

Quantitation of ultrashort- and short-chain PFAS in beverages by a direct injection LC-MS/MS method

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This technical note describes a direct injection LC-MS/MS method for the quantitation of ultrashort- and short-chain per- and polyfluoroalkyl substances (PFAS) in beverages. The sensitivity of the SCIEX 7500 system enabled a simple direct injection approach and the use of dilution and smaller injection volumes to reduce matrix effects. Application of the method to 24 beverage samples revealed the presence of several ultrashort- and short-chain PFAAs, where trifluoroacetic acid (TFA) dominated in detection frequency and concentration (Figure 1). TFA concentrations were at least an order of magnitude higher than the sum of all other PFAAs detected, with the highest levels observed in fruit- and vegetable-based juice and wine.

Key benefits of the SCIEX 7500 system for analyzing PFAS in beverages

- **Leveraging sensitivity for direct injection:** The SCIEX 7500 system enabled direct injection and the use of dilution and smaller injection volumes to counter matrix effects
- **Good quantitative performance in matrix spikes:** Recoveries of 80–120% and precision %CV <20% for most of the target PFAS were achieved in bottled water, tea, apple juice, sake and wine spiked at different concentrations.
- **Detection in real-world beverages:** Sub-to-100s of µg/L of TFA and ng/L levels of other PFAAs were detected in drinking water, juice, alcoholic beverages and other assorted drinks.
- **Interlaboratory corroboration of TFA levels:** Independent analysis showed good corroboration (<31% difference) of TFA levels between 2 different detection techniques.

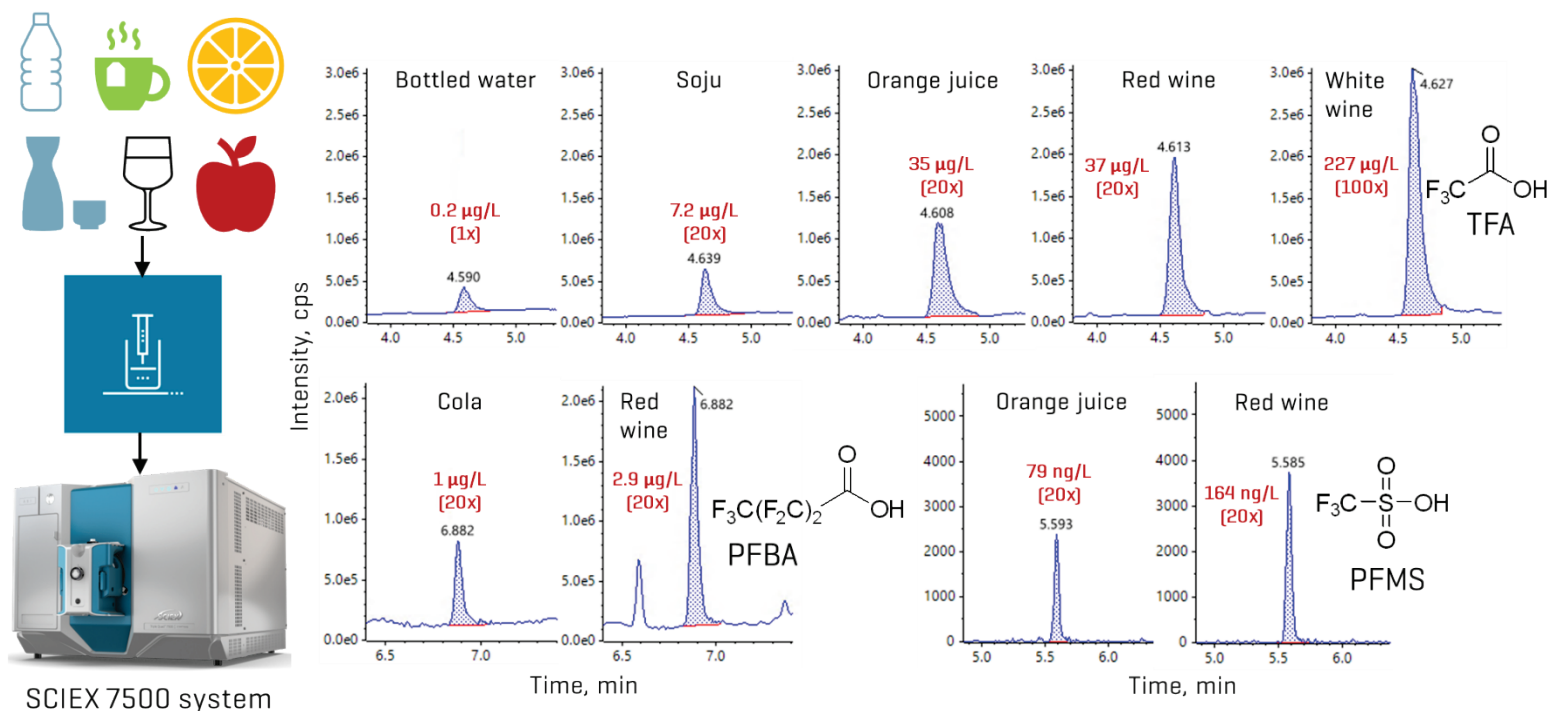


Figure 1. Detection of ultrashort- and short-chain PFAAs in beverages using a simple direct injection LC-MS/MS method on the SCIEX 7500 system.

Representative extracted ion chromatograms (XICs) of TFA, PFBA and PFMS demonstrate their presence in assorted beverage matrices at concentrations ranging from ng/L to µg/L levels. The values in brackets represent the dilution factors required to dilute the sample prior to injection.

