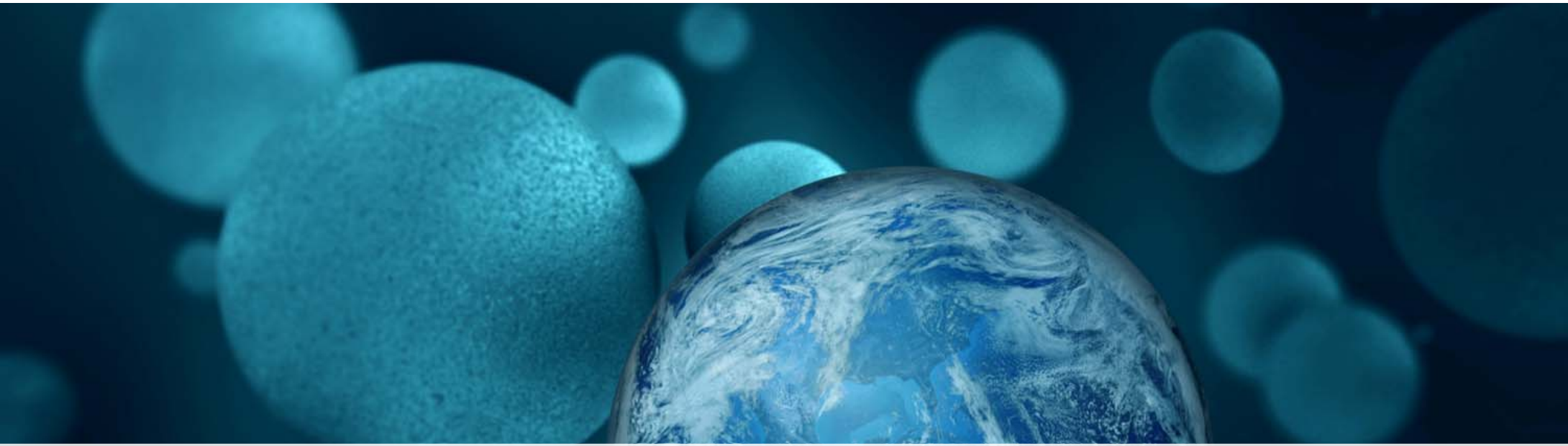

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EPA Validation for Per- and Polyfluorinated Compounds by LC-MS/MS

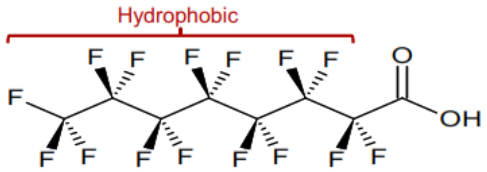
Richard Jack, Ph.D., Claudia Martins,
Cristina Jacob; Thermo Fisher Scientific

Ali Haghani, Andy Eaton
Eurofins Eaton
Monrovia, CA

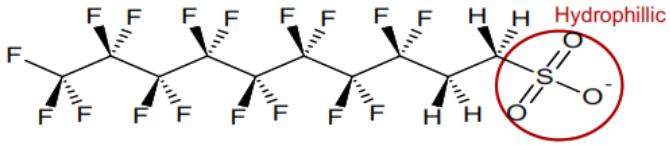
Background

What are PFAS?

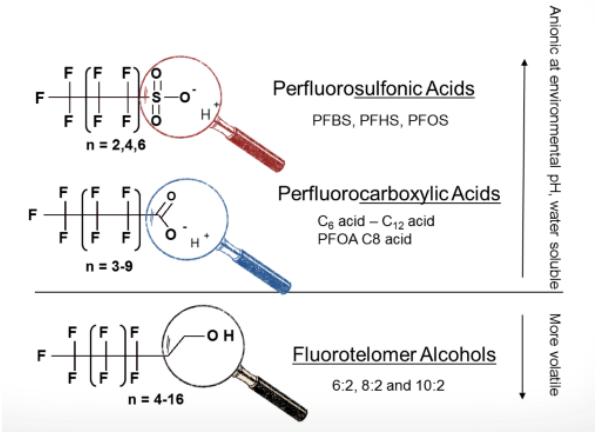
- PFASs are **P**er- and **P**oly**F**luorinated **A**lkyl **S**ubstances. Exclusively anthropogenic.
- Structures contain a hydrophobic perfluoroalkyl backbone and a hydrophillic end group
- Include a diverse range of compounds with a variety of chain lengths and end groups



Perfluorooctanoic acid
- PFOA
- Teflon®



8:2 Fluorotelomer sulfonate
- 8:2 FTS



Industrial Uses

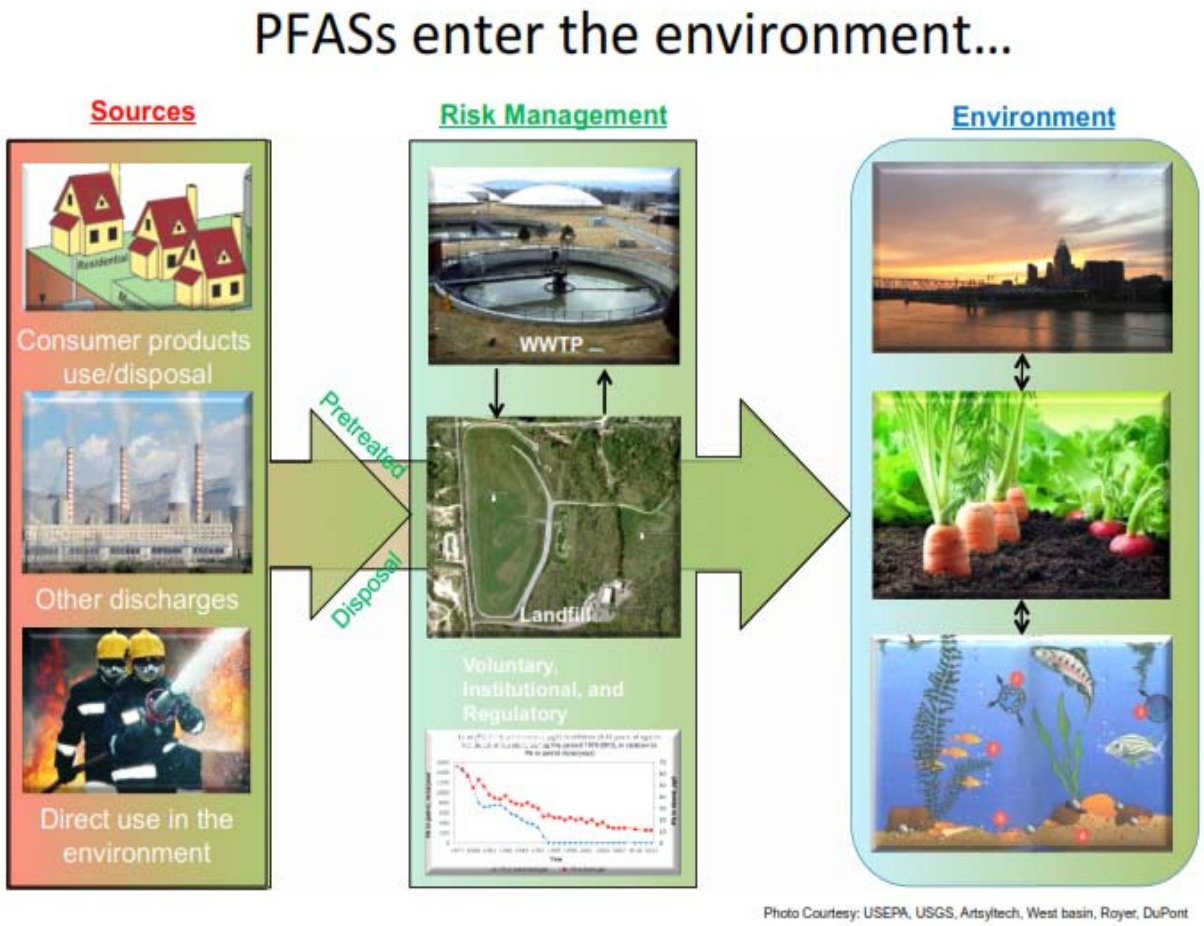
- PFAS are used in a variety of applications because of their chemical and physical properties. These include:
  - Industrial polymers (Teflon® - PFOA)
  - Stain repellants (Scotch Guard® - PFOS)
  - Aqueous film forming foams (AFFF) – fire fighting applications

Sources

- Can be found anywhere at differing (generally lower) concentrations,
- Areas of elevated concentration and concern are:
  - Airports
  - Run-off from incidents of fire
  - Landfill leachate
  - WWTP effluent

>4000 varieties compared to 75 PCB congeners

PFASs

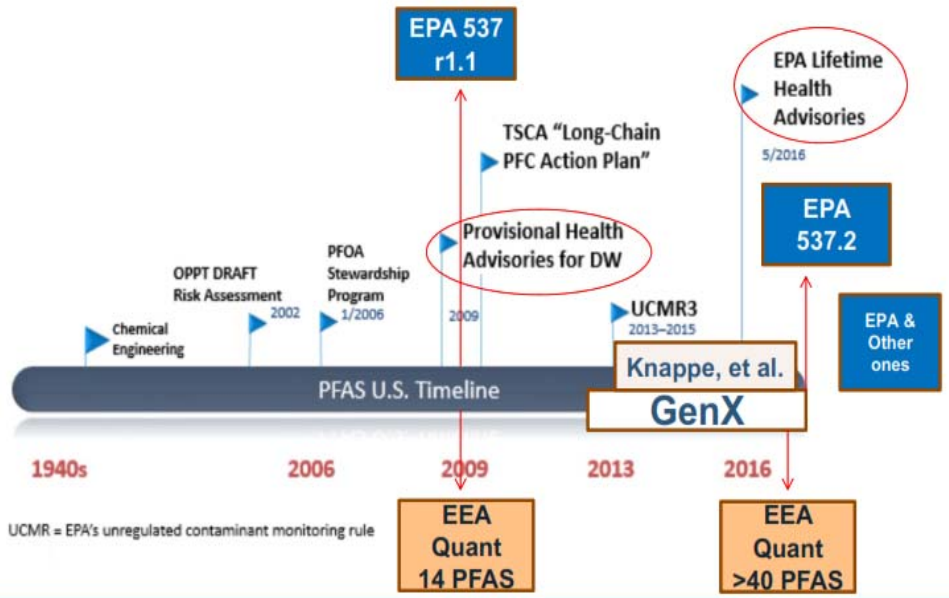


- Consumers may be exposed to PFASs in non-stick cookware, grease-resistant paper, fast food wrappers, microwave popcorn bags, stain-resistant carpets and fabrics, water-resistant clothing, cleaning products, and personal care products.
- PFAS are also used in industrial processes such as firefighting foams used by the military, airport authorities, and local fire and rescue agencies. The EPA says that it is these foams that are most often implicated when PFAS is found in groundwater or in the environment and that some PFAS take a very long time to break down in the environment and our bodies.

PFAA Toxicology and Regulatory timeline

- PFAS found in human hair
- Persistent and bioaccumulate
- Toxicity has been observed in some compounds
- Not regulated at this time, but still a “hot” topic Globally.
  - EPA
  - EU – Stockholm Conv. Persistent Organic Pollutant
  - Environmental chemists, epidemiologists and toxicologists are trying to deduce how many PFASs there are, track and assess potential harm.

- Toxicology > Concern > New Methods
- Health advisories are suggestions



eurofins | Eaton Analytical

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PFAA Drinking - , Wastewater and Soil Clean up > Non-targeted and targeted

- **FEDERAL LEVEL ACTIONS**
- Water and Soil Method Validations
- EPA Off. Of Ground Water and Drinking Water
- EPA Office of Water
- Approx. 600 military bases in US have PFC contamination

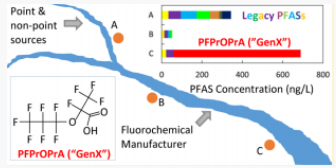
- **STATE LEVEL ACTIONS**
- PFOS and PFOA in WW regulated in 7 States
- **California** - "*Expressed support for including the **broader panel** of perfluoroalkyl and polyfluoroalkyl substances (PFASs).*"

BIOMONITORING CALIFORNIA
MEASURING CHEMICALS IN CALIFORNIANS

- **North Carolina** – New Legislation specifically focused on PFC/PFAA monitoring

SECTION 7.(d) The sum of eight million dollars ($8,000,000) …
(ii) …of essential scientific instruments,
(iii) …sample collection and analysis, training

Dr. P. Lee Ferguson
Assoc. Prof. of Civil
and Environmental Engineering
Duke University



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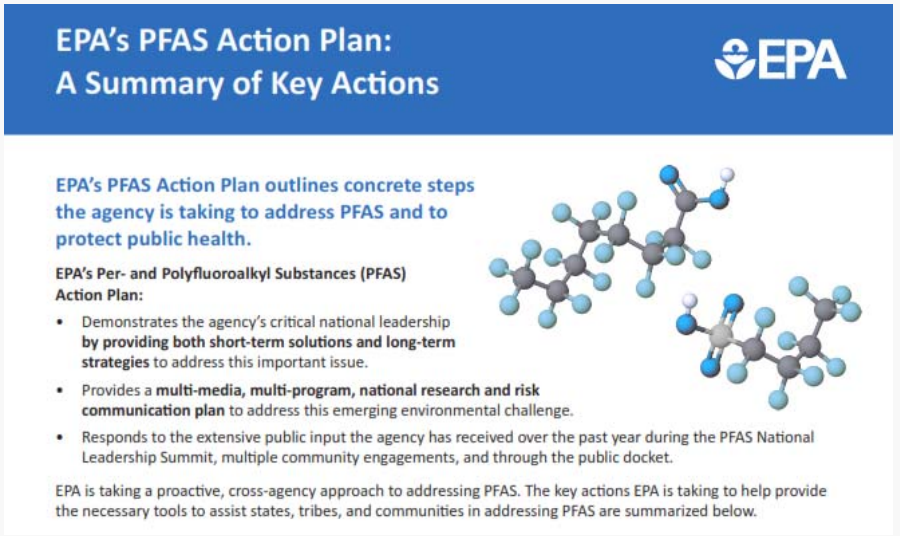
EPA is Proposal to Regulate PFAA in DW

U.S. ENVIRONMENTAL PROTECTION AGENCY
NEWS RELEASE
WWW.EPA.GOV/NEWSROOM

- Announced in Feb. 2019
- First ever comprehensive nationwide Action Plan to help states address concerns.
- Proposing a Federal Maximum Contaminant Level
- Begin the process to **propose** a regulation
- ***This doesn't mean PFAS are regulated!***


EPA's PFAS Action Plan:
A Summary of Key Actions

EPA

EPA's PFAS Action Plan outlines concrete steps the agency is taking to address PFAS and to protect public health.

EPA's Per- and Polyfluoroalkyl Substances (PFAS) Action Plan:

- Demonstrates the agency's critical national leadership **by providing both short-term solutions and long-term strategies** to address this important issue.
- Provides a **multi-media, multi-program, national research and risk communication plan** to address this emerging environmental challenge.
- Responds to the extensive public input the agency has received over the past year during the PFAS National Leadership Summit, multiple community engagements, and through the public docket.

