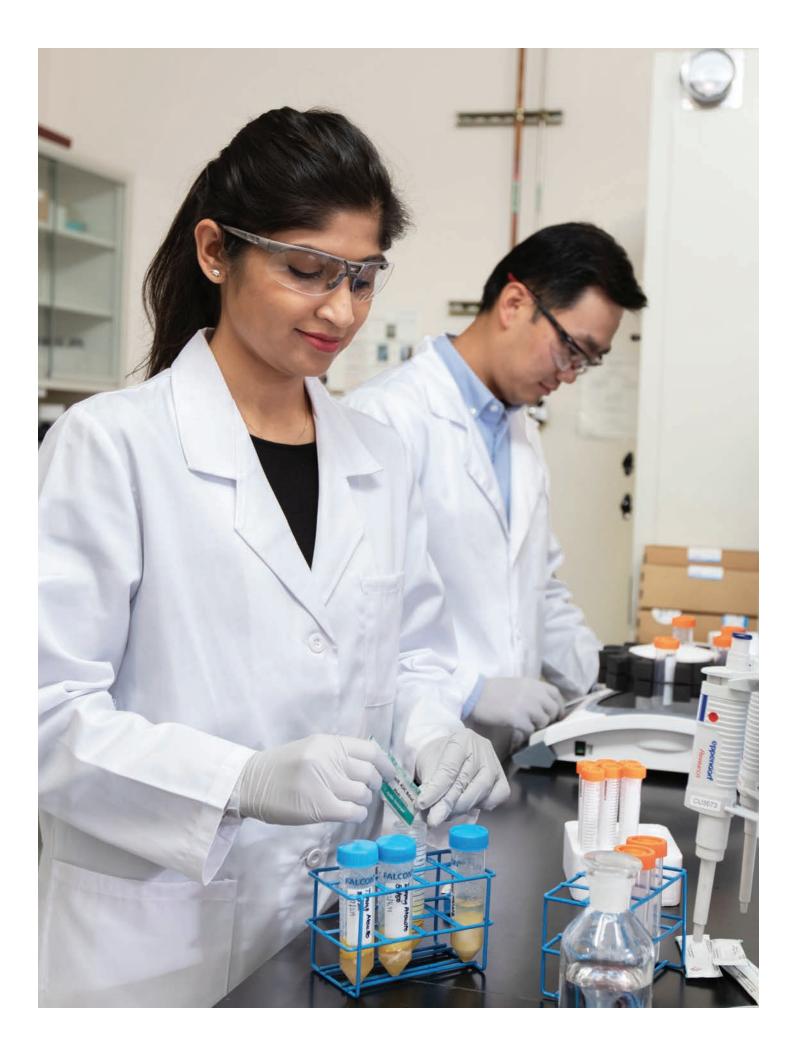


Prepare to Meet the Challenges of a Regulated PFAS Landscape





A Public Health Crisis Decades in the Making

Per- and polyfluoroalkyl substances (PFAS) are man-made substances widely used in industry and manufacturing because of their unique properties. These compounds have been used for several decades in many applications like nonstick cookware, stain-repellent clothing, food packaging materials, detergents, cleaning products, and firefighting foams. The widespread use of these compounds has led to their ubiquity in the environment. Studies have indicated that PFAS are also present in most humans. Research on these compounds has identified them as being persistent and bioaccumulative (especially PFAS with a carbon chain length $>C_7$). Toxic effects, including tumors and thyroid disruption, have also been attributed to some of them.¹ This has resulted in regulatory guidance for water and soil, as well as accelerated monitoring and identification of these compounds.

¹US EPA. 2020. Basic Information On PFAS | US EPA.



Firefighting foams often contain PFAS to assist in dousing flames.

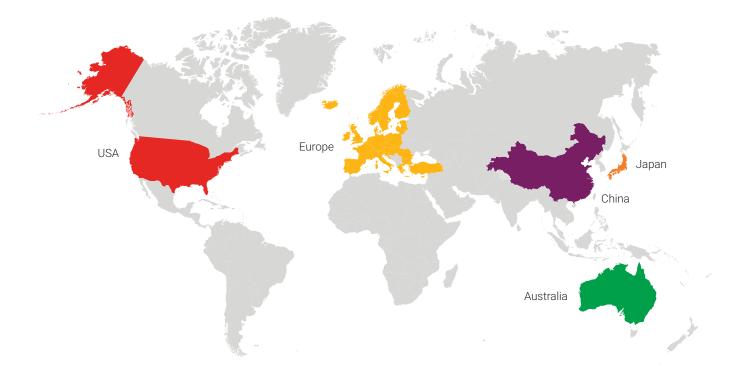
Regulatory Overview



There are >4,000 known PFAS compounds that have been created for commercial use. Regulatory guidance and restrictions exist for just a few of them, leading to unrestricted use for the rest.