Introduction

While PFAS detection in beverages has received far less attention than food matrices,¹ emerging data indicate the prevalence of ultrashort- and short-chain perfluoroalkyl acids [PFAAs] in beverages.²⁻⁵ Ultrashort- and short-chain PFAAs represent a subset of PFAS that are characterized by a chain length of 1–6 perfluorinated carbons [C_F] (**Figure 2**). Given their water solubility and documented phytoaccumulation⁶, these chemicals presumably accumulate in aquatic environments and terrestrial plant tissues, resulting in exposure through drinking water and plant-derived beverages. In particular, trifluoroacetic acid [TFA] has been reported at concentrations of 10s–100s $\mu\text{g/L}$ in fruit juices³ and wine⁴, compared to the ng/L levels typically observed for other PFAAs. This discrepancy is primarily due to multiple sources, such as the atmospheric degradation of fluorinated refrigerants, pharmaceuticals and pesticides,^{7,8} contributing to the increased presence of TFA in the environment.

Previously, we demonstrated a direct injection LC-MS/MS method with robust retention and quantitation of ultrashort-, short- and long-chain PFAAs in aqueous matrices.⁹ Here, further optimization enabled a similar direct injection approach, with the addition of dilution and a smaller injection volume to counter the matrix effects in more complex beverage matrices.

Methods

Chemical standards and samples: Native and isotopically-labeled standards were purchased from Wellington Laboratories and Cambridge Isotope Laboratories. Assorted water and beverages were sourced from Toronto, Ontario, Canada.

Sample preparation: MilliQ, bottled and tap water samples were spiked with isotopically-labeled internal standards at an in-vial concentration of 10 ng/L and directly injected without dilution. Pre-screened water with the lowest background levels of PFAS was used for the subsequent preparation of calibration standards and samples. For all other beverages, 10 mL of each sample was centrifuged at 4,000 rpm for 10 minutes, followed by diluting 1 mL of the supernatant with varying volumes of water, depending on the sample. Further in-vial dilution was performed with only water to maintain a 100% aqueous vial composition.

A subset of these samples was independently analyzed at York University by direct injection on an ion chromatograph coupled to a quadrupole mass spectrometer [IC-MS]. Experimental details of the IC-MS method are described elsewhere.¹⁰

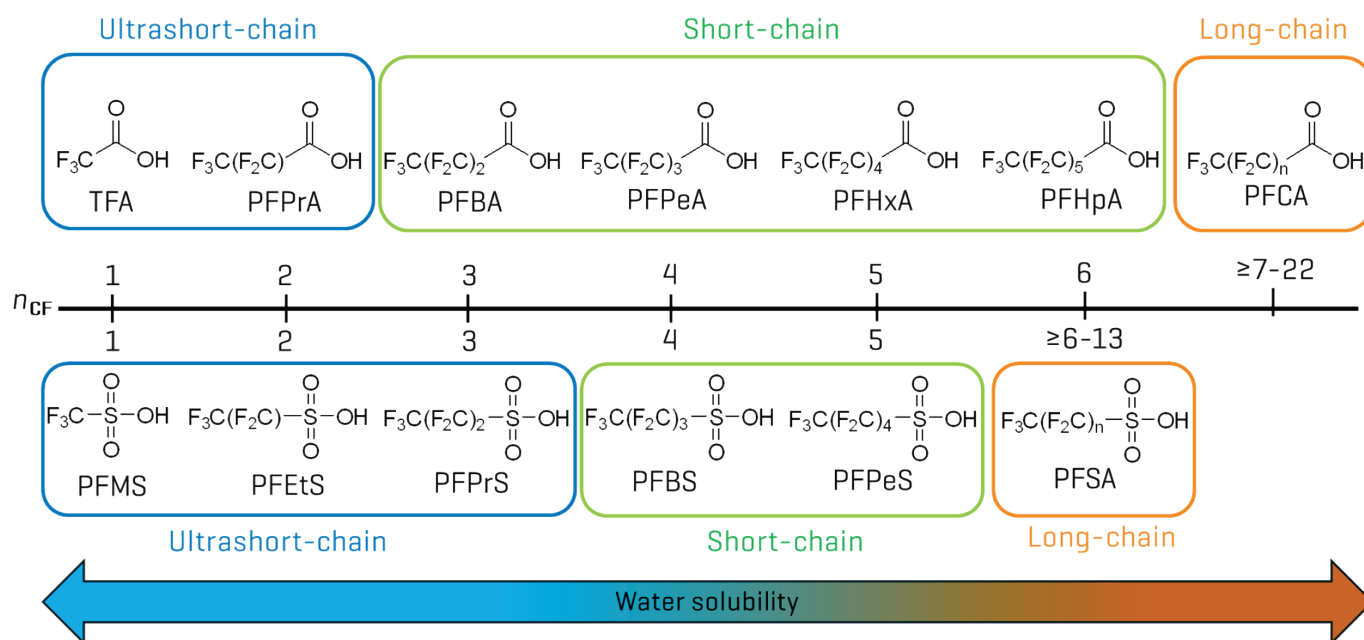


Figure 2. A structural overview of ultrashort-, short- and long-chain PFAAs. The varying chain length of perfluoroalkyl carboxylic acids [PFCAs, top] and perfluoroalkane sulfonic acids [PFSAs, bottom] is demonstrated by the number of C_F in their structures. The water solubility of the PFAA is inversely correlated with the number of C_F in the fluorinated chain.

Chromatography: Chromatographic separation was performed on a Shimadzu Prominence LC system using a Luna Omega PS C18 as the analytical column (150 x 2.1 mm, 3 μ m, [Phenomenex P/N: 00F-4758-AN](#)) and a combination of a Luna Omega PS C18 (50 x 3 mm, 3 μ m, [Phenomenex P/N: 00B-4758-YO](#)) and a Biozen Glycan (100 x 2.1 mm, 2.6 μ m, [Phenomenex P/N: 00D-4773-AN](#)) as the delay columns. A flow rate of 0.4 mL/min, an injection volume of 10 μ L and a column temperature of 45°C were used. The LC gradient used is shown in **Table 1**.

