

Incorporating Ultrashort-Chain PFAS into Comprehensive PFAS Analysis in Ready-to-Drink Teas and Fruit Juices

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Key Highlights

- A dilute-and-shoot LC-MS/MS workflow on the Ultra IBD Inert column simultaneously quantifies 43 PFAS—from ultrashort-chain through long-chain (C1–C14) and alternative PFAS—in a single, 12-minute run.
- The mixed-mode stationary phase packed in inert-coated hardware enables sufficient retention for highly polar compounds, such as TFA and TFMS, while maintaining optimal retention of long-chain PFAS, resulting in comprehensive PFAS coverage with a short analytical run time.
- Simple dilute-and-shoot sample preparation limits lab-introduced PFAS contamination and supports high sample throughput.
- Evaluated across five diverse ready-to-drink teas and juices, the method delivered recoveries of 71–122% and %RSD $\leq 12\%$ with LOQs as low as 2 ng/L for most analytes.
- Applied to 23 commercial beverages, the method revealed that ultrashort-chain PFAS—particularly TFA and TFMS—are the dominant PFAS contaminants in teas and juices, a class largely missed by conventional C18-based methods.

Abstract

Ultrashort-chain (USC) PFAS are a highly polar subset of PFAS with carbon chain lengths shorter than C4 that are difficult to retain using conventional reversed-phase LC methods, yet their detection is increasingly important in monitoring dietary and environmental PFAS exposure. This application note describes a straightforward, dilute-and-shoot LC-MS/MS workflow for the simultaneous determination of C1 to C14 perfluoroalkyl carboxylic and sulfonic acids, along with other PFAS classes, in diverse beverage matrices. Chromatographic separation used the Ultra IBD Inert column, a highly inert mixed-mode column that provides enhanced retention of highly polar USC compounds compared to traditional C18 columns while maintaining excellent performance for long-chain PFAS. The method was evaluated across five representative teas and juices for the quantification of 43 PFAS compounds and subsequently applied to the analysis of 23 commercially available beverages..

Introduction

Per- and polyfluoroalkyl substances (PFAS) are a large family of synthetic chemicals valued for their chemical stability and resistance to water, oil, and heat [1]. Their widespread use and persistence have led to global dissemination in soil, water, and the food supply, raising concerns about chronic dietary exposure [2–4]. While PFAS studies have historically emphasized short- and long-chain compounds, emerging evidence indicates that ultrashort-chain (USC) PFAS, which contain one to three perfluorinated carbon atoms, may contribute substantially to overall contamination because of their exceptional mobility, environmental persistence, and relevance to dietary exposure [5]. These C1–C3 compounds include trifluoroacetic acid (TFA); perfluoropropanoic acid (PFPrA); trifluoromethanesulfonic acid (TFMS); perfluoroethanesulfonic acid (PFETs); and perfluoropropanesulfonic acid (PFPrS), which are increasingly recognized as major contributors to overall PFAS burdens in aquatic environments [6].



Related Products

- Ultra IBD Inert column, 3.0 μm , 100 x 2.1 mm (cat.# 9175312-T)
- Ultra IBD column, 3.0 μm , 150 x 2.1 mm (cat.# 9175362)
- PFAS 28 calibration standard (cat.# 30734)
- Polypropylene vials (cat.# 23243)
- Polyethylene caps (cat.# 23244)

Due to analytical challenges, current methods for PFAS analysis in foods often exclude USC compounds from target lists, which underestimates the level and impact of dietary PFAS exposure [7]. Beverages are an important exposure route because they are consumed extensively across all age groups and, as predominantly water-based products, may contain elevated levels of polar USC PFAS. Although comprehensive PFAS analysis incorporating USC compounds has been reported for bottled water and ready-to-drink (RTD) milk products, PFAS surveillance data remains limited for other beverages, such as teas and fruit juices. These products are manufactured with ingredients and water sources that may already contain trace PFAS, with additional potential contamination through processing equipment, filtration systems, storage tanks, and packaging materials. Therefore, robust workflows capable of detecting both USC and long-chain compounds are essential for comprehensive monitoring of PFAS contamination in beverages.

Chromatographic analysis of USC PFAS is inherently challenging because of their high polarity, minimal retention on traditional reversed-phase LC columns, and susceptibility to loss during multistep sample preparation. Conventional LC-MS/MS methods using C18 columns are generally optimized for PFAS with chain lengths of C4 and longer and provide insufficient retention for USC compounds. Anion-exchange columns have been explored as an alternative but often suffer from long retention times and broad peak shapes that reduce sensitivity and sample throughput. In contrast, the Ultra IBD Inert column has previously demonstrated balanced retention of USC and long-chain PFAS in water and milk matrices [8,9] and is a promising approach for the development of new methods that can effectively cover the full range of PFAS chain lengths in beverage matrices.

Building on that chromatographic strategy, this study establishes a streamlined workflow for comprehensive PFAS determination—targeting 43 analytes encompassing C2–C14 perfluoroalkyl carboxylic acids, C1–C13 perfluoroalkyl sulfonic acids, fluorotelomer acids, perfluorooctane sulfonamides and sulfonamidoacetic acids, and per- and polyfluoroether acids—across a variety of RTD teas and fruit juices. The objectives were to (1) develop a simplified sample preparation procedure that minimizes contamination while enabling accurate quantification; (2) optimize chromatographic conditions to achieve efficient analysis of USC through long-chain PFAS within a short run time; and (3) apply the finalized workflow to assess PFAS contamination across a broader range of commercial beverages.

Experimental

Standard and Sample Preparation

Method performance was assessed using commercially purchased RTD green tea, black tea, apple juice, blended berry juice, and orange juice. Since matrix effect can vary significantly across sample types, isotopically labeled internal standards were used to correct for matrix interferences and ensure accurate, reliable quantification across the chemically diverse beverages analyzed in this study.

Calibration standards (500 µL) covering 1–2000 ng/L were prepared from Restek's PFAS 28 calibration standard (cat.# 30734) and standards obtained separately in a 1:1 mixture of ultrapure water and acetonitrile, fortified with 2.5 µL of a quantitative internal standard (QIS) working solution (10 ng/mL for each of the labeled analytes).

For teas and juices, 0.5 mL of sample was aliquoted into a 15-mL polypropylene centrifuge tube, spiked with 5.0 µL of QIS working solution, and mixed with 0.5 mL of acetonitrile by vortexing for 30 seconds—a simple, time-saving dilute-and-shoot approach with no extraction, evaporation, or cleanup steps. The tube was centrifuged at 4000 rpm, and the resulting supernatant was transferred directly to clean polypropylene vials for LC-MS/MS analysis.

Because orange juice samples exhibited stronger matrix effects than other beverages, they required an initial twofold dilution with water prior to the acetonitrile dilute-and-shoot step to maintain acceptable peak shape for early-eluting compounds. An in-depth discussion of matrix effects and method development is available in a separate publication detailing the complete study [10].

Instrumentation and Chromatographic Method

LC-MS/MS analysis was performed on a Waters ACQUITY I-Class UPLC coupled to a Xevo TQ-S triple-quadrupole mass spectrometer under negative electrospray ionization. Chromatographic separation of 43 target analytes and 13 quantitative internal standards was achieved using the Ultra IBD Inert column (100 × 2.1 mm, 3.0 µm; cat.# 9175312-T). An Ultra IBD column (150 × 2.1 mm, 3.0 µm; cat.# 9175362) was installed as a delay column to effectively sequester background PFAS contamination originating from the LC system and mobile phases.

Mobile phase A consisted of ultrapure water with 2 mM ammonium formate and 0.1% formic acid; mobile phase B was acetonitrile:water (95:5, v/v) with the same additives. The gradient began at 50% B, increased linearly to 100% B over 0–7 min, held at 100% B until 10 min, and then returned to 50% B for re-equilibration through 12 min. The column was held at 40 °C with a flow rate of 0.4 mL/min, and 20 µL of sample was injected per run.