- In 2009, perfluorooctanesulfonic acid (PFOS) and its salts were listed as persistent organic pollutants (POPs) under the *Stockholm Convention*. All parties are required to eliminate the release of these compounds into the environment.
- The European Union (EU) Water Framework Directive lists PFOS as a priority hazardous substance that poses a "significant risk to the aquatic environment." It has established an annual average environmental quality standard (AA-EQS) of 0.65 ng/L in inland surface waters, and an AA-EQS of 0.13 ng/L for other surface waters (Directive 2013/39/EU). The EU drinking water directive aims to have routine monitoring of up to 20 PFAS compounds in drinking water from 2021.
- The UK Chemical Investigation Program requires measurement of PFOS and perfluorooctanoic acid (PFOA) down to 0.09 ng/L. Similarly, in October 2018, the EU Parliament approved a proposal to recast its Drinking Water Directive with revised limits for monitoring PFOS and PFOA in drinking water. The new limits are 100 ng/L, with combined PFAS concentrations not to exceed 500 ng/L (COM (2017) 753 1.2.2018).
- Several European countries, including those in the *Nordic region*, have guidance levels for PFAS in drinking water and surface water. In *Sweden*, recommended levels for a sum of 11 PFAS in drinking water should not exceed 90 ng/L.
- In the United States, the US EPA has established a drinking water health advisory level for PFOS and PFOA at a combined 70 ppt (ng/L). Several states have their own advisories for PFOA, PFOS, and other PFAS—such as perfluorononanoic acid (PFNA) and GenX—at the low ppt range. Other initiatives are also in the works. These include the PFAS Action Act (Jan 2019), the US EPA PFAS Plan (Feb 2019), and the US EPA Commitment to PFAS Drinking Water Standards (Feb 2019).
- Australia, China, and several other countries are implementing restrictions (or establishing maximum amounts) for drinking water and receiving water regulations for PFOA, PFOS, and newer PFAS detected at low ng/L to pg/L levels.

As newer PFAS are identified in the environment, and as more toxicological information becomes available, further guidelines and regulations are almost certain.



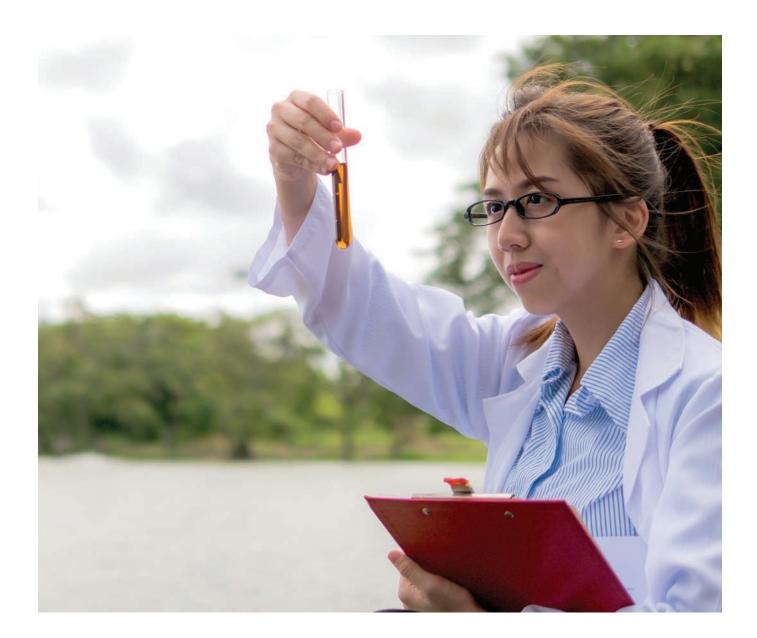
Worldwide regions where strict PFAS monitoring regulations are being enacted.

Current Standards and Consensus methods for PFAS analysis in the environment.

Method	Matrix Tested	No. of Analytes	Sample Preparation Procedure	Quantification Technique
EPA 533	Drinking water	25	Solid phase extraction	Isotope dilution
EPA 537	Drinking water	14	Solid phase extraction	Internal standard correction
EPA 537.1	Drinking water	18	Solid phase extraction	Internal standard correction
EPA 8327 (draft)	Surface water, groundwater, wastewater influent and effluent	24	Dilute and shoot	External calibration (isotope dilution also allowed)
ASTM 7979	Surface water, groundwater, wastewater influent and effluent	21	Dilute and shoot	External calibration (isotope dilution also allowed)
ASTM 7968	Soil and solids	21	Organic extraction with MeOH	External calibration
ISO/DIS 21675	Drinking water, sea water, fresh water, wastewater (<0.2% solids)	30	Solid phase extraction	Internal standard correction

Sample Preparation Techniques to Maximize PFAS Recoveries and Minimize Contamination

Due to their widespread use in clothing, protective gear, and consumer products, PFAS have been found in human and environmental samples in all regions of the world. Use these best practices to avoid contaminating your sample with PFAS during collection and storage.



Do:

- Wear well-washed lab coats and nitrile lab gloves.
- Use high-density polyethylene (HDPE) or polypropylene (PP) containers and caps as recommended in US EPA and ASTM methods.
- Refrigerate samples below 6 °C during storage.

Don't:

- Wear personal care products (such as sunscreen and hand creams) during sampling.
- Wear waterproof clothing or shoes that may be lined with PFAS or stain-repellent material.
- Use sample collection apparatus that may contain polytetrafluoroethylene (PTFE) or other plastics containing PFAS.
- Use aluminum foil to cover openings of sample containers, as PFAS can be transferred from foil.

Proper sample cleanup and concentration are essential to robust, accurate, and reliable analysis. As the world's chromatography leader, Agilent supports your efforts with innovative LC columns, solid phase extraction (SPE) cartridges, vials, and filters manufactured to demanding specifications. All are tested under strict conditions for reliable analysis of PFAS.



Extracting PFAS from water

Several regulatory methods, including EPA 537 and 533, call for extracting PFAS from drinking water using SPE cartridges followed by LC/TQ analysis. Typically, a weak anion exchange (WAX) cartridge is suggested due to its ability to extract both shorterand longer-chain PFAS with good recoveries as done in EPA 533 and ISO methods. EPA 537 uses an Agilent Bond Elut LMS cartridge, which provides high recoveries for medium- and long-chain PFAS.

From instruments, columns, and supplies, to fast, worldwide delivery, to decades of method development expertise—Agilent supports your entire workflow for PFAS testing.

