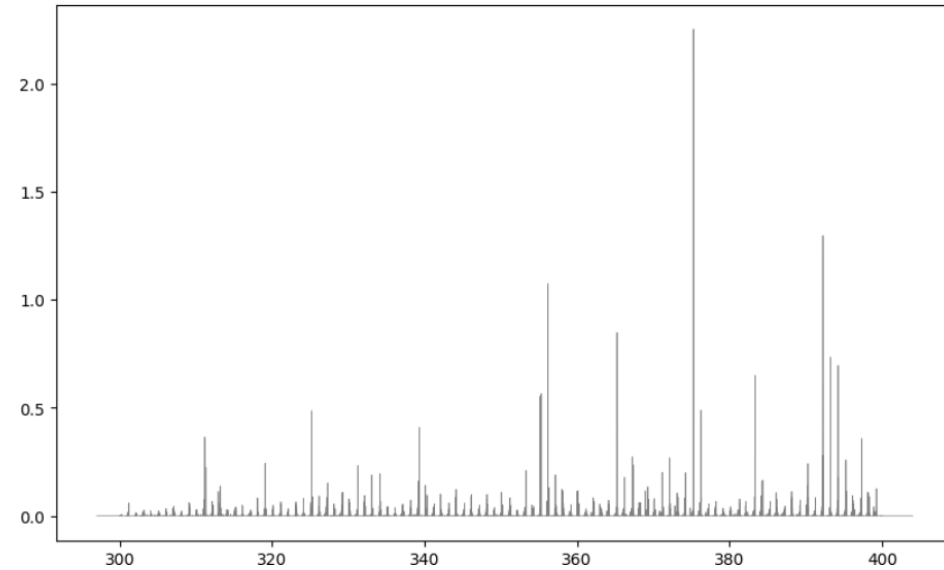
<https://github.com/Daitoueqaq/HRMS-modification>

Peak Selection Process

01



Peaks Assortment ($\geq 0.001RI_{IS}$);
Control and blank subtraction;
100~200 peaks selected in full scan mode



Example Spectra



3



Non-target
Screening

03

Fragment Matrix Match

Database developed contains all potential PFAS fragments from the fragment library & recent paper

The database list includes fragments like: $C_2F_5^-$, $C_3F_7^-$, $C_3F_5^-$, $C_5F_7^-$, $C_2HF_4^-$, $C_3F_5O^-$, $CO_2NF_4S^-$...