Retention times, MRM transitions, and cone and collision cell voltages are provided in Appendix I for all analytes, the surrogate, and internal standards.

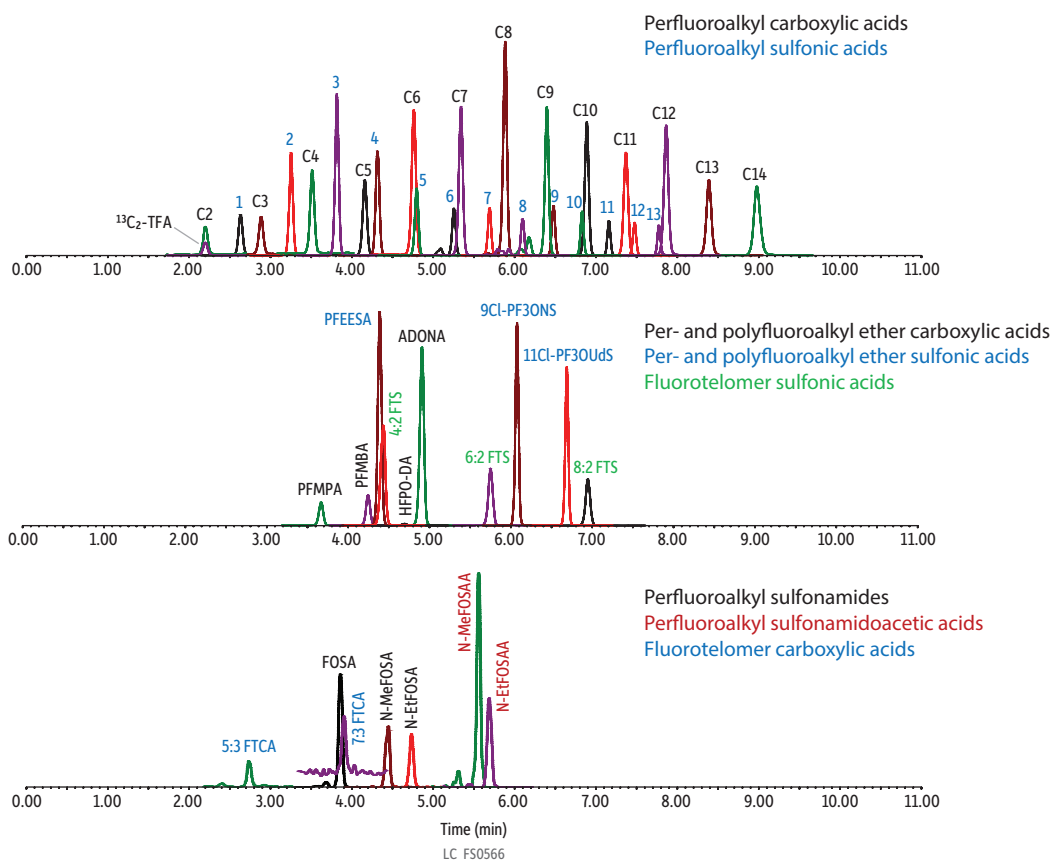
Results and Discussion

Chromatographic Performance

Building on the chromatographic strategies previously established for USC-inclusive PFAS analysis in water and milk matrices, this study applied the Ultra IBD Inert column to RTD beverages with diverse compositions. The optimized method conditions improved retention and separation of early-eluting USC compounds while also promoting faster elution of long-chain PFAS. The fast 12-minute total run time produced good chromatography for all analytes and did not sacrifice resolution for retention, which allows increased sample throughput—a meaningful advantage for laboratories running large numbers of samples.

Background contamination is a persistent challenge for PFAS analysis as it can originate from reagents, system components, and common lab materials. Use of the delay column and consumables that were previously shown to have low background levels were important factors in minimizing contamination. All labs performing PFAS analysis should prescreen solvents, reagents, and consumables for background PFAS contamination. The implementation of a delay column is highly recommended to help distinguish system-derived PFAS signals from those originating in the sample.

Figure 1: The Ultra IBD Inert column provided good retention and separation of both ultrashort chain and longer chain PFAS.



Column Ultra IBD Inert (cat.# 9175312-T)

Dimensions: 100 mm x 2.1 mm ID

Particle Size: 3 µm

Pore Size: 100 Å

Temp.: 40 °C

Standard/Sample

PFAS 28 calibration standard (cat.# 30734)

Other standards were obtained externally.

Diluent: 50:50 Water:acetonitrile

Conc.: The blend berry juice was fortified at 500 ng/L and diluted two-fold with acetonitrile.

Inj. Vol.: 20 µL

Mobile Phase

A: Water, 2mM ammonium formate, 0.1% formic acid

B: 95:5 Acetonitrile:water, 2mM ammonium formate, 0.1% formic acid

Time (min)	Flow (mL/min)	%A	%B
0.00	0.4	50	50
7.00	0.4	0	100
10.00	0.4	0	100
10.01	0.4	50	50
12.00	0.4	50	50

Max Pressure: 540 bar

Detector Waters Xevo TQ-S

Ion Source: Waters Zspray ESI

Ion Mode: ESI-

Mode: MRM

Instrument Waters ACQUITY UPLC I-Class

Sample Preparation The blend berry juice (0.5 mL) was transferred into a 15 mL polypropylene centrifuge tube, fortified at 500 ng/L, and mixed with 0.5 mL of acetonitrile by vortexing for 30 seconds. The mixture was then centrifuged at 4000 rpm, and the resulting supernatant was transferred to polypropylene HPLC vials for LC-MS/MS analysis.

Notes The confirmation ion peaks were not shown in the chromatogram.

An Ultra IBD column (150 x 2.1 mm, 3.0 µm; cat # 9175362) was used as the delay column.

For the chromatograms of perfluoroalkyl carboxylic and sulfonic acids, the peak numbers correspond to the carbon chain lengths of the PFAS compounds.

Evaluation of Linearity and LOD

Using quadratic regression with 1/x weighting, all analytes demonstrated strong linearity, with r^2 values greater than 0.995 and deviations below 30%. Calibration ranges were tailored by analyte: 1–1000 or 2–1000 ng/L for most compounds; 10–1000 ng/L for HFPO-DA; 10–2000 ng/L for TFA; and 4–1000 ng/L for fluorotelomer carboxylic acids and sulfonamidoacetic acids.

Limits of detection (LOD) were estimated from a signal-to-noise ratio of 3 in fortified beverage samples. A summary of linearity and LOD performance by matrix is given in Table I below; individual results for each analyte in each matrix are provided in Appendix II (Table IV).

Table I: Summary of LOD, Calibration Range, and Linearity Results by Beverage Type Across All 43 Target PFAS

Beverage Matrix	LOD Range (ng/L)	Calibration Range (ng/L)*	Analytes with $r^2 > 0.995$
Green tea	0.31 – 15.0	1–1000	43/43
Black tea	0.25 – 12.0	1–1000	43/43
Apple juice	0.18 – 12.7	1–1000	43/43
Blended berry juice	0.16 – 15.0	1–1000	43/43
Orange juice	0.30 – 12.5	1–1000	43/43

*The calibration range for most compounds was 1–1000 ng/L, although the lowest calibrator for some analytes was slightly above 1 ng/L. TFA was a notable exception and had a calibration range of 10–2000 ng/L.

Evaluation of Method Accuracy, Precision, and LOQ

Method accuracy and precision were evaluated by fortifying the five representative beverages with native analytes at 2, 4, 10, 20, 100, and 500 ng/L. Isotopically labeled $^{13}\text{C}_2$ -TFA was used as a surrogate for determining TFA recovery. Three analytical batches were conducted on separate days, with three replicates per fortified concentration in each batch, resulting in a total of nine replicates for each fortification level. Background (incurred) PFAS concentrations were subtracted from fortified sample results to calculate recovery.

