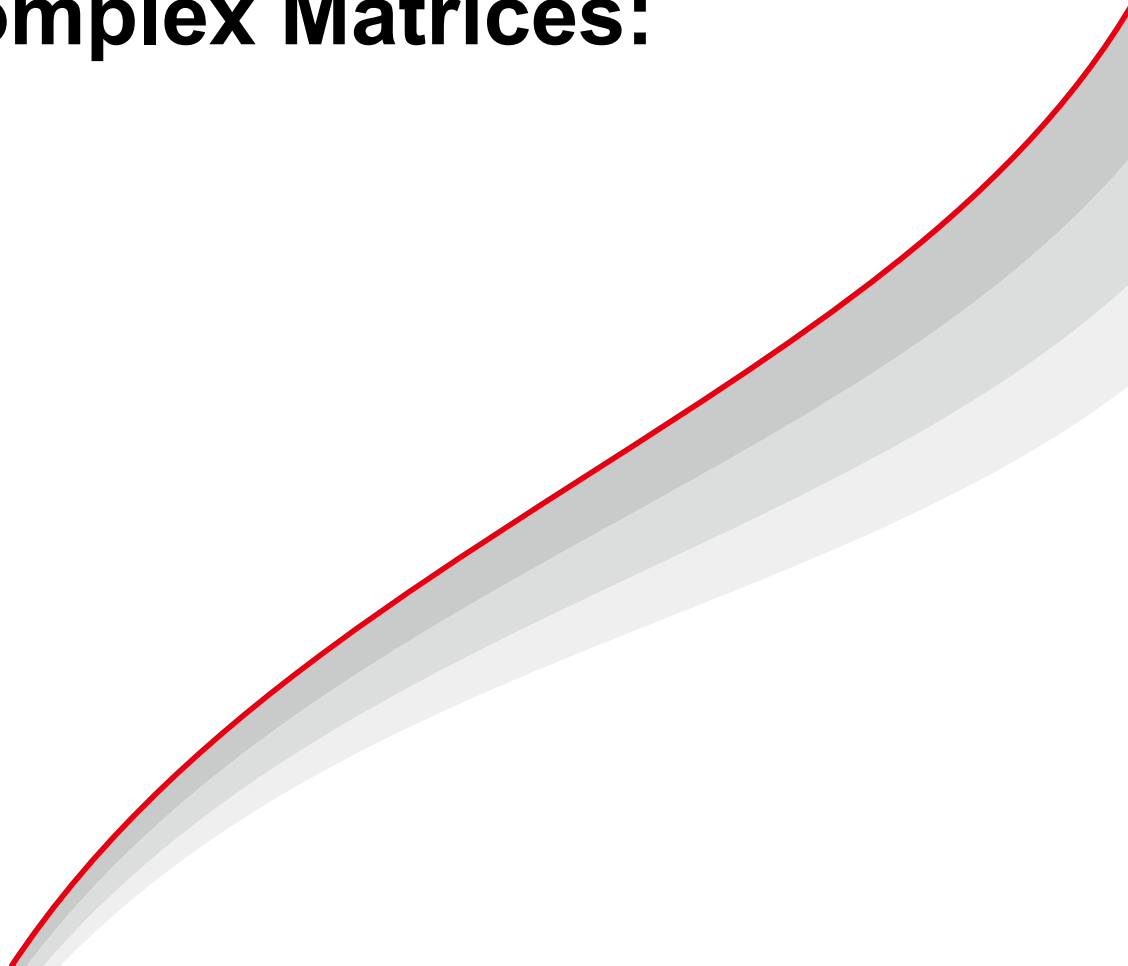
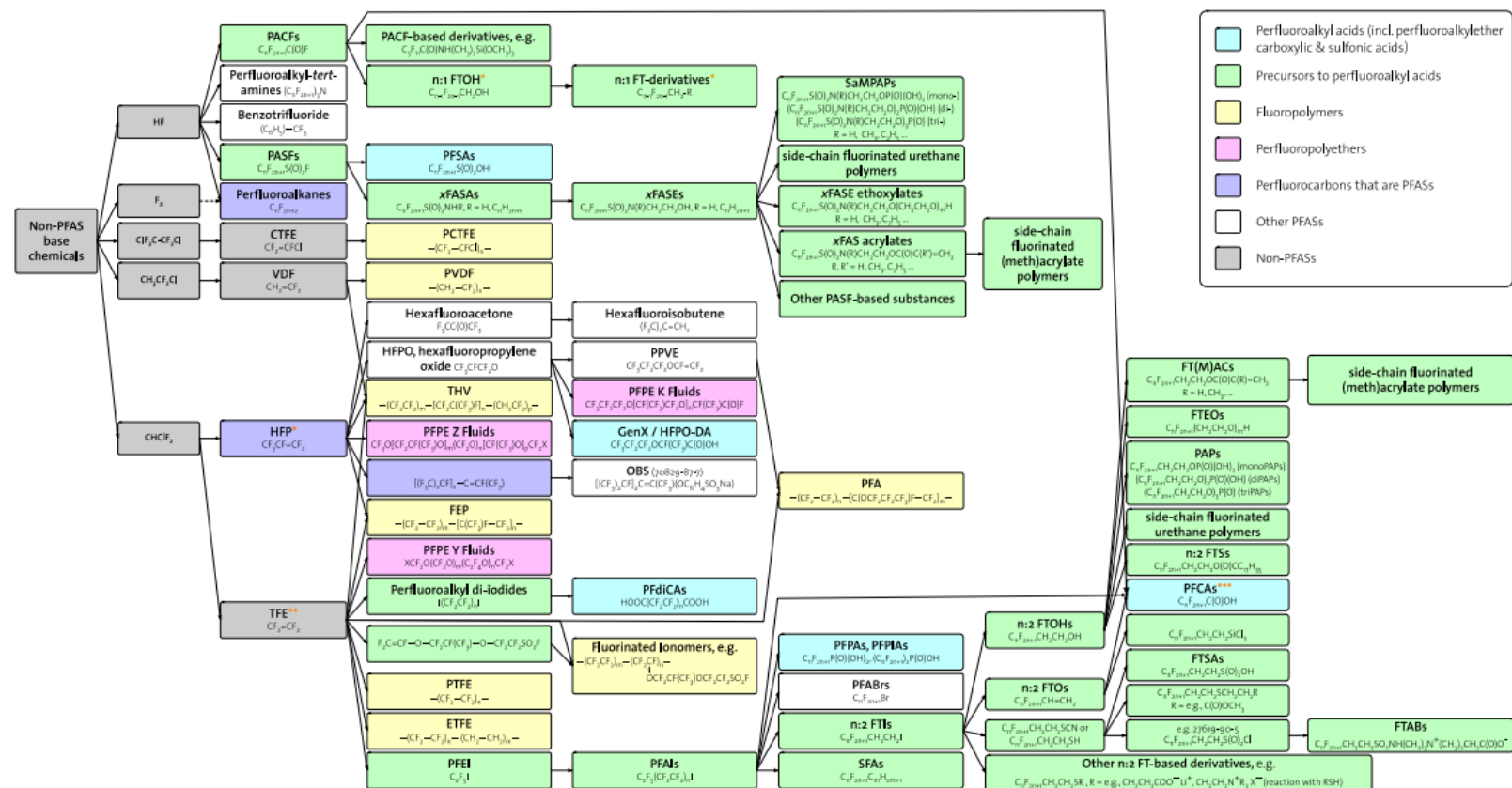


Navigating PFAS Analysis in Complex Matrices: The Role of Isotope Dilution

Andy Sandy, Evelyn Wang,
Ruth Marfil-Vega, **Alan Owens**



The PFAS Universe



* Strictly speaking, these substances are not fluorotelomers, as they are not derived from the telomerization process. Despite this, they are termed here "n:1 fluorotelomer-based" substances for readability. Future work may consider to identify more proper terminology for this group of PFASs.

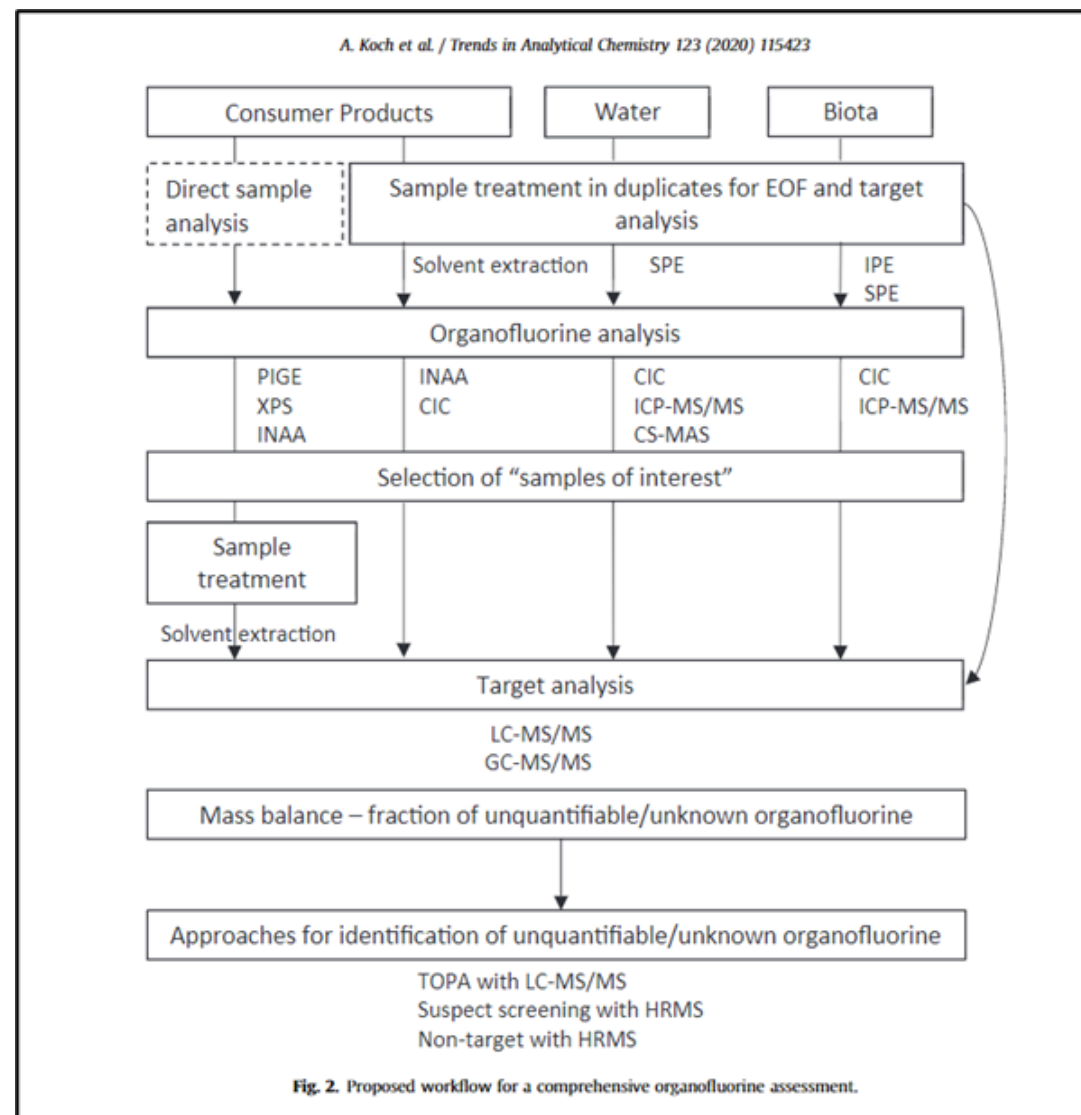
** Note that for many compounds such as HFP and TFE, there are different synthesis routes with different starting materials, and here shows only one of them.

*** Note that there are three synthesis routes shown here for manufacturing of PFCAs, from PACFs, PFAs and n:2 FTIs. Note that different synthesis routes may generate PFCAs with different perfluorocarbon chain lengths.