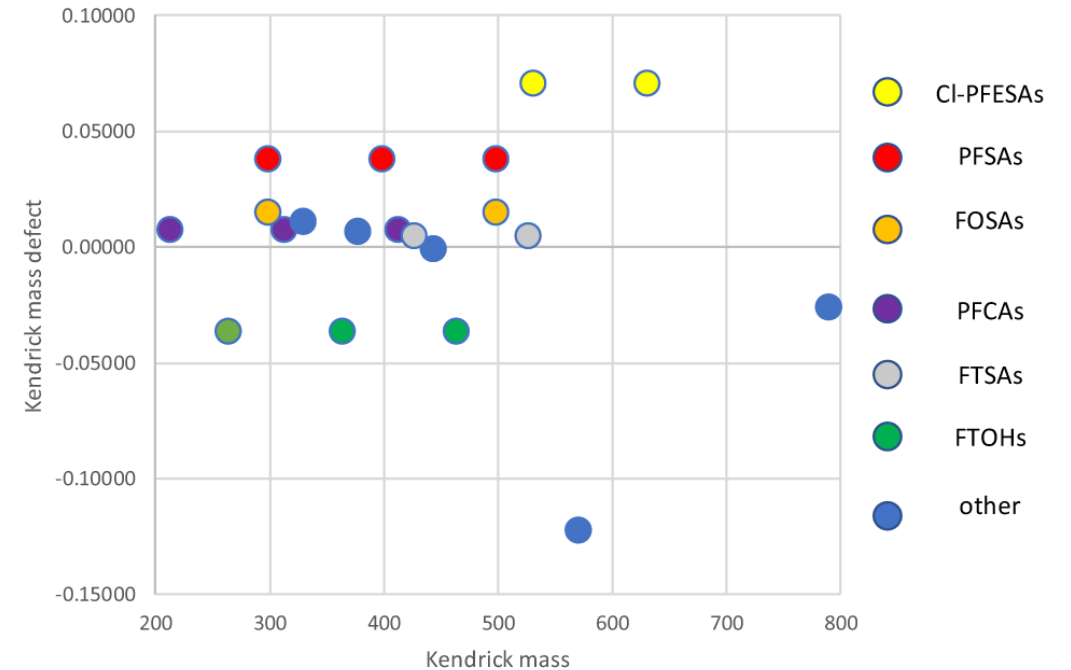
102	C2F5-	118.99202	Am-PFSM C13F17H12SO2N2-	583.0348
103	C8H9O-	121.06534	SCHEMBL776735 C9H9F3O3S	253.01462
104	C6H11O2N+	129.07898	Newly-Detected C13H3F8NO3+ SI Page 68	372.99852
105	C3F5-	130.99202	Branched-H-PFBA C4H2F6O2	194.98807
106	C3F5-	130.99202	CF2H-(CF2)7-O-(CF2)2-SO3H C10H2F20O4S	596.92762
107	C3F5-	130.99202	FPrSA C3HF7NO2S-	247.96162
108	C2F5O-	134.98693	SCHEMBL1766578 C3HF5O3	179.98458
109	C2F5O-	134.98693	CF3-O-CF2-CFH-SO3H C3H2F6O4S	247.9578
110	C8H7O2-	135.0446	SCHEMBL776735 C9H9F3O3S	253.01462
111	C2H2O4NS-	135.97045	FOSAA C10H4F17NO4S	555.95113
112	C4F5-	142.99202	6:2 FTSA C8H6F13NO2S	425.98334
113	CO2NF3S-	146.96018	Triflimide C2F6NO4S2-	279.91729
114	C3F5O-	146.98693	CF3-O-CF2-CFH-SO3H C3H2F6O4S	247.9578
115	CO2NF4S-	165.95859	Triflimide C2F6NO4S2-	279.91729