Recovery and %RSD results, summarized in Table II, demonstrate that the method meets or exceeds typical regulatory expectations [11] for PFAS accuracy and precision across all five beverage types. Complete accuracy and precision data for all 43 analytes at each of the six fortification levels, in each of the five beverage matrices, are provided in Appendix III (Tables V–IX).

Limits of quantitation (LOQ) for each analyte were defined as the lowest fortified concentration that could be quantified with acceptable accuracy [11]. Overall, the majority of the 43 targeted PFAS were accurately quantifiable at LOQs of 2 or 4 ng/L, with orange juice (which required additional dilution during preparation) requiring somewhat higher LOQs. A few compounds with lower MS sensitivity or stronger matrix interference (TFA, TFMS, HFPO-DA; fluorotelomer carboxylic acids; perfluorooctane sulfonamides; and sulfonamidoacetic acids) exhibited LOQs of 10–20 ng/L depending on beverage type. Individual LOQs for each analyte in each matrix are the lowest fortification levels shown in Appendix III (Tables V–IX).

Table II: Summary of Accuracy and Precision for Fortified Beverage Samples Across All Spike Levels and Days

Beverage Matrix	Average Recovery Range (%)	Max %RSD	Typical LOQ (ng/L)
Green tea	75.3–115	≤12	2 – 20
Black tea	71.1–118	≤12	2 – 20
Apple juice	83.6–117	≤12	2 – 20
Blended berry juice	78.5–121	≤12	2 – 20
Orange juice	83.9–122	≤12	4 – 20

Screening for PFAS in More Commercial Beverage Matrices

The method was used to profile PFAS in 23 commercial beverages purchased from local grocery stores, including unsweetened and sweetened green and black teas; several fruit-flavored black teas; and an expanded variety of fruit juices (apple, grape, cranberry, pineapple, orange, and multiple mixed-fruit blends).

Ultrashort- and short-chain PFAS were the primary contributors to PFAS contamination across the expanded beverage panel. Every beverage tested contained TFA at substantially higher concentrations than any other PFAS. In several samples, TFA levels were so high that they exceeded the upper calibration limit and required additional dilution for accurate quantification. TFMS, PFPrA, and PFPrS were also commonly detected, but long-chain PFAS were rarely found, with PFOA and PFOS appearing in only a few samples. Detailed methodology and quantitative results are available in the full study [10].

These results reinforce the central finding of this work: ultrashort-chain PFAS, not conventional long-chain PFAS, are the predominant contaminants in tea and juice beverages, and they will likely go undetected if labs use traditional workflows that cannot retain and quantify them.

Conclusion

This study establishes a simple, reliable, and broadly applicable LC-MS/MS method for the comprehensive determination of ultra-short-chain, long-chain, and alternative PFAS in diverse RTD tea and fruit juice beverages. The Ultra IBD Inert column provides increased retention of USC PFAS, resolving the fundamental analytical gap that leaves these compounds undetected by conventional C18 methods. In addition, an Ultra IBD delay column keeps background contamination from compromising low-level quantification. Combined with a minimal-handling dilute-and-shoot sample preparation procedure, the workflow minimizes contamination risk and turnaround time, delivering accurate, precise results (71–122% recovery, %RSD $\leq$ 12%) across five chemically distinct beverage matrices at LOQs as low as 2 ng/L.

Application of the qualified method to 23 commercial beverages revealed that ultrashort-chain PFAS, particularly TFA and TFMS, are the predominant contaminants in RTD teas and fruit juices, with long-chain PFAS only sporadically detected. This finding underscores why comprehensive food and beverage safety testing must include USC PFAS: methods that target only C4-and-longer compounds risk missing the majority of PFAS burden in these products [12].

The workflow described here provides laboratories, CROs, and food safety programs with a practical, single-injection solution for complete PFAS characterization in beverages, supporting ongoing surveillance and regulatory efforts as USC PFAS gain increasing scrutiny.

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Appendix I: MS/MS Ion Transitions and Parameters

Table III: MS/MS Ion Transitions, Parameters, and Chromatographic Retention Times of Target Analytes, Surrogate Standards, and Internal Standards

Compound	RT (min)	Precursor Ion	Product Ions (Quantifier/Qualifier)	Cone (V)	Collision (V)	Quant. IS
Perfluoroalkyl Carboxylic Acids						
Trifluoroacetic acid (TFA)	2.20	113.03 [M-H]-	69.01	10	10	¹³ C ₃ -PFPrA
Perfluoropropanoic acid (PFPrA)	2.88	162.97 [M-H]-	119.02	10	8	¹³ C ₃ -PFPrA
Perfluorobutanoic acid (PFBA)	3.51	213.03 [M-H]-	168.98	14	8	¹³ C ₄ -PFBA
Perfluoropentanoic acid (PFPeA)	4.16	262.97 [M-H]-	218.97	2	6	¹³ C ₅ -PFPeA
Perfluorohexanoic acid (PFHxA)	4.76	313.10 [M-H]-	268.97/118.99	2	8/20	¹³ C ₅ -PFHxA
Perfluoroheptanoic acid (PFHpA)	5.34	363.16 [M-H]-	319.09/169.06	8	10/18	¹³ C ₆ -PFHpA
Perfluorooctanoic acid (PFOA)	5.88	413.10 [M-H]-	368.96/168.90	2	10/16	¹³ C ₈ -PFOA
Perfluorononanoic acid (PFNA)	6.40	463.10 [M-H]-	419.01/219.02	4	10/16	¹³ C ₉ -PFNA
Perfluorodecanoic acid (PFDA)	6.89	513.17 [M-H]-	469.16/219.06	4	12/16	¹³ C ₆ -PFDA
Perfluoroundecanoic acid (PFUnA)	7.37	563.23 [M-H]-	519.24/269.07	6	12/18	¹³ C ₂ -PFTeDA
Perfluorododecanoic acid (PFDoA)	7.86	613.23 [M-H]-	569.19/169.06	8	12/26	¹³ C ₂ -PFTeDA
Perfluorotridecanoic acid (PFTriDA)	8.38	663.23 [M-H]-	619.21/169.06	8	14/28	¹³ C ₂ -PFTeDA
Perfluorotetradecanoic acid (PFTeDA)	8.98	712.67 [M-H]-	668.69/168.94	10	12/26	¹³ C ₂ -PFTeDA
Perfluoroalkyl Sulfonic Acids						
Trifluoromethanesulfonic acid (TFMS)	2.63	148.97 [M-H]-	79.93/98.92	62	13/18	¹³ C ₃ -PFBS
Perfluoroethanesulfonic acid (PFETS)	3.25	198.90 [M-H]-	79.92/98.91	38	22/22	¹³ C ₃ -PFHxS
Perfluoropropanesulfonic acid (PFPrS)	3.81	248.97 [M-H]-	79.92/98.91	2	24/24	¹³ C ₅ -PFPeA
Perfluorobutanesulfonic acid (PFBS)	4.32	298.97 [M-H]-	79.97/98.89	2	26/26	¹³ C ₃ -PFBS
Perfluoropentanesulfonic acid (PFPeS)	4.79	349.10 [M-H]-	79.98/98.98	6	32/30	¹³ C ₃ -PFHxS
Perfluorohexanesulfonic acid (PFHxS)	5.25	398.90 [M-H]-	79.97/98.89	56	32/34	¹³ C ₃ -PFHxS
Perfluoroheptanesulfonic acid (PFHpS)	5.69	449.17 [M-H]-	79.98/98.97	4	42/38	¹³ C ₃ -PFHxS
Perfluorooctanesulfonic acid (PFOS)	6.11	499.03 [M-H]-	79.92/98.90	8	40/40	¹³ C ₈ -PFOS
Perfluorononanesulfonic acid (PFNS)	6.48	549.10 [M-H]-	79.92/98.83	12	42/40	¹³ C ₈ -PFOS
Perfluorodecanesulfonic acid (PFDS)	6.83	599.17 [M-H]-	79.98/98.83	8	44/46	¹³ C ₈ -PFOS
Perfluoroundecanesulfonic acid (PFUDS)	7.16	648.73 [M-H]-	79.94/98.94	38	50/44	¹³ C ₈ -PFOS
Perfluorododecanesulfonic acid (PFDoS)	7.47	698.77 [M-H]-	79.95/98.94	10	60/44	¹³ C ₈ -PFOS
Perfluorotridecanesulfonic acid (PFTriDS)	7.77	748.73 [M-H]-	79.94/98.94	8	76/52	¹³ C ₈ -PFOS
Fluorotelomer Sulfonic Acids						
1H,1H,2H,2H-Perfluorohexane sulfonic acid (4:2 FTS)	4.44	327.10 [M-H]-	307.08/80.83	50	18/24	¹³ C ₃ -PFHxS
1H,1H,2H,2H-Perfluorooctane sulfonic acid (6:2 FTS)	5.75	427.17 [M-H]-	407.18/80.71	2	22/32	¹³ C ₈ -PFOA
1H,1H,2H,2H-Perfluorodecane sulfonic acid (8:2 FTS)	6.94	527.17 [M-H]-	507.16/80.83	66	26/32	¹³ C ₃ -PFHxS
Fluorotelomer Carboxylic Acids						
3-perfluoropentyl propanoic acid (5:3 FTCA)	2.73	340.93 [M-H]-	216.96/236.93	2	24/14	¹³ C ₃ -PFPrA
3-perfluoroheptyl propanoic acid (7:3 FTCA)	3.92	440.90 [M-H]-	336.88/316.91	20	12/22	¹³ C ₄ -PFBA
Perfluoroalkyl Sulfonamides						
Perfluorooctanesulfonamide (FOSA)	3.87	498.17 [M-H]-	77.97/477.76	8	28/26	¹³ C ₈ -FOSA
N-methyl perfluorooctanesulfonamide (NMeFOSA)	4.45	511.77 [M-H]-	168.95/218.91	2	26/24	¹³ C ₅ -PFPeA
N-ethyl perfluorooctanesulfonamide (NEtFOSA)	4.73	525.83 [M-H]-	168.96/218.92	10	26/24	¹³ C ₅ -PFHxA