Table 1: Chromatographic gradient for the analysis of ultrashort- and short-chain PFAS in beverages.

Time [min]	Mobile phase A [%]	Mobile phase B [%]
0.0	98	2
0.5	98	2
3.0	70	30
7.0	30	70
7.5	4	96
7.6	98	2
11	98	2

Mobile phase A: Water with 0.1% (v/v) acetic acid

Mobile phase B: 90:10 (v/v) acetonitrile/water with 10mM ammonium acetate

Mass spectrometry: Analysis was performed using negative electrospray ionization on the [SCIEX 7500 system](#). Data was acquired by scheduled multiple reaction monitoring (sMRM) with optimized source and gas conditions (**Table 2**) and compound-dependent parameters, which are reported elsewhere.⁹

Table 2: Source and gas parameters for the analysis of ultrashort- and short-chain PFAS on the SCIEX 7500 system.

Parameter	Value
Polarity	Negative
Ion source gas 1	40 psi
Ion source gas 2	70 psi
Curtain gas	40 psi
Source temperature	380°C
Ion spray voltage	-2000 V
CAD gas	9 psi

Data processing: Data acquisition and processing were performed using [SCIEX OS software](#) (version 3.4).

Gradient optimization for different analyte panels

The mixed-mode selectivity from the Luna Omega PS C18 column previously enabled the development of a 20-minute gradient for the simultaneous analysis of ultrashort-, short- and long-chain PFAAs.⁹ The current method focused on a smaller subset of the ultrashort- and short-chain PFAAs due to their expected higher prevalence in beverages as compared to their longer-chain analogues. Gradient optimization resulted in shorter LC runs for different target PFAS based on the assay needs (**Figure 3**). The final gradient was reduced by almost half to focus on the ultrashort- and short-chain PFAAs in beverages. Despite the shorter runtime, the gradient still retained the analytes (>4 min), had excellent separation and reproducible retention times (RTs, <1 %CV) for the early eluting TFA and perfluoromethane sulfonic acid [PFMS] from the interference-prone void region.

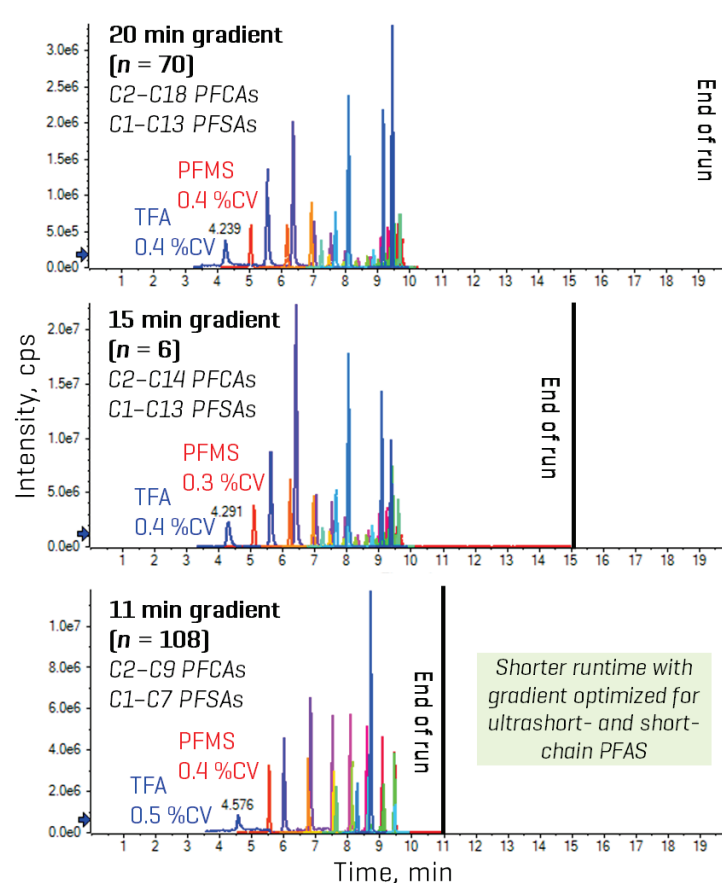


Figure 3. Chromatographic optimization for different PFAS panels. Gradient modifications resulted in different runtimes (20 min, 15 min and 11 min) catered for the analysis of different PFAS, while still maintaining robust retention (RT %CV <1%) of the earliest eluting TFA and PFMS. The RT %CV was calculated from all standards and spiked quality control (QC) samples, as indicated by the injection count in brackets for each batch.