EPA is taking a proactive, cross-agency approach to addressing PFAS. The key actions EPA is taking to help provide the necessary tools to assist states, tribes, and communities in addressing PFAS are summarized below.

- Drinking Water
- Clean up
- Monitoring
- Research – *Water and Toxicology*
- Enforcement

PFAA Workflows

- **Drinking Water – EPA 537.1**
- Offline SPE

AutoTrace – Peek free

- **Surface and Ground Water – EPA 8327**
- Direct Injection

Chromeleon

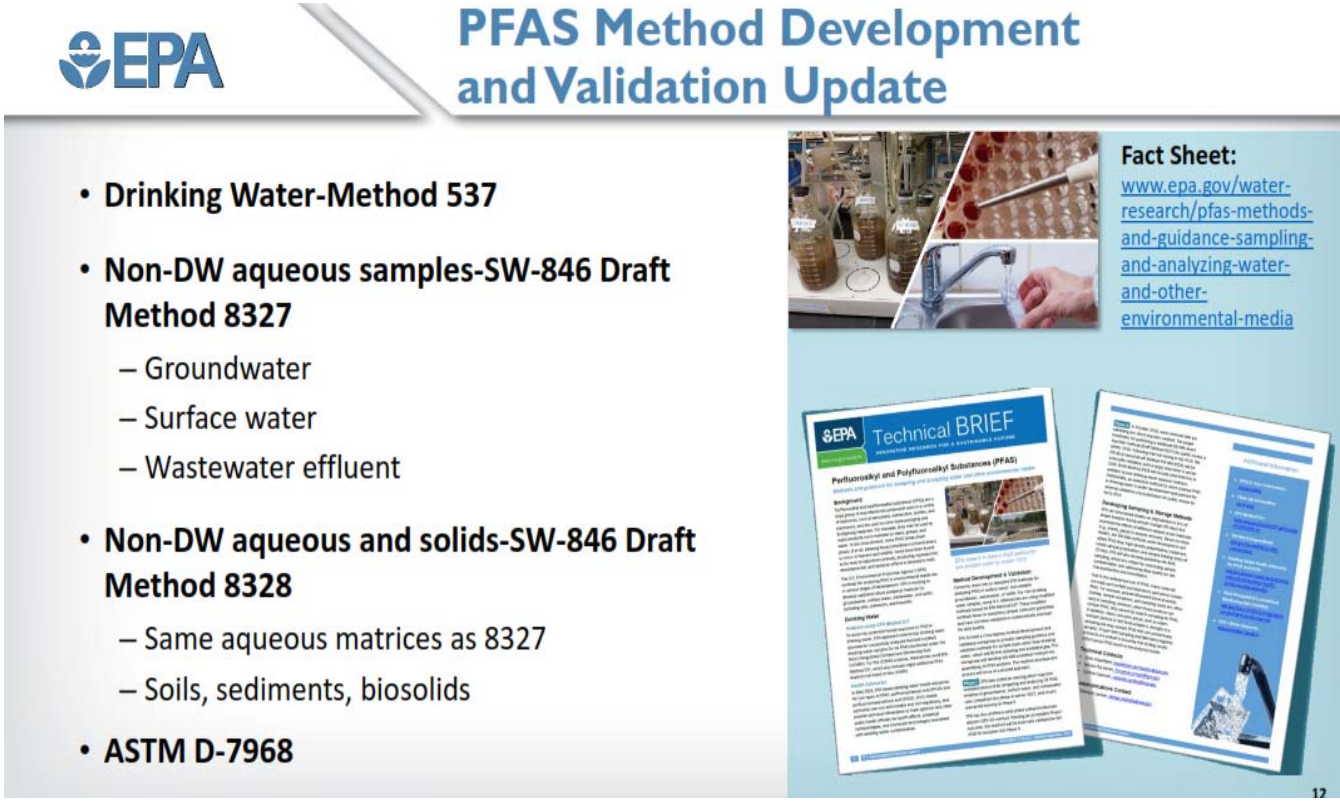
Tracefinder

Peek Free trap columns and tubing kits available

EPA Methods Development

A validated method is needed to ….

- Propose a DW regulation at federal level
- Monitoring source waters
- Start cleaning up cont. sites
  - Superfund sites (military bases)
- Enforcement from violations
- Research



Regulatory Participation – Surface and Ground Water

- Method Validation of EPA 8327 – 10 labs
- Claudia Martins MS Product mgmt
- Cristina Jacob MS Product mgmt.

Thermo Scientific Vanquish™ Flex Binary UHPLC System fitted with PFC-free kit and interfaced with Thermo Scientific **TSQ Altis™** Mass Spectrometer

EPA

Non Drinking Water: SW-846 Draft Method 8327

24 PFAS (including all target analytes in EPA Method 537)

- Commercially available standards ("neat" and isotopically labeled)

Direct injection based on EPA Region 5/Chicago Regional Lab Method

- Similar to draft American Society for Testing and Materials (ASTM) Method D7979
- Phase 1: Six internal (EPA) lab validation (Completed December 2017)
- Phase 2: Ten external lab validation (ongoing)
  - Initial demonstration of capability complete (7 labs "in" and 3 "out")
  - August 2018: Shipped samples (60 unknowns: surface, ground, and waste waters)
  - January 2019: Draft method posted for public comment

Target Quantitation Limits: 10 nanogram/L

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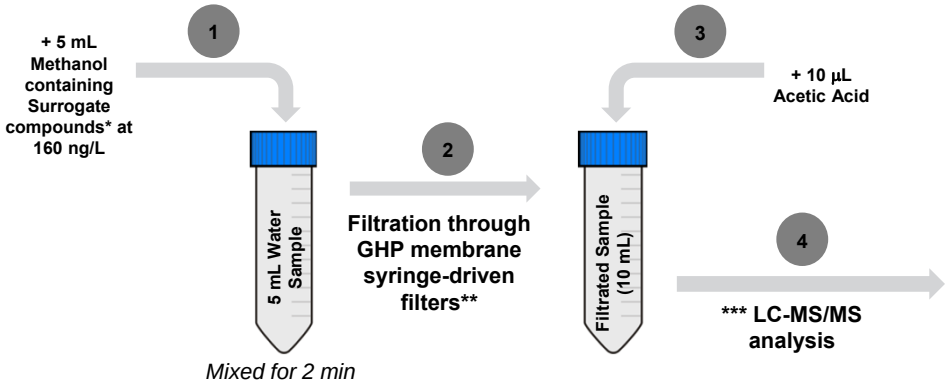
Sample preparation

❑ EPA Draft SW-846 Method 8327



Thermo Scientific Vanquish™ Flex Binary UHPLC System fitted with PFC-free kit and interfaced with Thermo Scientific **TSQ Altis™** Mass Spectrometer

* All standards were obtained form Wellington Laboratories

**Acrodisc GxF/0.2 µm GHP membrane syringe-driven filters were washed twice with LC-MS grade methanol (2x 10 mL) and acetonitrile (2x 10 mL)

*** Silanized-amber glass autosampler vials sealed with polypropylene caps were free of contaminants and interferences

SW846 Scope and Application

- A water sample (5 mL) is diluted 1:1 with methanol spiked with isotopically labeled surrogates and hand-shaken or vortexed for 2 min.
- The samples are then filtered through a membrane syringe driven filter unit. Acetic acid (10 µL) is added to all the samples to adjust to pH ~3 - 4 and then analyzed by LC/MS/MS. 2.2 The target compounds are identified by comparing the multiple reaction monitoring (MRM) transitions in the sample to the MRM transitions in the standards (Table 3). The retention time (RT) for the analytes of interest must also agree with the RT of the mid-level standard by ±5%. The target compounds are quantitated using the quantifier MRM transition of the target compounds utilizing external calibration.
- PFAS Sulfonic Acids – 10
- PFAS Carboxylic Acids – 11
- PFAS sulfonamides and sulfonamidoacetic acids – 3
- Surrogates - 19

SW846 8327 method aspects

- Standards and Surrogates can be used for 1 yr. If they fall within +/- 20% of original cal.
- 19 Surrogates are spiked into each sample
- Lower Limit Of Quantification final conc. Is 10 ng/L.

EPA Field Samples – External validation study

60 EPA water samples

Reagent Water	Ground Water	Surface Water	Waste Water
• 5x 5 mL native analytes • 5x 5 mL low spike • 5x 5 mL high spike	• 5x 5 mL native analytes • 5x 5 mL low spike • 5x 5 mL high spike	• 5x 5 mL native analytes • 5x 5 mL low spike • 5x 5 mL high spike	• 5x 5 mL native analytes • 5x 5 mL low spike • 5x 5 mL high spike

- Field samples divided into 3 batches of 20 samples
- 2 Method blanks, 2 LLOQs levels (10 and 20 ppt) and 2 Lab controls (LCS) were prepared for each batch

Standard Preparation according draft SW-846 Method 8327

- ✓Calibration standards were prepared from a 2mg/L (targets) and 1mg/L (surrogates) reference standards

	LV1 5 ppt	LV2 10 ppt	LV3 20 ppt	LV4 40 ppt	LV5 60 ppt	LV6 80 ppt	LV7 100 ppt	LV8 150 ppt	LV9 200 ppt
Solution A (μL)	25	50	100	200	300	400	500	750	1000
Solution B (μL)	975	950	900	800	700	600	500	250	0

Solution A: Level 9 stock solution prepared according to Section 7.4.4

Solution B: 50:50 methanol and water with 0.1% acetic acid.

* These values are the nominal concentrations in the calibration standards. The concentration obtained from the instrument is then corrected for the 2-fold dilution made during the sample preparation process

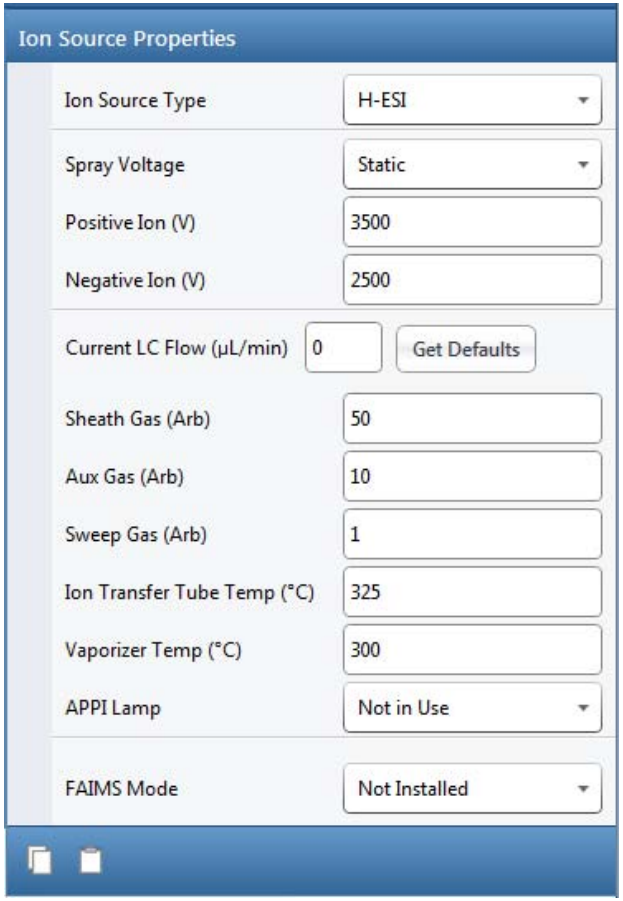
LC Conditions

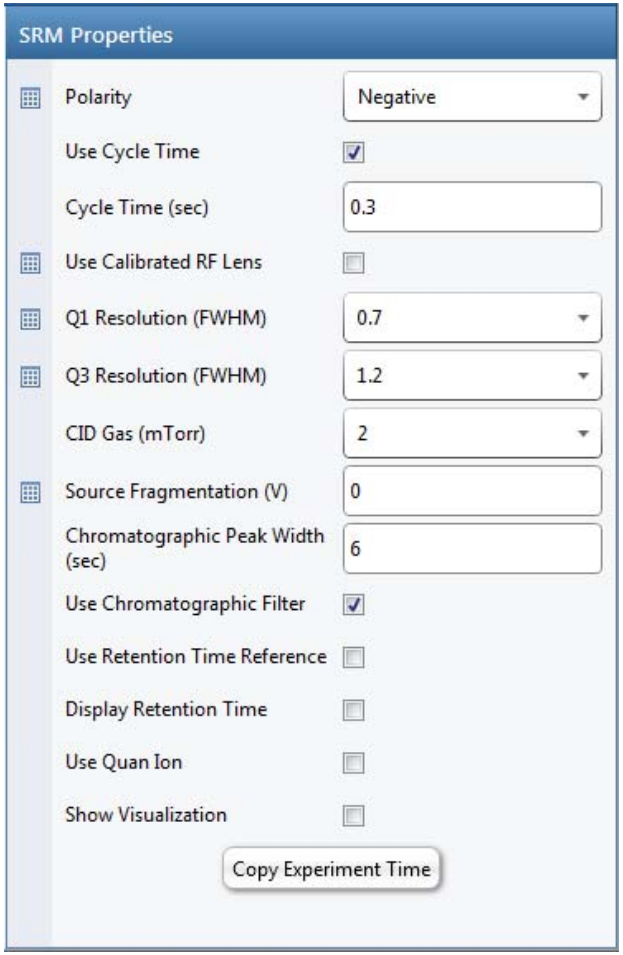
- **Analytical Column** Thermo Accucore RP*, 2.1 x 100 mm, 2.6 μm
- **Isolator column** Thermo BDS Hypersil C18, 2.1 x 50 mm, 5 μm
- **Column temperature** 45 °C
- **Flow rate** 500 μL/min
- **Solvent A** Water containing 2mM ammonium acetate, 2% methanol and 0.1% acetic acid
- **Solvent B** Methanol containing 2mM ammonium acetate, 2% water and 0.1% Acetic acid
- **Injection volume** 25 μL

No	Time	Flow [ml/min]	%B	Curve
1	0.000	Equilibration		
2	0.000	0.500	0.0	5
3	*New Row*			
4	0.000	Run		
5	0.000	0.500	0.0	5
6	1.000	0.500	30.0	5
7	6.000	0.500	45.0	5
8	13.000	0.500	80.0	5
9	14.000	0.500	100.0	5
10	17.000	0.500	100.0	5
11	18.000	0.500	0.0	5
12	21.000	0.500	0.0	5
13	*New Row*			
14	21.000	Stop Run		

*Similar performance was achieved with both Thermo Scientific™ Accucore™ RP and Waters Acquity CSH Phenyl-hexyl as described in EPA draft SW-846 method 8327 – However the Accucore column benefits from significantly lower back pressure

Source Parameters – TSQ Altis





Monitored SRM transitions (1 of 4)