Sources: (1) Siegemund G, Schwertfeger W, Feiring A, Smart B, Behr F, Vogel H, McKusick B. *Fluorine Compounds*, Organic, 3rd ed., Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 2000; Vol. 33. (2) Banks RE, Smart BE, Tatlow JC. *Organofluorine Chemistry: Principles and Commercial Applications*. New York: Plenum, 1994. (3) Buck RC, Franklin J, Berger U, Conder JM, Cousins IT, De Voogt P, Jensen AA, Kannan K, Mabury SA, van Leeuwen SPI. Perfluoroalkyl and polyfluoroalkyl substances in the environment: terminology, classification, and origins. *Integr Environ Assess Manag* 2011, 7 (4), 533–541. (4) Wang Z, Cousins IT, Scheringer M, Buck RC, Hungerbühler K. Global emission inventories for C4–C14 perfluoroalkyl carboxylic acid (PFCA) homologues from 1951 to 2030, Part I: production and emissions from quantifiable sources. *Environ Int* 2014, 70, 62–75. (5) Moffett RH, Howell JL, Hoerter JM, Shtarow AB, Jannerfeldt G, Johnston SB, Keenan J, Warriner C, Closser DM. *Perfluoroalkylpolyethers in Synthetics, Mineral Oils, and Bio-Based Lubricants: Chemistry and Technology* (third edition), Edited by Rudnick LR. 2020. CRC Press. ISBN: 978-1-138-06821-6. (6) Grot W. *Fluorinated Ionomers*. William Andrew 2011. ISBN: 978-1-437-74457-6.

Figure 10. An overview of some common synthesis routes of different individual or groups of PFASs based on publicly accessible source

The Analytical Instrumentation Universe for PFAS



Growing Interest in Neutral and Volatile PFAS

Established PFAS analytical methodologies currently include EPA Methods 533, 537.1, 8327, and 1633A, as well as Other Test Methods (OTMs) 45 and 50. Most of these methods are LCMS based methods used to measure neutral PFAS.



LC/MS Triple Quadrupole Mass Spectrometer

- Unfortunately, **LCMS is unable to measure some PFAS**.
 - Bach et al. in Journal of Chromatography A indicate that using LCMS, the simultaneous analysis of non-ionic and ionic PFAS (**FTOH**) is impeded by ionization suppression caused by the buffered mobile phase.
 - In addition, compounds such as **FTIs** cannot generate protonated and deprotonated molecules by electrospray-ionization.

GC-MS for Volatile PFAS Analysis



GCMS-NX Series

- **Unlike LCMS, GCMS is suitable** to analyze these problematic compounds. Therefore, GCMS is paramount as a **complementary technique** to LCMS in providing a **total solution** for measurement of PFAS.
- **GCMS Advantages:**
 - Capable of analyzing volatile PFAS
 - Minimal sample preparation
 - Automated SPME

Sample Introduction Techniques for GC/MS

Sample Introduction Technique	Sensitivity (GC-MS)	Extraction Mode	Liquid Injection Compatible
Static Headspace (SHS)	ppb-ppm level	Static equilibrium gas extraction	✓
Dynamic Headspace (DHS)*	ppt-ppb level	Dynamic non-equilibrium gas extraction	✓
Solid Phase Microextraction (SPME)	ppt-ppb level	Sorptive extraction	✓
Thermal Desorption (TD)	ppt-ppb level	Sorptive extraction	
Direct Thermal Desorption (Direct-TD)	ppt-ppm level	Direct thermal extraction	
Liquid Injection (Liq)	ppb level		✓
Pyrolysis (Py)	µg level	Destructive thermal decomposition	
Direct Injection (DI)	ng level		

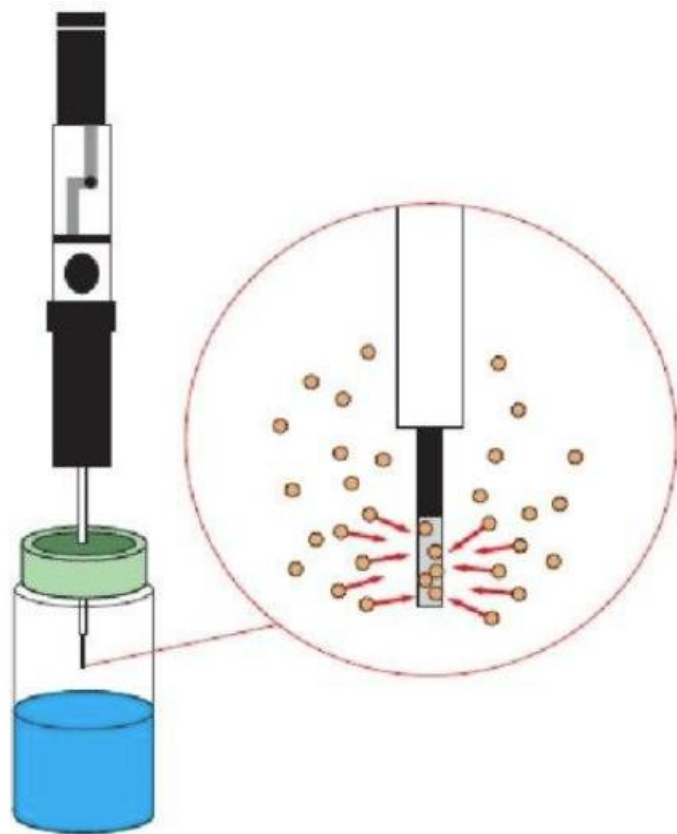
* Purge & Trap

Thermal Desorption – GC/MS



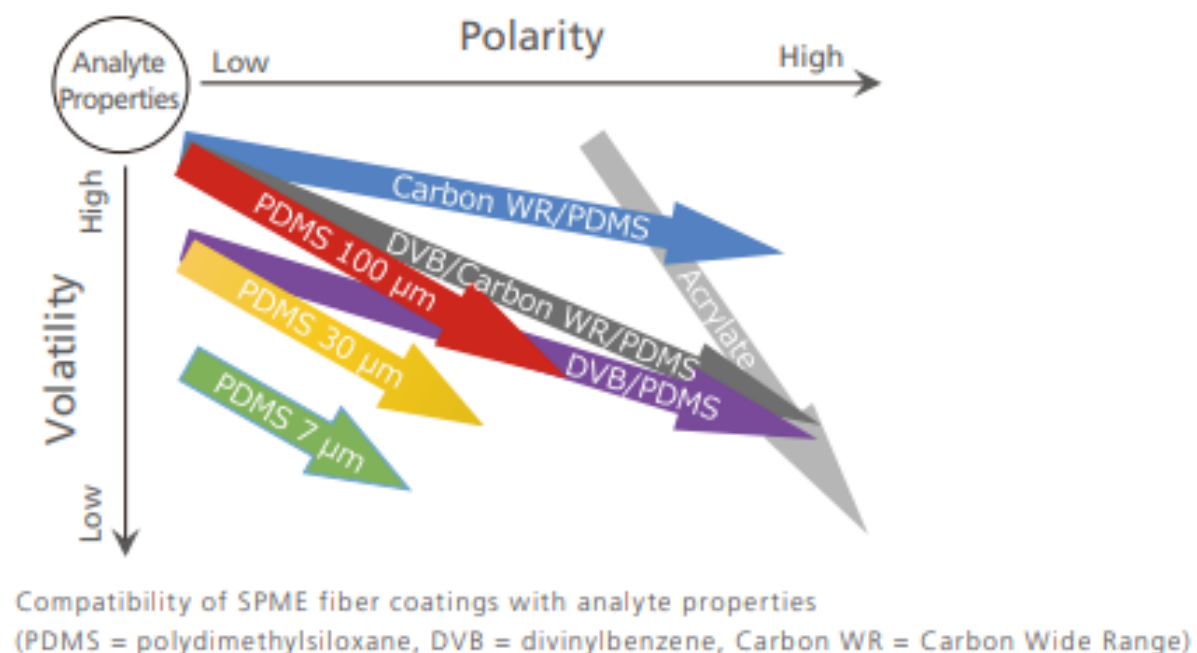
- **Direct Air Sample Analysis**
 - Avoids solvent-related contaminations and losses
 - Preserves analyte integrity, especially for volatile and semi-volatile PFAS
- **Increased Sensitivity and Lower Detection Limits**
 - Concentrates large air volumes onto sorbent tubes
 - Enables detection of trace-level PFAS (ppt or lower) not easily captured by liquid injection
- **Minimizes Sample Handling and Contamination Risk**
 - Fewer steps = less chance of background PFAS contamination (e.g., from labware or solvents)
- **Improved Recovery of Volatile and Thermally Labile PFAS**
 - Gentle desorption conditions reduce analyte degradation
 - Ideal for ultra-volatile or thermally sensitive compounds (e.g., FTOHs, fluorotelomer acrylates)

Head Space – Solid Phase Micro Extraction – GC/MS



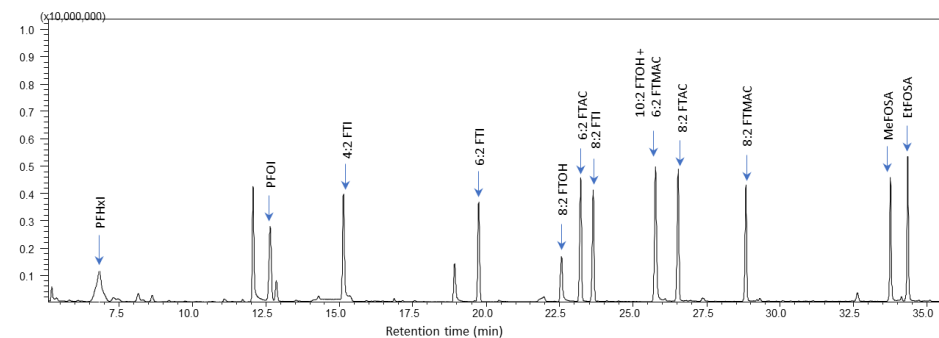
Head Space(HS) SPME and the sorption of compounds on to the fiber

Occurrence of volatile PFAS in **liquid** and solids samples of diverse origin (**environmental, food, consumer products**)



Experimental Plan

- Compound identification
- Chromatographic and MS methods: development by liquid injection
- SPME parameters - optimization
- Calibration curve and linear range
- Carry-over
- PFAS in the background
- Analysis of different liquid samples
 - Precision and accuracy
 - **Matrix effects**

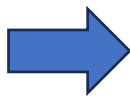


Background on Workflow

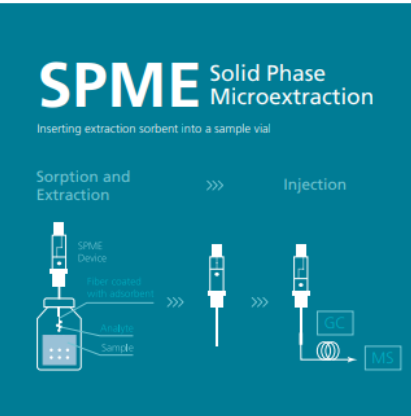
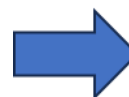
Sample collection



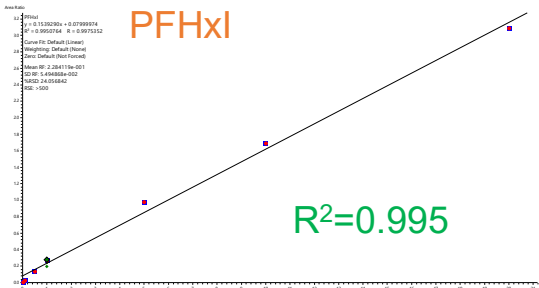
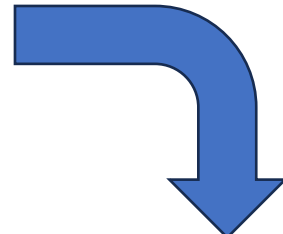
10 ml water pipetted