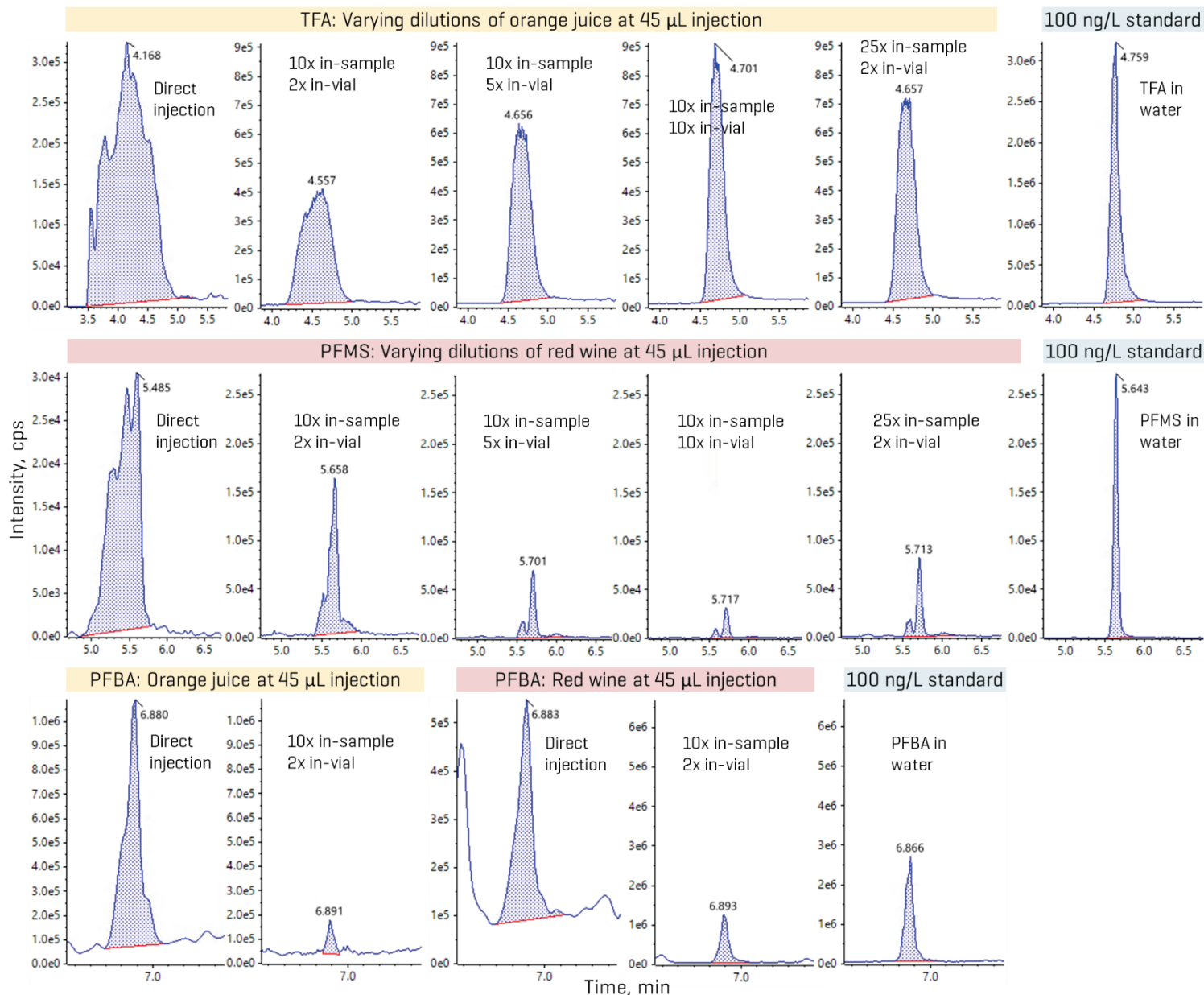


Figure 4. Impact of dilution on the chromatography of TFA, PFMS and PFBA injected at 45 μ L in orange juice and red wine. The top panel shows representative XICs of TFA in orange juice injected directly, at varying in-vial dilutions [2x, 5x and 10x] and in-sample dilutions [1 mL of juice diluted to 10 mL [10x] and 25 mL [25x]], while the middle panel shows the same for PFMS in red wine. Similar data is shown for PFBA detected in juice and red wine. A 100 ng/L standard is included to provide reference RTs and peak shapes for TFA, PFMS and PFBA in water.

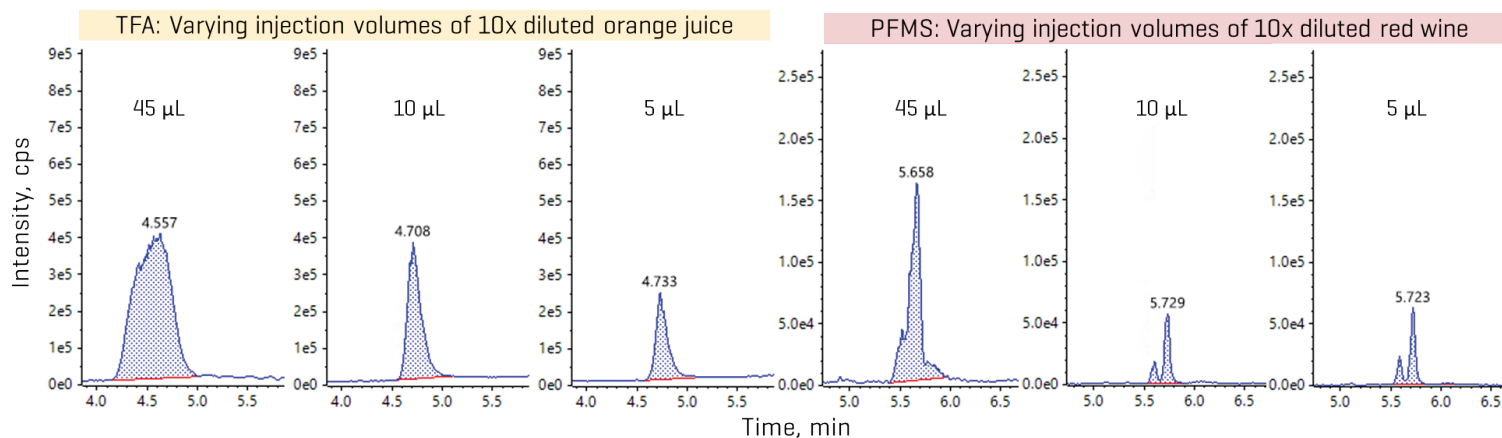


Figure 5. Impact of injection volume on the chromatography of TFA in orange juice and PFMS in red wine. The left panel shows XICs of TFA injected at varying injection volumes [45, 10 and 5 μ L] in orange juice, while the right panel shows similar data for PFMS in red wine.