Average recovery is between 40% and 70%
RSD is greater than 19%

All 30 PFAS were recovered, and US EPA 537 compounds had recoveries between 70 and 130% with RSD <15% for both water qualities. These results comply with US EPA method QA/QC requirements. In addition, only 4 of the 30 compounds had recoveries below 70%, but all 4 were above 40%. The 14 compounds in the US EPA method produced acceptable recovery using the Agilent WAX SPE cartridge. The 16 other PFAS, including compounds on the ASTM list, also had good recoveries and can be analyzed with this method.

Name	LC Grade Water Average Recovery	LC Water RSD (%)	Tap Water Average Recovery	Tap Water RSD (%)
EPA 537 Compou	inds			
PFBS	85	14	99	1
PFDA	101	5	95	6
PFDoA	86	3	88	2
PFHpA	105	10	101	3
PFHxS	97	15	102	1
PFHxA	104	8	107	2
PFNA	100	5	104	3
PFOS	92	13	94	3
PFOA	102	10	106	2
PFTrDA	91	3	103	15
PFUdA	100	6	102	3
PFTrDA	91	3	103	15
N-MeFOSAA	84	11	79	10
N-EtFOSAA	84	9	89	3
Additional Comp	ounds			
PFDoA	86	3	88	2
PFTeDA	96	10	86	8
FOSA	57	14	67	20
FHEA	107	6	90	8
FOEA	61	13	52	14
FDEA	56	21	58	15
PFHpPA	47	27	46	14
4-2 FTS	91	10	91	13
6-2 FTS	87	16	100	6
8-2 FTS	104	10	101	10
6-2 FTUA	118	8	106	3
8-2 FTUA	96	11	78	13
PFPeS	97	15	104	2
PFHpS	83	11	83	3
PFNS	93	12	91	8
PFDS	85	4	81	6

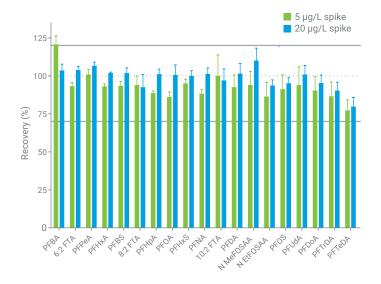
Want a closer look?

Read application note **5994-0250EN**: Extraction of Per/Polyfluoroalkyl Substances in Water Using Agilent Offline Solid Phase Extraction

Extracting PFAS in biota

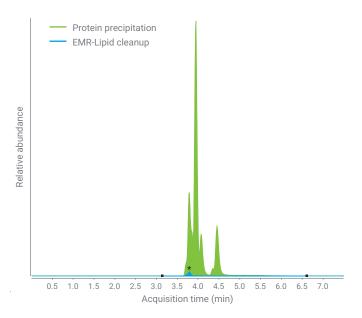
PFAS compounds are readily absorbed into animal and human tissue. Since these substances have been used in industry for many years, their existence in human blood and serum—as well as presence in fish, salmon, and other wildlife—is pervasive. Research has shown that longer chain PFAS (>C7) have the potential to bioaccumulate, increasing both the need and urgency to test and analyze for PFAS levels in biota and biological fluids.

SPE and supported liquid extraction (SLE) can be time consuming and complicated to perform on biological samples. Agilent Captiva EMR—Lipid makes it easy to remove interferences, particularly phospholipids, in minutes without PFAS loss. Its pass-through format is fast, repeatable, and delivers a clean extract with minimal ion suppression, extending column life and reducing the frequency of MS cleaning.



PFAS recovery fell between 70 and 130% with most compounds having an extraction recovery of >90%. The full procedure for extraction with Agilent Captiva EMR—Lipid is detailed in application note **5991-8656EN**, and shows how this simple technique can be performed in minutes.





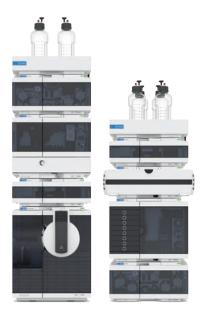
Chromatographic baseline of EMR—Lipid phospholipid cleanup compared to protein precipitation. We reduced MS cleaning and increased column life without sacrificing PFAS recovery.

Want a closer look?

Read application note 5991-8656EN: Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ

Configure Your LC for Success: PFAS Elimination

Fluoropolymers are commonly found in many industrial products, including those used in the lab for analysis, extraction, and cleanup. Lab supplies such as solvents, syringes, pipettes, and SPE devices can contain trace PFAS levels that may contaminate your samples and interfere with your results. Some LC instrument parts can also contribute to trace-level contamination.



InfinityLab LC instruments: Efficiency for any application and budget

Agilent InfinityLab HPLC and UHPLC systems feature the latest technology while maintaining full compatibility with legacy LC instrumentation.

- The Agilent 1260 Infinity II LC is the flexible choice for operational efficiency.
- The Agilent 1290 Infinity II LC is the next generation of liquid chromatography—delivering ultrahigh performance for superior analytical results.

Is PFC background noise hurting your PFAS analysis?

The InfinityLab PFC-free HPLC conversion kit for the Agilent 1290 Infinity II LC helps keep your flow path free from perfluorinated compounds, so you can minimize PFAS background noise and meet stringent regulations.

To request your kit, simply use our easy ordering guide that links to a prefilled shopping cart at the Agilent online store.

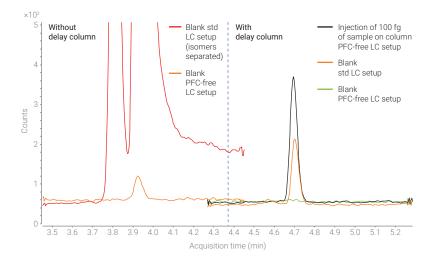


Consumables solutions for analyzing trace-level PFAS with confidence

Agilent's new InfinityLab PFC-free HPLC conversion kit includes everything needed to ensure that the 1290 Infinity II HPLC systems and high-speed pumps are free of PFAS contamination. This includes various replacement parts, tubing, inline filters, solvent bottle assembly, and an InfinityLab Delay column with Quick Connect HPLC fitting.