#C	Compound		Start Time (min)	End Time (min)	Quantifier/Qualifier	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Min Dwell Time (ms)	RF Lens (V)
C4	Perfluorobutanoic acid	PFBA	2	3.5	Quantifier	212.979	168.97	9	148.63	30
	Perfluoro-n-[1,2,3,4-$^{13}C_4$]butanoic acid	MPFBA	2	3.5	Quantifier	216.993	172	9	148.63	30
C5	Perfluoropentanoic acid	PFPeA	4.2	5.3	Quantifier	262.976	219.042	9	148.63	31
	Perfluoro-n-[1,2,3,4,5-$^{13}C_5$]pentanoic acid	M5PFPeA	4.2	5.3	Quantifier	267.993	222.99	9	148.63	32
C4	Perfluorobutanesulfonate	PFBS	5	6	Quantifier	298.943	79.957	34	25.82	116
	Perfluorobutanesulfonate	PFBS	5	6	Qualifier	298.943	98.956	29	25.82	116
	Sodium perfluoro-1-[2,3,4-$^{13}C_3$]butanesulfonate	M3PFBS	5	6	Quantifier	301.953	79.96	34	25.82	119
	Perfluorohexanoic acid	PFHxA	7	8.2	Qualifier	312.973	119.042	18.76	25.82	39
	Perfluorohexanoic acid	PFHxA	7	8.2	Quantifier	312.973	268.97	9	25.82	39
	Perfluoro-n-[1,2,3,4,6-$^{13}C_5$]hexanoic acid	M5PFHxA	7	8.2	Quantifier	317.99	273	9	25.82	37
C6	Fluorotelomer sulfonate 4:2	FtS 4:2	7	8	Qualifier	326.974	81.042	26.07	25.82	115
	Fluorotelomer sulfonate 4:2	FtS 4:2	7	8	Qualifier	326.974	286.958	23	25.82	115
	Fluorotelomer sulfonate 4:2	FtS 4:2	7	8	Quantifier	326.974	307.042	18.11	25.82	115
	Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$]hexane sulfonate (4:2)	M2-4:2FTS	7	8	Quantifier	328.981	308.96	18	25.82	103
	Perfluoropentansulfonate	PFPeS	7.5	8.5	Quantifier	348.94	80.042	33.66	41.57	145
	Perfluoropentansulfonate	PFPeS	7.5	8.5	Qualifier	348.94	99	31	41.57	145
	Perfluoropentansulfonate	PFPeS	7.5	8.5	Qualifier	348.94	119.054	31.42	41.57	145
C7	Perfluoroheptanoic acid	PFHpA	9.5	10.1	Qualifier	362.97	119.054	19.52	41.42	43
	Perfluoroheptanoic acid	PFHpA	9.5	10.1	Qualifier	362.97	168.97	15.53	41.42	43
	Perfluoroheptanoic acid	PFHpA	9.5	10.1	Quantifier	362.97	319.042	9	41.42	43
	Perfluoro-n-[1,2,3,4-$^{13}C_4$]heptanoic acid	M4PFHpA	9.5	10.5	Quantifier	366.983	321.98	9	41.42	43
C6 SO_4	Perfluorohexanesulfonate	PFHxS	9	10.2	Quantifier	398.937	79.957	39	25.81	135
	Perfluorohexanesulfonate	PFHxS	9	10.2	Qualifier	398.937	98.956	35	25.81	135
	Sodium perfluoro-1-[1,2,3-$^{13}C_3$]hexanesulfonate	M3PFHxS	9.5	10.5	Quantifier	401.947	79.957	39	25.81	133

"Quantifier": target compounds are quantitated using the quantifier MRM transition of the target compounds utilizing external calibration. Qualifiers are used to help with identification

Monitored SRM transitions (2 of 4)

Compounds		Start Time (min)	End Time (min)	Quantifier/Qualifier	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Min Dwell Time (ms)	RF Lens (V)
Perfluorooctanoic acid	PFOA	10.5	11.3	Qualifier	412.966	219	14.55	16.35	49
Perfluorooctanoic acid	PFOA	10.5	11.3	Quantifier	412.966	369.042	9	16.35	49
Perfluoro-n-[$^{13}C_8$]octanoic acid	M8PFOA	10.5	11.5	Quantifier	420.993	376	9	16.35	48
Fluorotelomer sulfonate 6:2	FtS 6:2	10.5	11.3	Qualifier	426.968	81.042	29.94	25.81	123
Fluorotelomer sulfonate 6:2	FtS 6:2	10.5	11.3	Qualifier	426.968	386.97	26.72	25.81	123
Fluorotelomer sulfonate 6:2	FtS 6:2	10.5	11.3	Quantifier	426.968	406.988	21.45	25.81	123
Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$]octane sulfonate (6:2)	M2-6:2FTS	10.5	11.5	Quantifier	428.975	408.96	21	25.81	123
Perfluoroheptanesulfonate	PFHpS	10.5	11.5	Quantifier	448.933	80.012	37.6	16.35	131
Perfluoroheptanesulfonate	PFHpS	10.5	11.5	Qualifier	448.933	98.97	36.2	16.35	131
Perfluoroheptanesulfonate	PFHpS	10.5	11.5	Qualifier	448.933	169.03	31.04	16.35	131
Perfluorononanoic acid	PFNA	11.5	12.3	Qualifier	462.963	169	17.51	16.35	52
Perfluorononanoic acid	PFNA	11.5	12.3	Qualifier	462.963	219.012	15.23	16.35	52
Perfluorononanoic acid	PFNA	11.5	12.3	Quantifier	462.963	418.97	9	16.35	52
Perfluoro-n-[$^{13}C_9$]nonanoic acid	M9PFNA	11.5	12.5	Qualifier	471.993	426.97	9	16.35	52
Perfluorooctanesulfonate	PFOS	11.5	12.5	Quantifier	498.93	79.957	47	15.33	159
Perfluorooctanesulfonate	PFOS	11.5	12.5	Qualifier	498.93	98.956	40	15.33	159
Sodium perfluoro-[$^{13}C_8$]octanesulfonate	M8PFOS	11.5	12.6	Quantifier	506.957	79.957	40	15.33	160
Perfluorodecanoic acid	PFDA	12.5	13.2	Qualifier	512.96	219.012	16.14	14.36	56
Perfluorodecanoic acid	PFDA	12.5	13.2	Qualifier	512.96	269.042	15.8	14.36	56
Perfluorodecanoic acid	PFDA	12.5	13.2	Quantifier	512.96	469.042	9	14.36	56
Perfluoro-n-[1,2,3,4,5,6-$^{13}C_6$]decanoic acid	M6PFDA	12.5	13.5	Quantifier	518.98	473.97	9	14.36	56
Fluorotelomer sulfonate 8:2	FtS 8:2	12.5	13.2	Qualifier	526.962	81.012	34.83	14.36	137
Fluorotelomer sulfonate 8:2	FtS 8:2	12.5	13.2	Qualifier	526.962	487	28.92	14.36	137
Fluorotelomer sulfonate 8:2	FtS 8:2	12.5	13.2	Quantifier	526.962	506.97	24.37	14.36	137
Sodium 1H,1H,2H,2H-perfluoro-1-[1,2-$^{13}C_2$]decane sulfonate (8:2)	M2-8:2FTS	12.5	13.5	Quantifier	528.968	508.96	24	14.36	137
Perfluorononanesulfonate	PFNS	12.5	13.5	Quantifier	548.927	80.071	42.34	14.36	148

C8

C10

Monitored SRM transitions (3 of 4)

C10

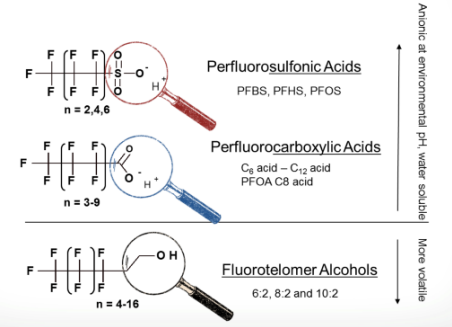
C14

Compounds		Start Time (min)	End Time (min)	Quantifier/Qualifier	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Min Dwell Time (ms)	RF Lens (V)
Perfluorononanesulfonate	PFNS	12.5	13.5	Qualifier	548.927	98.97	40.67	14.36	148
Perfluorononanesulfonate	PFNS	12.5	13.5	Qualifier	548.927	229.958	41.66	14.36	148
Perfluoroundecanoic acid	PFUdA	13	14	Qualifier	562.957	219	17.32	11.57	62
Perfluoroundecanoic acid	PFUdA	13	14	Qualifier	562.957	269.03	16.94	11.57	62
Perfluoroundecanoic acid	PFUdA	13	14	Quantifier	562.957	518.97	9	11.57	62
N-(Heptadecafluorooctylsulfonyl)-N-methylglycine	NMeFOSAA	13	14	Quantifier	569.967	418.97	18.42	11.57	107
N-(Heptadecafluorooctylsulfonyl)-N-methylglycine	NMeFOSAA	13	14	Qualifier	569.967	512	19.55	11.57	107
Perfluoro-n-[1,2,3,4,5,6,7-$^{13}C_7$]undecanoic acid	M7PFUdA	13	14	Quantifier	569.98	524.97	9	11.57	62
N-methyl-d3-perfluoro-1-octanesulfonamidoacetic acid	d3-N-MeFOSAA	13	14	Quantifier	572.986	418.97	18	11.57	107
Perfluorooctanesulfonamide	PFOSA	13	14	Quantifier	497.946	78.071	29.37	11.57	127
Perfluorooctanesulfonamide	PFOSA	13	14	Qualifier	497.946	169.03	25.85	11.57	127
Perfluorooctanesulfonamide	PFOSA	13	14	Qualifier	497.946	478.042	22.51	11.57	127
Perfluoro-1-[$^{13}C_8$]octanesulfonamide	M8FOSA-I	13	14	Quantifier	505.973	77.97	29	11.57	127
N-ethyl-N-((heptadecafluorooctyl)sulfonyl)glycine	NEtFOSAA	13	14	Qualifier	583.983	418.97	18.34	11.57	101
N-ethyl-N-((heptadecafluorooctyl)sulfonyl)glycine	NEtFOSAA	13	14	Qualifier	583.983	482.958	13.9	11.57	101
N-ethyl-N-((heptadecafluorooctyl)sulfonyl)glycine	NEtFOSAA	13	14	Quantifier	583.983	526.03	18.26	11.57	101
N-ethyl-d5-perfluoro-1-octanesulfonamidoacetic acid	d5-N-EtFOSAA	13	14	Quantifier	589.014	418.97	18	11.57	101
Perfluorodecanesulfonate	PFDS	13.2	14.2	Quantifier	598.924	80.042	44.92	11.57	169
Perfluorodecanesulfonate	PFDS	13.2	14.2	Qualifier	598.924	98.929	43.48	11.57	169
Perfluorodecanesulfonate	PFDS	13.2	14.2	Qualifier	598.924	229.929	46.09	11.57	169

Monitored SRM transitions (4 of 4)

Compounds		Start Time (min)	End Time (min)	Quantifier/Qualifier	Precursor (m/z)	Product (m/z)	Collision Energy (V)	Min Dwell Time (ms)	RF Lens (V)
Perfluorododecanoic acid	PFDoA	13.6	14.4	Qualifier	612.954	169.03	23.69	11.57	67
Perfluorododecanoic acid	PFDoA	13.6	14.4	Qualifier	612.954	319.042	17.54	11.57	67
Perfluorododecanoic acid	PFDoA	13.6	14.4	Quantifier	612.954	569	9	11.57	67
Perfluoro-n-[1,2-$^{13}C_2$]dodecanoic acid	MPFDoA	13.5	14.5	Quantifier	614.96	569.97	9	11.57	67
Perfluorotridecanoic acid	PFTriA	14	14.9	Qualifier	662.95	168.97	25.16	15.25	71
Perfluorotridecanoic acid	PFTriA	14	14.9	Qualifier	662.95	369.071	17.85	15.25	71
Perfluorotridecanoic acid	PFTriA	14	14.9	Quantifier	662.95	619.042	9	15.25	71
Perfluorotetradecanoic acid	PFTreA	14	14.9	Qualifier	712.947	319.054	19.86	41.51	74
Perfluorotetradecanoic acid	PFTreA	14	14.9	Qualifier	712.947	369.042	18.87	41.51	74
Perfluorotetradecanoic acid	PFTreA	14	14.9	Quantifier	712.947	668.97	9	41.51	74
Perfluoro-n-[1,2-$^{13}C_2$]tetradecanoic acid	M2PFTeDA	14	14.9	Quantifier	714.954	669.96	9	41.51	74

C14



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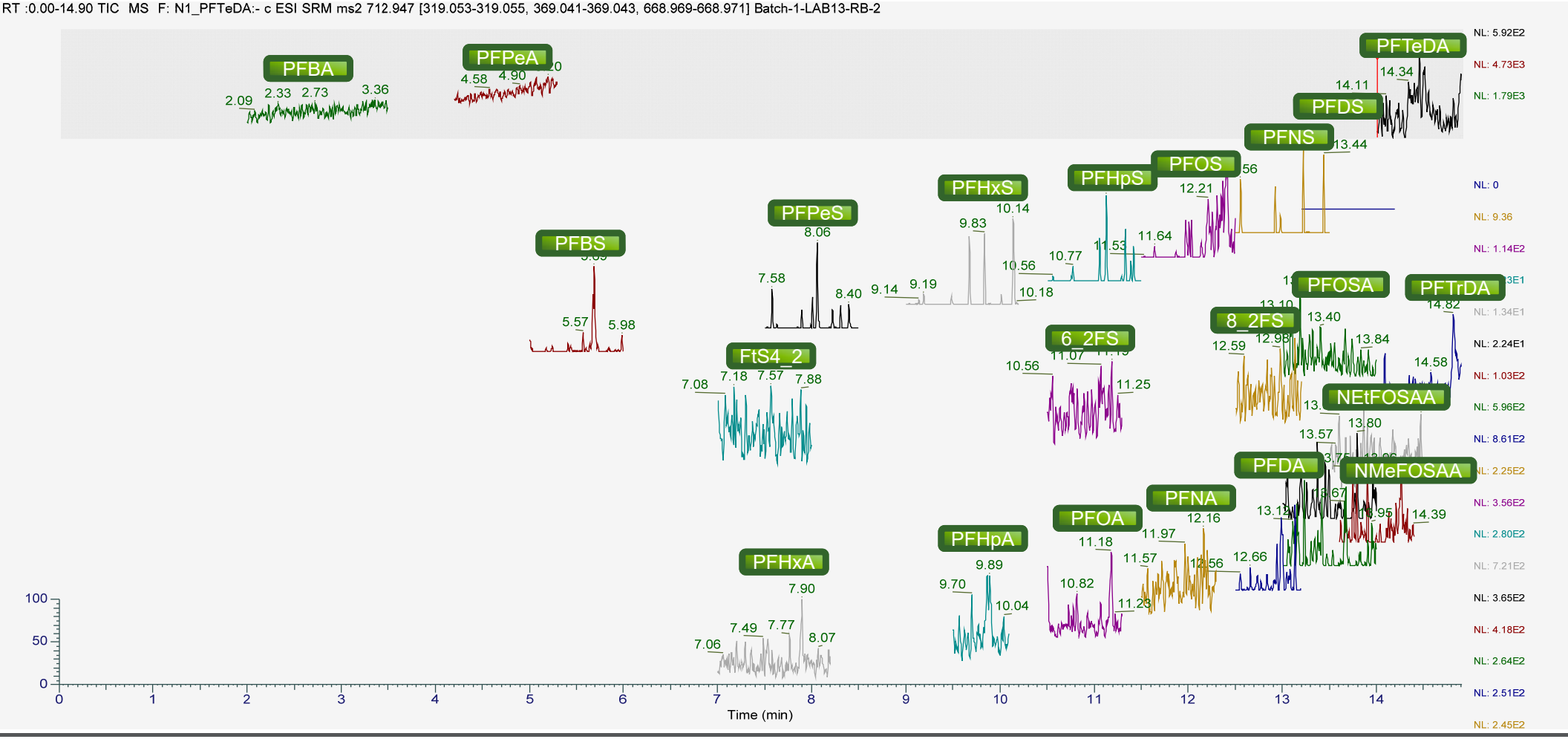
TSQ Altis: Reagent Blank