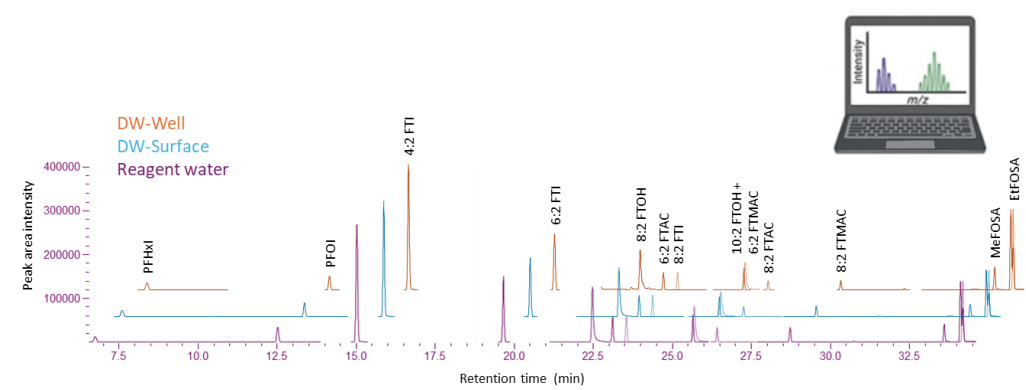
Sample Preparation



Sample Analysis



Data Analysis



GC/MS-NX Series

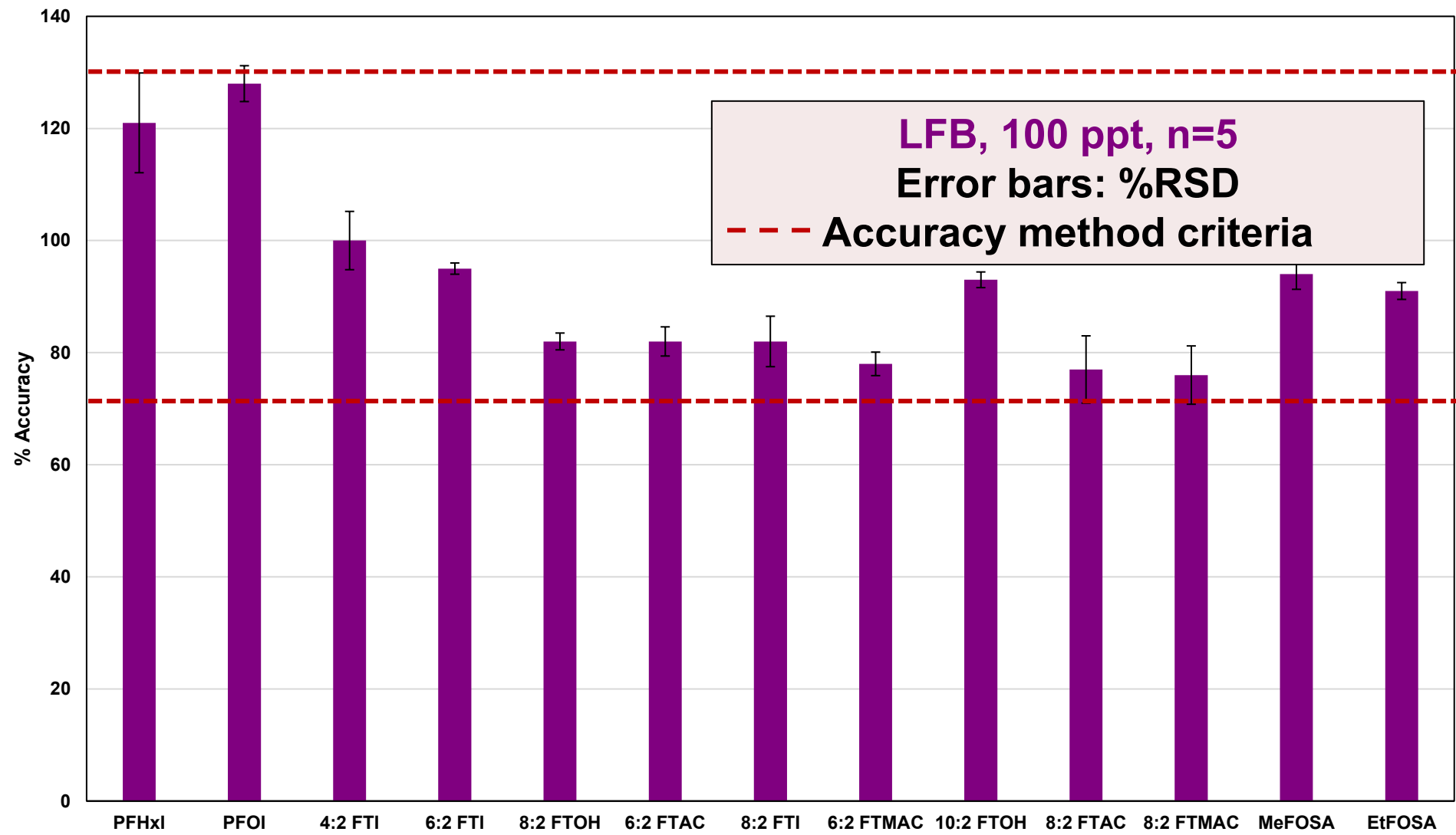
Method condition

Gas Chromatography	Nexis GC-2030
Injection port mode	Splitless
Carrier gas	Helium
Injection port temperature (°C)	240
Column	SH-I-624Sil MS Capillary, 30 m x 0.25 mmID x 1.40 µm
Flow control mode (cm/sec)	Linear velocity: 45
Oven Temperature	40 °C (7 min.), 5 °C/min. to 190 °C (0 min.), 40 °C/min. to 300 °C, (5 min.)
Mass Spectrometer	GCMS-TQ8040 NX
Interface Temperature (°C)	280
Ion Source Temperature (°C)	200
Detector Voltage (kV)	Relative to Tune 0.4
Threshold	0
Acquisition mode	Acquisition mode: MRM, Loop time: 0.5 sec.
Tuning mode	Normal mode
SPME analysis	AOC-6000 Plus
SPME Fiber	50/30 µm DVB/CAR/PDMS
Incubation time (min)	5
Extraction time (min)	30
Desorption time (min)	7
Agitation speed (rpm)	300
Extraction Temperature (°C)	50
Sample volume (mL)	10
Desorption temperature (°C)	240
Sampling salinity	2% NaCl (w/v)

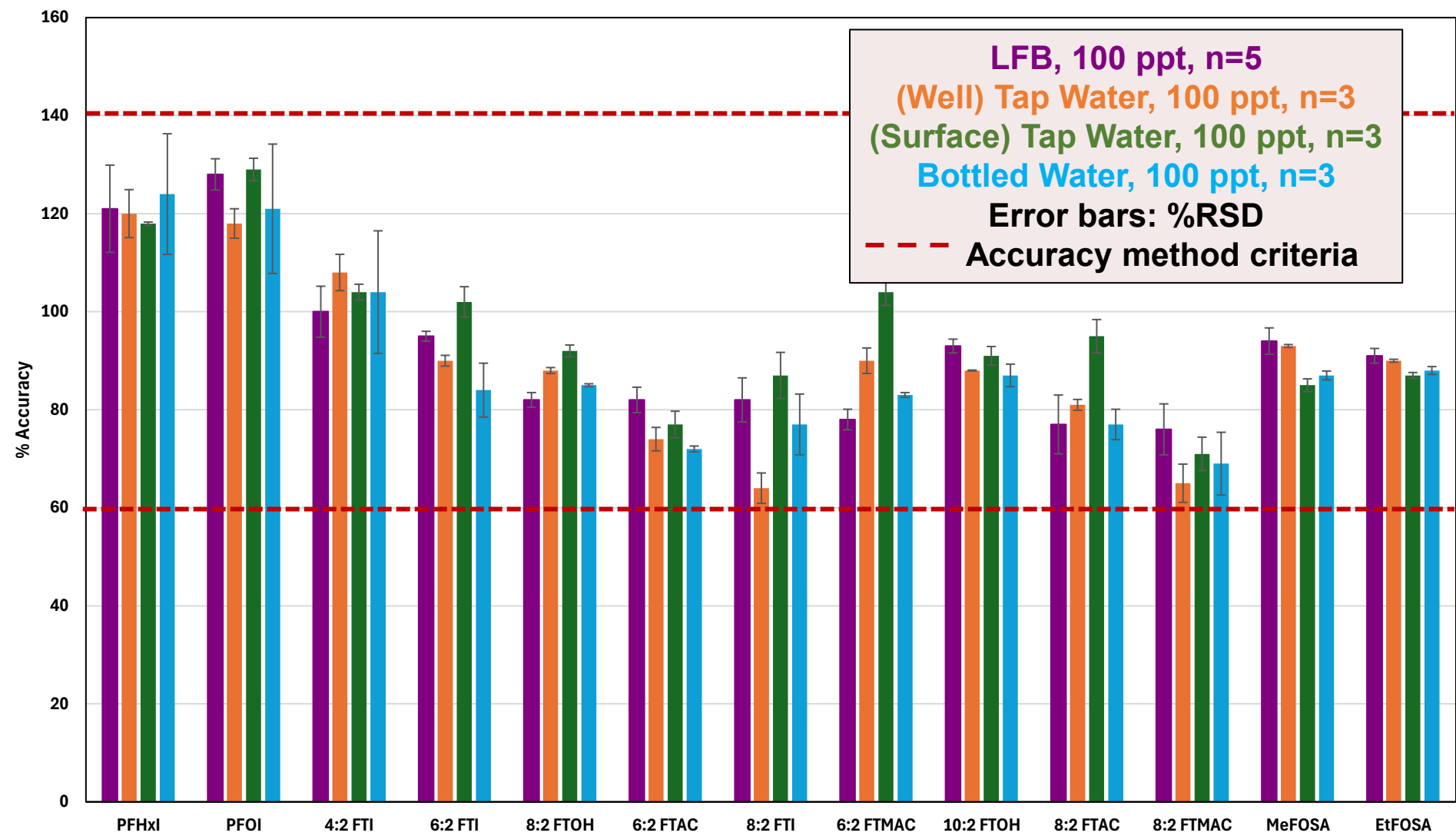
Compound table and ISTD grouping for drinking water matrix

	Compound	Ret. Time (min)	Quantifier (m/z)	CE	Qualifier #1 (m/z)	CE	Qualifier #2 (m/z)	CE	Internal standard group
Targets	PFHxI	6.7	119.0>69.0	12	319.0>69.1	24	319.0>231.0	6	3
	PFOI	12.5	169.0>69.0	21	119.0>69.0	21	419.0>69.1	27	3
	4:2 FTI	15.0	373.9>227.0	9	373.9>163.1	21	373.9>113.1	27	3
	6:2 FTI	19.6	473.9>326.9	12	69.0>50.0	27	473.9>263.0	21	1
	8:2 FTOH	22.5	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27	1
	6:2 FTAC	23.1	418.1>99.1	15	99.1>43.1	9	99.1>57.1	12	2
	8:2 FTI	23.5	574.0>426.9	15	169.0>69.0	9	574.0>65.1	24	2
	10:2 FTOH	25.7	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27	3
	6:2 FTMAC	25.6	86.1>68.1	6	432.1>113.1	12	432.1>86.1	21	1
	8:2 FTAC	26.4	518.0>99.1	15	99.1>57.1	12	99.1>43.1	9	1
	8:2 FTMAC	28.7	86.0>68.1	6	86.0>41.1	15	532.00>113.1	21	2
	MeFOSA	33.6	131.1>69.1	24	169.0>69.0	12	94.00>91.8	57	4
	EtFOSA	34.2	108.1>80.0	6	448.0>69.1	27	108.10>44.1	3	4
Internal Standards	8:2 FTOH ¹³ C ₂	22.4	98.0>69.0	15	131.1>81.1	15	98.00>48.1	27	1
	6:2 FTAC d ₃	23.1	101.1>57.1	12	101.1>45.0	9	102.00>45.0	9	2
	10:2 FTOH ¹³ C ₂	25.6	98.0>69.0	12	131.1>81.1	12	98.00>48.1	27	3
	EtFOSA d ₅	34.1	113.1>81.0	6	81.0>64.0	24	450.10>69.0	27	4