Several regulatory methods, including EPA 537 and 533, call for extracting PFAS from drinking water using SPE cartridges followed by LC/MS/MS analysis. Agilent's SPE cartridge portfolio includes both ultraclean divinylbenzene sorbent for EPA 537, as well as the weak anion exchange or WAX cartridge required for analyzing shorter-chain and emerging PFAS compounds. Captiva syringe filters with regenerated cellulose (RC) membranes are ideal for PFAS analysis described in EPA 8327 and ASTM D7979 methods for non-potable waters.

Agilent ZORBAX RRHD columns, based on a fully porous particle, increase resistance to strong sample injection solvents and allow for high-volume injections, making them ideal for analyzing PFAS compounds in water.



PFHpA blank and sample chromatograms from different LC system setups. We tested Agilent PFCfree conversion kits using 38 analytes representing standard and regulatory methods—including US EPA 533, 537.1, 8327, and ISO 21675. No background was detected for 36 out of the 38 analytes.

Want a closer look?

Read these application notes:

5994-2291EN: Reduce PFAS Background with the Agilent PFC-Free HPLC Conversion Kit
5994-2151EN: Filtration for the Analysis of Per- and Polyfluoroalkyl Substances in Environmental Extracts
5994-0250EN: Extraction of Per/Polyfluoroalkyl Substances in Water Using Agilent Offline Solid Phase Extraction

Meet Regulatory Guidance Levels with Robust Results

Global regulations for PFOS and PFOA

PFOS and PFOA are the two most commonly measured PFAS and have regulatory guidance levels in regions including China, Europe, the United States, Japan, and Australia.

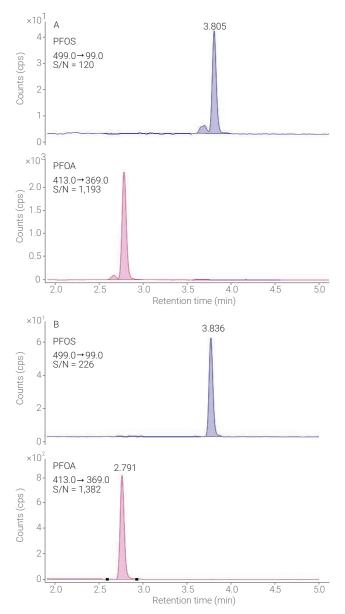
PFOS and its formulations are listed as priority substances in the Stockholm Convention. The EPA safe drinking water guidelines for PFOS and PFOA are not to exceed 70 ng/L. However, several regulatory and municipal bodies require monitoring and detection of PFAS at low single-digit ng/L levels in water and soil.

General PFAS analysis with SPE cleanup

The sensitivity, robustness, and reliability of Agilent triple quadrupole LC/MS systems (LC/TQ) make them ideal for analyzing general and regulated PFAS targets. An Agilent Ultivo can quantify low levels (ppt) of PFOA and PFAS in water and soil using WAX SPE cartridge concentration and cleanup.

Here, we used Agilent WAX SPE cartridges to extract PFOA and PFOS from water and soil.

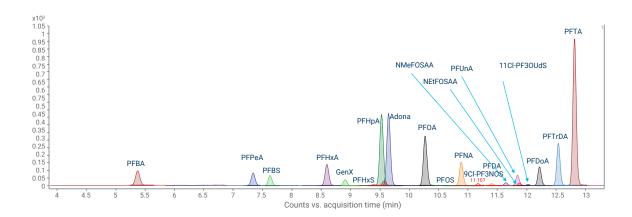
The Agilent InfinityLab Poroshell 120 EC-C18 $(2.1 \times 100 \text{ mm}, 2.7 \mu \text{m})$ column allows for effective separation of linear and branched isomers for PFOA. Recoveries between 80 and 120% for both compounds in surface water, wastewater (2.5, 40, and 200 ng/L), soil, and sediment (0.5, 5, and 20 ng/g) were achieved at different spiking levels.



Chromatograms for PFOA and PFOS spiked at 2.5 ng/L in water (A) and 0.5 μ g/kg in blank soil (B). Note: Only a quantitative ion chromatogram is shown for each compound.

US EPA drinking water methods

US EPA method 537.1 analyzes 18 PFAS, including PFOS and PFOA, in drinking water using SPE followed by LC/TQ analysis. EPA 537 uses an Agilent Bond Elut LMS solid phase extraction cartridge (p/n 12255021) to extract 500 mL of drinking water. This process is followed by evaporation and creation of the final extract with ~96% methanol. The following chromatogram shows the separation and detection of PFAS using an Agilent ZORBAX Eclipse Plus C18, 3.0×50 mm, 1.8μ m column (p/n 959757-302). Samples were analyzed on the Agilent Ultivo triple quadrupole LC/MS.

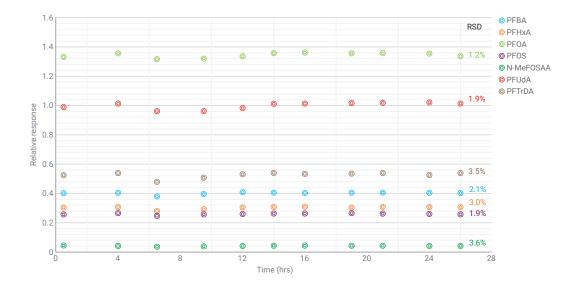


Want a closer look?

Read application note 5994-0437EN: LC/TQ Determination of PFOS and PFOA in Water and Soil Matrices

In addition to meeting and exceeding reporting levels required by the US EPA method, you must also achieve robustness across a batch of real water samples. Here, we show a relative response in area counts for 11 continuous calibration water samples run over a 26-hour batch for EPA 537.