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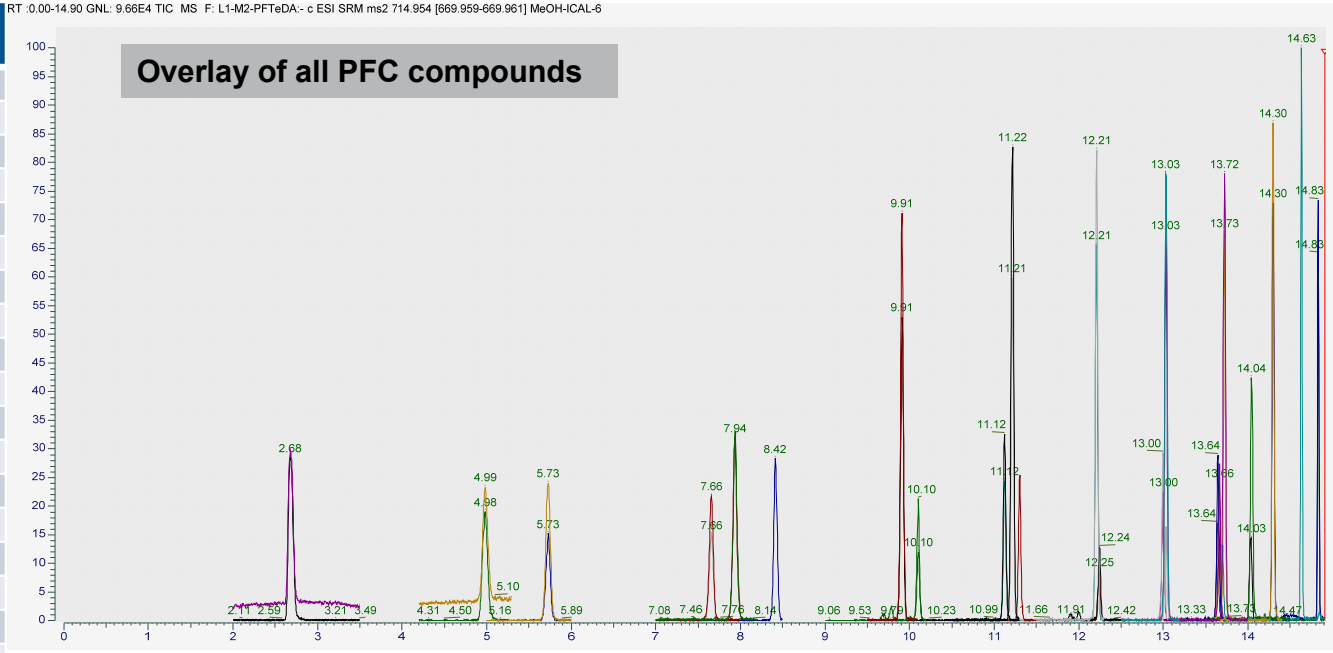
TSQ Altis – Calibration curves: range 5 – 200 ppt

Compounds		LV 1 – 5 ppt % Deviation	LV2 - 10 ppt % Deviation	LV3 – 20 ppt % Deviation	RT (min)	R^2
N-1	PFTreA	15%	7%	-2%	14.83	0.9906
N-2	PFTriA	2%	2%	4%	14.63	0.9966
N-3	PFDoA	-8%	4%	7%	14.3	0.9989
N-4	PFUnA	-3%	4%	-1%	13.72	0.9996
N-5	PFDA	12%	1%	-5%	13.03	0.9979
N-6	PFNA	3%	6%	-2%	12.21	0.9983
N-7	PFOA	13%	-1%	-2%	11.22	0.9972
N-8	PFHpA	1%	6%	-2%	9.91	0.9991
N-9	PFHxA	8%	0%	-1%	7.94	0.9983
N-10	PFPeA	-16%	4%	14%	4.98	0.9984
N-11	PFBA	0%	-1%	3%	2.68	0.9993
N-12	PFDS	4%	-14%	11%	13.7	0.9939
N-13	PFNS	0%	-6%	15%	13.04	0.9976
N-14	PFOS	-7%	-4%	9%	12.24	0.9981
N-15	PFHpS	16%	-7%	-9%	11.3	0.9979
N-16	PFHxS	13%	-5%	0%	10.11	0.9985
N-17	PFPeS	5%	4%	-3%	8.42	0.9991
N-18	PFBS	2%	1%	-2%	5.73	0.9995
N-19	PFOSA	10%	5%	-4%	13.66	0.9931
N-20	FtS 8:2	6%	-3%	-1%	13	0.9997
N-21	FtS 6:2	7%	3%	-7%	11.12	0.9977
N-22	FtS 4:2	23%	-10%	-9%	7.66	0.9976
N-23	NEtFOSAA	4%	-13%	9%	14.04	0.9985
N-24	NMeFOSAA	-10%	8%	6%	13.64	0.9993



Calibration curves

- ✓ Linearity over the range 5 – 200 ppt
  (2-fold dilution not taken into consideration)
- ✓ R^2 > 0.99 for all compounds
- ✓ Deviation < 20%

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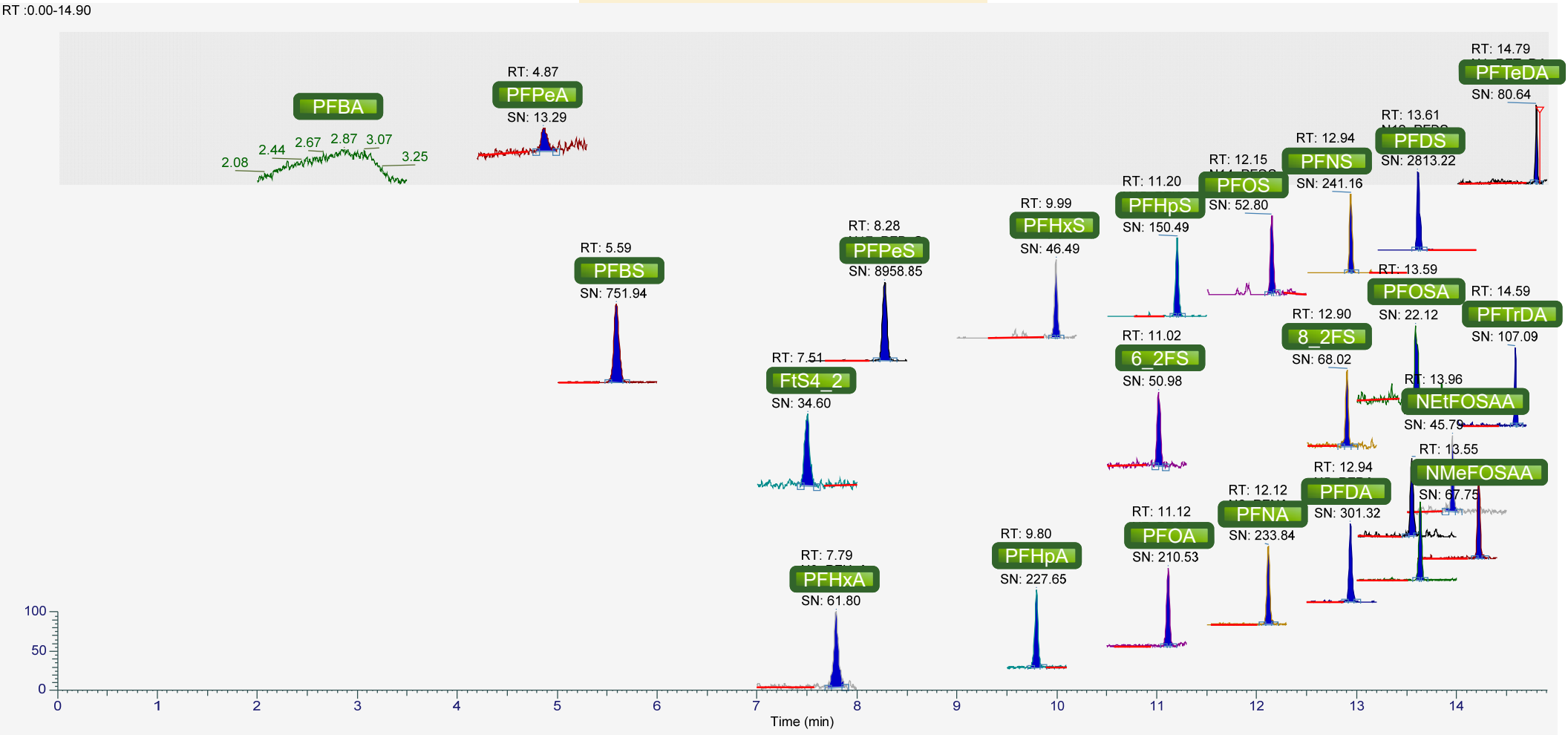
TSQ Altis – PFC target compounds spike at 10 ppt in water samples



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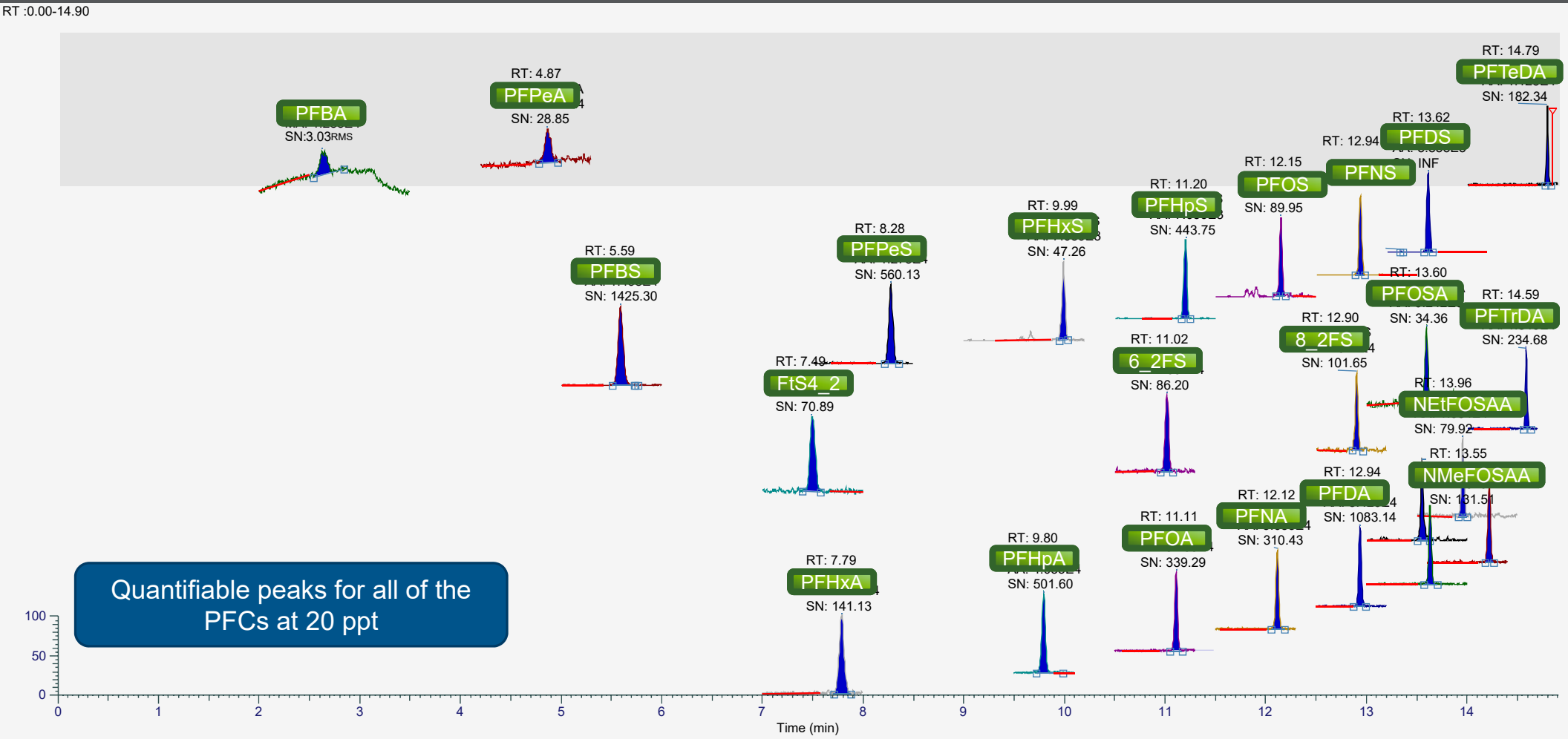
TSQ Altis – PFC target compounds spike at 20 ppt in water samples



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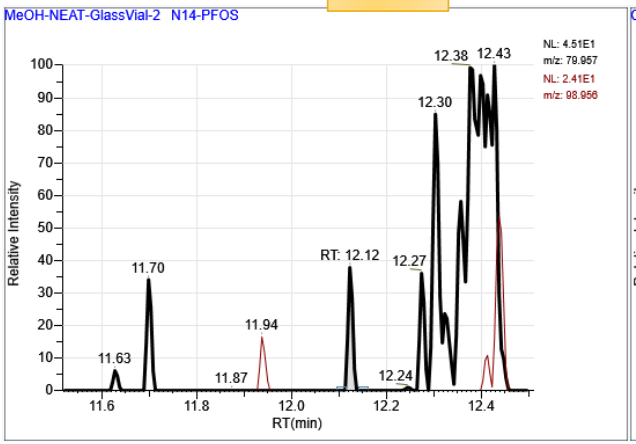
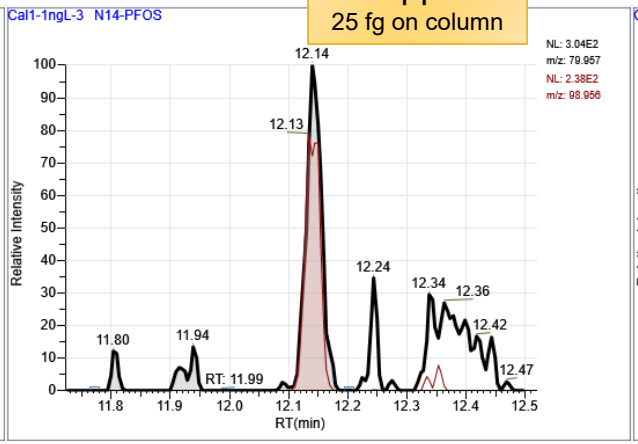
PFOS – Quan Ion and confirming ion overlay at different concentrations