Leveraging sensitivity for reducing matrix load

Quantitative performance in aqueous standards

Preliminary direct injections of beverage samples revealed poor chromatography and retention time [RT] shifts for certain PFAAs due to significant matrix effects (**Figures 4 and 5**). The high sensitivity of the SCIEX 7500 system enabled the use of dilutions and smaller injection volumes to reduce the matrix load on the column. **Figures 4 and 5** demonstrate how in-sample and in-vial dilutions and smaller injection volumes were able to recover the peak shapes and RT shifts for TFA and PFMS in orange juice and red wine. Based on their reported occurrences in beverages,²⁻⁴ subsequent method development prioritized these two compounds, resulting in sample-specific dilutions to stay within the calibration range. An injection volume of 10 μL was selected to balance between sensitivity and peak quality. These optimizations may not be necessary for all PFAAs, as demonstrated for PFBA, which retained good peak shape even with 45 μL injections of both the undiluted and diluted beverage samples (**Figure 4**). This suggests the need to optimize sample preparation based on the different sensitivity limits and matrix responses of the analytical method across the target PFAS panel, which may result in running separate injections.

Table 3 summarizes the quantitative performance of the aqueous calibration standards. Linearity with $r^2 \geq 0.99$ was achieved for all analytes, with 2–3 orders of dynamic range. The LOQ selection was based on the lowest standard achieving a signal-to-noise [S/N] ratio ≥ 10 , accuracy within $\pm 30\%$ and %CV of $< 30\%$. The in-vial LOQs ranged from 0.5 ng/L to 50 ng/L. Endogenous levels in the filtered tap water used as the diluent resulted in higher LOQs of 50 ng/L for TFA and 25 ng/L for PFBA. Overall, acceptable accuracies within $\pm 30\%$ and %CV $< 30\%$ were achieved at the LOQ level, while accuracies within $\pm 25\%$ and %CV $< 20\%$ were achieved at all other levels for most analytes. Replicate injections of a mid-level standard also exhibited good accuracy ($\pm 15\%$) and precision [%CV $< 10\%$] for most analytes (**Table 3**).

Figure 6 shows example XICs of the quantifier and qualifier transitions of TFA at the LOQ and in various beverage matrices. Despite its lower sensitivity, the qualifier transition based on the F^- fragment (m/z 19) can be used to confirm TFA detection, especially in beverages with mid-to-high $\mu\text{g/L}$ levels.

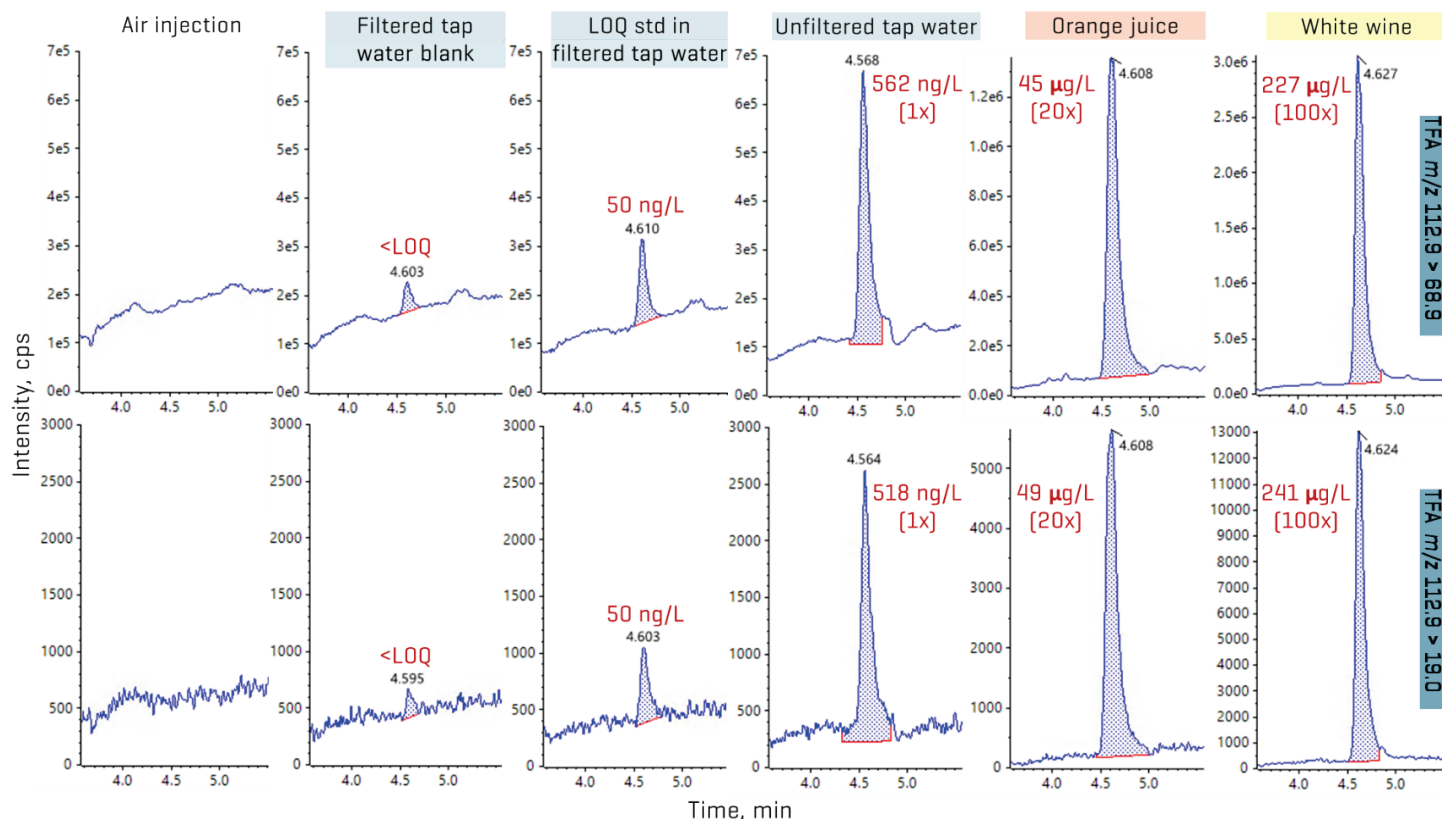


Figure 6. Representative XICs of the quantifier (top) and qualifier (bottom) transitions of TFA in various beverage matrices. The XICs represent the levels of TFA observed in an air injection from an empty vial, a solvent blank comprised of filtered tap water, the LOQ standard, unfiltered tap water, orange juice and white wine. All water samples were directly injected on the instrument, while the beverage samples were diluted [dilution factor in brackets] prior to injection.