The Ultivo LC/TQ system allows you to continuously run routine EPA methods for PFAS with the desired sensitivity and reproducibility. Its small footprint lets you fit approximately three Ultivo systems in the space needed for one traditional LC/TQ instrument.



Want a closer look?

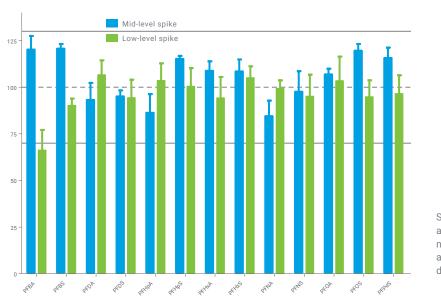
Read application note **5991-8969EN**: Analysis of Per/Polyfluoroalkyl Substances (PFAS) in Drinking Water Using the Agilent Ultivo Triple Quadrupole LC/MS

Eliminating sample preparation for US EPA 537

SPE sample preparation and extraction is a critical step for cleanup and interference removal. However, it is time consuming and tedious, and can introduce sources of PFAS contamination into the sample.

For labs looking to monitor the PFAS listed on EPA method 537, the Agilent 6495 LC/TQ system is an ideal choice. It eliminates the hassle of sample preparation in clean water samples and gets you from sample collection to data reporting quickly. The 6495 offers excellent sensitivity and increased throughput without any sacrifice in method reporting levels.

A method developed on the 6495 LC/TQ quantified 14 PFAS present in EPA 537. The analysis took less than six minutes, with a direct injection of 80 μ L of sample diluted slightly with methanol to achieve detection levels of 0.83 to 3.3 ng/L.



The following graph shows the recovery of these PFAS at two spiking levels.

To learn more about the challenges and mitigation strategies in detection of PFAS in water, watch this **on-demand webinar** by Dr. Arjun Venkatesan, Stony Brook University.

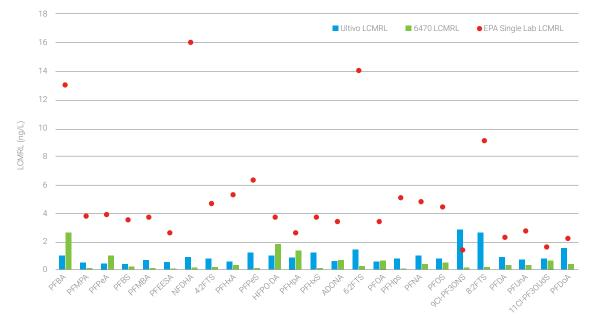
Spike recoveries of PFAS at low level (10 ng/L; 2 ng/L for PFOS and PFOA) and mid level (40 ng/L) in drinking water samples.

Analyzing challenging compounds with EPA 533

EPA method 533 addresses some of the challenging compounds in EPA methods 537 and 537.1 for C_4 and C_5 acids and sulfonates. It also limits chain length to C_{12} acids, while adding some emerging PFAS.

Agilent's sample preparation, consumables, and Ultivo LC/TQ provide the tools needed to achieve the detection limits required by EPA 533 while offering ultimate robustness and easy-maintenance features for novice mass spectrometry users too.

An Agilent 6470 LC/TQ with Agilent Jet Stream ESI source delivers sensitivity, precision, and accuracy exceeding EPA requirements, allowing users to future-proof their lab against dropping regulatory limits that could be expected. Recoveries were between 87% and 103% for all PFAS in reagent and tap water.



LCMRLs calculated according to EPA for all analytes in EPA 533 with Ultivo and 6470 LC/MS compared to EPA single lab LCMRL.

Want a closer look?

Read these application notes:

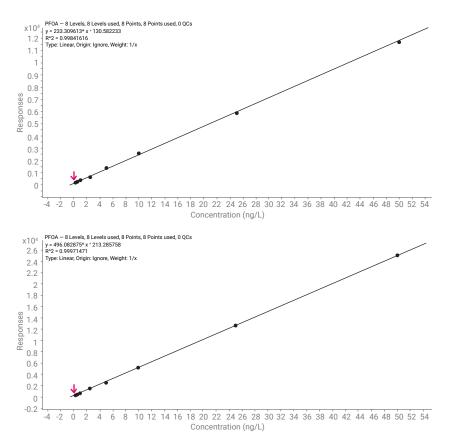
5994-1628EN: EPA Method 533 for Analysis of Per/Polyfluoroalkyl Substances in Drinking Water Using Agilent 6470 LC/TQ

5994-1920: Analysis of Per/Polyfluoroalkyl Substances (PFAS) in Drinking Water by EPA 537.1 and EPA 533 Using the Agilent Ultivo Triple Quadrupole LC/MS

EU regulations

The EU has an environmental quality standard of 0.65 ng/L in water bodies for PFOS, and researchers anticipate similarly low reporting levels for PFOA in water. The high sensitivity of the Agilent 6495 triple quadrupole LC/TQ lets you achieve these low levels by direct aqueous injection and run your analysis in a "dilute-and-shoot" manner, so you can skip laborious, time-consuming sample concentration.

We generated these linear calibration curves for PFOS and PFOA standards (0.25, 0.5, 1, 2.5, 5, 10, 25, and 50 ng/L with $R^2 > 0.99$) using direct aqueous injection on the 6495 LC/TQ.



Calibration curves for PFOS and PFOA, standards at 0.25, 0.5, 1, 2.5, 5, 10, 25, and 50 ng/L.