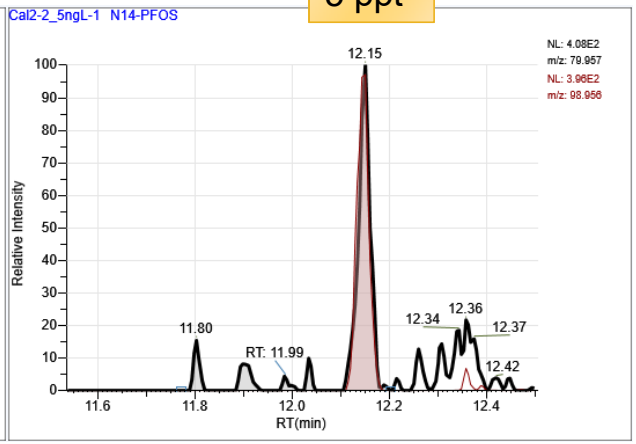
Blank



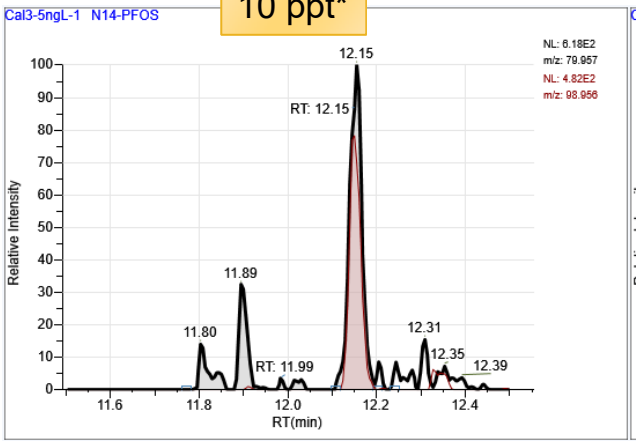
2 ppt*
25 fg on column



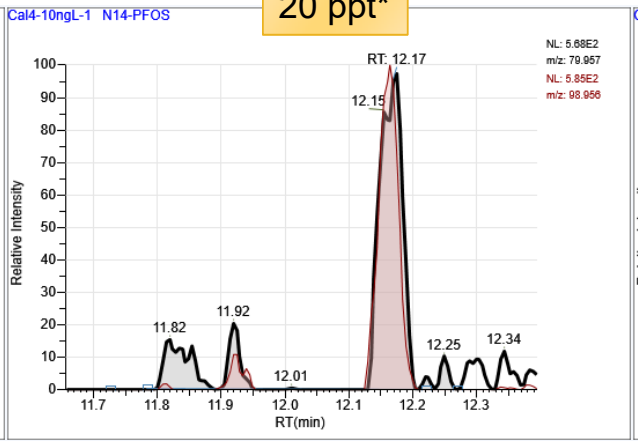
5 ppt*



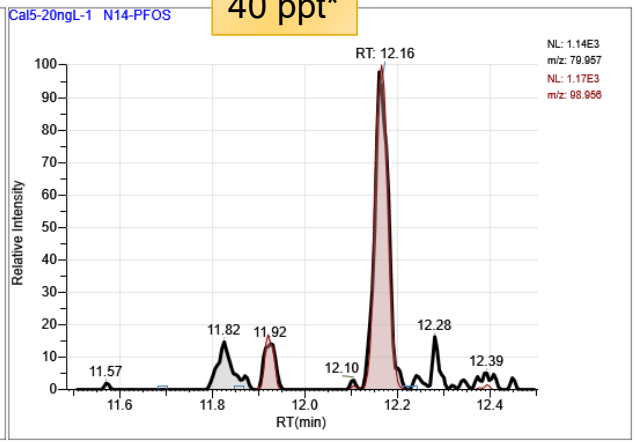
10 ppt*



20 ppt*



40 ppt*



*2-fold dilution was taken into consideration

Quantifiable amount at 2 ppt which is 5 times lower than EPA required lower reporting limit

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EPA Draft SW-846 Method 8327 Criteria for Control Samples

	Reagent Blanks	Method Blanks	LLOQ Verification	Laboratory Control Sample LCS/LCSD
	Methanol: Water (50:50, v/v) + 0.1% Acetic acid	Reagent Water + surrogates. Taken through sample preparation	Reagent water + targets at LOQ + surrogates at LOQ. Taken through sample preparation	Reagent water + targets + surrogates. (80 ppt) Taken through sample preparation
	Concentration must be one half the LLOQ	**Concentration must be one half the LLOQ**	**S/N ratio ≥ 3 for all quantitative ions & Target Recoveries < 50% deviation**	**Target Recoveries < 30% deviation**
Thermo Scientific TSQ ALTIS	Target compounds **NOT DETECTED OR BELOW <LLOQ**	Target compounds **NOT DETECTED OR BELOW LLOQ**	**LLOQ at 10 ppt** Recoveries <30% deviation for most of the compounds **LOQ at 20 ppt** Recoveries <30% deviation for most of the compounds	Target Recoveries <30% deviation for most of the compounds

Evaluate reagent water, instrument, sample prep, DL and Quantitation limit – excluding matrix effects

EPA Field Samples Results

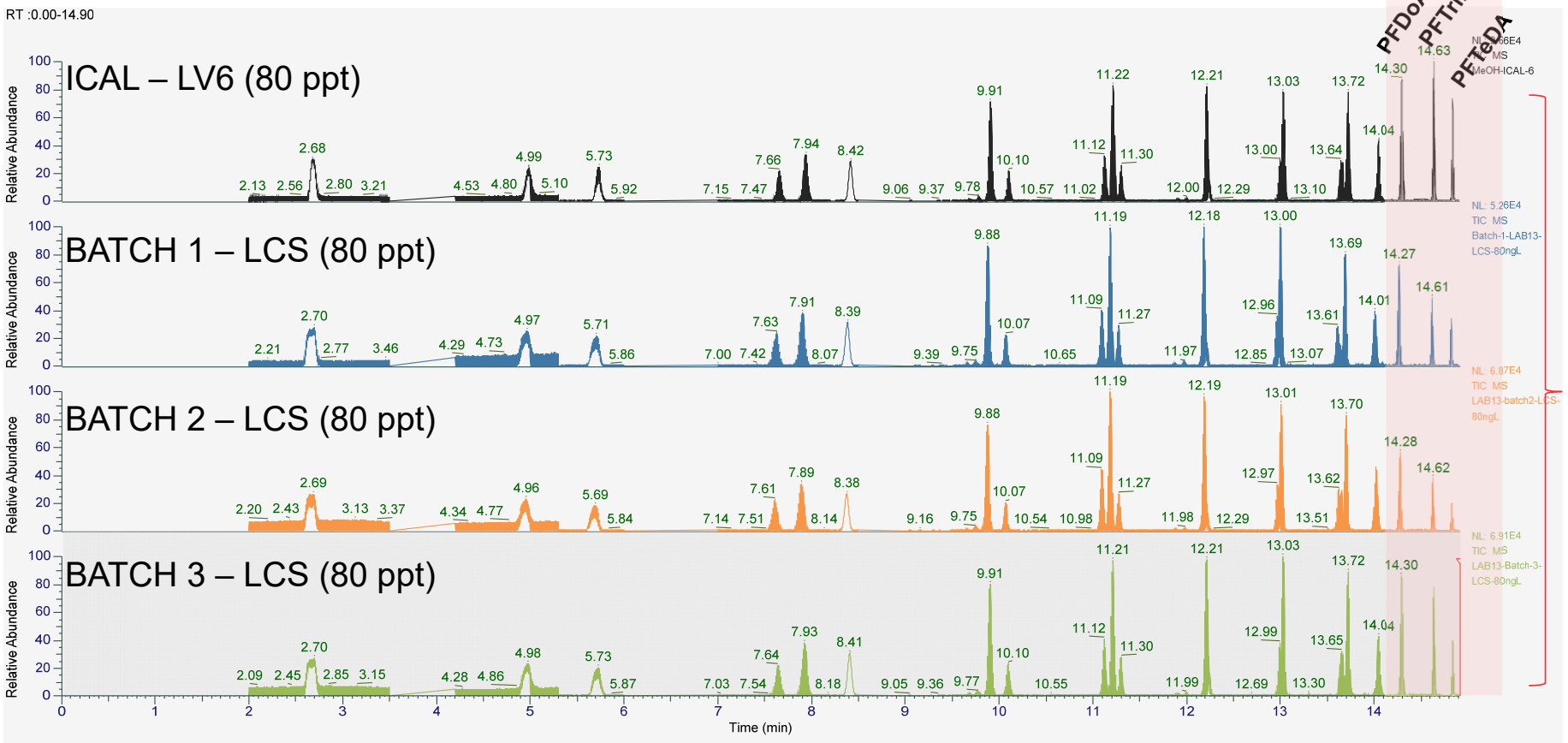
RSD < 20% for majority of the compounds among different water matrices.
All of the Reagent Water RSD <20%

	GROUND WATER				REAGENT WATER				SURFACE WATER				WASTE WATER			
N = 5	Low level spike		High level spike		Low level spike		High level spike		Low level spike		High level spike		Low level spike		High level spike	
Target compounds	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %	Average (ppt)	RSD %
N1_PFTeDA	26.13	12%	69.5	12%	24.43	10%	71.84	6%	26.78	18%	82.63	13%	23.92	11%	77.91	4%
N2-PFTrDA	22.81	11%	65.76	12%	22.29	9%	74.45	6%	23.8	17%	76.87	15%	22.24	8%	77.47	7%
N3-PFDoA	21.22	8%	64.08	12%	20.01	9%	73.25	9%	22.17	19%	71.55	14%	20.54	13%	75.8	9%
N4_PFUdA	22.05	11%	65.41	7%	21.23	12%	72.08	9%	23.19	21%	69.81	11%	21.74	12%	74.95	9%
N5_PFDA	22.98	9%	64.83	8%	21.63	11%	72.83	8%	23.55	17%	69.98	11%	23.16	3%	76.89	7%
N6-PFNA	22.29	8%	66.83	8%	21.21	9%	73.4	7%	23.15	16%	70.65	10%	22.7	9%	75.64	7%
N7-PFOA	22.89	12%	65.88	10%	21.26	9%	71.72	9%	24.15	15%	69.87	9%	27.08	8%	79.79	7%
N8-PFHpA	23.34	11%	65.96	11%	21.89	10%	72.23	8%	25.51	18%	69.48	11%	26.35	12%	77.48	9%
N9-PFHxA	22.33	12%	64.9	10%	21.05	8%	71.47	8%	23.36	16%	69.43	11%	40.48	7%	93.5	8%
N10_PFPeA	27.41	13%	63.44	11%	23.42	12%	71.5	10%	32.24	23%	67.87	9%	38.32	3%	84.01	10%
N11_PFBA	18.99	24%	64.11	4%	21.04	10%	70.09	6%	19.59	16%	63.82	6%	14.01	45%	66.61	6%
N12-PFDS	20.79	14%	58.96	20%	18.2	14%	60.87	12%	22.02	24%	56.67	13%	19.43	24%	69.12	14%
N13-PFNS	20.32	27%	56.17	16%	19.67	8%	59.42	10%	20.08	17%	57.1	12%	18.19	20%	63.55	9%
N14-PFOS	22.57	20%	60.07	8%	21.26	16%	63.04	9%	24.71	14%	62.52	10%	24.29	10%	75.43	13%
N15-PFHpS	20.81	12%	61.61	9%	19.53	11%	67.95	10%	21.7	17%	63.27	10%	19.43	15%	71.37	10%
N16-PFHxS	19.69	15%	59.56	10%	18.38	10%	63.56	9%	20.89	14%	61.66	7%	19.94	11%	67.58	9%
N17-PFPeS	20.32	11%	62.4	9%	19.35	6%	65.83	9%	21.52	18%	63.48	8%	19.87	10%	68.3	9%
N18-PFBS	22.55	13%	61.07	10%	19.98	11%	63.39	10%	21.34	26%	61.46	9%	24.88	15%	52.03	36%
N19-PFOSA	20.51	15%	60.19	12%	18	10%	60.89	12%	22.6	17%	63.44	10%	19.66	10%	67.62	9%
N20_FtS8_2	22.18	7%	63.6	6%	21.55	10%	69.86	8%	20.12	18%	66.8	8%	21.51	8%	71.42	7%
N21-FtS6_2	20.64	13%	64.29	11%	21.46	17%	69.2	7%	29.54	37%	80.12	13%	33.15	25%	82.55	11%
N22-FtS4_2	21.11	6%	62.04	5%	20.4	11%	69.78	6%	21.02	15%	65.49	11%	19.75	7%	69.17	8%
N23_NEtFOSAA	23.66	12%	63.56	11%	22.96	18%	70.55	7%	23.72	25%	70.56	14%	22.16	16%	76.7	8%
N24_NMeFOSAA	23.88	9%	65.42	9%	21.8	8%	73.34	7%	23.97	17%	71.28	8%	22.9	10%	73.38	7%

Perfluorotri- and tetradecanoic acids (PFTriDA and PFTeDA): solubility issues

Variable recoveries obtained due to their low solubility in water (highest spike concentration was diluted in 50:50 methanol: water)

Increasing proportion of methanol or changing to acetonitrile could improve recovery



variable recoveries at same concentration

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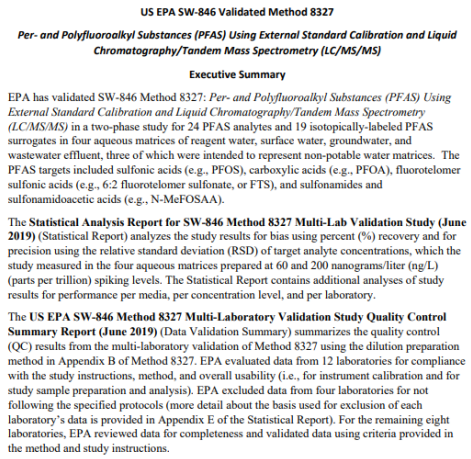
Summary

- ✓ **TSQ Altis** is able to quantitate at 5 ppt the list of PFCs listed in EPA draft SW-846 method 8327 using direct injection (2-fold dilution not taken into consideration)
- ✓ **TSQ Altis** is able to quantitate certain PFCs 5 times lower than the LLOQ reported by EPA
- ✓ **Thermo Accucore RP** provides excellent performance as described in EPA draft SW-846 method 8327
- ✓ Retention time stability was very good inter-batch
- ✓ Large injection volumes overload the analytical columns and chromatographic peak fronting is observed. Reduced injection volumes maintain sensitivity and improve assay robustness.
- ✓ Longest chain perfluorocarboxylic acids showed high variability within batches mainly due their low solubility in water (higher spike concentration)
- ✓ EPA field samples showed RSDs below 20% for most of the compounds among different water matrices

Update EPA SW-846 Validation Study Conclusions

- *…. The performance for 6:2 fluorotelomer sulfonate (6:2 FTS) was erratic, with high average recovery and high RSDs in some matrices and spike levels.*
- *With the exception of 6:2 FTS, the target analytes in the **study generally met the precision and bias criteria defined in the method and study instructions.** The principal problems laboratories encountered with preparation and analysis of study samples were retention of the target analytes and surrogates in solution*



US EPA SW-846 Validated Method 8327

Per- and Polyfluoroalkyl Substances (PFAS) Using External Standard Calibration and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS)

Executive Summary

EPA has validated SW-846 Method 8327: *Per- and Polyfluoroalkyl Substances (PFAS) Using External Standard Calibration and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS)* in a two-phase study for 24 PFAS analytes and 19 isotopically-labeled PFAS surrogates in four aqueous matrices of reagent water, surface water, groundwater, and wastewater effluent, three of which were intended to represent non-potable water matrices. The PFAS targets included sulfonic acids (e.g., PFOS), carboxylic acids (e.g., PFOA), fluorotelomer sulfonic acids (e.g., 6:2 fluorotelomer sulfonate, or FTS), and sulfonamides and sulfonamidoacetic acids (e.g., N-MeFOSAA).