Results – Laboratory Control Samples (LCS) Accuracy and Repeatability



Results – Environmental and Bottled Water Samples



From Simple to Complex: Expanding Matrix Complexity



Proven Durability Across Drinking Water Matrices

- Tap water
- Bottled water



But These Are Relatively Simple Matrices

- Low in matrix complexity
- Fewer interfering substances



Increase
Complexity



Introducing a More Complex Matrix: Juice

- Natural product with high complexity
- Contains:
 - Sugars & salts
 - Food colorings
 - Preservatives & vitamins
 - Other additives

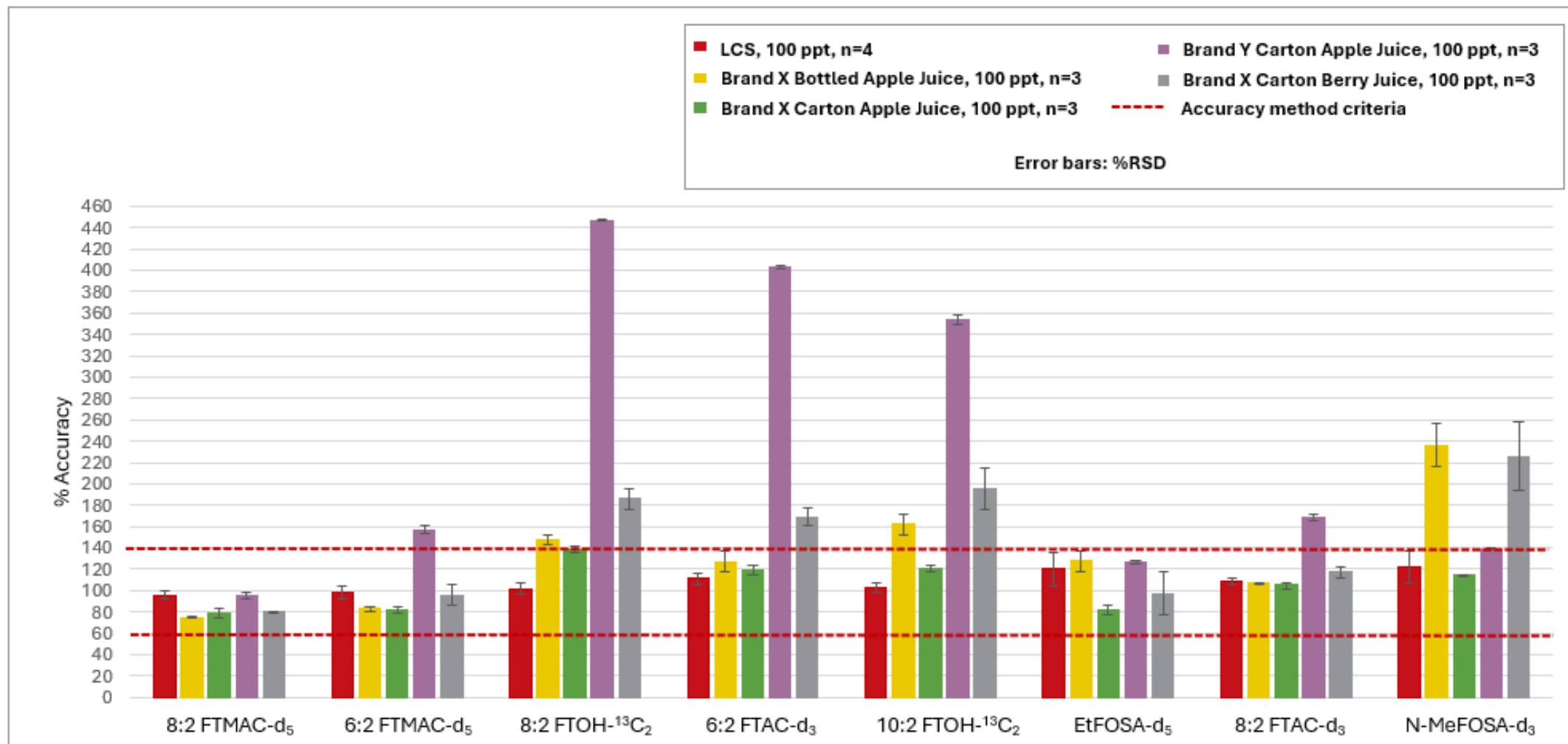


Compound table and ISTD grouping for drinking water matrix

Internal standard group	Compound	Ret. Time (min)	Quantifier (m/z)	CE	Qualifier #1 (m/z)	CE	Qualifier #2 (m/z)	CE
1	6:2 FTI	19.6	473.9>326.9	12	69.0>50.0	27	473.9>263.0	21
	8:2 FTOH	22.5	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27
	6:2 FTMAC	25.6	86.1>68.1	6	432.1>113.1	12	432.1>86.1	21
	8:2 FTAC	26.4	518.0>99.1	15	99.1>57.1	12	99.1>43.1	9
	8:2 FTOH ¹³C₂	22.4	98.0>69.0	15	131.1>81.1	15	98.00>48.1	27
2	6:2 FTAC	23.1	418.1>99.1	15	99.1>43.1	9	99.1>57.1	12
	8:2 FTI	23.5	574.0>426.9	15	169.0>69.0	9	574.0>65.1	24
	8:2 FTMAC	28.7	86.0>68.1	6	86.0>41.1	15	532.00>113.1	21
	6:2 FTAC d₃	23.1	101.1>57.1	12	101.1>45.0	9	102.00>45.0	9
3	PFHxI	6.7	119.0>69.0	12	319.0>69.1	24	319.0>231.0	6
	PFOI	12.5	169.0>69.0	21	119.0>69.0	21	419.0>69.1	27
	4:2 FTI	15.0	373.9>227.0	9	373.9>163.1	21	373.9>113.1	27
	10:2 FTOH	25.7	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27
	10:2 FTOH ¹³C₂	25.6	98.0>69.0	12	131.1>81.1	12	98.00>48.1	27
4	MeFOSA	33.6	131.1>69.1	24	169.0>69.0	12	94.00>91.8	57
	EtFOSA	34.2	108.1>80.0	6	448.0>69.1	27	108.10>44.1	3
	EtFOSA d₅	34.1	113.1>81.0	6	81.0>64.0	24	450.10>69.0	27

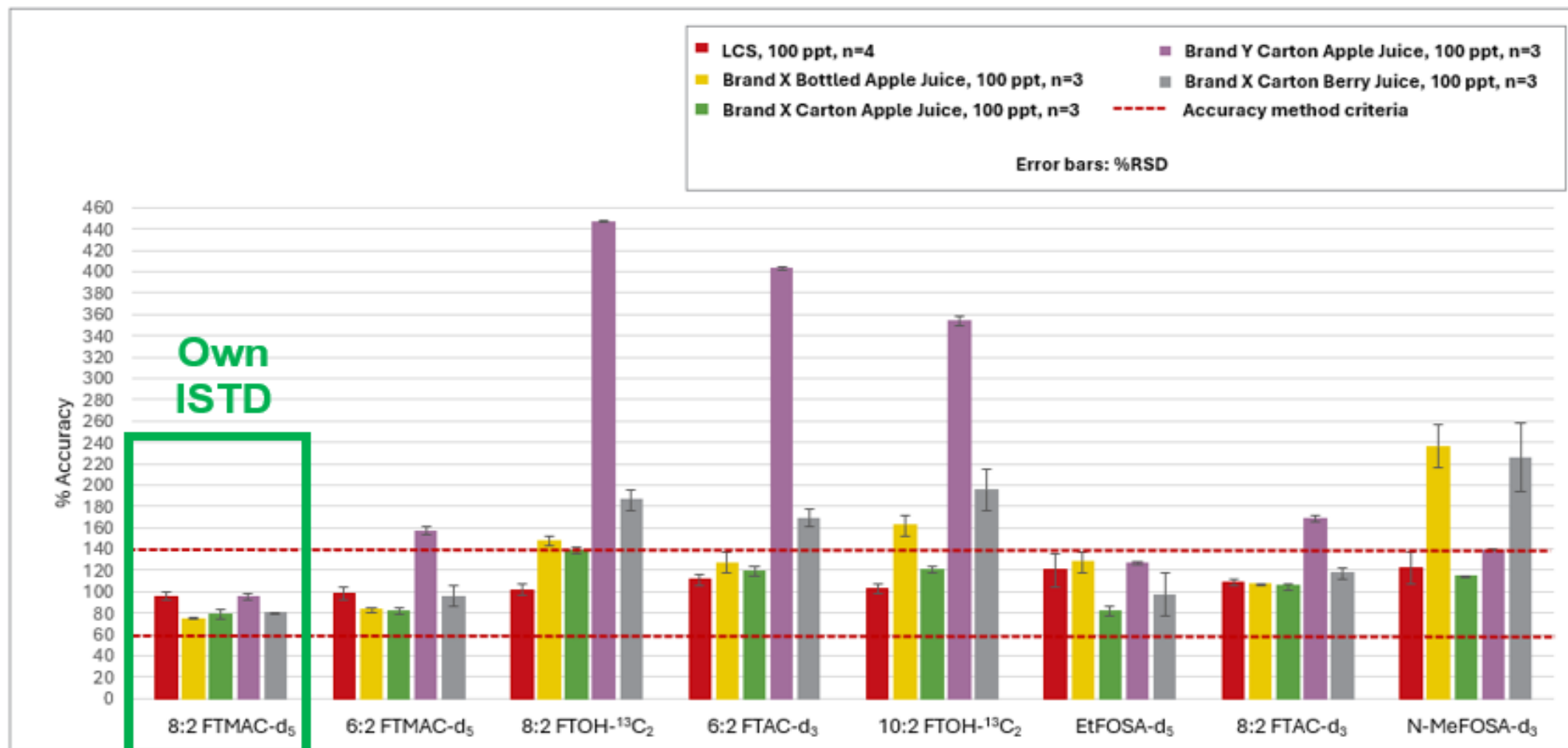
Accuracy is drastically different with different ISTD

8:2 FTMAC accuracy results using multiple isotopic labelled internal standards



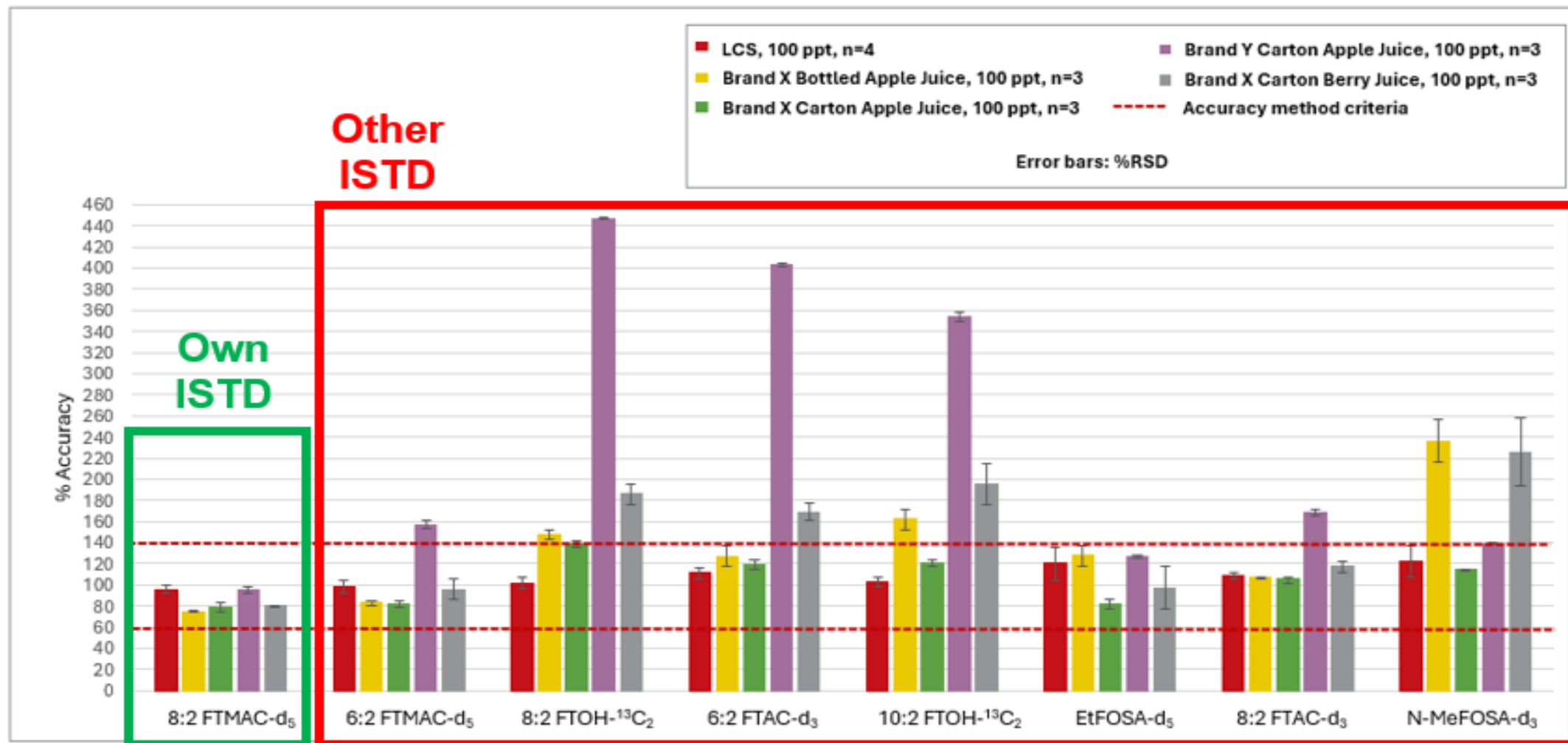
Accuracy is drastically different with different ISTD