	0.5 ng/L	. Standard	1.0 ng/L Standard		
Compound	Average Area	RSD (%)	Average Area	RSD (%)	
PFOS	423.3	5.3	668.3	4.9	
PFOA	280.1	5.0	387.7	4.4	

Enhanced sensitivity allows you to measure PFAS at extremely low levels without any loss in reproducibility or robustness. The RSD for both PFOS and PFOA at a 0.5 ng/L concentration was <6%.

ASTM and EPA 8327 methods

ASTM method 7979-17 analyzes 21 PFAS in nonpotable waters—including surface water, groundwater, and wastewater. It uses a simplified methanol dilution and large-volume (30 μ L) injection onto an LC/TQ. EPA 8327 follows identical sample preparation and analytical protocols.

Briefly, the method requires 5 mL of sample to be diluted with 5 mL of methanol, acidified, filtered, and injected onto an LC/TQ. This sample preparation technique increases throughput and reduces contamination sources. Reporting levels for most compounds in this method are 10 ng/L with an expected calibration range of up to 400 ng/L. Analysis at low ng/L levels demands a sensitive mass spectrometer with good robustness to deal with different water matrices. It also requires strategies to eliminate any PFAS contamination present in glass containers and consumables.

A simple technique for background removal or background delay

To perform the ASTM 7979 efficiently, we eliminated PFAS contamination quickly and easily using an Agilent delay column and replacing any PTFE-containing tubing with PEEK. The Agilent 6470 LC/TQ achieved the detection limits required for all 21 PFAS in ASTM 7979. It also detected seven other PFAS, including ADONA and 9CI-PF3ONS (component in F53-B), that are being monitored as "emerging" PFAS.

The following table shows recoveries for 28 PFAS, including those in the ASTM 7979 and EPA 8327 methods, at the low limit of quantification (LLOQ) levels of 10 and 20 ng/L with the Agilent 6470 LC/TQ. It includes six replicates with recoveries between 50% and 150%, as stated in the ASTM method for all compounds. Most compounds showed recoveries between 80% to 120%, and the relative standard deviation (RSD) was below 20% for all compounds.

Compound	Spike Recover	y, % at 10 ng/L	Spike Recovery, % at 20 ng/L	
	Average	RSD (%)	Average	RSD (%)
I1CI-PF30UdS	119	1.8	116	3.6
4:2 FTS	115	5.8	96	8.6
B:2 FTS	103	15.2	114	0.8
9CI-PF30NS	110	10.5	108	6.8
ADONA	107	11.1	102	4.6
N-EtFOSAA	122	12.3	111	2.7
N-MeFOSAA	118	16.4	117	17.1
PFBA	101	10.7	104	10.6
PFBS	108	8.4	117	3.2
PFDA	110	17.1	107	6.6
PFDoA	101	13.3	106	13.3
PFDS	65	36.0	90	16.7
PFEESA	55	2.3	125	6.1
PFHpA	125	15.4	114	13.6
PFHpS	83	15.5	129	8.7
PFHxA	104	5.0	118	11.7
PFHxS	114	12.6	100	11.3
PFMBA	141	4.2	125	4.6
PFNA	102	18.8	106	9.4
PFNS	100	19.4	106	18.2
PFOA	121	11.1	108	9.1
PFOS	97	9.9	116	16.3
PFOSA	94	11.1	94	10.0
PFPeA	105	3.9	111	2.9
PFPeS	106	9.3	99	15.6
PFTreA	100	8.0	102	8.4
PFTriA	105	10.1	106	6.6
PFUnA	116	12.4	106	1.1

Spike recoveries and RSD (%) at 10 ng/L and 20 ng/L for all 28 PFAS, including those in ASTM 7979. Consult application note **5994-0678EN** for full method parameters.

Want a closer look?

Read application note **5994-0678EN**: Simplified and Fast Analysis of Per- and Polyfluoroalkyl Substances in Nonpotable Waters

Future-Proof Your Lab to Address the Growing List of PFAS

More than 4,000 PFAS are currently known to have been used, and this list continues to expand. But current regulatory monitoring lists globally only look at a very limited subset of PFAS. While regulatory lists may vary across regions, it is safe to assume that many additional PFAS will be monitored across the globe in time.

The following table shows method detection and method quantification levels (MDLs and MQLs) of more than 50 PFAS representing 16 different classes of legacy and emerging PFAS analyzed in water. We used a single analytical method that covered both legacy and emerging PFAS, including diPAPs, ADONA, and PFESAs (components of F-53B). Samples were analyzed on the 6495 LC/TQ, making use of its enhanced sensitivity to analyze all these PFAS in one injection without compromising detection levels.

The results can be summarized as follows:

- Instrument detection limits (IDLs) ranged from 2.5 to 469 fg on column for all compounds.
- Calculated IDLs were below 10 fg on column for 22 compounds from the classes PFCA, PFSA, FTS, FOSAA, and CI-PFAES—plus the compounds FOSA, diSAmPAP, and ADONA.
- MDLs ranged from 0.28 to 18 ng/L. MQLs ranged from 0.35 to 26 ng/L, with 46 PFAS having quantification levels below 5 ng/L.
- Run time was less than 12 minutes.

MDLs for the 53 PFAS were calculated based on US EPA 40 CFR Part 136, Appendix B, Revision 2. Seven 250 mL aliquots of ultrapure water were spiked at 5 ng/L for all compounds except FTCAs, FOSEs, and PFDPA, which were spiked at 20 ng/L.

PFAS analysis using SPE extraction and triple quadrupole LC/MS.