116	C8H7ON2F+	166.05424	N-hydroxyethyl dimethylammonioethyl perfluorohexane sulfonamido propylsulfonate C16H24F13N2O6S2+	651.08682
117	C3HF6O-	166.99316	CF3-O-CF2-CFH-SO3H C3H2F6O4S	247.9578
118	C3F7-	168.98882	N-MeFOSA C9H4F17NO2S	511.9613
119	C3F7-	168.98882	PFOA C8HF15O4	412.96588
120	C3F7-	168.98882	PFOS C8HF17O3S	498.92967
121	C3F7-	168.98882	perfluorooctane sulfinate C8HF17O2S	482.93475
122	C3F7-	168.98882	FHpSA C7H2F15NO2S	447.94885
123	C3F7-	168.98882	FOSAA C10H4F17NO4S	555.95113
124	C3F7-	168.98882	DTXSID801033084 C10H6F15NO4S	519.96998
125	C3F7-	168.98882	H-PFHpA C7HF12O2-	344.97849
126	C3F7-	168.98882	H-PFOA C8HF14O2-	394.9753

Database

Building Kendrick Exact Mass Difference Network

Non-target
Screening

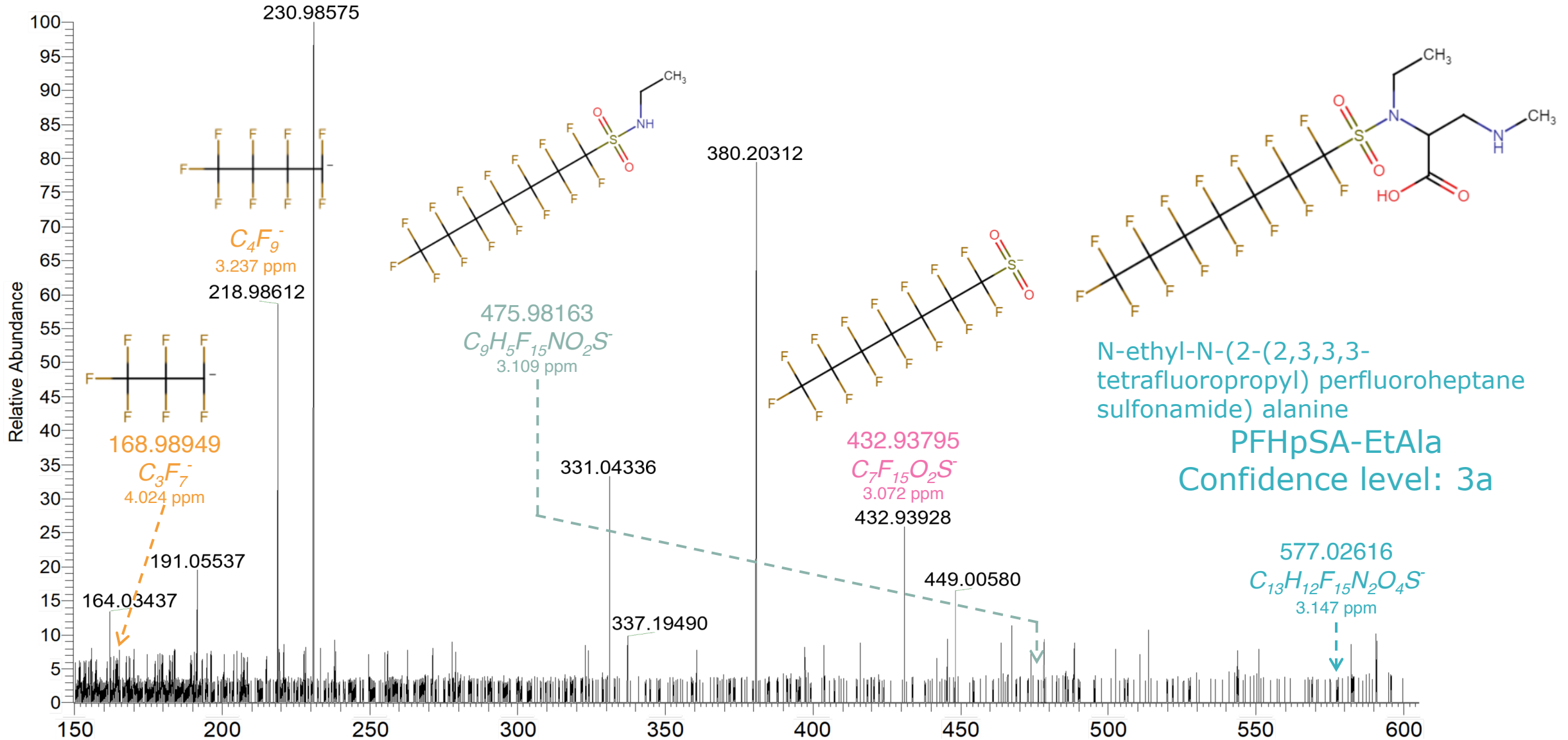
Other than fragments, MS¹ spectra was used to build Kendrick defect network based on the moiety addition/substitution : CF₂, CHF, F₂, H/F, Cl/F, SF₅/CF₃...