8:2 FTMAC accuracy results using multiple isotopic labelled internal standards



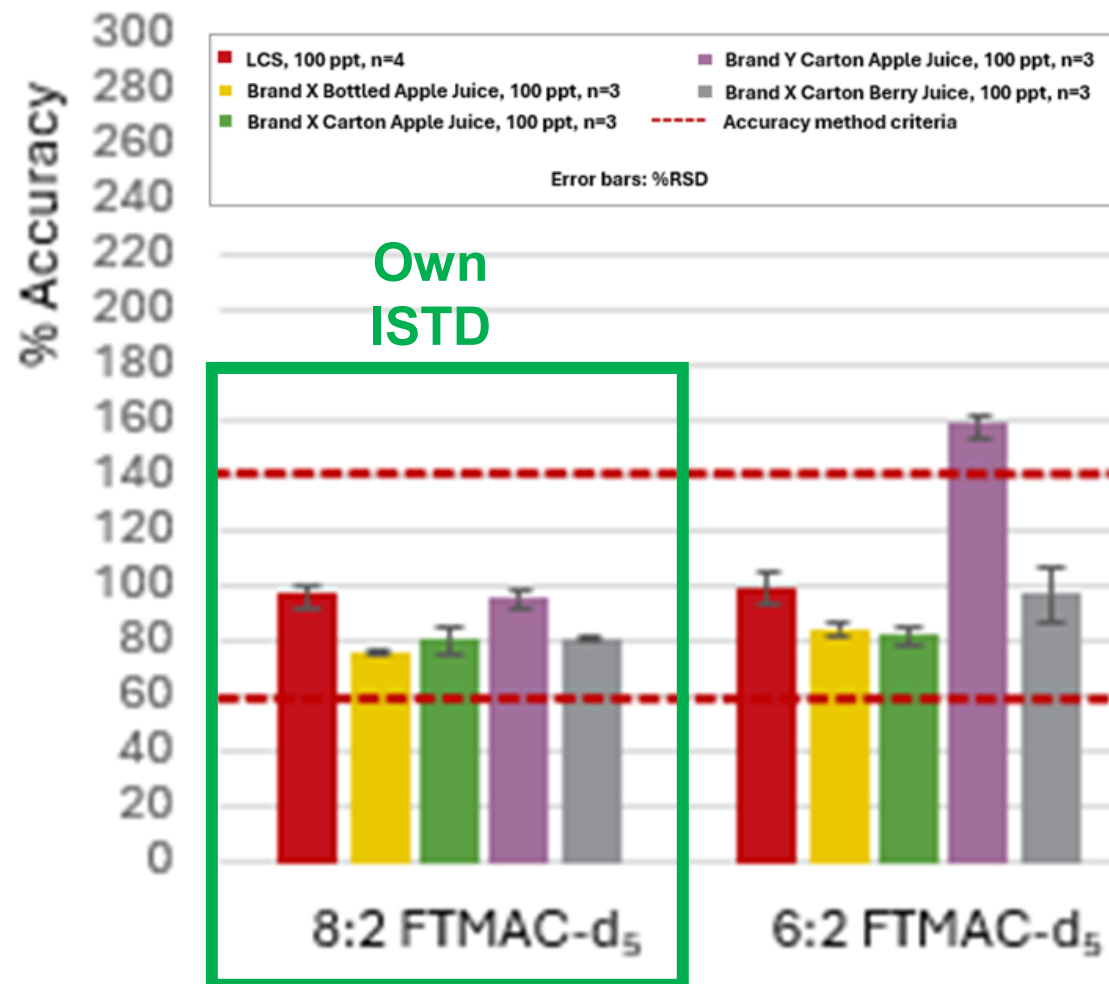
Accuracy is drastically different with different ISTD

8:2 FTMAC accuracy results using multiple isotopic labelled internal standards



Accuracy is drastically different with different ISTD

8:2 FTMAC accuracy results using multiple isotopic labelled internal standards



Compound table and ISTD grouping for complex matrix

	Compound	Ret. Time (min)	Quantifier (m/z)	CE	Qualifier #1 (m/z)	CE	Qualifier #2 (m/z)	CE	Internal standard group
Targets	6:2 FTI	19.6	473.9>326.9	12	69.0>50.0	27	473.9>263.0	21	1
	8:2 FTOH	22.4	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27	1
	6:2 FTAC	23.1	418.1>99.1	15	99.1>43.1	9	99.1>57.1	12	2
	8:2 FTI	23.5	574.0>426.9	15	169.0>69.0	9	574.0>65.1	24	2
	10:2 FTOH	25.6	95.0>69.0	15	127.1>77.1	15	95.0>45.1	27	3
	6:2 FTMAC	25.6	86.1>68.1	6	432.1>113.1	12	432.1>86.1	21	5
	8:2 FTAC	26.4	518.0>99.1	15	99.1>57.1	12	99.1>43.1	9	6
	8:2 FTMAC	28.7	86.0>68.1	6	86.0>41.1	15	532.00>113.1	21	7
	MeFOSA	33.5	430.00>91.10	33	94.00>91.80	57	448.00>78.00	33	8
	EtFOSA	34.1	108.1>80.0	6	448.0>69.1	27	108.10>44.1	3	4
Internal Standards	8:2 FTOH ¹³ C ₂	22.3	98.0>69.0	15	131.1>81.1	15	98.00>48.1	27	1
	6:2 FTAC d ₃	23.0	101.1>57.1	12	101.1>45.0	9	102.00>45.0	9	2
	10:2 FTOH ¹³ C ₂	25.5	98.0>69.0	12	131.1>81.1	12	98.00>48.1	27	3
	EtFOSA d ₅	34.1	113.1>81.0	6	81.0>64.0	24	450.10>69.0	27	4
	6:2 FTMAC d ₅	25.6	91.1>73.1	6	437.1>118.2	12	437.1>91.1	18	5
	8:2 FTAC d ₃	26.4	521.1>102.1	15	102.1>58.1	12	102.1>74.1	6	6
	8:2 FTMAC d ₅	28.7	91.1>73.1	6	537.1>91.1	21	537.1>118.1	21	7
	N-MeFOSA d ₃	33.5	433.1>114.0	25	433.1>94.3	33	97.1>94.1	57	8

Compounds in red bold font lack their own ISTD

Recovery in various complex matrices

Column	Brand X Bottled AJ		Brand X Carton AJ		Brand Y Carton AJ		Brand X Carton BJ	
	Mean % Recovery	%RSD	Mean % Recovery	%RSD	Mean % Recovery	%RSD	Mean % Recovery	%RSD
6:2 FTI	105	3.3	120	3.8	76	1.4	84	4.2
8:2 FTOH	90	0.6	87	2.1	83	0.9	86	0.7
6:2 FTAC	70	3.0	69	5.8	74	2.9	79	5.5
8:2 FTI	88	7.9	79	10.9	70	2.5	91	11.6
6:2 FTMAC	95	0.3	95	1.4	99	1.7	94	2.2
10:2 FTOH	101	2.5	93	1.9	117	1.9	92	3.2
8:2 FTAC	115	1.9	114	2.7	104	0.4	112	2.6
8:2 FTMAC	75	1.0	79	5.1	95	3.1	80	0.8
MeFOSA	96	0.9	91	2.5	95	4.0	86	3.7
EtFOSA	87	1.3	88	0.5	88	0.3	86	0.2

Conclusion



- The HS-SPME GC-MS/MS method demonstrates an effective and reliable workflow for the quantification of volatile PFAS in complex matrices, as shown using juice as a representative sample.
- The workflow offers key advantages in terms of simplicity, speed, precision, and accuracy that is critical for routine monitoring in challenging matrices.



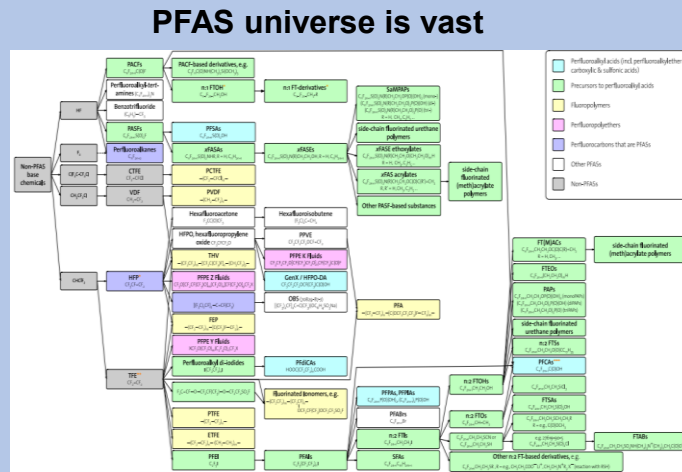
Conclusion



- Accurate quantification in complex matrices requires that each target compound be paired with its own isotopically labeled internal standard to account for compound-specific matrix effects.
- For certain analytes (e.g., 6:2 FTI and 8:2 FTI), appropriate internal standards are not commercially available. This underscores the need for expanded availability of isotopically labeled standards from suppliers.
- In the absence of compound-specific internal standards, those with similar matrix behavior may be used cautiously, provided their suitability is supported by thorough validation.



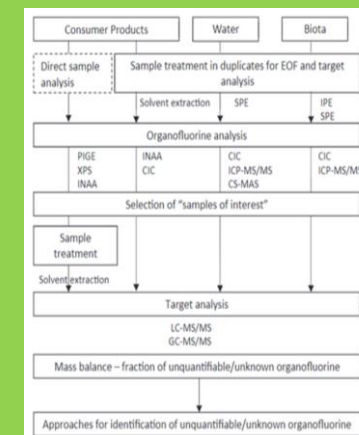
Take Home Message – How to Measure Volatile PFAS?



LCMS is unable to measure some PFAS, such as some volatile PFAS.