(Continued)

Table III (continued)

Compound	RT (min)	Precursor Ion	Product Ions (Quantifier/Qualifier)	Cone (V)	Collision (V)	Quant. IS
Perfluoroalkyl Sulfonamidoacetic Acids						
N-methyl perfluorooctanesulfonamidoacetic acid (NMeFOSAA)	5.55	570.20 [M-H]-	419.17/483.16	46	20/14	¹³ C ₃ -PFPrA
N-ethyl perfluorooctanesulfonamidoacetic acid (NEtFOSAA)	5.68	584.20 [M-H]-	419.18/483.11	6	20/16	¹³ C ₃ -PFPrA
Per- and Polyfluoroether Carboxylic Acids						
Perfluoro-3-methoxypropanoic acid (PFMPA)	3.68	228.93 [M-H]-	84.97/198.94	10	10/14	¹³ C ₄ -PFBA
Perfluoro-4-methoxybutanoic acid (PFMBA)	4.24	278.87 [M-H]-	84.96/234.93	8	10/6	¹³ C ₅ -PFHxA
Hexafluoropropylene oxide dimer acid (HFPO-DA)	4.68	285.03 [M-COOH]-	169.02/185.02	2	6/16	¹³ C ₃ -PFHxS
4,8-Dioxa-3H-perfluorononanoic acid (ADONA)	4.90	376.90 [M-H]-	250.93/84.97	22	12/26	¹³ C ₄ -PFHpA
Per- and Polyfluoroether Sulfonic Acids						
Perfluoro(2-ethoxyethane)sulfonic acid (PFEEESA)	4.09	314.83 [M-H]-	134.94/83.01	4	22/16	¹³ C ₃ -PFHxS
9-Chlorohexadecafluoro-3-oxanonane-1-sulfonic acid (9Cl-PF3ONS)	6.08	530.78 [M-H]-	350.85/82.96	12	26/24	¹³ C ₂ -PFTeDA
11-Chloroeicosafluoro-3-oxaundecane-1-sulfonic acid (11Cl-PF30UdS)	6.69	630.78 [M-H]-	450.80/82.95	8	26/32	¹³ C ₂ -PFTeDA
Surrogate						
¹³ C ₂ -TFA (surrogate)	2.20	114.90 [M-H]-	69.95	14	8	¹³ C ₃ -PFPrA
Quantification Internal Standards (QIS)						
¹³ C ₃ -PFPrA	2.88	165.97 [M-H]-	120.96	10	11	–
¹³ C ₄ -PFBA	3.51	217.03 [M-H]-	171.98	2	8	–
¹³ C ₅ -PFPeA	4.16	267.97 [M-H]-	222.99	2	6	–
¹³ C ₅ -PFHxA	4.76	318.03 [M-H]-	272.93	2	7	–
¹³ C ₄ -PFHpA	5.34	366.90 [M-H]-	321.93	2	10	–
¹³ C ₈ -PFOA	5.88	420.97 [M-H]-	375.94	2	10	–
¹³ C ₉ -PFNA	6.40	471.97 [M-H]-	426.87	4	12	–
¹³ C ₆ -PFDA	6.89	518.90 [M-H]-	473.87	4	13	–
¹³ C ₂ -PFTeDA	8.98	714.78 [M-H]-	669.80	8	14	–
¹³ C ₃ -PFBS	4.32	301.97 [M-H]-	79.97	2	28	–
¹³ C ₃ -PFHxS	5.25	401.90 [M-H]-	79.97	2	36	–
¹³ C ₈ -PFOS	6.11	506.84 [M-H]-	79.97	4	42	–
¹³ C ₈ -FOSA	3.87	505.91 [M-H]-	77.95	4	32	–

Appendix II: Linearity and Limit of Detection by Beverage Matrix

Table IV: Linearity Range and Matrix-Specific LOD in Matrix for Target Analytes

Analyte	Linear Calibration Range (ng/L)	LOD Green Tea	LOD Black Tea	LOD Apple Juice	LOD Berry Juice	LOD Orange Juice
TFA (via ¹³ C ₂ -TFA) ¹	10 – 2000	1.11	1.85	1.76	1.71	1.76
PFPrA	1 – 1000	1.2	2.40	1.00	0.86	2.20
PFBA	1 – 1000	1.81	1.90	0.92	1.00	1.09
PFPeA	1 – 1000	1.36	1.50	1.35	0.83	1.44
PFHxA	1 – 1000	1.09	1.42	0.83	0.86	1.30
PFHpA	1 – 1000	0.52	0.81	0.43	0.36	0.72
PFOA	1 – 1000	1.03	1.10	0.52	0.55	1.25
PFNA	1 – 1000	1.25	1.33	0.48	0.51	1.35
PFDA	1 – 1000	0.71	1.00	0.44	0.45	0.71
PFUnA	1 – 1000	0.74	1.21	0.41	0.40	1.14
PFDoA	1 – 1000	0.68	0.73	0.26	0.34	0.87
PFTTrDA	1 – 1000	0.57	0.82	0.27	0.28	0.71
PFTeDA	1 – 1000	0.41	0.52	0.27	0.26	0.44
TFMS	1 – 1000	0.48	0.67	0.42	0.32	0.60
PFEtS	1 – 1000	0.38	0.50	0.33	0.35	0.53
PFPrS	1 – 1000	0.39	0.73	0.27	0.27	0.79
PFBS	1 – 1000	0.62	0.65	0.39	0.30	0.69
PFPeS	1 – 1000	0.33	0.63	0.31	0.23	0.55
PFHxS	1 – 1000	0.78	0.59	0.90	0.79	0.97
PFHpS	1 – 1000	0.81	0.92	0.58	0.57	0.53
PFOS	1 – 1000	1.12	1.83	1.15	1.28	1.80
PFNS	1 – 1000	0.95	1.12	0.46	0.51	1.23
PFDS	1 – 1000	0.91	1.11	0.47	0.96	1.13
PFUDS	1 – 1000	0.50	0.55	0.71	0.78	0.77
PFDoS	1 – 1000	0.45	0.43	0.54	0.56	0.85
PFTTrDS	1 – 1000	0.80	0.71	0.70	0.71	0.80
4:2 FTS	1 – 1000	0.54	0.41	0.38	0.44	0.63
6:2 FTS	1 – 1000	0.75	1.00	1.49	1.57	1.60
8:2 FTS	1 – 1000	0.46	0.63	0.5	0.49	0.85
5:3 FTCA	4 – 1000	6.67	7.50	11.72	7.50	10.0
7:3 FTCA	4 – 1000	15.0	12.0	12.71	15.0	8.33
FOSA	2 – 1000	2.00	2.11	1.58	1.12	2.31
NMeFOSA	2 – 1000	5.00	5.25	3.11	3.13	4.29
NEtFOSA	2 – 1000	7.10	8.25	2.66	4.50	6.00
NMeFOSAA	4 – 1000	8.21	6.64	5.77	7.50	10.0
NEtFOSAA	4 – 1000	6.98	5.24	3.00	7.73	6.67
PFMPA	1 – 1000	1.09	1.33	1.00	1.36	1.42
PFMBA	1 – 1000	0.78	0.91	0.73	0.65	1.20
HFPO-DA	10 – 1000	4.29	11.2	4.62	4.29	12.5
ADONA	1 – 1000	0.45	0.42	0.48	0.41	0.91
PFEESA	1 – 1000	0.31	0.31	0.18	0.16	0.34
9Cl-PF3ONS	1 – 1000	0.50	0.57	0.29	0.39	0.55
11Cl-PF3OUdS	1 – 1000	0.43	0.25	0.20	0.21	0.30