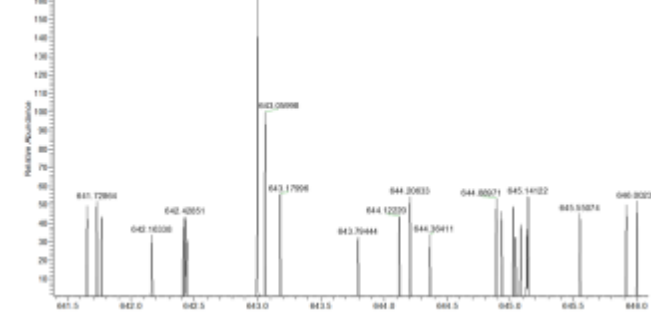
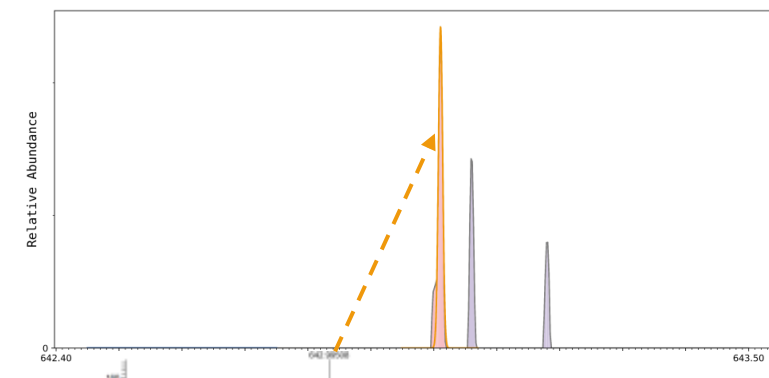
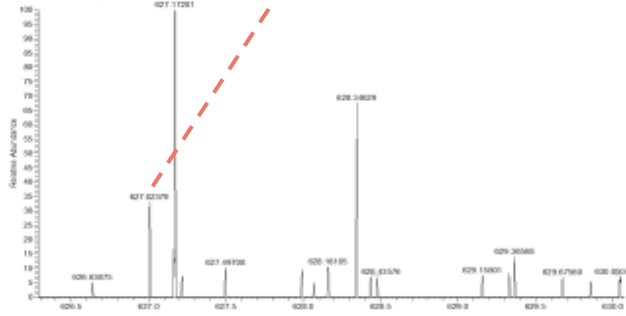
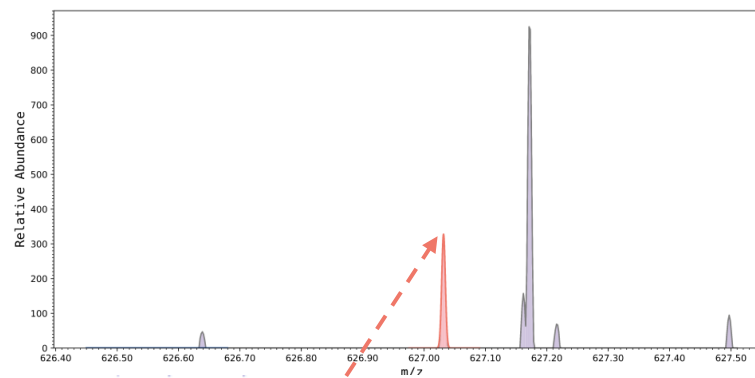
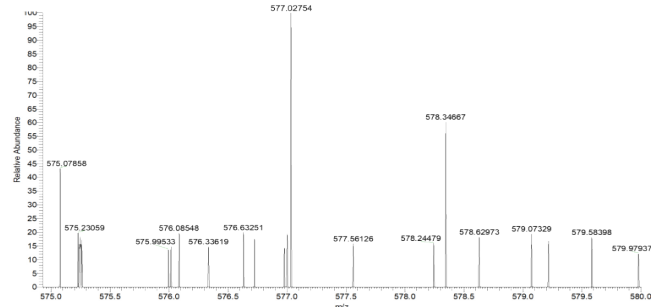
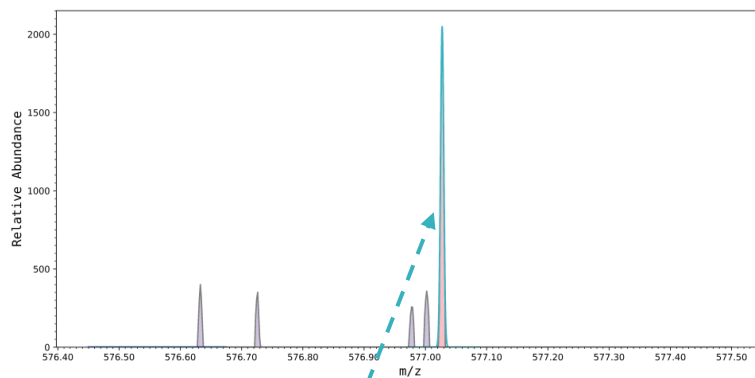
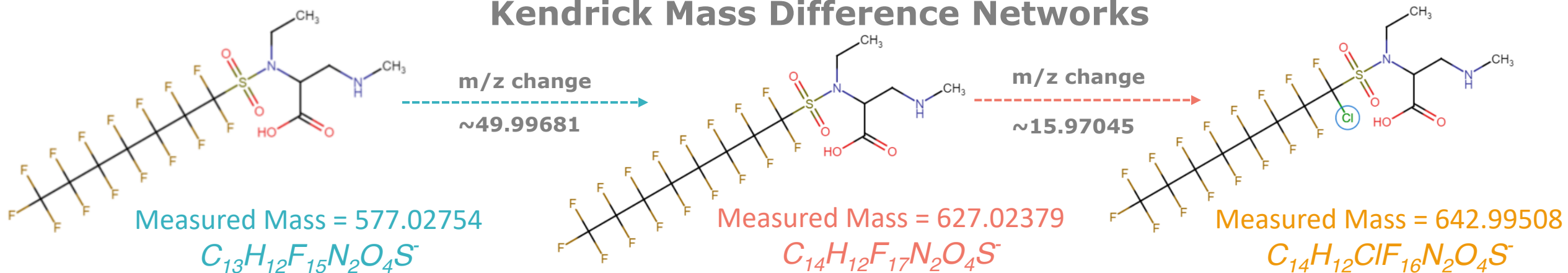
Strynar et al., JESEE, 2023