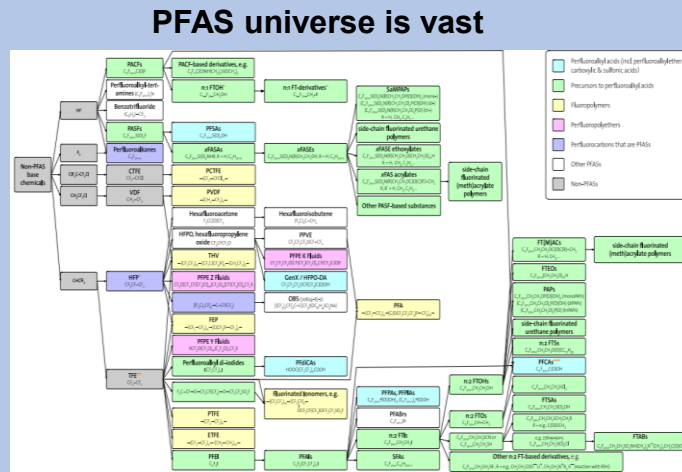
LC/MS Triple Quadrupole Mass Spectrometer



Multiple instrumentation is required:

- various matrices
- sample prep techniques

Take Home Message – GC-MS can be the Solution



GCMS is suitable to analyze volatile PFAS compounds.

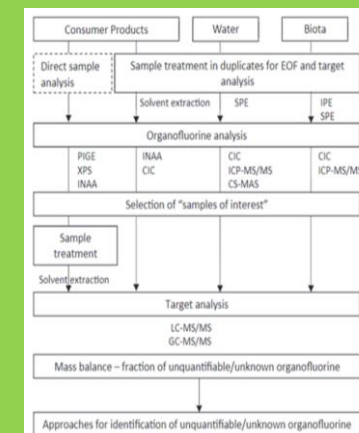


GCMS-NX Series

LCMS is unable to measure some PFAS, such as some volatile PFAS.



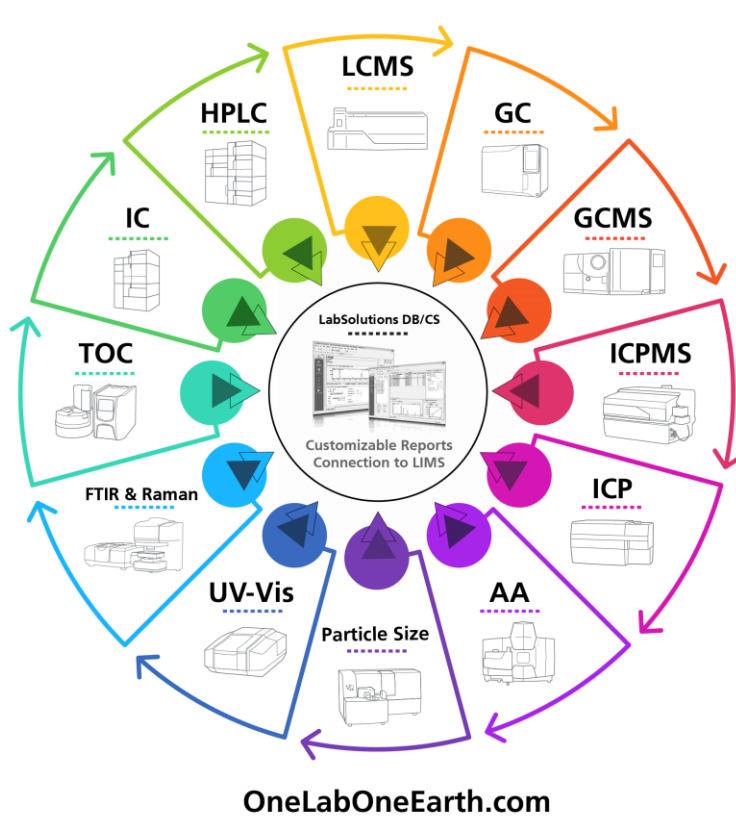
LC/MS Triple Quadrupole Mass Spectrometer



Multiple instrumentation is required:

- various matrices
- sample prep techniques

HPLC	Carbamate Diquat Glyphosate
IC	Anions Chromium VI Ammonia
TOC	Nitrogen Organic Carbon Phosphorous
FTIR & Raman	Microplastics
UV-Vis	Chlorine UV254 Others
Particle Size	Solids



LCMS	Cyanotoxins PFAS Pesticides Emerging Contaminants Unknowns (QTOF)	
GC	HAA's Herbicides Pesticides	Phenols Other Organics PCBs
GCMS	1,4-dioxane Dioxins & Furans Nitrosamines Other Organics Microplastics	Semivolatiles Taste & Odor Volatiles THMs
ICPMS	Metals	
ICP	Metals	
AA	Metals	

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End of the
presentation

Don't change logo, don't put things over the “Craftech Wing”



SHIMADZU Red

Spot color : PANTONE 185C
Process color : M100% + Y100%
RGB : R255 + G0 + B0
Similar color: DIC 156 : DIC 156 • To be used only when the spot color is unavailable, for any reason.

Black

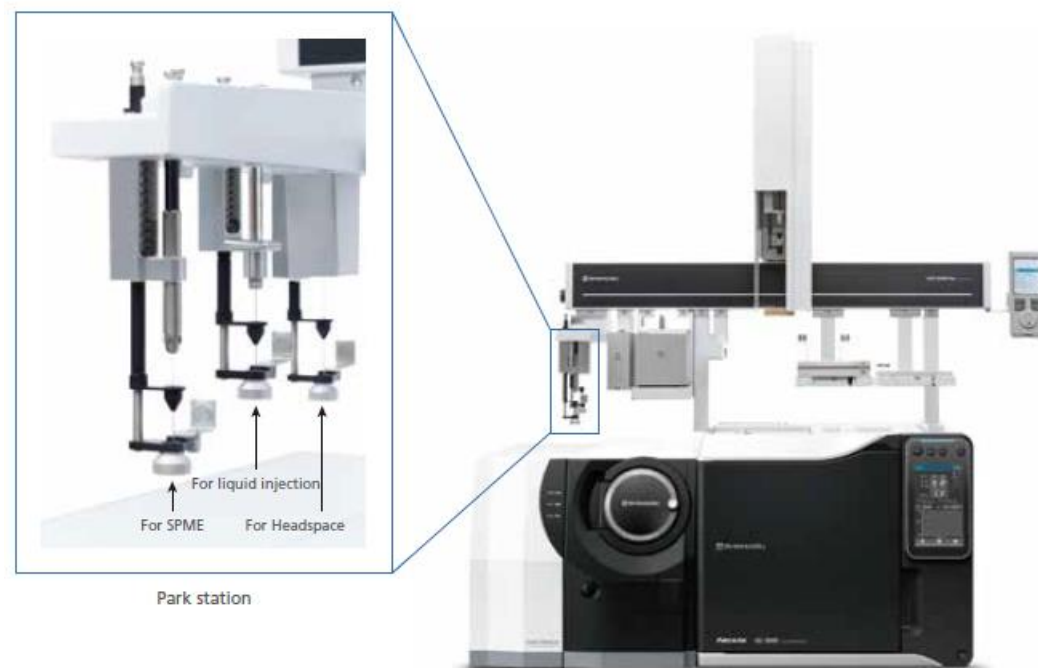
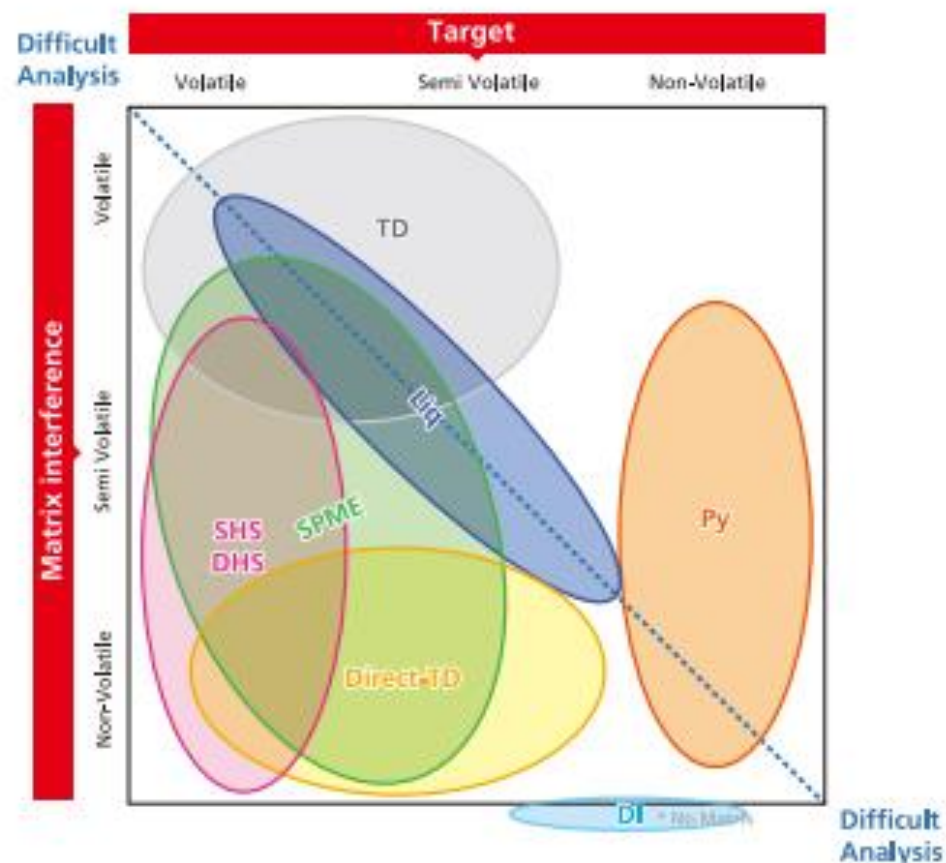
Process color : K100%
RGB : R0 + G0 + B0

	Color Name	Process Colors (CMYK) Reproduction	RGB Color Reproduction
Subordinate Colors	Purple	C40 % + M65 % + Y15 % + K0 %	R167 / G107 / B154
	Carmin	C20 % + M85 % + Y95 % + K0 %	R203 / G70 / B34
	Orange	C5 % + M55 % + Y100 % + K0 %	R234 / G139 / B0
	Glass green	C70 % + M18 % + Y100 % + K0 %	R83 / G157 / B53
	Blue green	C70 % + M10 % + Y40 % + K0 %	R62 / G172 / B164
	Sky blue	C80 % + M10 % + Y0 % + K0 %	R0 / G165 / B228
	Dark blue	C80 % + M50 % + Y10 % + K0 %	R50 / G113 / B174
	Blue gray	C40 % + M20 % + Y20 % + K20 %	R143 / G162 / B169
	Yellow ocher	C20 % + M40 % + Y60 % + K0 %	R210 / G163 / B108
	Yellow	C0 % + M10 % + Y100 % + K10 %	R241 / G212 / B0