Table 3: Quantitative performance of the aqueous calibration standards at the in-vial LOQ and a mid-level concentration. All analytes are listed with their in-vial calibration range, linear regression coefficient (r^2), accuracy and precision from replicate injections of the LOQ and a mid-level standard. Quantifier transitions are listed first for each analyte, followed by the qualifier transitions. Additional qualifier transitions were included for analytes prone to matrix interferences.

Analyte	m/z	In-vial range (ng/L)	r^2	LOQ (In-vial)		Mid-level standard (In-vial)	
				Conc (ng/L)	Accuracy [%CV] ($n = 3$)	Conc (ng/L)	Accuracy [%CV] ($n = 8$)
TFA 1	112.9 > 68.9	50 - 10000	0.9938	50	105 [12]	250	105 [9.4]
TFA 2	112.9 > 19.0	100 - 10000	0.9944	100	114 [7.3]	250	107 [10]
PFPrA 1	163.0 > 118.9	10 - 10000	0.9973	10	85 [12]	250	108 [3.5]
PFPrA 2	163.0 > 68.9	10 - 10000	0.9983	10	105 [23]	250	103 [6.3]
PFPrA 3	163.03 > 19.1	10 - 10000	0.9990	10	97 [13]	250	105 [3.8]
PFBA 1	213.0 > 169.0	25 - 5000	0.9930	25	81 [11]	250	109 [2.6]
PFBA 2	213.0 > 19.0	25 - 10000	0.9981	25	94 [4.9]	250	101 [3.5]
PFPeA 1	263.0 > 219.0	5 - 5000	0.9960	5	87 [3]	250	109 [5.8]
PFPeA 2	263.0 > 19.0	1 - 10000	0.9996	1	101 [29]	250	102 [5.1]
PFHxA 1	313.0 > 269.0	10 - 5000	0.9930	10	80 [15]	250	109 [4.2]
PFHxA 2	313.0 > 118.9	5 - 10000	0.9992	5	101 [14]	250	101 [4.7]
PFHpA 1	363.0 > 319.0	5 - 5000	0.9973	5	116 [9.5]	250	109 [3.3]
PFHpA 2	363.0 > 169.0	5 - 10000	0.9988	5	120 [15]	250	106 [4.4]
PFOA 1	413.0 > 369.0	2.5 - 5000	0.9989	2.5	98 [21]	250	109 [3.4]
PFOA 2	413.0 > 169.0	5 - 10000	0.9986	5	98 [11]	250	106 [3.8]
PFNA 1	463.0 > 419.0	5 - 10000	0.9950	5	97 [19]	250	106 [2.3]
PFNA 2	463.0 > 219.0	5 - 10000	0.9982	5	130 [3.2]	250	104 [4.0]
PFMS 1	149.0 > 80.0	0.5 - 10000	0.9919	0.5	85 [7.1]	25	103 [4.5]
PFMS 2	149.0 > 99.0	0.5 - 10000	0.9950	0.5	105 [13]	25	101 [3.8]
PFMS 3	149.0 > 83.0	5 - 10000	0.9940	5	91 [4.6]	25	103 [3.5]
PFEtS 1	199.0 > 79.9	0.5 - 5000	0.9969	0.5	104 [2.3]	25	102 [6.4]
PFEtS 2	199.0 > 99.0	2.5 - 10000	0.9949	2.5	71 [31]	25	102 [8.0]
PFEtS 3	199.0 > 82.9	5 - 10000	0.9948	5	102 [22]	25	96 [25]
PFPrS 1	249.0 > 79.9	2.5 - 5000	0.9962	2.5	91 [11]	25	103 [4.8]
PFPrS 2	249.0 > 99.0	2.5 - 10000	0.9939	2.5	97 [8.3]	25	106 [5.4]
PFPrS 3	249.0 > 119.0	2.5 - 10000	0.9934	2.5	85 [21]	25	104 [6.1]
PFPrS 4	249.0 > 169.0	5 - 10000	0.9933	5	102 [12]	25	107 [9.9]
PFBS 1	298.7 > 79.9	5 - 5000	0.9968	5	87 [12]	25	99 [5.6]
PFBS 2	298.7 > 98.8	5 - 10000	0.9941	5	66 [23]	25	99 [9.5]
PFPeS 1	349.0 > 79.9	2.5 - 10000	0.9922	2.5	116 [9.4]	25	109 [6.6]
PFPeS 2	349.0 > 98.8	2.5 - 10000	0.9957	2.5	89 [17]	25	104 [5.5]
PFHxS 1	398.7 > 79.9	0.5 - 10000	0.9924	0.5	105 [2.8]	25	102 [5.2]
PFHxS 2	398.7 > 98.8	2.5 - 5000	0.9914	2.5	116 [7.6]	25	100 [8.6]
PFHpS 1	449.0 > 79.9	1 - 10000	0.9904	1	86 [23]	25	101 [7.0]
PFHpS 2	449.0 > 98.8	2.5 - 5000	0.9935	2.5	124 [7.5]	25	107 [6.8]
HFPO-DA 1	284.9 > 168.9	2.5 - 1000	0.9948	2.5	98 [17]	25	109 [8.2]
HFPO-DA 2	284.9 > 184.9	5 - 1000	0.9962	5	91 [8.4]	25	104 [5.5]
ADONA 1	376.9 > 250.9	0.5 - 2500	0.9963	0.5	89 [6.3]	25	114 [6.8]
ADONA 2	376.9 > 84.8	1 - 5000	0.9979	1	110 [19]	25	104 [6.0]