Result-Non Target Analysis

9

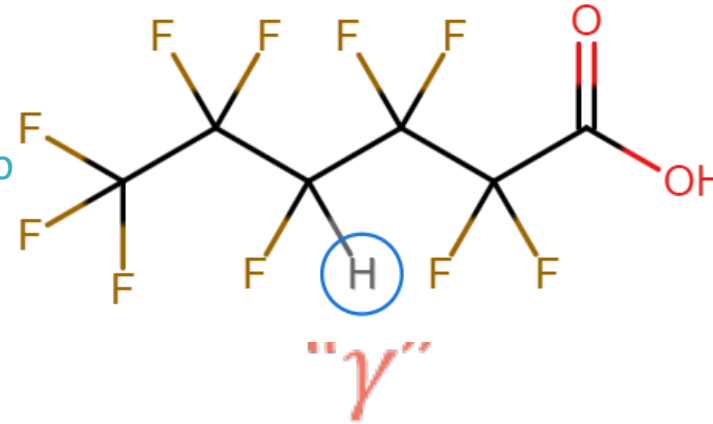
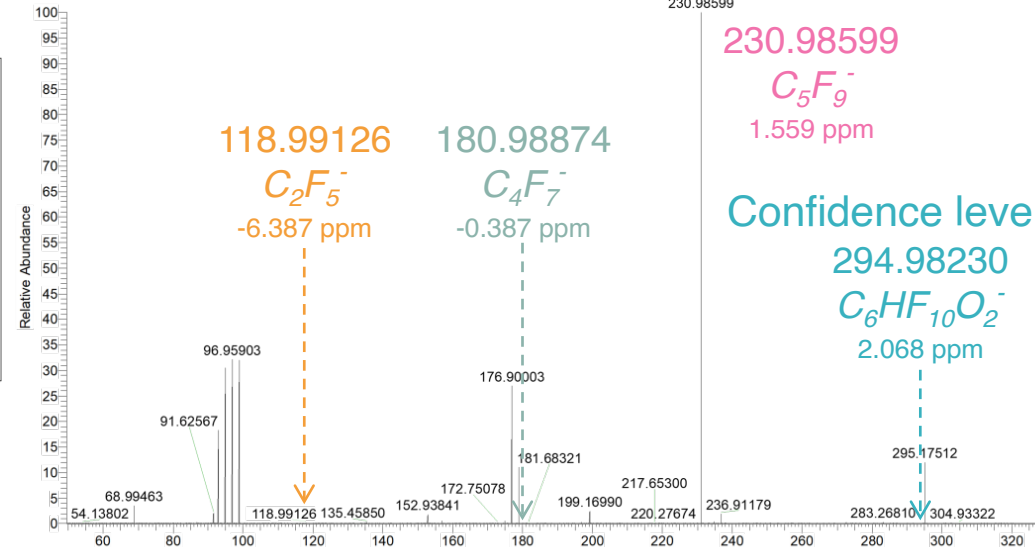
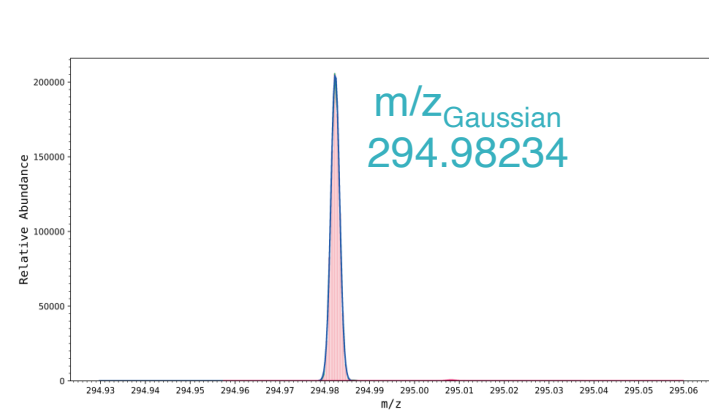