The **Statistical Analysis Report for SW-846 Method 8327 Multi-Lab Validation Study (June 2019)** (Statistical Report) analyzes the study results for bias using percent (%) recovery and for precision using the relative standard deviation (RSD) of target analyte concentrations, which the study measured in the four aqueous matrices prepared at 60 and 200 nanograms/liter (ng/L) (parts per trillion) spiking levels. The Statistical Report contains additional analyses of study results for performance per media, per concentration level, and per laboratory.

The **US EPA SW-846 Method 8327 Multi-Laboratory Validation Study Quality Control Summary Report (June 2019)** (Data Validation Summary) summarizes the quality control (QC) results from the multi-laboratory validation of Method 8327 using the dilution preparation method in Appendix B of Method 8327. EPA evaluated data from 12 laboratories for compliance with the study instructions, method, and overall usability (i.e., for instrument calibration and for study sample preparation and analysis). EPA excluded data from four laboratories for not following the specified protocols (more detail about the basis used for exclusion of each laboratory's data is provided in Appendix E of the Statistical Report). For the remaining eight laboratories, EPA reviewed data for completeness and validated data using criteria provided in the method and study instructions.

https://www.epa.gov/hw-sw846/validated-test-method-8327-and-polyfluoroalkyl-substances-pfas-using-external-standard

PFAA Workflows

- **Drinking Water – EPA 537.1**
- Offline SPE

AutoTrace – Peek free

- **Surface and Ground Water – EPA 8327**
- Direct Injection

Chromeleon

Tracefinder

Peek Free trap columns and tubing kits available

Secondary validation study for EPA Method 537.1 using automated SPE followed by LC-Q Exactive Orbitrap MS

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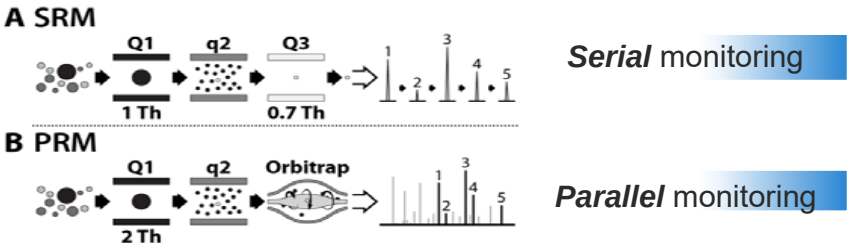

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EPA 537.1 Method Aspects

- 250 mL Water sample fortified with Surrogates and passed through SPE cartridge. (polystyrenedivinylbenzene) Solex HRPHS
- Concentrated to 1 mL in methanol:water (96%:4%)
- 10 µL injection
- 18 PFAS compounds including ADONA
- Calibration with 3 internal Standards
- Extraction efficiency calibrated with 4 Surrogates
- Changes cannot be made to:
  - Sample collection
  - Preservation
  - Sample extraction steps
  - QC requirements
- LC recommend flushing with Methanol for 20 min. prior to injection + Trap column

EPA 537.1 Method Validation Requirements

- Demonstration of low background is below 1/3 the MRL.
- Demonstrate precision 4 to 7 lab reagent blanks for RSD < 20%
- Recoveries of 4-7 lab fortified blank recoveries are 70% - 130%
- Precision and accuracy for mid lab fortified matrix and lab fortified sample matrix (LFSM) and duplicate (LFSMD) recoveries between 70-130% and RSD < 30%.
- Perform the Lowest Concentration Minimum Reporting Level (LCMRL). The LCMRL is the lowest spiking concentration where the probability of spike recovery in the 50% to 150% range is at least 99%. It differs from MDL studies because it also accounts for accuracy beside precision.

Spike Recoveries from blank reagent water using Orbitrap® Technology

Compound	Average Concentration (ng/L)	Theoretical Concentration (ng/L)	% Difference	% Recovery	Limit	% RSD
PFBS	26.719	25.000	6.87	107%	70-130%	4.76
PFHxA	26.166	25.000	4.66	105%	70–130%	3.59
GenX	25.459	25.000	1.83	102%	70–130%	4.61
PFHxS	25.739	25.000	2.95	103%	70–130%	2.13
PFHpA	24.744	25.000	-1.02	99%	70–130%	2.77
ADONA	22.629	25.000	-9.48	91%	70–130%	5.52
PFOA	28.394	25.000	13.57	114%	70–130%	3.24
PFOS	27.329	25.000	9.32	109%	70–130%	2.89
PFNA	26.596	25.000	6.39	106%	70–130%	4.60
9Cl-PF3ONS	25.982	25.000	3.93	104%	70–130%	5.49
PFDA	25.791	25.000	3.16	103%	70–130%	5.08
11CL-PF3OUdS	24.883	25.000	-0.47	100%	70–130%	5.49
NMeFOSAA	25.722	25.000	2.89	103%	70–130%	5.36
PFUnA	27.007	25.000	8.03	108%	70–130%	5.64
NEtFOSAA	25.534	25.000	2.14	102%	70–130%	6.66
PFDoA	26.028	25.000	4.11	104%	70–130%	5.36
PFTrDA	24.620	25.000	-1.52	98%	70–130%	5.13
PFTA	25.489	25.000	1.96	102%	70–130%	3.70

Spike Recoveries from 4 Tap water samples using Orbitrap® Technology

	Spike (ng/L)	LFSM	LFSM	LFSM	LFSM	Average	STDEV	%REC.	%RSD
PFBS	25	19.8	21.4	25.1	25.5	23.0	2.8	91.9%	12%
11CL-PF3OUdS	25	21.1	22.7	24.2	24.8	23.2	1.7	92.9%	7%
9Cl-PF3ONS	25	22.0	22.1	26.7	25.9	24.2	2.5	96.6%	10%
ADONA	25	18.2	19.8	19.4	19.6	19.2	0.7	77.0%	4%
GenX	25	22.0	23.0	24.4	24.4	23.4	1.2	93.8%	5%
NEtFOSAA	25	21.2	21.8	24.2	24.4	22.9	1.6	91.6%	7%
NMeFOSAA	25	20.6	22.4	24.3	26.0	23.3	2.3	93.3%	10%
PFDA	25	21.7	22.7	24.6	25.7	23.7	1.8	94.7%	8%
PFDoA	25	21.6	24.0	24.8	26.0	24.1	1.9	96.3%	8%
PFHpA	25	19.6	21.3	24.0	24.2	22.3	2.2	89.1%	10%
PFHxA	25	20.9	22.0	24.4	25.1	23.1	2	92.3%	9%
PFHxS	25	20.6	22.2	23.5	23.5	22.5	1.4	89.8%	6%
PFNA	25	23.5	23.5	25.9	26.2	24.8	1.5	99.2%	6%
PFOA	25	22.0	23.1	24.8	25.3	23.8	1.5	95.2%	6%
PFOS	25	22.5	24.0	25.6	26.2	24.6	1.7	98.3%	7%
PFTA	25	21.9	23.2	26.9	28.0	25.0	2.9	100.0%	12%
PFTrDA	25	21.3	23.1	25.5	25.4	23.8	2	95.3%	9%
PFUnA	25	22.2	24.8	26.1	26.5	24.9	1.9	99.5%	8%

DL and LCMRL comparisons

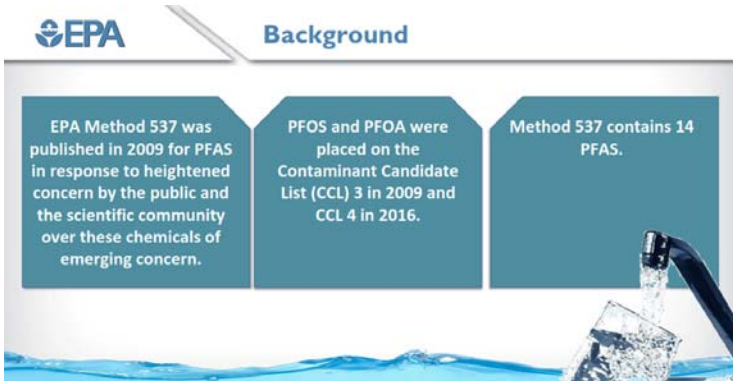
Analyte	DL (ng/L)	LCMRL (ng/L)
PFBS	0.42	2.5
PFHxA	0.22	0.71
GenX	0.34	1.1
PFHpA	0.18	1.3
PFHxS	0.17	0.38
ADONA	0.15	0.25
PFOA	0.16	0.73
PFOS	0.11	0.5
PFNA	0.3	0.58

Analyte	DL (ng/L)	LCMRL (ng/L)
9Cl-PF3ONS	0.14	0.29
PFDA	0.26	0.34
NMeFOSAA	0.24	0.44
PFUnA	0.45	0.64
NEtFOSAA	0.21	0.34
11CL-PF3OUdS	0.33	0.43
PFDoA	0.78	2.5
PFTrDA	0.13	0.58
PFTA	0.1	0.56

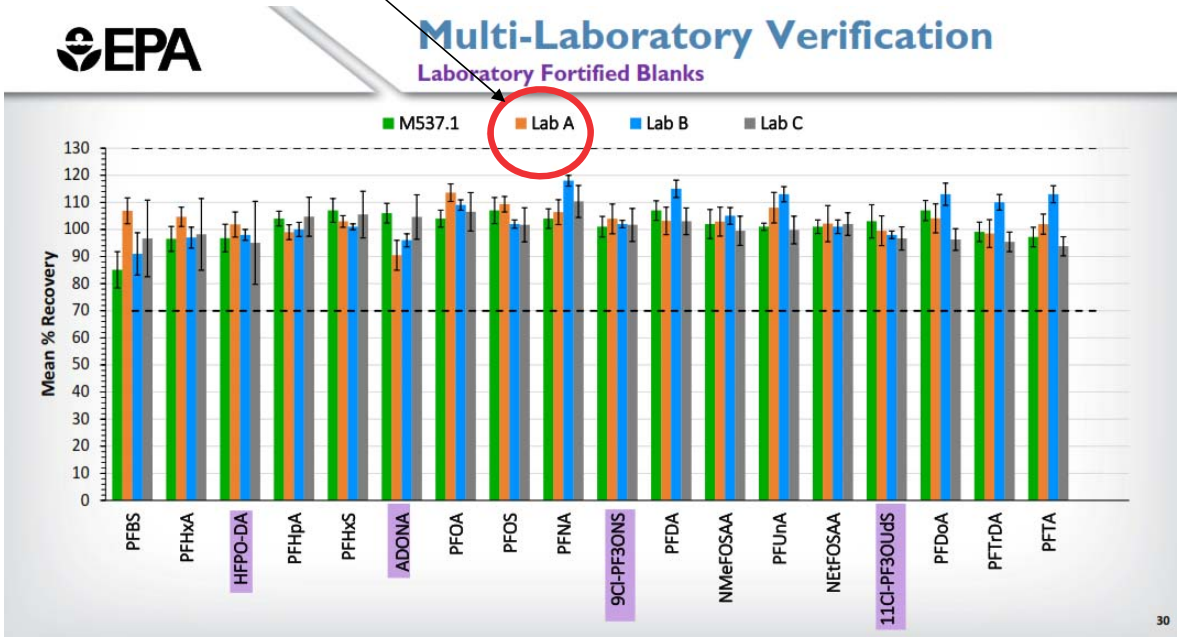
- For the LCMRL calculation, four replicates at concentrations of 0, 0.25, 0.5, 1, 2, 4, 8, 12, and 16 ng/L were extracted and analyzed. The LCMRL and DL were calculated using the LCMRL calculator from the EPA website: http://water.epa.gov/scitech/drinkingwater/labcert/analyticalmethods_ogwdw.cfm

Regulatory Participation – Drinking Water EPA 537.1

- Method Validation - 4 labs
  - QE+; PRM mode (lab A)
  - NJ Dept of public health
    - QQQ
  - EPA region 2
    - QQQ
  - EPA OGWDW
    - QQQ



Ali Haghani,
Eurofins Eaton



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What Type of MS can I use?

- 6.12.2. LC/TANDEM MASS SPECTROMETER –

- …capable of negative ion electrospray ionization (ESI) near the suggested LC flow rate of 0.3 mL/min.
- …capable of performing MS/MS to produce unique product ions … within specified retention time segments.
- A minimum of 10 scans across the chromatographic peak.

Environmental Solutions: Equipping customers to detect regulated and emerging contaminants

Mass spectrometry for regulatory method validation

- Active engagement with global regulatory agencies in co-development of methods
- Latest technology and applications
- Compliance monitoring
- Address emerging concerns over PFAS in:
  - Drinking water
    - EPA 537.1
    - Method validation – 14 PFAS, 3 labs
  - Ground, surface and waste water
    - EPA 8327
    - Method validation – 24 PFAs

"*We use the Q Exactive for both unknown screening and accurate quantitation for environmental contaminants in potable water, recently for the validation of updated EPA 537.1 for Perfluorinated organics with the EPA Office of Ground Water and Drinking Water. We've found it to be a flexible tool for our needs.*"

eurofins

Ali Haghani, R&D Manager
Eurofins Eaton Analytical, LLC

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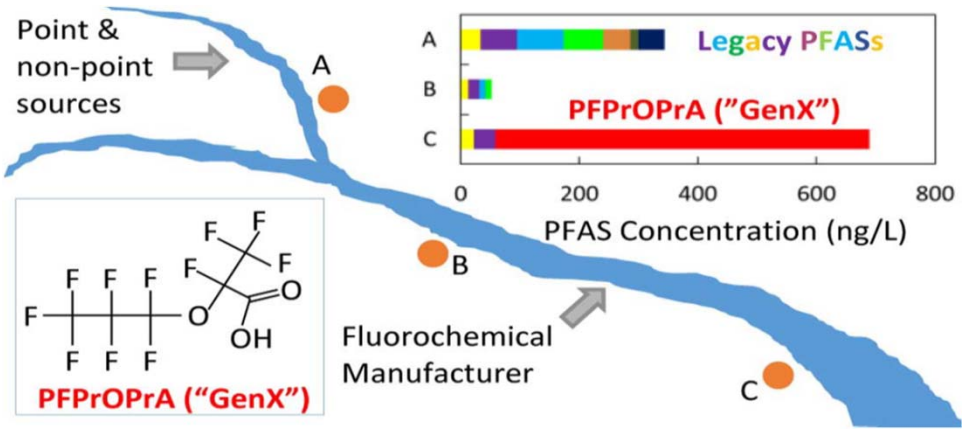
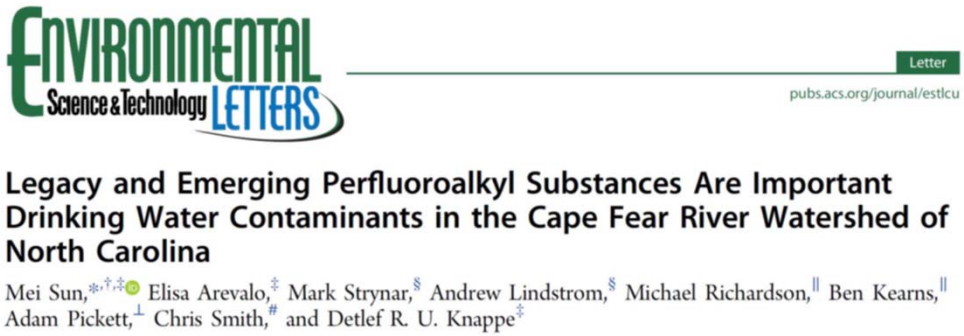
High Resolution Mass Spectrometry for Site Specific Emerging Contaminants.