Quantitative performance in beverages

Table 4 summarizes the quantitative performance in bottled water. Replicates of bottled water spiked at 1–10x the in-vial solvent LOQs were used to calculate the method detection limit (MDL). The MDL is defined as the lowest measured concentration of an analyte that can be measured with 99% confidence as distinguishable from the method blanks.¹¹ The MDL was calculated by multiplying the standard deviation from 8 replicates by the Student's t-value at the 99% confidence level based on this equation: $MDL = s \times t_{(n-1, 1-\alpha=0.99)}$

Overall, recoveries within $\pm 30\%$ of the nominally spiked concentration and %CV <25% were achieved in the MDL spikes. The calculated MDLs ranged from 0.7 ng/L to 60 ng/L for most analytes, except for TFA with a higher MDL of 130 ng/L [Table 4]. For aqueous beverages with less matrix effects, opting for a higher injection volume can improve method range limits, as shown by the lower MDLs previously achieved in 45 μ L injections of tap water spikes [Table 4].⁹

Table 4: Quantitative performance of bottled water spikes at the MDL based on a 10 μ L injection. All analytes are listed with their in-vial LOQ and MDL spike levels prepared at 1–10x of the LOQ. The recovery and precision achieved at the resulting in-sample MDLs are included. Tap water MDLs from a previous study⁹ based on a 45 μ L injection are included for comparison.

Analyte	In-vial		In-sample		
			10 μ L		45 μ L
	LOQ (ng/L)	Spike level (ng/L)	MDL (ng/L)	Rec [%CV]	MDL (ng/L)
TFA	50	100	130	80 [5.6]	190
PFPrA	10	50	21	96 [7.2]	3.9
PFBA	25	100	60	89 [11]	63
PFPeA	5	10	3.6	80 [7.5]	0.6
PFHxA	10	10	5.5	92 [10]	1.0
PFHpA	5	50	14	78 [6.0]	0.4
PFMS	0.5	2	0.7	108 [5.2]	-
PFEtS	0.5	2	1.0	106 [8.2]	0.7
PFPrS	2.5	2	1.6	91 [15]	0.4
PFBS	5	10	3.8	86 [7.3]	0.9
PFPeS	2.5	10	11	76 [24]	2.5
PFHxS	0.5	2	1.5	96 [13]	0.6
PFHpS	1	2	1.3	70 [16]	0.8
HFPO-DA	2.5	10	5.1	94 [9.1]	0.3
ADONA	0.5	2	0.7	90 [6.6]	0.1

Drinking water matrices were directly injected onto the LC-MS/MS. However, as demonstrated in **Figures 4** and **5**, other beverages exhibit significantly different matrix effects and concentration ranges, depending on the PFAAs. While TFA typically requires higher dilution, this may not be needed for other PFAAs. This complicates back-calculation of their in-sample MDLs, as the dilution factor can vary significantly for different PFAAs from sample to sample. **Table 5** lists the in-vial MDLs calculated for 4 representative PFAAs from various beverages that were spiked at 2–5x the in-vial LOQ and their corresponding recoveries and precision. In-vial MDLs were presented to demonstrate the quantitative performance in matrix spiked at near-LOQ levels.

Table 5: Quantitative performance of TFA, PFBA, PFMS and PFBS in beverage spikes at the in-vial MDL. Example in-vial MDLs and their corresponding recovery and precision are listed for TFA, PFBA and PFMS.

Analyte	In-vial MDL					
	Green tea		Apple juice		Sake	
	MDL (ng/L)	Rec [%CV]	MDL (ng/L)	Rec [%CV]	MDL (ng/L)	Rec [%CV]
TFA	18	74 [8.4]	39	100 [13]	28	98 [4.9]
PFBA	45	114 [2.6]	19	82 [16]	21	78 [9.1]
PFMS	0.5	110 [7.1]	0.5	120 [7.2]	-	-
PFBS	2.9	92 [10]	4.2	91 [15]	2.1	88 [8.0]

Beverage spikes were performed at two spike levels [2–100 ng/L and 10–500 ng/L] in green tea, apple juice, sake and white wine.

Figure 7 shows the violin plot distribution of the recoveries obtained in each beverage matrix. Overall, most of the target PFAS compounds showed excellent recovery [80–120%] and precision [%CV <20%]. Recoveries were impacted at the lower spiking level for some analytes in white wine due to matrix effects and/or endogenous background levels. No recoveries were reported for TFA in white wine, because its concentration in the unspiked sample was too high [$\sim 100 \mu$ g/L] to allow for over-spiking.