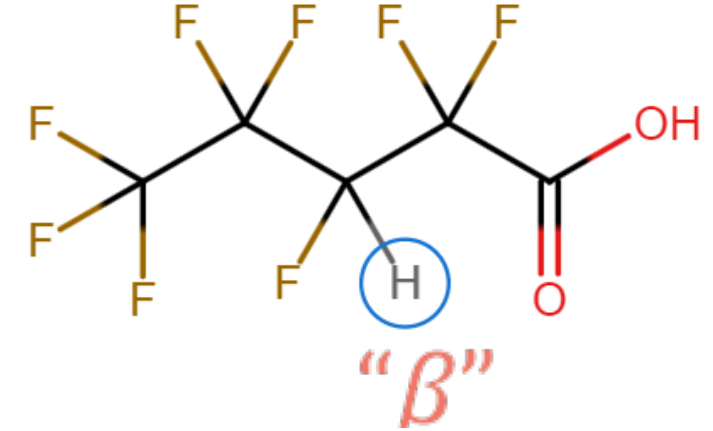
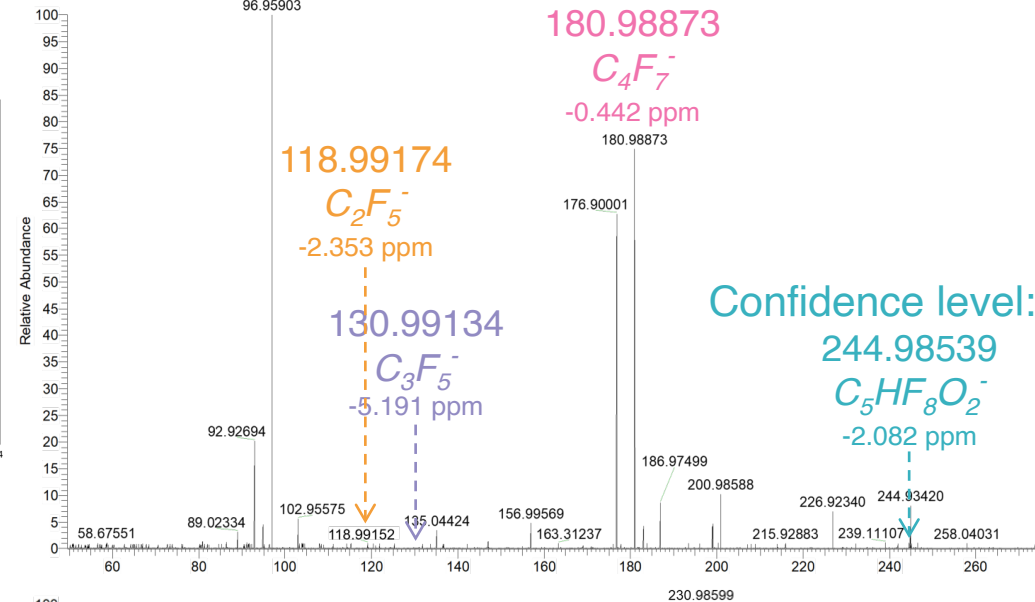
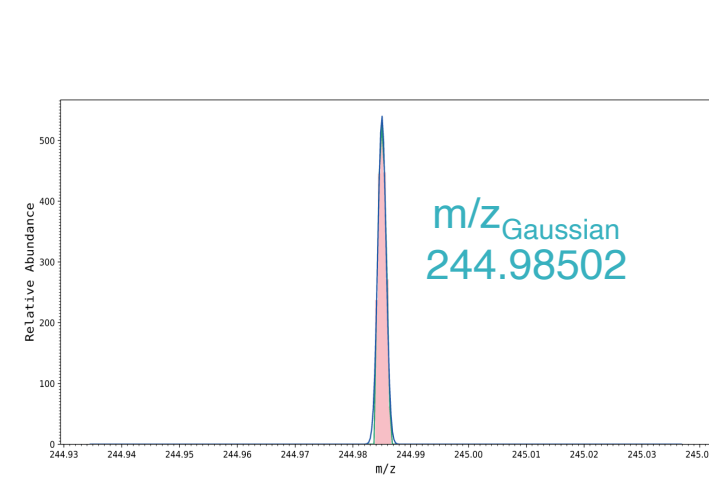