- EPA methods search for known PFAA's
  - 24 in 8327
- However there are > 4000 PFAA possible forms
- There are also precursors, unknown breakdown products.
  - Toxicity and prevalence are unknown
  - Standards are not available

- HRAM is the only approach capable to determine "what's out there"





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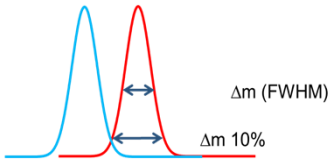
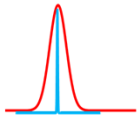
Two Important Aspects of High Resolution Accurate Mass. (Q Exactive Orbitrap ®)

Resolution

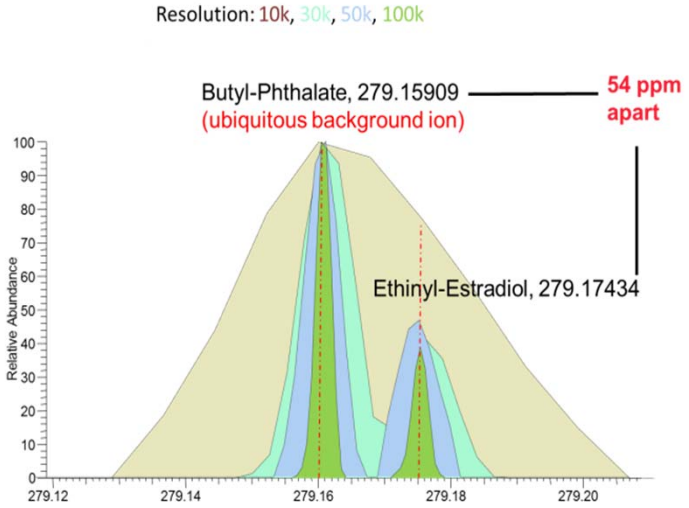
$$R = \frac{m}{\Delta m}$$



- Quadrupole MS $R = \frac{m}{\Delta m} = \frac{500}{0.6} = 833$



- Orbitrap MS $R = \frac{m}{\Delta m} = \frac{500}{0.0035} = 140000$



Mass Accuracy

$$\Delta m / z = \frac{m_{meas} - m_{true}}{m_{true}} \cdot 10^6$$

- Quadrupole MS $\Delta m / z = \frac{500.1 - 500.0}{500} \cdot 10^6 = 200 ppm$

- Orbitrap MS TOF MS $\Delta m / z = \frac{500.10314 - 500.10214}{500.10314} \cdot 10^6 = 2 ppm$

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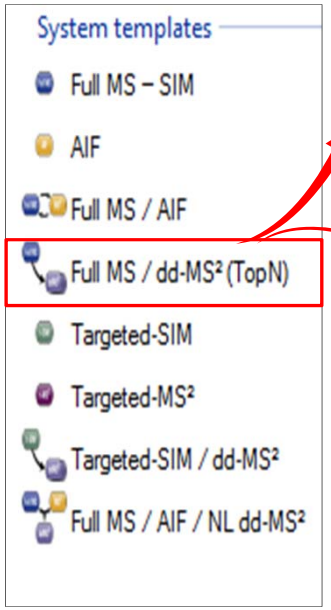
Q Exactive Analysis Set Up

- Step 1.
  - Full MS/data dependent MS^2
- Step 2.
  - Rescreen for suspected contaminant classes



- full MS:resolution 140,000 FWHM
  scan range100-1500 m/z
- ddMS^2:resolution 35,000 FWHM
  Inclusion list on
  isolation 1 m/z
  exclusion 5 s
  NCE 10,40,200

List of 146 PFAS target analytes

	Mass [m/z]	Formula [M]	Formula type	Species	CS [z]	Polarity
1	178.97731	C3HF5O3	Chemical formula	M-H	1	Negative
2	112.9857	C2HF3O2	Chemical formula	M-H	1	Negative
3	148.9526	CF3SO3H	Chemical formula	M-H	1	Negative
4	162.9823	C3F5O2H	Chemical formula	M-H	1	Negative
5	178.9773	C3HF5O3	Chemical formula	M-H	1	Negative
6	197.9654	C2HF5SO2NH	Chemical formula	M-H	1	Negative
7	198.9494	C2HF5SO3	Chemical formula	M-H	1	Negative
8	212.9792	C4HF7O2	Chemical formula	M-H	1	Negative
9	228.97411	C4HF7O3	Chemical formula	M-H	1	Negative
10	241.9916	C4H5F5NSO3H	Chemical formula	M-H	1	Negative
11	242.01723	C6H5F7O2	Chemical formula		1	Negative
12	244.96903	C4HF7O4	Chemical formula	M-H	1	Negative
13	247.9616	C3HF7NSO2H	Chemical formula	M-H	1	Negative
14	247.9622	C3HF7SO2NH	Chemical formula	M-H	1	Negative
15	248.9461	C3HF7SO3	Chemical formula	M-H	1	Negative
16	262.97601	C5HF9O2	Chemical formula	M-H	1	Negative
17	264.02022	C6H5F9O	Chemical formula		1	Negative
18	276.9411	C4F7SO4H	Chemical formula	M-H	1	Negative
19	278.97092	C5HF9O3	Chemical formula	M-H	1	Negative
20	282.9481	C4HF9SO2	Chemical formula	M-H	1	Negative
21	291.9884	C5H5F7NSO3H	Chemical formula	M-H	1	Negative
22	297.9584	C4HF11NSO2H	Chemical formula	M-H	1	Negative
23	298.94299	C4F9SO3	Chemical formula		1	Negative
24	310.9607	C5HF9O5	Chemical formula	M-H	1	Negative
25	310.96075	C5HF9O5	Chemical formula	M-H	1	Negative
26	312.97281	C6HF11O2	Chemical formula	M-H	1	Negative
27	325.96647	C6H4F9SO3	Chemical formula	M-H	1	Negative

…
…
…
146

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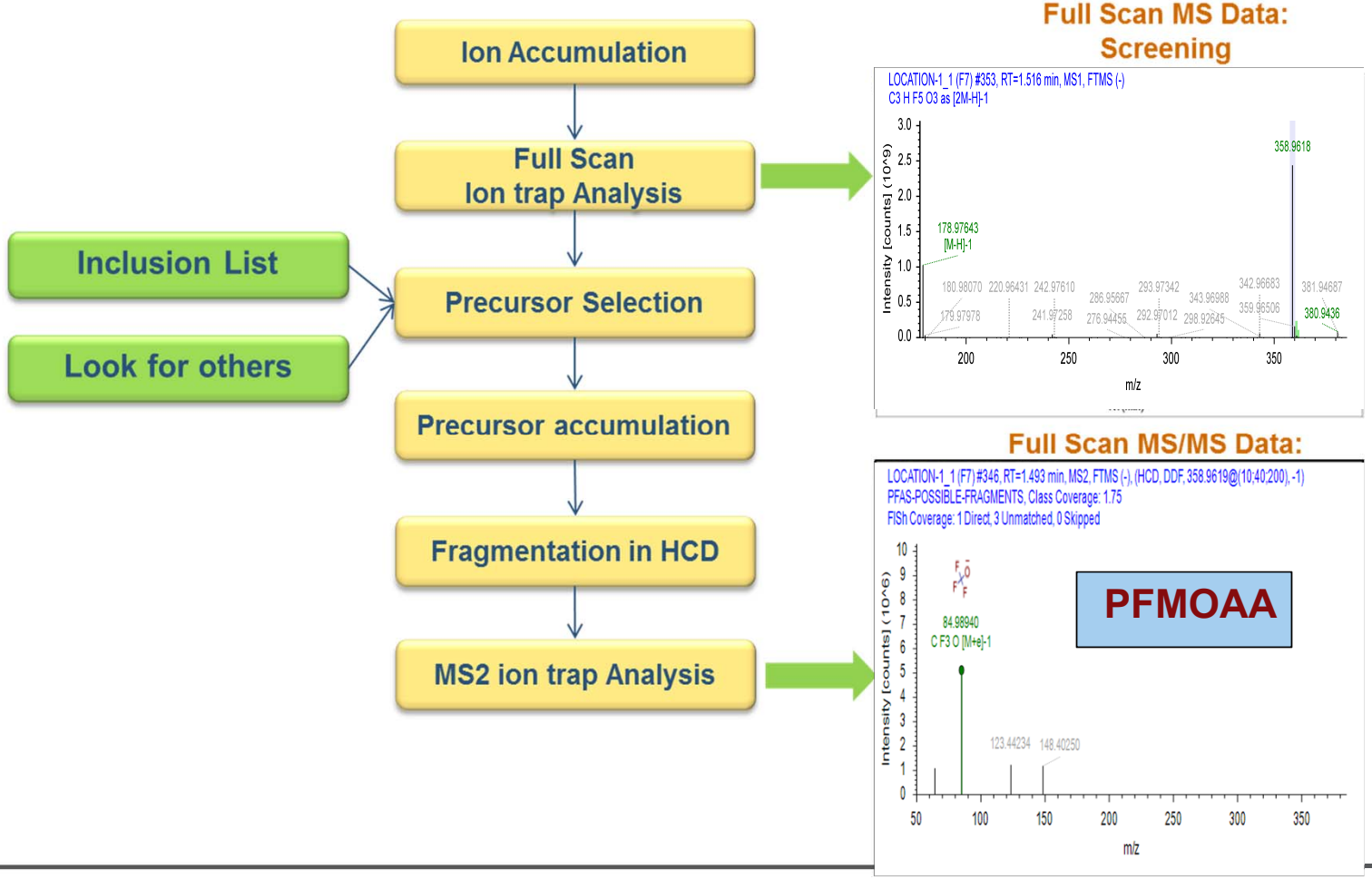
FS-ddMS2 Screening Process



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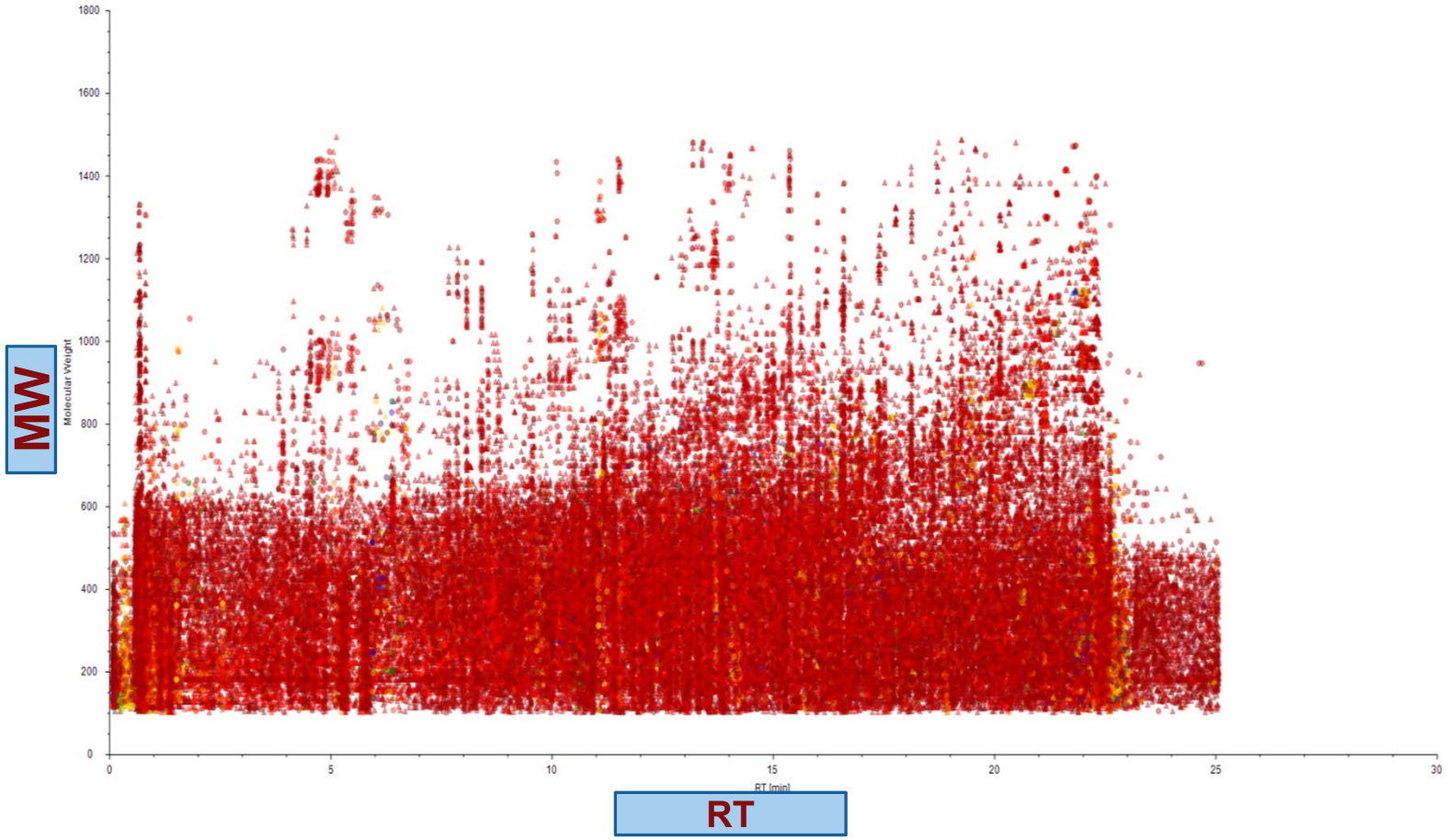
Large Data Files Showing > 83000 Data Points To Mine Through.