¹Due to background levels of TFA, ¹³C₂-TFA is used as a surrogate for TFA to generate the calibration curve.

Appendix III: Full Accuracy and Precision Data by Beverage Matrix

The following tables report average recovery (%RSD, n=9) at each fortification level (2, 4, 10, 20, 100, and 500 ng/L) for all 43 target analytes in each of the five representative beverage matrices. A dash (–) indicates the fortification level was below the analyte's LOQ in that matrix.

Table V: Accuracy and Precision for Green Tea

Analyte	2 ng/L	4 ng/L	10 ng/L	20 ng/L	100 ng/L	500 ng/L
¹³ C ₂ -TFA	–	–	–	101 (6.01)	97.8 (8.72)	113 (3.76)
PFPPrA	–	105 (6.54)	105 (5.99)	108 (3.90)	107 (2.95)	111 (4.51)
PFBA	–	107 (5.66)	98.0 (5.67)	102 (7.19)	107 (4.64)	110 (2.45)
PFPeA	–	98.2 (7.18)	97.6 (8.27)	94.9 (8.82)	104 (7.73)	97.8 (4.89)
PFHxA	–	106 (5.53)	108 (3.28)	105 (7.67)	113 (3.28)	112 (5.54)
PFHpA	95.3 (8.89)	93.4 (8.32)	94.8 (7.10)	98.5 (3.49)	106 (2.38)	90.2 (2.60)
PFOA	–	109 (8.46)	107 (7.81)	109 (7.91)	104 (8.73)	109 (6.47)
PFNA	–	106 (7.63)	110 (5.85)	111 (6.41)	105 (6.69)	109 (3.72)
PFDA	109 (3.55)	94.5 (7.33)	89.5 (7.12)	99.1 (4.35)	100 (4.29)	90.1 (5.56)
PFUnA	110 (6.51)	106 (8.12)	98.8 (7.02)	107 (5.46)	114 (4.04)	109 (5.62)
PFDoA	109 (5.62)	110 (6.66)	103 (6.74)	109 (4.25)	104 (5.74)	101 (8.09)
PFTTrDA	99.0 (8.03)	103 (8.56)	107 (8.41)	114 (4.09)	107 (7.30)	100 (8.00)
PFTeDA	113 (7.51)	105 (3.06)	115 (3.26)	106 (7.68)	108 (7.45)	109 (5.41)
TFMS	–	–	105 (4.55)	108 (3.03)	106 (3.74)	111 (3.47)
PFETs	104 (5.11)	98.2 (8.56)	99.9 (5.89)	97.4 (6.70)	108 (6.50)	107 (6.73)
PFPPrS	102 (6.95)	100 (3.67)	107 (5.77)	99.6 (7.01)	104 (6.67)	98.0 (10.1)
PFBS	113 (3.63)	108 (5.07)	110 (5.95)	102 (8.78)	113 (2.56)	104 (4.80)
PFPeS	103 (8.22)	103 (4.62)	102 (2.89)	106 (3.80)	108 (3.27)	112 (8.41)
PFHxS	112 (8.41)	103 (9.71)	98.5 (4.13)	99.5 (7.79)	105 (3.03)	104 (4.54)
PFHpS	111 (5.52)	97.7 (6.31)	99.0 (8.59)	98.3 (9.38)	105 (5.27)	88.7 (6.48)
PFOS	–	100 (8.90)	104 (5.40)	100 (9.13)	111 (4.76)	104 (5.18)
PFNS	–	103 (8.62)	107 (5.07)	113 (5.69)	111 (5.45)	105 (4.31)
PFDS	–	103 (10.2)	100 (9.92)	109 (6.48)	112 (4.47)	100 (6.20)
PFUDs	109 (9.79)	108 (6.41)	103 (7.23)	109 (4.61)	104 (5.29)	100 (2.91)
PFDoS	100 (9.44)	106 (8.64)	107 (7.05)	109 (6.32)	108 (7.18)	107 (3.77)
PFTTrDS	–	99.7 (10.0)	98.4 (10.3)	103 (4.11)	110 (7.00)	108 (5.14)
4:2 FTS	102 (10.7)	105 (6.42)	97.0 (8.35)	97.2 (6.37)	110 (5.97)	107 (6.41)
6:2 FTS	113 (3.95)	107 (6.25)	105 (9.47)	100 (9.47)	106 (5.97)	98.5 (7.66)
8:2 FTS	111 (6.32)	105 (10.6)	97.6 (10.7)	101 (8.33)	103 (4.80)	89.4 (9.41)
FOSA	–	–	104 (9.57)	91.8 (10.6)	101 (10.0)	93.4 (7.50)
NMeFOSA	–	–	109 (8.85)	102 (9.02)	96.4 (9.18)	89.0 (6.37)
NEtFOSA	–	–	–	104 (8.60)	107 (6.61)	95.6 (8.79)
5:3 FTCA	–	–	–	104 (8.59)	99.8 (8.23)	86.6 (9.52)
7:3 FTCA	–	–	–	95.1 (4.81)	98.8 (5.82)	86.0 (6.81)
NMeFOSAA	–	–	–	92.9 (11.0)	87.9 (11.5)	75.3 (10.4)
NEtFOSAA	–	–	–	92.2 (10.4)	95.9 (8.36)	83.7 (10.0)
PFMPA	–	95.7 (5.69)	96.3 (8.57)	94.8 (4.06)	107 (4.69)	104 (5.62)
PFMBA	103 (7.98)	101 (8.80)	106 (6.65)	109 (7.77)	109 (5.97)	113 (3.08)
HFPO-DA	–	–	–	105 (5.97)	100 (9.22)	103 (4.26)
ADONA	109 (7.76)	104 (9.97)	104 (6.68)	102 (9.77)	112 (3.25)	105 (2.95)
PFEESA	105 (6.83)	100 (8.27)	101 (8.66)	101 (8.66)	110 (4.99)	106 (6.19)
9Cl-PF3ONS	110 (5.62)	107 (7.20)	101 (6.31)	112 (5.55)	111 (5.64)	93.0 (2.54)
11Cl-PF3OUdS	112 (6.11)	111 (4.29)	105 (5.28)	108 (6.78)	110 (4.00)	94.6 (1.68)