Kendrick Mass Difference Networks

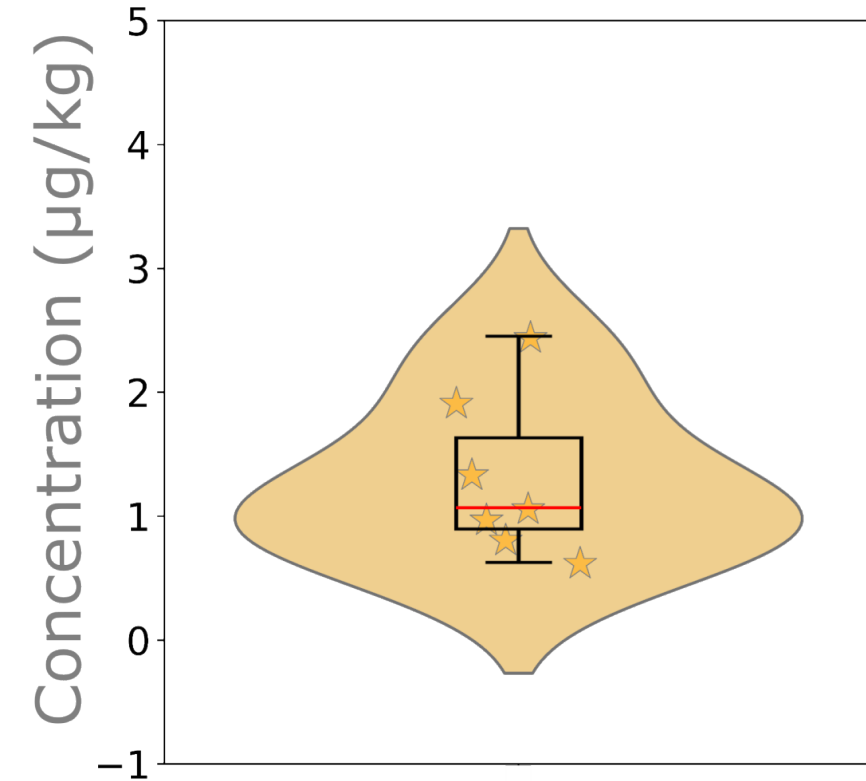


Result-Non Target Analysis

11



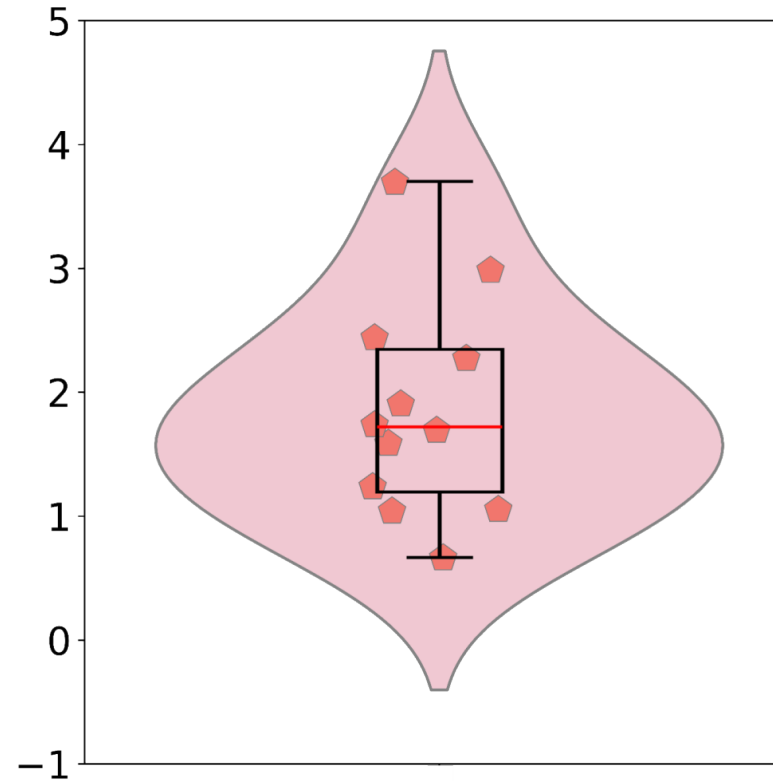
PFHpSA-EtAla



$n=7$

$\text{Conc}_{\text{Avg.}} = 1.202 \mu\text{g/kg}$

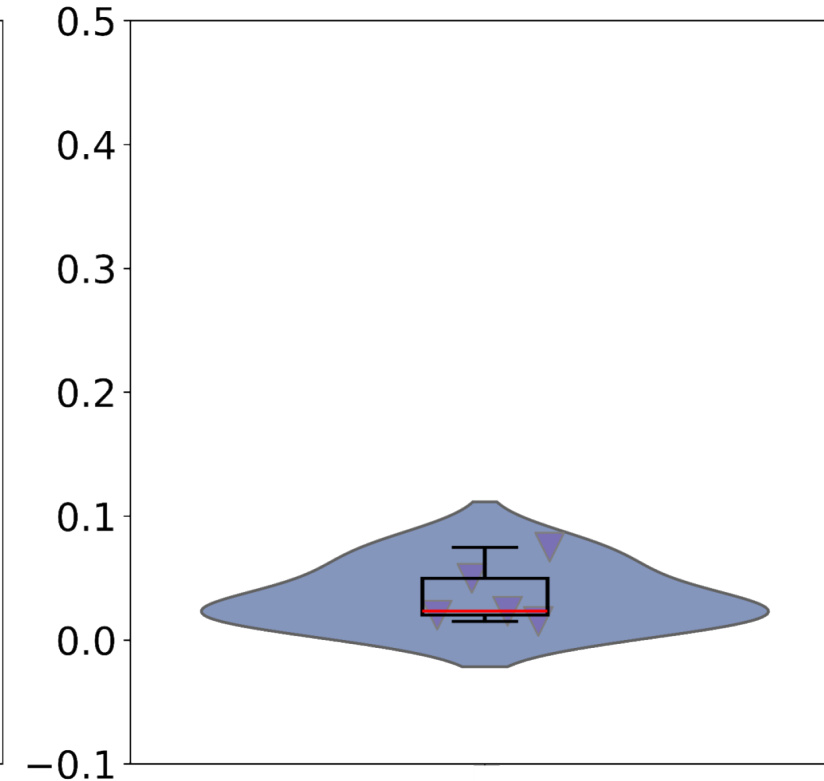
H-PFHxA



$n=12$

$\text{Conc}_{\text{Avg.}} = 1.858 \mu\text{g/kg}$

H-PFPeA



$n=5$

$\text{Conc}_{\text{Avg.}} = 0.047 \mu\text{g/kg}$



Summary

13

Target Analysis

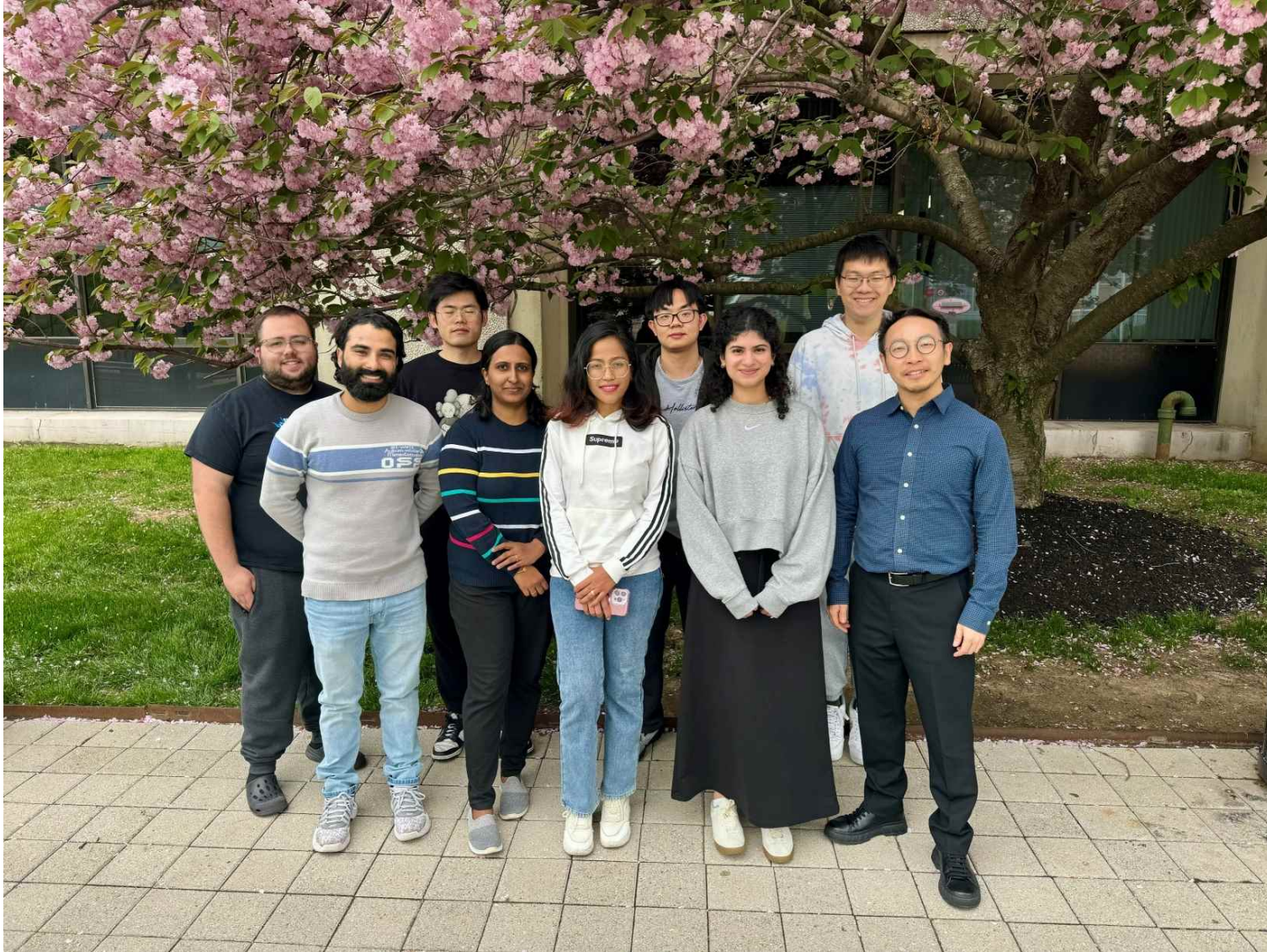
PFOA, PFHxA, and PFOS were dominant in the farmland area of the superfund site.

Non-Target Analysis

Novel PFAS: PFHpSA-EtAla, H-PFPeA and H-PFHxA were widely detected in soil matrix at high concentrations.

Environmental Impacts

PFAS Profiles at Ringwood Superfund Site revealed potential health risks to the indigenous residents



Advisor: Dr. Mengyan "Ian" Li

Current & Previous Colleague

- Jose Antunes
- Sumbel Yaqoob
- Chao Li
- Chen Wu
- Dung Ngoc Pham
- Jason Ong
- Manish Baskota
- Sowmiya Sukumar
- Devi Dhakal Gaudel



Welcome to our platforms/posters

15

Title	Presenter	Location and Time
Identification of Fluorotelomer Carboxylic Acid Degradors from Long Term Enriched Sludge Consortia	Sumbel Yaqoob NJIT	Poster #90 E7: PFAS and Bugs: The Search Continues 6/5/2024 4:30 PM Exhibit Hall
Substrate-Mediated Biodefluorination of Fluorotelomer-Based PFAS by <i>Rhodococcus jostii</i> RHA1	Sumbel Yaqoob NJIT	Poster #91 E7: PFAS and Bugs: The Search Continues 6/5/2024 4:30 PM Exhibit Hall
Distinct Biodefluorination Pathways of 6:2 versus 5:3 Fluorotelomer Carboxylic Acids (FTCAs) by Municipal Activated Sludge	Dr. Mengyan Li NJIT	Poster #85 E7: PFAS and Bugs: The Search Continues 6/5/2024 4:30 PM Exhibit Hall