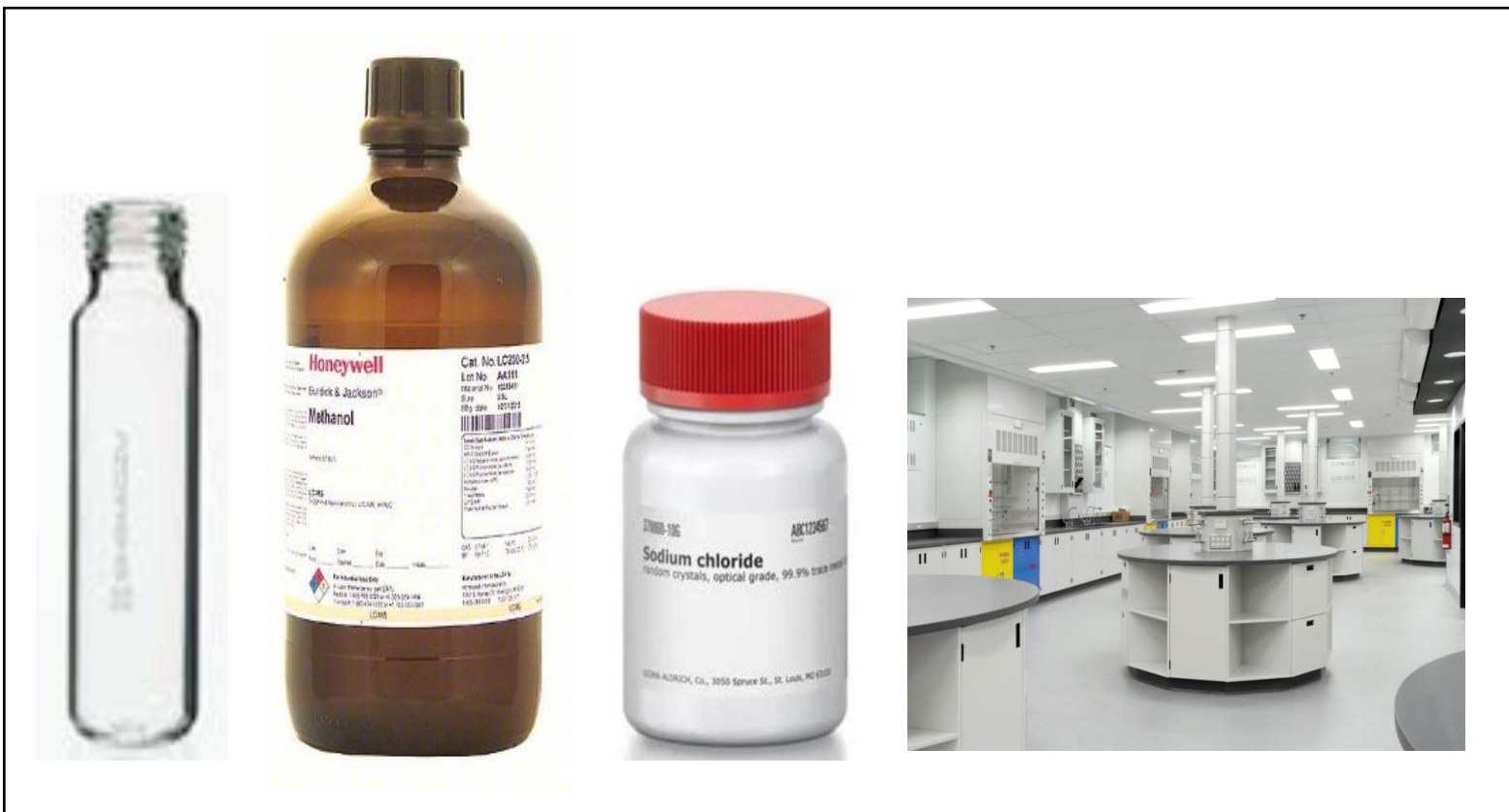
	Black	SHIMADZU Red + Black
Support Colors	Black80%	SHIMADZU Red + Black80%
	Black65%	SHIMADZU Red + Black65%
	Black50%	SHIMADZU Red + Black50%
	Black40%	SHIMADZU Red + Black35%
	Black35%	SHIMADZU Red + Black20%
	Black30%	
	Black20%	

HS-SPME-GCMS

Occurrence of volatile PFAS in **liquid** and solids samples of diverse origin (**environmental**, food, consumer products) with same set-up



PFAS in the Background



Consumables and reagents

- HS vials
- SPME fibers
- Salt
- Solvents
- Commercial standards

✓ **No fluorinated components
in sample flow path**

Background and carryover

- None of the target PFAS in the laboratory blank samples showed quantifiable results
- The area of peaks of in the blanks were less than 1/5 of the lowest calibration standard
- The carryover effect was evaluated by analyzing a blank immediately after the highest calibration standard: <0.2%



Instrumentation and targets



Shimadzu's GCMS QP-2020NX



Shimadzu's GCMS TQ-8040

Chemical Class	Compound	Acronym	CAS Number
Perfluoroalkyl iodides (PFIs)	Perfluorohexyl iodide	PFHxI	355-43-1
	Perfluorooctyl iodide	PFOI	507-63-1
(n:2) Fluorotelomer iodides (FTIs)	4:2 Fluorotelomer iodide	4:2 FTI	2043-55-2
	6:2 Fluorotelomer iodide	6:2 FTI	2043-57-4
	8:2 Fluorotelomer iodide	8:2 FTI	2043-53-0
(n:2) Fluorotelomer acrylates (FTACs)	6:2 Fluorotelomer acrylate	6:2 FTAC	17527-29-6
	8:2 Fluorotelomer acrylate	8:2 FTAC	27905-45-9
	1H,1H,2H,2H-Perfluoro-n-octyl acrylate-d3	6:2 FTAC d3	7527-29-6
(n:2) Fluorotelomer methacrylates (FTMACs)	6:2 Fluorotelomer methacrylate	6:2 FTMAC	2144-53-8
	8:2 Fluorotelomer methacrylate	8:2 FTMAC	1996-88-9
(n:2) Fluorotelomer alcohols (FTOHs)	8:2 Fluorotelomer alcohol	8:2 FTOH	678-39-7
	10:2 Fluorotelomer alcohol	10:2 FTOH	865-86-1
	2-perfluorooctyl-[1,1-2H2-1,2- ¹³ C2]-ethanol	8:2 FTOH ¹³ C2	872398-73-7
	2-perfluorodecyl-[1,1-2H2-1,2- ¹³ C2]-ethanol	10:2 FTOH ¹³ C2	865-86-1
Perfluoroalkane sulfonamides (FASAs)	N-Methyl perfluorooctane sulfonamide	MeFOSA	31506-32-8
	N-Ethyl perfluorooctane sulfonamide	EtFOSA	4151-50-2
	n-ethyl-d5-perfluoro-1-octanesulfonamide	EtFOSA d5	936109-40-9

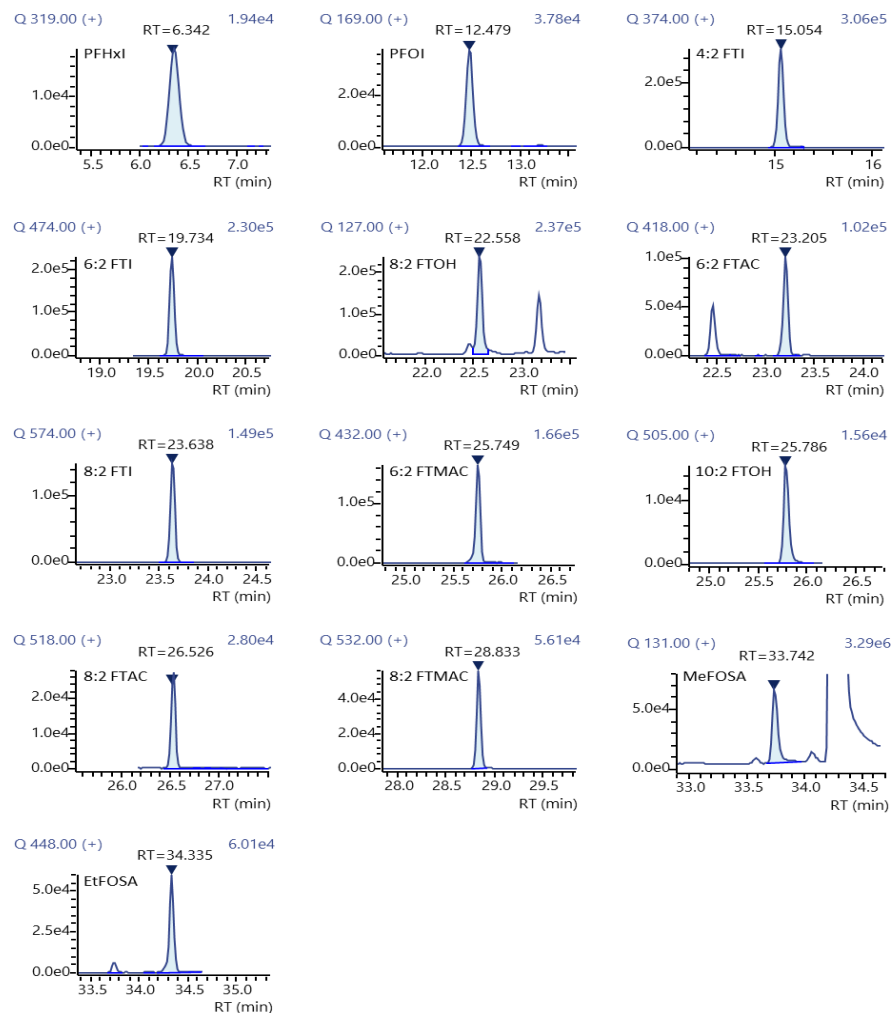
Optimized Method Conditions

Gas Chromatography	Nexis GC-2030
Injection mode	Splitless
Carrier gas	Helium
Injection port temperature (°C)	240
High pressure injection	Auto, 250 kPa, 1 min
Column	SH-I-624Sil MS Capillary, 30 m x 0.25 mmID x 1.40 µm
Flow control mode (cm/sec)	Linear velocity, 44.4
Total flow (mL/min)	50
Oven temperature	40°C (7 min.), 5°C/min. to 188°C (0 min.), 40°C/min. to 300°C, (5 min.)
SPME analysis	AOC-6000 Plus
SPME Fiber	50/30 µm DVB/CAR/PDMS
Incubation time (min)	5
Extraction time (min)	30
Desorption time (min)	7
Agitation speed (rpm)	300
Extraction temperature (°C)	50
Sample volume (mL)	10
Desorption temperature (°C)	240
Sampling salinity	2 % NaCl (w/v)

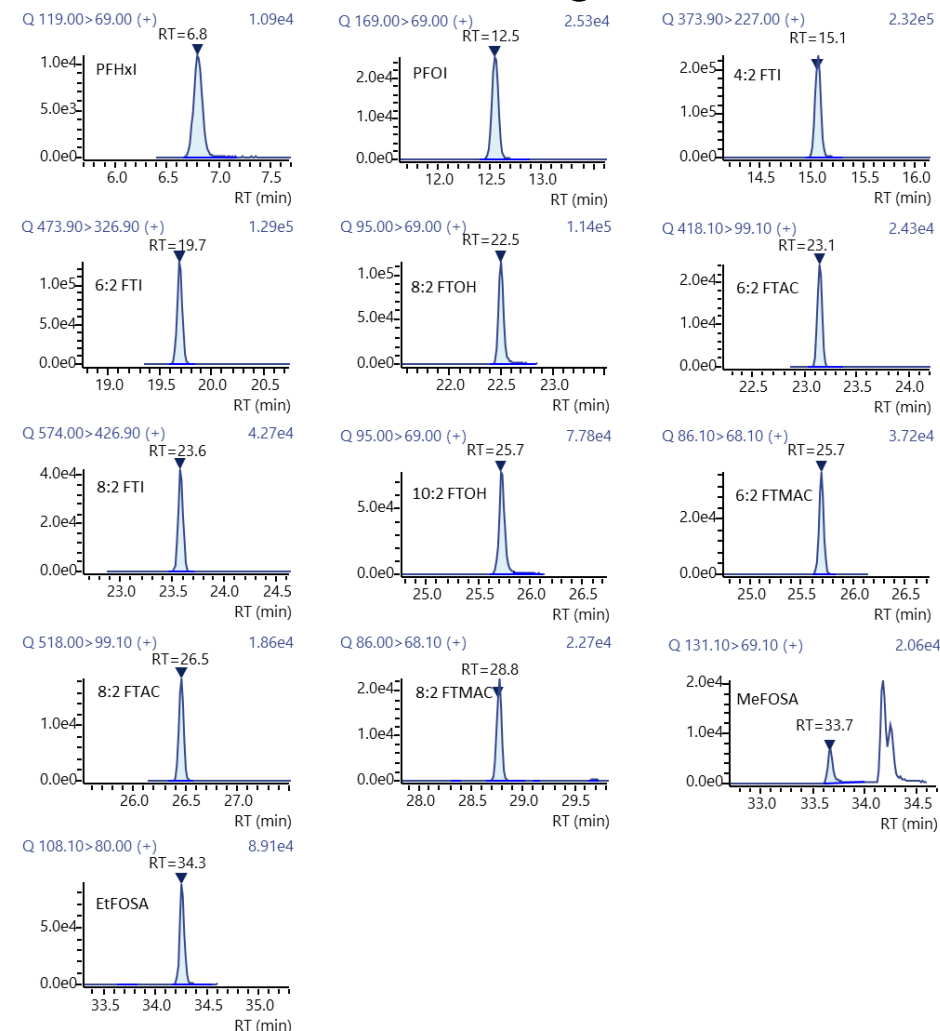
Mass Spectrometer	Common Parameters
Interface temperature (°C)	280
Ion source temperature (°C)	200
Detector voltage (kV)	Relative to Tune 0.4
Threshold	0
Mass Spectrometer	QP-2020NX
Acquisition mode	Qualitative analysis: Full scan: m/z 50 to 600 Quantitative analysis: SIM, Event time 0.3 sec.
Tuning mode	High Sensitivity
Mass Spectrometer	TQ-8040 NX
Acquisition mode	Qualitative analysis: Full scan: m/z 50 to 600 Quantitative analysis: MRM, Loop time: 0.3 sec.
Tuning mode	Normal mode