Compound	MDL (ng/L)	MQL (ng/L)	Extraction Method Accuracy (%)	Method Precision RSD (%)
PFBA	0.59	0.75	93	4
PFPeA	0.71	0.89	92	5
PFHxA	0.87	1.1	90	6
PFHpA	0.84	1.1	96	6
PFOA	0.28	0.35	93	2
PFNA	0.61	0.77	98	4
PFDA	0.71	0.89	98	4
PFUnA	0.80	1.0	85	6
PFDoA	1.2	1.5	93	8
PFTrA	1.4	1.8	78	12
PFTeA	0.67	0.84	93	5
PFBS	0.49	0.62	89	3
PFPeS	1.2	1.5	100	9
PFHxS	0.69	0.88	91	5
PFHpS	0.79	1.0	99	6
PFOS	0.78	1.0	95	5
PFNS	1.0	1.3	87	7
PFDS	1.1	1.3	83	8
PFDoS	1.4	1.8	72	13
ADONA	0.82	1.0	88	6
6:2 FTCA	13	17	103	16
8:2 FTCA	16	19	92	23
10:2 FTCA	17	21	67	28
6:2 FTUCA	1.7	2.1	121	9
8:2 FTUCA	1.6	2.0	111	10
10:2 FTUCA	2.8	3.6	87	19
3:3 FTCA	1.4	1.7	118	7

Want a closer look?

Read application note ${\rm 5994-0919EN}$: Analysis of >50 Legacy and Emerging PFAS in Water Using the Agilent 6495C LC/TQ

Ultrapure water blanks (n=7) were extracted alongside method validation samples. Method accuracy was expressed as the mean recovery of method validation samples for the expected concentration as a percentage and relative standard deviation.

The versatility, accuracy, and robustness of our LC/TQ systems let you add several PFAS to your method without sacrificing sensitivity or throughput. If you need to add new or novel PFAS to your methods, Agilent LC/MS compound optimizer automates the process and provides reliable compound parameters in minutes.

In addition, Agilent consultants can help make your PFAS analysis hassle free. Our decades of experience, combined with our MRM and method data capabilities, can get your lab up to speed quickly.

Compound	MDL (ng/L)	MQL (ng/L)	Extraction Method Accuracy (%)	Method Precision RSD (%)
5:3 FTCA	1.8	2.3	103	11
7:3 FTCA	2.4	3.1	75	20
PFHxPA	2.9	3.4	104	17
PFOPA	4.6	5.8	100	26
PFDPA	18	26	82	10
6:2 diPAP	1.9	2.4	81	14
6:2/8:2 diPAP	1.9	2.4	123	11
8:2 diPAP	0.83	1.1	93	6
6:2 CI-PFESA	1.3	1.7	88	9
8:2 CI-PFESA	1.1	1.4	80	9
4:2 FTS	2.7	3.4	93	16
6:2 FTS	0.56	0.7	90	4
8:2 FTS	1.3	1.7	87	9
10:2 FTS	1.4	1.8	66	13
FOSA	0.76	1.0	70	7
MeFOSA	4.0	5.0	127	18
EtFOSA	2.1	2.7	80	19
FOSAA	3.2	4.0	91	17
MeFOSAA	1.4	1.7	106	8
EtFOSAA	1.5	1.9	93	10
MeFOSE	2.9	3.7	96	5
EtFOSE	4.9	6.2	93	9
6:6 PFPiA	1.2	1.5	74	10
6:8 PFPiA	1.8	2.3	95	12
8:8 PFPiA	3.1	4.0	138	11
diSAmPAP	3.3	3.0	76	19

PFAS analysis using SPE extraction and triple quadrupole LC/MS.

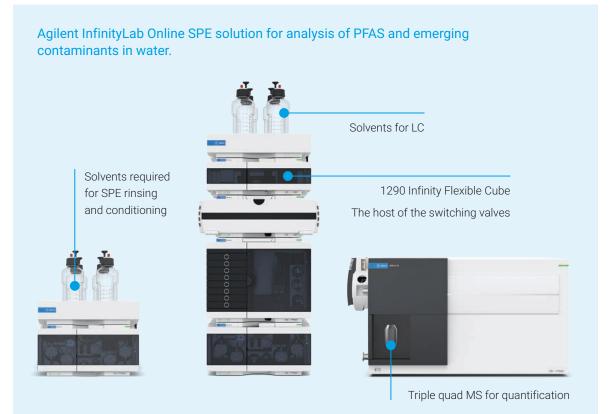


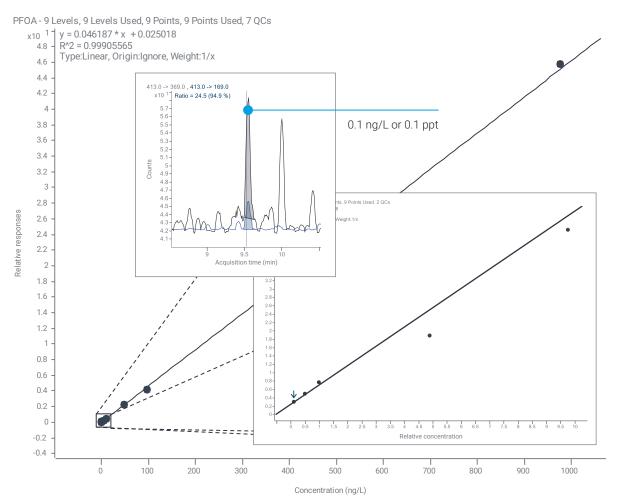


For more information on the analysis, fate, and removal of PFAS in water treatment plants using the 6495C LC/TQ, please watch this **on-demand webinar** by Prof. Bradley Clarke, University of Melbourne, Australia.

Automate PFAS sample preparation with online SPE

Solid phase extraction for PFAS can be time consuming and tedious, and offers the potential of adding contamination while reducing reproducibility of the overall analysis. Automated online SPE can provide similar detection limits while using a fraction of the water sample while completely automating sample extraction and analysis which reduces labor time, increases accuracy of results and drastically improves throughput. Further, it also reduces costs of expensive and environmentally unfriendly solvent usage and the amount of isotopically labelled standards needed. While automation can seem complicated, Agilent's online SPE setup coupled to the most reliable and robust Agilent mass spectrometers provide seamless software interface to make the process much simpler, letting you reduce the loads of doing manual and tiresome offline extractions.