Table VI: Accuracy and Precision for Black Tea

Analyte	2 ng/L	4 ng/L	10 ng/L	20 ng/L	100 ng/L	500 ng/L
¹³ C ₂ -TFA	–	–	–	99.4 (5.47)	91.8 (3.33)	95.0 (4.11)
PFPrA	–	93.0 (7.52)	103 (9.72)	99.1 (7.80)	115 (5.92)	110 (2.92)
PFBA	–	98.6 (7.36)	100 (9.20)	95.4 (7.10)	110 (6.93)	106 (2.97)
PFPeA	–	106 (9.50)	92.0 (7.30)	95.1 (9.03)	108 (4.32)	90.4 (3.90)
PFHxA	–	107 (8.90)	101 (9.22)	100 (6.33)	112 (3.85)	103 (4.62)
PFHpA	103 (7.55)	99.6 (8.09)	91.5 (9.38)	92.8 (5.09)	99.8 (3.77)	85.7 (5.22)
PFOA	–	105 (8.15)	102 (9.20)	93.4 (8.04)	96.0 (9.55)	94.0 (9.17)
PFNA	–	104 (9.44)	105 (8.42)	104 (8.33)	102 (9.58)	96.6 (9.69)
PFDA	107 (4.85)	96.2 (6.76)	93.2 (9.95)	91.8 (7.02)	97.4 (8.89)	88.6 (7.49)
PFUnA	–	98.4 (9.41)	91.2 (7.66)	102 (9.44)	100 (10.1)	100 (8.96)
PFDoA	–	109 (5.39)	101 (9.69)	108 (3.90)	109 (6.28)	111 (5.41)
PFTrDA	93.2 (9.53)	105 (8.03)	101 (9.83)	103 (8.29)	110 (8.85)	103 (5.66)
PFTeDA	115 (5.91)	113 (6.22)	114 (3.43)	109 (6.73)	113 (5.98)	113 (2.38)
TFMS	–	–	104 (6.51)	110 (4.55)	108 (7.52)	110 (8.31)
PFETs	112 (8.35)	100 (10.0)	102 (7.37)	98.4 (9.90)	103 (8.86)	100 (10.3)
PFPrS	101 (8.73)	99.1 (7.37)	103 (5.91)	101 (3.42)	105 (3.07)	108 (4.04)
PFBS	110 (9.58)	100 (9.93)	99.2 (9.05)	102 (7.77)	111 (7.82)	103 (2.68)
PFPeS	–	–	104 (6.34)	100 (5.59)	107 (7.03)	102 (3.90)
PFHxS	105 (9.74)	97.1 (5.50)	97.2 (5.88)	97.9 (8.12)	106 (6.39)	102 (5.89)
PFHpS	103 (8.93)	93.1 (9.22)	98.3 (8.71)	91.0 (6.18)	103 (5.98)	86.7 (8.88)
PFOS	–	108 (8.98)	100 (9.15)	98.3 (5.19)	108 (5.13)	109 (5.53)
PFNS	–	118 (7.54)	99.8 (8.86)	101 (8.79)	115 (6.06)	110 (5.99)
PFDS	–	110 (8.97)	100 (8.63)	105 (9.99)	107 (7.70)	103 (7.84)
PFUDs	109 (11.8)	108 (9.72)	101 (9.71)	105 (7.29)	106 (6.34)	105 (4.41)
PFDoS	–	114 (8.33)	104 (6.72)	106 (7.27)	109 (7.51)	111 (4.69)
PFTrDS	106 (9.37)	111 (4.99)	108 (9.24)	101 (7.75)	108 (7.26)	109 (6.00)
4:2 FTS	95.0 (7.72)	94.6 (10.0)	90.7 (5.21)	94.6 (9.67)	109 (7.20)	94.8 (5.73)
6:2 FTS	97.0 (6.81)	93.8 (9.89)	93.6 (10.6)	88.6 (9.93)	105 (8.29)	89.9 (8.03)
8:2 FTS	94.7 (7.66)	110 (5.56)	102 (8.86)	106 (7.60)	112 (4.14)	102 (9.42)
FOSA	–	–	86.4 (5.30)	100 (8.73)	106 (8.86)	109 (9.15)
NMeFOSA	–	–	–	101 (5.95)	107 (9.34)	88.8 (8.29)
NEtFOSA	–	–	–	99.1 (7.83)	109 (2.97)	90.8 (6.63)
5:3 FTCA	–	–	–	100 (7.89)	95.9 (7.54)	81.3 (4.23)
7:3 FTCA	–	–	–	94.8 (10.6)	89.4 (9.19)	86.9 (6.49)
NMeFOSAA	–	–	–	–	76.4 (8.76)	71.1 (4.74)
NEtFOSAA	–	–	–	–	75.0 (8.01)	74.1 (11.0)
PFMPA	108 (7.29)	98.8 (9.85)	94.5 (7.70)	92.2 (7.52)	100 (6.58)	85.4 (3.52)
PFMBA	106 (9.72)	102 (9.42)	104 (9.19)	105 (8.71)	111 (5.86)	111 (6.33)
HFPO-DA	–	–	–	102 (9.32)	111 (8.12)	111 (6.47)
ADONA	107 (9.56)	104 (9.56)	98.6 (8.03)	102 (9.91)	111 (4.21)	113 (7.52)
PFEESA	101 (9.34)	100 (7.72)	105 (8.36)	105 (5.85)	112 (5.12)	106 (4.67)
9Cl-PF3ONS	111 (9.82)	106 (9.47)	94.7 (7.67)	91.3 (8.82)	96.9 (5.88)	95.9 (6.71)
11Cl-PF3OUdS	111 (5.78)	112 (5.65)	86.4 (5.54)	101 (9.05)	100 (6.18)	98.7 (5.68)