Data provided by Eurofins Eaton

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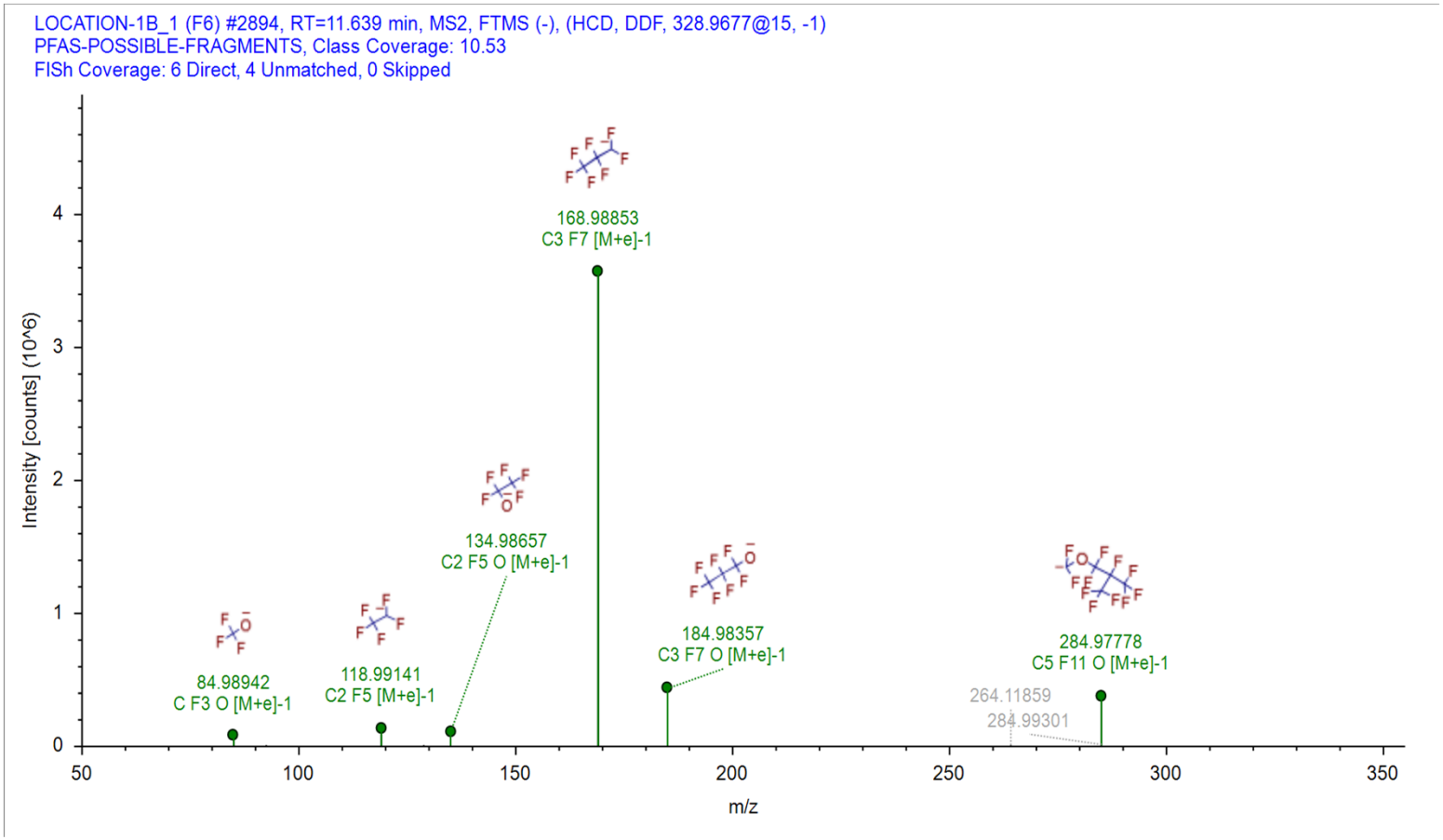
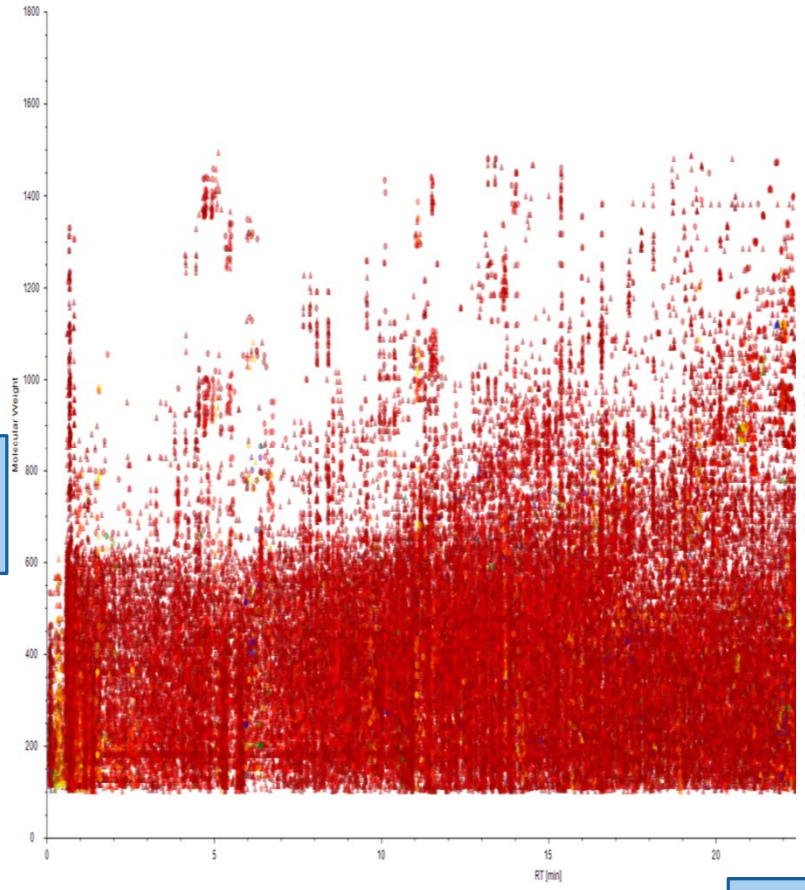
GenX Continued: Fragments From a Std are Shown

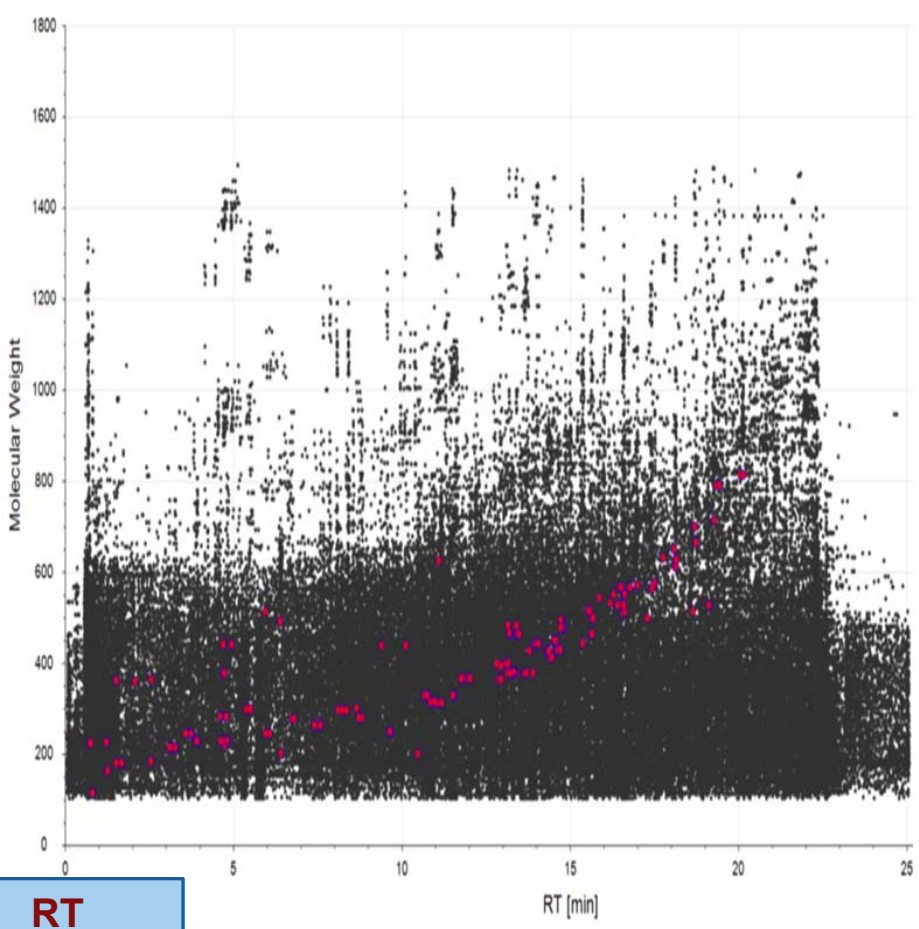


Data provided by Eurofins Eaton

Showing the Non Target Candidates on the Right.

MW





RT

Data provided by Eurofins Eaton

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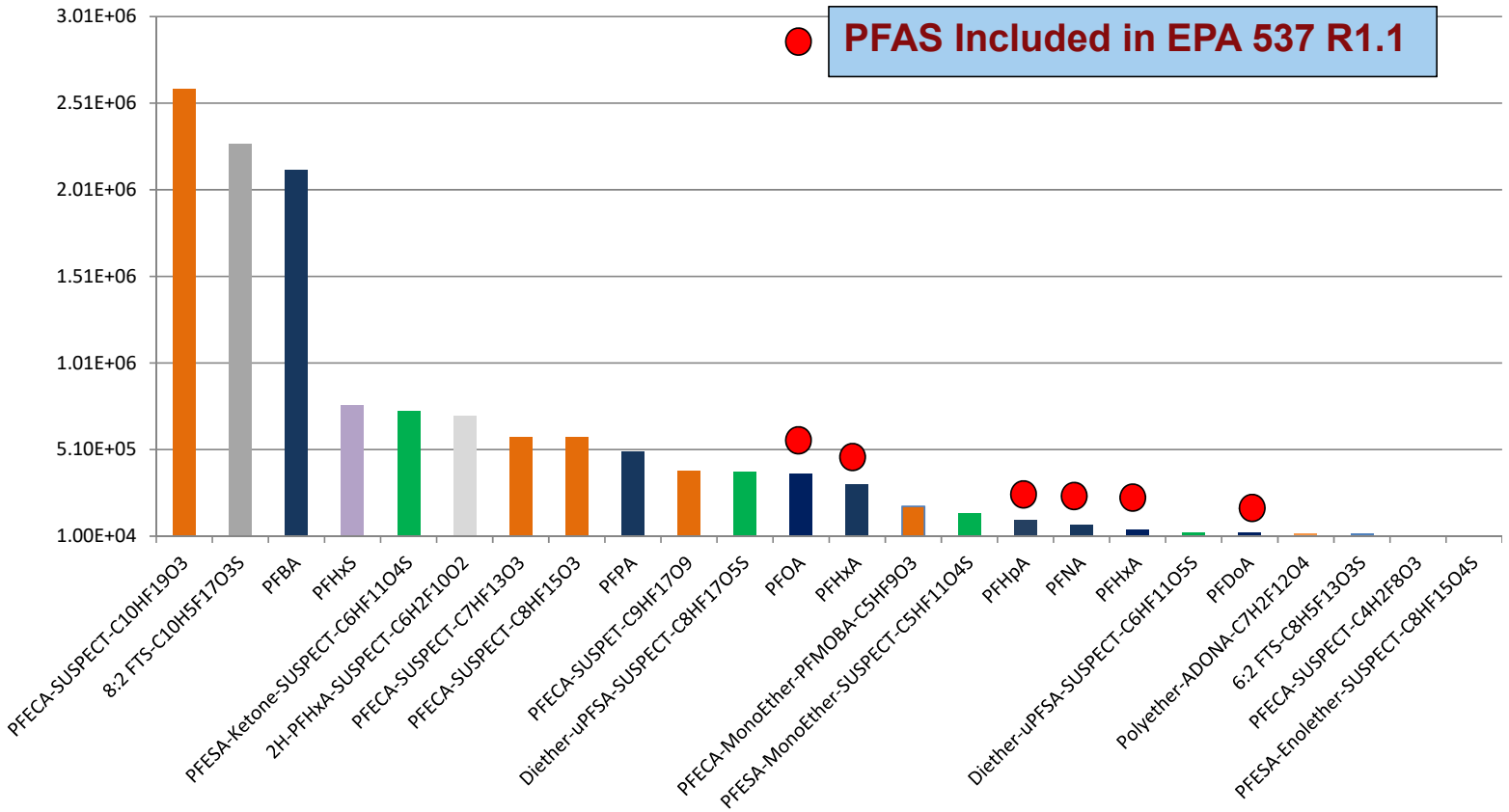
PFAA's found in > Conc. than required by EPA 537.1/8327



Data provided by Eurofins Eaton

44 Total suspects/hits from a single sample (NC).

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In-house SB Test Results of DW (NC)

- 39 legacy and GenX were quantitated.
  - 13 PFAS were detected.
  - 26 PFAS were not detected.
- Four **new** PFECA and two Nafion BPs were estimated.
  - 5 new PFAS were detected.
  - 1 new PFAS was not detected.

Data provided by Eurofins Eaton

In-House Results of 147 DW Samples (NC)

- PFAA in red are those measure in EPA 537.1
- Health effects known *only* for PFOA and PFOS
- Only by using Orbitrap ® technology can we find unknowns present.
- There are unknowns:
  - > conc.
  - whose health effects are unknown
- The discovery of unknowns can't be determined using MS/MS technology

Compound	Highest Conc. ng/L	Mean Conc. ng/L	% of Results ≥ MRL	% of Results > HA
PFPeA	59	25	95	---
PFHxA	74	25	90	---
PFBA	26	14	86	---
PFHpA	50	13	79	---
PFOA	24	6	77	0
PFBS	12	2	60	---
PFOS	52	4	35	0
PFHxS	43	<2	30	---
PFNA	6	<2	21	---
PFDA	6	< 2	15	---
PFPeS	8	<2	0.7	---
NEtFOSAA	10	< 2	0.1	---

Data provided by Eurofins Eaton

EPA 537 & In-house SB Test Results: Emerging PFAS (NC)

Compound	# of Sample	Highest Conc. ng/L	Mean Conc. ng/L	Median Conc. ng/L	% of Results ≥ 5 ng/L
GenX (DW)	288	230	14	< 5	43
GenX (GW)	181	179	16	< 5	48

MRL Confirmation Study

	Mean	sd	HPIR	Lower PIR >50%	Upper PIR <150%
GenX	4.58	0.334	1.322	65	118

Data provided by Eurofins Eaton

In-house SB Test: 6 Non-Target PFAS (PFECAs)

Compound	Acronym	Reference	Highest Conc. ng/L	% of Results ≥ 5 ng/L
Perfluoro-2-methoxyacetic acid	PFMOAA	GenX	5560	98
Perfluoro (3,5-dioxahexanoic) acid	PFO2HxA	GenX	180	80
Perfluoro (3,5,7-trioxaoctanoic) acid	PFO3OA	GenX	109	55
Perfluoro (3,5,7,9-tetraoxadecanoic) acid	PFO4DA	GenX	31	33
Nafion Byproduct 1	Nafion BP1	---	< 5	0
Nafion Byproduct 2	Nafion BP2	Nafion BP1	33	35

Data provided by Eurofins Eaton

Conclusion

Mass spectrometry for regulatory method validation

- MS/MS and Orbitrap® MS systems have been shown to provide equivalent quantitation for EPA method validation studies.
- Address emerging concerns over PFAS in:
  - Drinking water
    - EPA 537.1
  - Ground, surface and waste water
    - EPA 8327
- Orbitrap® Technology is ideal for both nontargeted screening and quantitation of PFAS compounds.

Thank you