Linearity, dynamic range (0.1-1000 ng/L), and sensitivity of PFOA analysis using Agilent InfinityLab Online SPE with a 6470 LC/MS/MS.

Discovering New PFAS Using High-Resolution LC/Q-TOF

Triple quadrupole LC/MS is a great tool for measuring known PFAS at extremely low levels. However, several thousand PFAS are used in commerce, and many have yet to be identified in the environment. This is where a quadrupole time-of-flight (Q-TOF) mass spectrometer shows its value.

LC/Q-TOF instruments allow you to perform untargeted analysis and to identify unknown PFAS. You can also use libraries to screen for PFAS without the need for analytical reference standards. In addition, LC/Q-TOF technology lets you acquire data over a wide dynamic range. That means you can analyze trace sample amounts next to abundant peaks in the same spectrum. Together with simultaneous high sensitivity and high resolution, Agilent LC/Q-TOF instruments are ideal for identifying unknown PFAS in environmental samples.

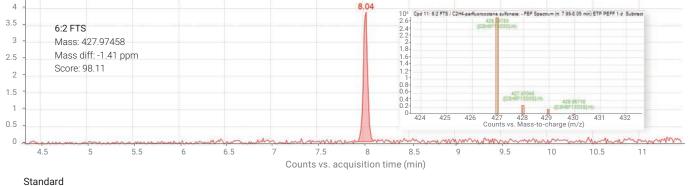


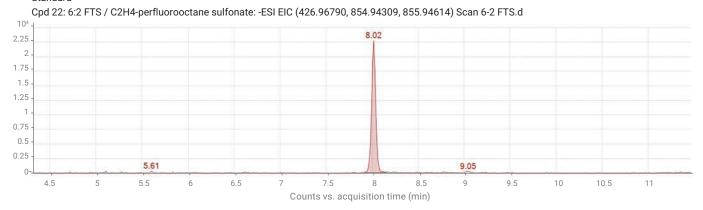
In the following spectra, we identified 6:2 FtS with high mass accuracy and isotope fidelity in a wastewater sample. The compound was later verified with a reference standard to have the same retention time by LC/Q-TOF.

Identification of PFAS PCDL + Std ID.

WWTP1 Final Effluent

Cpd 11: 6:2 FTS / C2H4-perfluorooctane sulfonate: -ESI EIC (426.96790, 854.94309, 855.94614) Scan Frag=350.0V ETP FEFF 1.d

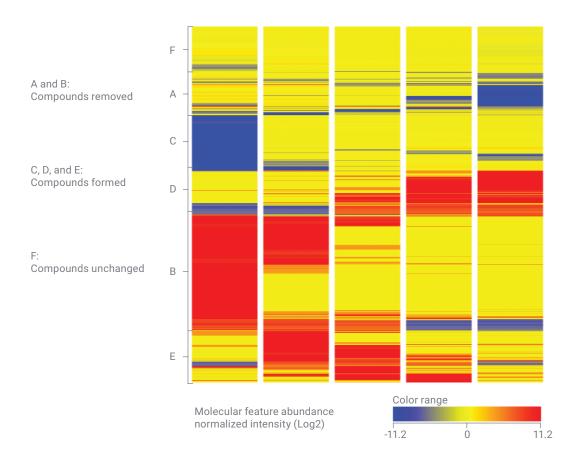




Since LC/Q-TOF collects all ionizable species in the analysis, you are able to retroactively mine for data and identify compounds without sample reinjection. Here, 6:2 FtS samples were identified at all treatment stages of the wastewater plant samples. Therefore, the abundance of this compound could be plotted to track efficacy in the wastewater treatment plant.

Alternatively, an LC/Q-TOF system can be used for fingerprinting PFAS sources, or for studying PFAS composition in aqueous film-forming foams (AFFF).

Mass Profiler Professional (MPP) software can be used to identify new PFAS and perform source appropriation and fingerprinting studies. It includes statistical profiling tools like principal component analysis (PCA), hierarchical clustering, and Kendrick mass defect plots.



Capture, Analyze, and Share Water Quality Data

The advanced data mining and processing tools in the Agilent MassHunter software suite let you quickly and accurately extract available information from the analytes in your samples.

- Take advantage of powerful data collection, processing, and reporting tools. Breeze through application-specific workflows with comprehensive support of GC, GC/MS, and LC/MS technology.
- Use one software for all Agilent GC, GC/MS, and LC/MS instruments, including single quadrupole, tandem quadrupole, and Q-TOF.
- Analyze complex environmental samples with compound-based analysis and reporting workflows, using Agilent MassHunter Quantitative Analysis with Quant-My-Way customization.
- Simplify target and suspect screening with highly confident compound identification using Agilent Personal Database and Libraries.
- Quickly build targeted screening and quantitation acquisition methods using the Agilent PFAS MRM database for triple quadrupole LC/MS of a few—or a few dozen—PFAS compounds.



Agilent CrossLab services

CrossLab is an Agilent capability that integrates services and consumables to support workflow success and important outcomes like improved productivity and operational efficiency. Through CrossLab, Agilent strives to provide insight in every interaction to help you achieve your goals. CrossLab offers method optimization, flexible service plans, and training for all skill levels. We have many other products and services to help you manage your instruments and your lab for best performance.

Learn more about Agilent CrossLab and see examples of insight that leads to great outcomes at www.agilent.com/crosslab



Learn more: www.agilent.com/chem/environmental

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