Table VII: Accuracy and Precision for Apple Juice

Analyte	2 ng/L	4 ng/L	10 ng/L	20 ng/L	100 ng/L	500 ng/L
¹³ C ₂ -TFA	–	–	–	100 (8.34)	95.6 (7.39)	116 (4.89)
PFPrA	–	103 (5.33)	109 (6.40)	104 (5.05)	107 (4.58)	115 (4.46)
PFBA	–	100 (9.92)	105 (9.86)	101 (9.06)	101 (5.41)	112 (8.78)
PFPeA	–	103 (7.73)	105 (7.77)	110 (6.49)	98.0 (4.20)	108 (5.33)
PFHxA	105 (8.21)	100 (8.48)	107 (9.32)	105 (5.56)	101 (8.88)	111 (9.21)
PFHpA	103 (8.42)	104 (8.64)	109 (7.15)	108 (8.42)	108 (3.76)	112 (8.68)
PFOA	105 (10.5)	104 (7.28)	111 (8.64)	113 (7.04)	102 (7.24)	110 (9.30)
PFNA	99.5 (8.21)	103 (9.73)	107 (7.87)	108 (5.42)	98.2 (9.41)	100 (6.70)
PFDA	100 (9.26)	101 (6.55)	106 (9.75)	111 (3.84)	92.8 (8.63)	102 (4.88)
PFUnA	105 (9.15)	107 (9.54)	110 (9.40)	114 (4.80)	98.6 (4.51)	105 (5.11)
PFDoA	100 (9.71)	109 (6.91)	114 (4.47)	114 (6.60)	103 (6.14)	110 (2.07)
PFTrDA	105 (4.88)	109 (3.75)	109 (7.75)	111 (4.93)	106 (5.96)	108 (8.77)
PFTeDA	106 (7.72)	109 (5.79)	108 (7.63)	114 (5.80)	109 (6.67)	110 (7.47)
TFMS	–	–	110 (3.57)	110 (6.49)	107 (3.28)	112 (4.25)
PFETs	111 (6.55)	104 (9.68)	112 (7.92)	113 (4.56)	96.2 (9.75)	105 (7.20)
PFPrS	102 (9.57)	113 (4.99)	113 (5.94)	113 (6.68)	110 (7.61)	112 (6.55)
PFBS	111 (7.77)	103 (9.12)	111 (8.36)	113 (5.16)	102 (9.78)	108 (4.99)
PFPeS	107 (7.80)	109 (6.29)	115 (6.03)	114 (4.66)	101 (8.29)	111 (4.08)
PFHxS	115 (5.37)	100 (9.99)	107 (9.81)	105 (7.65)	100 (6.73)	109 (2.40)
PFHpS	103 (8.96)	103 (8.83)	110 (7.81)	114 (4.11)	103 (8.55)	107 (8.21)
PFOS	100 (9.28)	105 (7.20)	108 (7.07)	110 (7.20)	109 (7.24)	112 (6.52)
PFNS	94.3 (9.44)	95.7 (8.01)	108 (8.01)	108 (5.01)	103 (8.24)	106 (3.87)
PFDS	114 (9.37)	108 (7.91)	106 (10.1)	114 (3.49)	100 (5.96)	108 (4.84)
PFUDs	108 (9.03)	106 (9.85)	106 (8.80)	112 (4.96)	103 (7.50)	111 (5.14)
PFDoS	117 (7.01)	112 (4.44)	111 (7.11)	110 (7.82)	106 (7.68)	110 (8.99)
PFTrDS	98.1 (7.20)	104 (10.2)	102 (7.95)	107 (5.62)	106 (4.43)	106 (4.68)
4:2 FTS	113 (2.78)	107 (8.03)	113 (4.82)	111 (4.07)	106 (7.23)	108 (7.46)
6:2 FTS	–	103 (5.75)	108 (8.96)	106 (6.80)	113 (2.87)	111 (3.83)
8:2 FTS	98.1 (9.26)	109 (5.66)	108 (8.65)	112 (2.95)	103 (6.38)	110 (8.67)
FOSA	–	113 (7.22)	93.1 (8.26)	108 (6.88)	101 (8.20)	112 (4.83)
NMeFOSA	–	–	98.9 (8.53)	111 (7.32)	100 (10.8)	104 (7.25)
NEtFOSA	–	–	102 (7.18)	109 (6.10)	83.6 (3.59)	98.5 (6.59)
5:3 FTCA	–	–	–	104 (8.88)	104 (8.63)	107 (9.66)
7:3 FTCA	–	–	–	107 (8.80)	97.8 (9.49)	91.5 (9.88)
NMeFOSAA	–	–	94.9 (9.09)	109 (9.19)	105 (9.36)	112 (4.56)
NEtFOSAA	–	–	108 (9.13)	106 (8.94)	93.7 (10.6)	111 (5.95)
PFMPA	–	92.4 (8.56)	98.4 (9.49)	103 (7.70)	95.5 (4.59)	105 (8.86)
PFMBA	97.6 (5.16)	102 (5.63)	109 (9.29)	110 (8.37)	94.5 (7.43)	104 (5.55)
HFPO-DA	–	–	117 (3.35)	112 (4.40)	110 (7.84)	113 (3.93)
ADONA	93.9 (7.70)	98.7 (9.16)	106 (8.27)	106 (9.42)	97.2 (4.43)	103 (9.28)
PFEESA	109 (7.55)	104 (4.63)	110 (8.58)	108 (6.43)	95.9 (9.48)	104 (3.72)
9Cl-PF3ONS	102 (7.89)	110 (10.0)	112 (6.40)	110 (6.53)	94.9 (7.97)	100 (3.36)
11Cl-PF3OUdS	109 (5.77)	108 (4.73)	110 (7.77)	109 (6.35)	99.0 (5.55)	105 (3.19)

Table VIII: Accuracy and Precision for Blended Berry Juice

Analyte	2 ng/L	4 ng/L	10 ng/L	20 ng/L	100 ng/L	500 ng/L
¹³ C ₂ -TFA	–	–	–	94.3 (5.65)	104 (1.94)	114 (0.88)
PFPrA	–	110 (9.34)	110 (5.05)	107 (7.17)	111 (4.92)	105 (3.80)
PFBA	–	109 (8.06)	110 (8.65)	108 (6.62)	104 (9.48)	94.1 (6.35)
PFPeA	–	102 (8.13)	106 (8.92)	94.8 (9.61)	105 (4.38)	101 (8.78)
PFHxA	106 (8.34)	99.1 (9.69)	97.6 (9.07)	95.6 (5.25)	104 (2.97)	99.6 (7.18)
PFHpA	106 (9.74)	104 (8.49)	110 (7.86)	107 (9.03)	107 (8.88)	103 (7.69)
PFOA	106 (6.78)	107 (8.53)	105 (7.54)	108 (5.82)	102 (5.41)	101 (9.17)
PFNA	106 (9.47)	106 (6.45)	103 (4.80)	108 (6.15)	97.2 (8.85)	96.3 (5.25)
PFDA	100 (8.41)	109 (8.62)	112 (4.56)	114 (4.42)	104 (9.84)	108 (5.66)
PFUnA	104 (8.55)	106 (5.85)	103 (8.94)	110 (5.94)	96.5 (6.33)	101 (7.31)
PFDoA	111 (6.98)	109 (7.06)	108 (6.30)	115 (3.95)	97.9 (6.15)	104 (7.28)
PFTrDA	102 (4.85)	108 (6.37)	97.2 (9.78)	111 (6.43)	99.6 (6.35)	108 (9.52)
PFTeDA	106 (4.73)	105 (4.56)	96.6 (7.63)	114 (3.89)	102 (3.29)	109 (8.41)
TFMS	–	–	105 (4.65)	109 (3.53)	111 (5.55)	114 (4.54)
PFETs	113 (5.75)	109 (6.75)	111 (6.78)	112 (6.59)	109 (7.19)	112 (4.10)
PFPrS	104 (9.93)	105 (7.84)	110 (8.21)	106 (6.13)	110 (4.55)	110 (9.02)
PFBS	110 (9.59)	101 (9.58)	106 (5.83)	98.5 (6.93)	108 (5.87)	96.8 (2.27)
PFPeS	102 (8.01)	103 (8.47)	100 (4.04)	104 (7.94)	111 (8.67)	100 (4.41)
PFHxS	121 (2.63)	97.9 (7.91)	102 (7.27)	97.3 (7.45)	101 (5.40)	98.7 (7.35)
PFHpS	104 (9.71)	107 (7.04)	110 (6.22)	112 (4.28)	111 (4.77)	99.3 (5.76)
PFOS	109 (8.60)	104 (9.08)	99.4 (9.43)	107 (4.43)	105 (6.60)	109 (9.20)
PFNS	106 (10.0)	106 (9.05)	103 (9.53)	113 (3.87)	99.4 (5.39)	102 (8.75)
PFDS	117 (5.26)	115 (7.64)	104 (10.1)	110 (6.35)	99.2 (7.59)	106 (8.96)
PFUDs	110 (9.55)	99.4 (9.91)	102 (8.31)	114 (3.77)	97.7 (5.54)	105 (9.64)
PFDoS	112 (8.38)	114 (7.34)	106 (7.36)	111 (6.22)	98.5 (4.55)	109 (7.70)
PFTrDS	118 (5.45)	105 (8.22)	107 (9.63)	111 (7.64)	98.6 (5.14)	109 (9.31)
4:2 FTS	113 (4.84)	96.7 (9.18)	100 (9.62)	93.7 (9.99)	92.5 (9.98)	95.4 (9.41)
6:2 FTS	–	97.9 (9.49)	103 (9.92)	95.8 (5.54)	95.3 (7.85)	101 (9.59)
8:2 FTS	97.9 (8.92)	94.9 (9.01)	108 (4.02)	99.4 (7.84)	92.5 (6.18)	93.1 (5.47)
FOSA	–	112 (9.69)	95.8 (10.3)	108 (9.65)	100 (9.18)	96.5 (7.23)
NMeFOSA	–	–	107 (6.32)	108 (9.18)	105 (9.20)	107 (5.20)
NEtFOSA	–	–	97.5 (9.70)	114 (4.09)	99.2 (9.06)	104 (8.33)
5:3 FTCA	–	–	–	107 (9.06)	110 (5.34)	101 (6.95)
7:3 FTCA	–	–	–	103 (8.73)	100 (6.43)	87.6 (9.60)
NMeFOSAA	–	111 (5.76)	106 (3.40)	102 (3.10)	78.5 (7.91)	111 (2.71)
NEtFOSAA	–	–	102 (9.91)	108 (8.12)	95.2 (9.76)	94.2 (9.68)
PFMPA	103 (9.19)	98.1 (9.01)	98.2 (8.02)	90.9 (8.82)	100 (9.17)	91.6 (4.13)
PFMBA	106 (3.93)	95.0 (6.39)	106 (9.20)	92.8 (8.93)	104 (3.69)	96.8 (4.67)
HFPO-DA	–	–	–	108 (9.00)	99.1 (10.3)	113 (4.02)
ADONA	111 (9.21)	103 (9.02)	95.7 (9.26)	92.8 (8.61)	99.0 (7.31)	92.0 (4.84)
PFEESA	101 (9.28)	95.8 (9.76)	101 (6.99)	100 (7.70)	107 (3.21)	95.1 (3.23)
9Cl-PF3ONS	102 (8.98)	101 (9.11)	97.8 (7.91)	109 (5.06)	99.3 (4.23)	101 (7.61)
11Cl-PF3OUds	109 (6.95)	117 (3.67)	109 (6.38)	115 (5.11)	97.3 (2.80)	103 (7.69)