Results- SIM and MRM Chromatograms

QP-2020NX Chromatogram Results

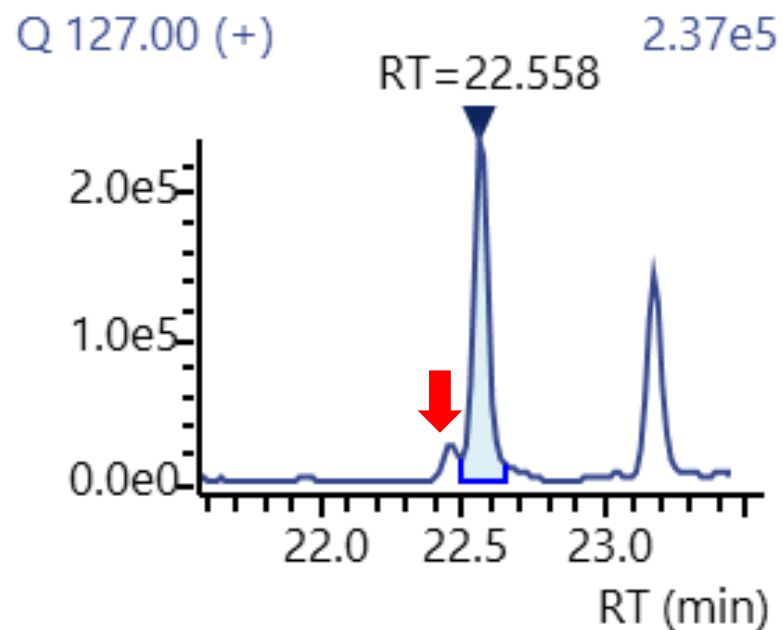


TQ-8040NX Chromatogram Results

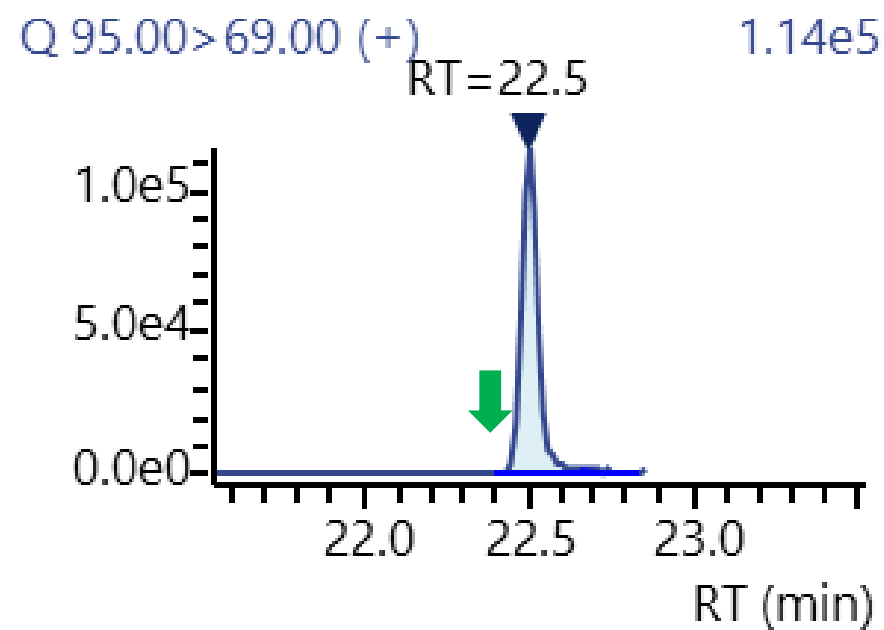


Results- SIM and MRM 8:2 FTOH Chromatograms

QP-2020NX SIM Chromatogram Results



TQ-8040NX MRM Chromatogram Results



Summary of Calibration Range and Linearity Results

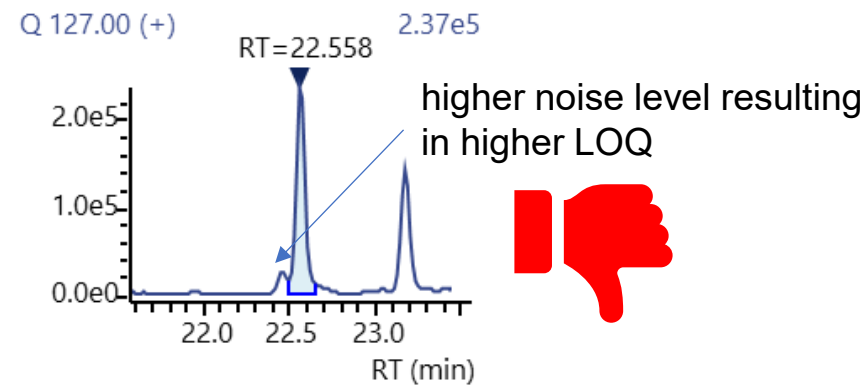
Compound	QP-2020NX (SIM)			TQ-8040 (MRM)		
	Calibration Range (ng/L)	R ²	RF (Response Factor) %RSD	Calibration Range (ng/L)	R ²	RF (Response Factor) %RSD
PFHxI	2.5-2000	0.993	10.89	2.5-2000	0.999	13.68
PFOI	2.5-2000	0.997	10.26	2.5-1000	0.998	18.94
4:2 FTI	2.5-800	0.993	8.28	2.5-2000	0.997	9.30
6:2 FTI	25-800	0.994	13.53	1-2000	0.998	17.18
8:2 FTOH	25-2000	0.997	5.37	2.5-2000	>0.999	6.31
6:2 FTAC	25-2000	0.998	19.87	2.5-2000	0.998	4.03
8:2 FTI	2.5-800	0.996	13.59	2.5-2000	0.999	9.05
10:2 FTOH	2.5-2000	0.999	10.38	2.5-2000	>0.999	6.45
6:2 FTMAC	2.5-800	0.995	12.43	2.5-2000	0.998	10.41
8:2 FTAC	5-250	0.995	14.81	2.5-2000	0.999	11.32
8:2 FTMAC	2.5-250	0.998	19.51	2.5-2000	0.999	9.98
MeFOSA	5-2000	>0.999	17.79	2.5-2000	0.999	6.85
EtFOSA	10-2000	0.999	11.40	1-2000	>0.999	7.17

Sensitivity: SQ: 2.5 - 25 ppt; TQ: 1 – 2.5 ppt

Calibration Range of 8:2 FTOH

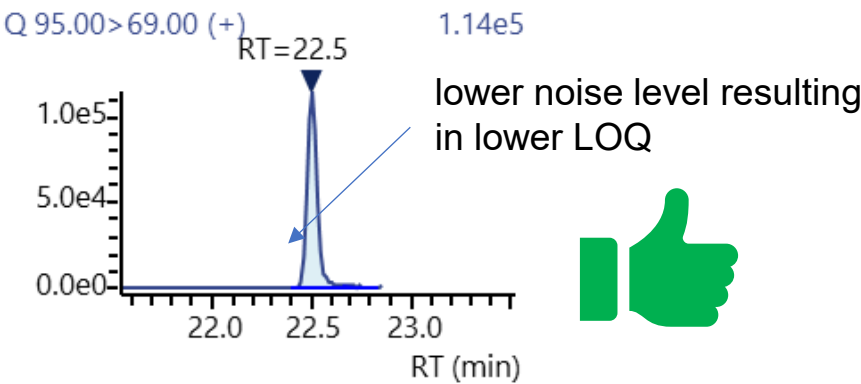
Compound	QP-2020NX (SIM)			TQ-8040 (MRM)		
	Calibration Range (ng/L)	R2	RF (Response Factor) %RSD	Calibration Range (ng/L)	R ²	RF (Response Factor) %RSD
PFHxI	2.5-2000	0.993	10.89	2.5-2000	0.999	13.68
PFOI	2.5-2000	0.997	10.26	2.5-1000	0.998	18.94
4:2 FTI	2.5-800	0.993	8.28	2.5-2000	0.997	9.30
6:2 FTI	25-800	0.994	13.53	1-2000	0.998	17.18
8:2 FTOH	25-2000	0.997	5.37	2.5-2000	>0.999	6.31

QP-2020NX Chromatogram Results



8:2 FTOH **SIM** Chromatogram

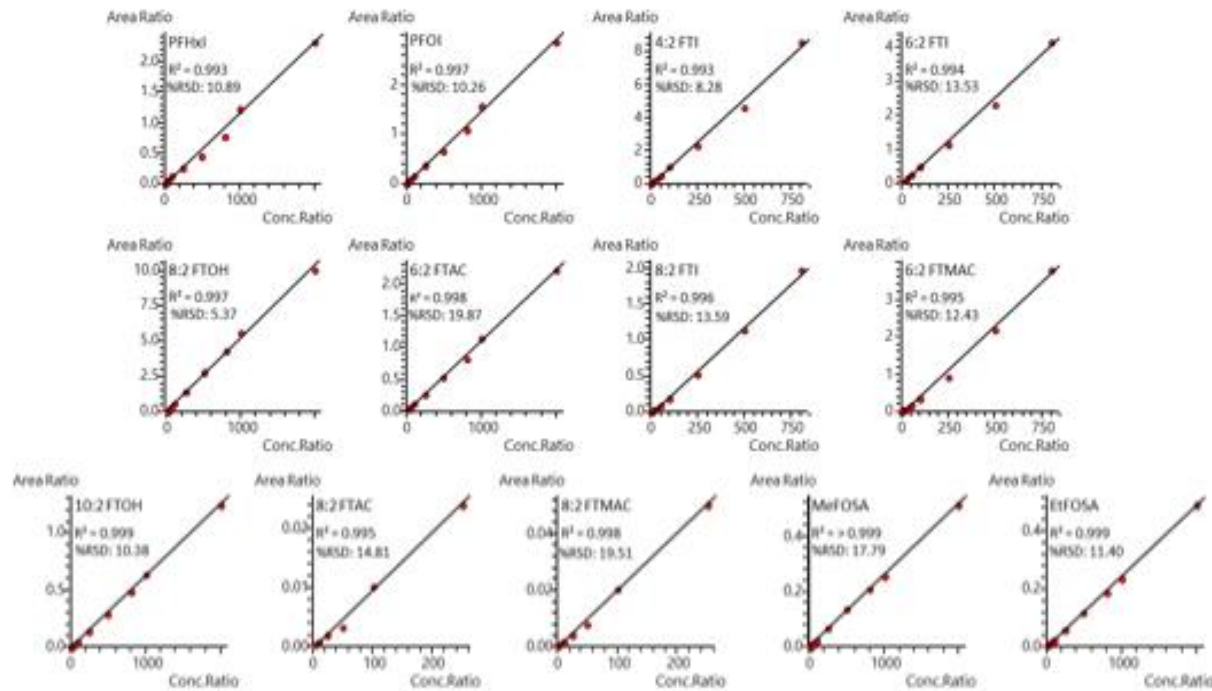
TQ-8040 Chromatogram Results



8:2 FTOH **MRM** Chromatogram

SIM and MRM Calibration Curves

Single Quadrupole Chromatogram Results



Triple Quadrupole Chromatogram Results