Table IX: Accuracy and Precision for Orange Juice

Analyte	2 ng/L	4 ng/L	10 ng/L	20 ng/L	100 ng/L	500 ng/L
¹³ C ₂ -TFA	–	–	–	109 (4.78)	97.0 (7.06)	114 (3.48)
PFPrA	–	–	112 (9.01)	101 (8.91)	111 (4.88)	113 (2.79)
PFBA	–	104 (6.26)	102 (6.19)	106 (5.90)	109 (6.11)	105 (2.32)
PFPeA	–	112 (8.29)	107 (8.34)	97.6 (8.75)	103 (5.43)	104 (3.63)
PFHxA	–	108 (8.53)	102 (7.96)	98.7 (9.41)	106 (7.22)	102 (5.65)
PFHpA	–	107 (9.56)	104 (8.25)	109 (4.34)	113 (9.31)	114 (2.85)
PFOA	–	112 (5.83)	101 (9.36)	93.8 (8.96)	99.2 (7.07)	90.8 (3.00)
PFNA	–	107 (7.92)	97.1 (9.17)	95.0 (7.20)	99.3 (8.94)	95.3 (4.97)
PFDA	–	105 (9.58)	97.1 (8.98)	89.6 (7.06)	103 (4.58)	95.3 (5.14)
PFUnA	–	103 (8.83)	102 (7.80)	98.7 (9.25)	104 (7.57)	92.3 (2.80)
PFDoA	–	118 (4.35)	104 (9.54)	103 (9.09)	111 (5.50)	97.7 (2.60)
PFTrDA	–	111 (4.93)	101 (8.79)	95.7 (8.87)	96.6 (4.50)	86.5 (2.11)
PFTeDA	–	115 (6.24)	106 (5.81)	101 (6.93)	111 (6.56)	104 (1.60)
TFMS	–	–	–	105 (7.35)	108 (5.60)	102 (3.51)
PFETs	–	110 (6.57)	108 (5.56)	109 (5.22)	108 (2.56)	112 (4.06)
PFPrS	–	109 (5.62)	110 (6.21)	105 (9.07)	107 (7.16)	109 (5.84)
PFBS	–	107 (9.79)	102 (7.49)	99.6 (9.76)	105 (6.19)	102 (3.54)
PFPeS	–	106 (9.30)	105 (7.37)	108 (8.49)	107 (6.11)	112 (7.53)
PFHxS	–	111 (7.18)	99.0 (7.59)	96.0 (6.94)	95.9 (9.08)	101 (6.24)
PFHpS	–	111 (5.92)	98.3 (9.71)	102 (8.34)	100 (6.60)	102 (2.52)
PFOS	–	114 (8.86)	103 (9.19)	94.3 (8.99)	96.8 (6.13)	98.9 (4.38)
PFNS	–	120 (7.66)	86.8 (5.72)	102 (10.1)	95.2 (8.09)	92.4 (3.12)
PFDS	–	111 (7.72)	97.2 (8.59)	95.7 (10.7)	95.1 (6.71)	83.9 (3.69)
PFUDs	–	112 (6.21)	99.7 (8.65)	96.1 (9.44)	100 (6.93)	90.4 (3.81)
PFDoS	–	109 (6.06)	98.3 (9.53)	98.8 (9.43)	106 (6.57)	93.6 (3.54)
PFTrDS	–	115 (5.44)	109 (6.27)	95.9 (10.6)	104 (7.01)	95.0 (5.06)
4:2 FTS	–	102 (8.22)	104 (8.92)	93.0 (6.36)	98.4 (9.32)	93.4 (6.29)
6:2 FTS	–	104 (3.08)	97.7 (7.27)	94.4 (9.75)	110 (7.26)	109 (5.80)
8:2 FTS	–	108 (8.43)	96.5 (8.58)	103 (8.41)	108 (8.02)	115 (3.39)
FOSA	–	116 (8.38)	101 (7.95)	102 (9.79)	101 (8.26)	107 (8.98)
NMeFOSA	–	–	103 (9.25)	107 (9.74)	109 (7.03)	115 (3.60)
NEtFOSA	–	–	107 (4.13)	106 (7.54)	104 (9.22)	100 (9.16)
5:3 FTCA	–	–	–	94.5 (9.06)	100 (8.37)	100 (6.81)
7:3 FTCA	–	–	–	99.3 (9.08)	109 (6.13)	111 (3.62)
NMeFOSAA	–	–	122 (2.96)	99.4 (8.85)	106 (8.90)	109 (6.56)
NEtFOSAA	–	–	–	94.7 (9.55)	102 (9.15)	102 (9.44)
PFMPA	–	100 (7.26)	95.7 (7.44)	93.5 (7.34)	93.1 (7.00)	87.3 (4.14)
PFMBA	–	111 (4.98)	107 (8.50)	91.7 (6.34)	110 (6.47)	103 (5.88)
HFPO-DA	–	–	–	91.9 (8.61)	104 (9.74)	88.5 (8.47)
ADONA	–	102 (9.87)	99.4 (8.22)	94.4 (6.41)	109 (5.66)	107 (4.46)
PFEESA	–	110 (6.86)	96.9 (9.85)	91.4 (9.96)	102 (7.64)	98.9 (1.32)
9Cl-PF3ONS	–	111 (3.64)	97.8 (8.46)	104 (9.83)	107 (6.47)	103 (2.06)
11Cl-PF3OUdS	–	108 (5.31)	91.8 (7.72)	93.0 (7.28)	98.4 (3.61)	87.3 (1.49)

Featured Products



Ultra IBD Inert, 3 μ m, 100 x 2.1 mm HPLC Column

- Inert LC column technology reduces nonspecific binding of chelating analytes, enabling sensitive analysis and smooth integration of peaks.
- Increased response and analyte recovery, allowing lower detection limits.
- Improved peak shape without passivation or mobile phase additives.
- Specialized columns for mixed polar and nonpolar compounds.
- Part of Restek's Ultra LC column line, our broadest selection of stationary phases on a single silica support.

Catalog No.	Product Name	Units
9175312-T	Ultra IBD Inert, 3 μ m, 100 x 2.1 mm HPLC Column	ea.



Ultra IBD HPLC Column

Catalog No.	Product Name	Units
9175362	Ultra IBD, 3 μ m, 150 x 2.1 mm HPLC Column	ea.



PFAS 28 Calibration Standard

Catalog No.	Product Name	Units
30734	PFAS 28 Calibration Standard, 1 μ g/mL, Methanol (1 mM KOH), 1 mL/ampul	ea.