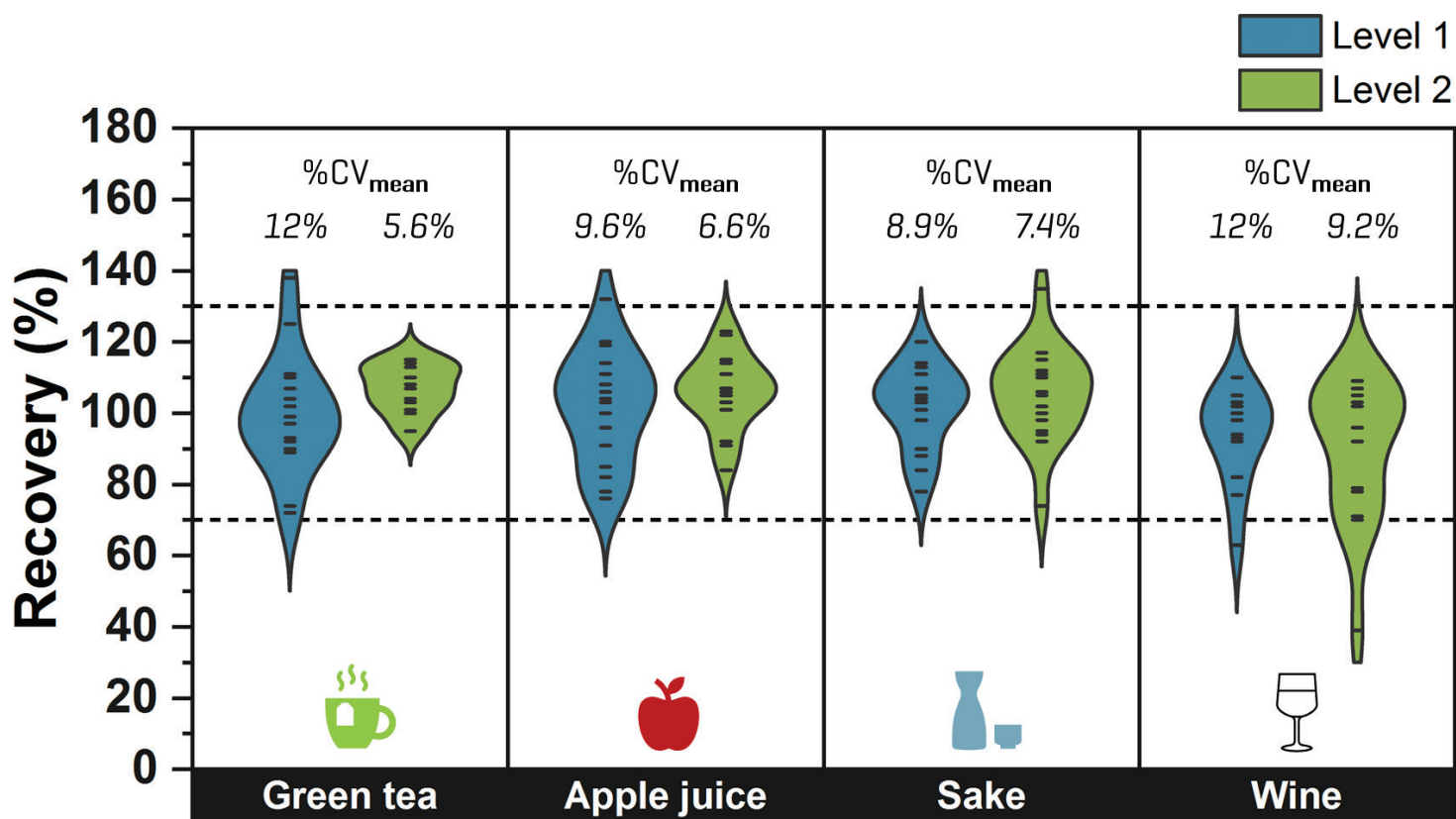


Figure 7. Violin plots of recovery distribution of the target PFAS spiked in green tea, apple juice, sake and white wine. The blue and green data represent the recoveries obtained at in-vial spike levels of 2–100 ng/L and 10–500 ng/L, respectively. The dotted black lines represent $\pm 30\%$ tolerance on recovery. The $\%CV_{\text{mean}}$ at the top represents the average $\%CV$ calculated across the target PFAS panel based on 8 replicate spikes of each beverage matrix.

Quantitation in real-world beverages

The method applicability was tested in assorted beverages from Toronto, Ontario. Overall, TFA accounted for the majority of the PFAS detected in the samples (Figures 1 and 8). Concentrations of TFA spanned several orders of magnitude depending on the matrix, ranging from ng/L levels in drinking water to tens and hundreds of $\mu\text{g/L}$ levels in juice and wine, respectively. PFMS was the second most prevalent PFAA, primarily detected in juice, followed by PFBA. PFPrS and PFHxS were also observed in 2 wine samples and an unfiltered tap water, but their detection could not be confirmed due to the absence of their qualifier transitions at the low levels measured. No other PFAAs were detected in the beverage samples. Detections of TFA, PFBA and PFMS were confirmed using their qualifier transitions, as shown in Figures 6 and 9. Optimization on the SCIEX 7500 system enabled the use of the F^- fragment [m/z 19] as the qualifier transition of TFA, PFPrA, PFBA and PFPeA. Given the historical precedence of monitoring PFBA and PFPeA with only the M-44

transition [loss of CO_2], the ability to use this second qualifier transition greatly simplifies their detection by removing the need for orthogonal confirmation using high-resolution mass spectrometry or a second chromatographic gradient.

The TFA concentrations in juice [0.8–47 $\mu\text{g/L}$] and wine [39–227 $\mu\text{g/L}$] are consistent with the levels previously reported in similar matrices.^{3,4} PFMS was detected as the predominant perfluoroalkane sulfonic acid (PFSA), with concentrations ranging from 16 ng/L in unfiltered tap water to 13–79 ng/L in juice, with the highest concentration observed at 164 ng/L in a red wine sample.

For the PFAAs detected, the recoveries of the labeled internal standards spiked into the beverages were calculated against those in the aqueous standards to assess matrix effects. The recoveries of $^{13}\text{C}_2$ -TFA, $^{13}\text{C}_4$ -PFBA, $^{13}\text{C}_3$ -PFBS and $^{13}\text{C}_3$ -PFHxS were in the ranges of 59–109%, 93–106%, 90–114%, 111–114% and 98%, respectively. The lower recoveries of $^{13}\text{C}_2$ -TFA [59–68%] typically occurred in the juice samples at 20x dilution, but improved to 78–85% at 100x dilution with water.

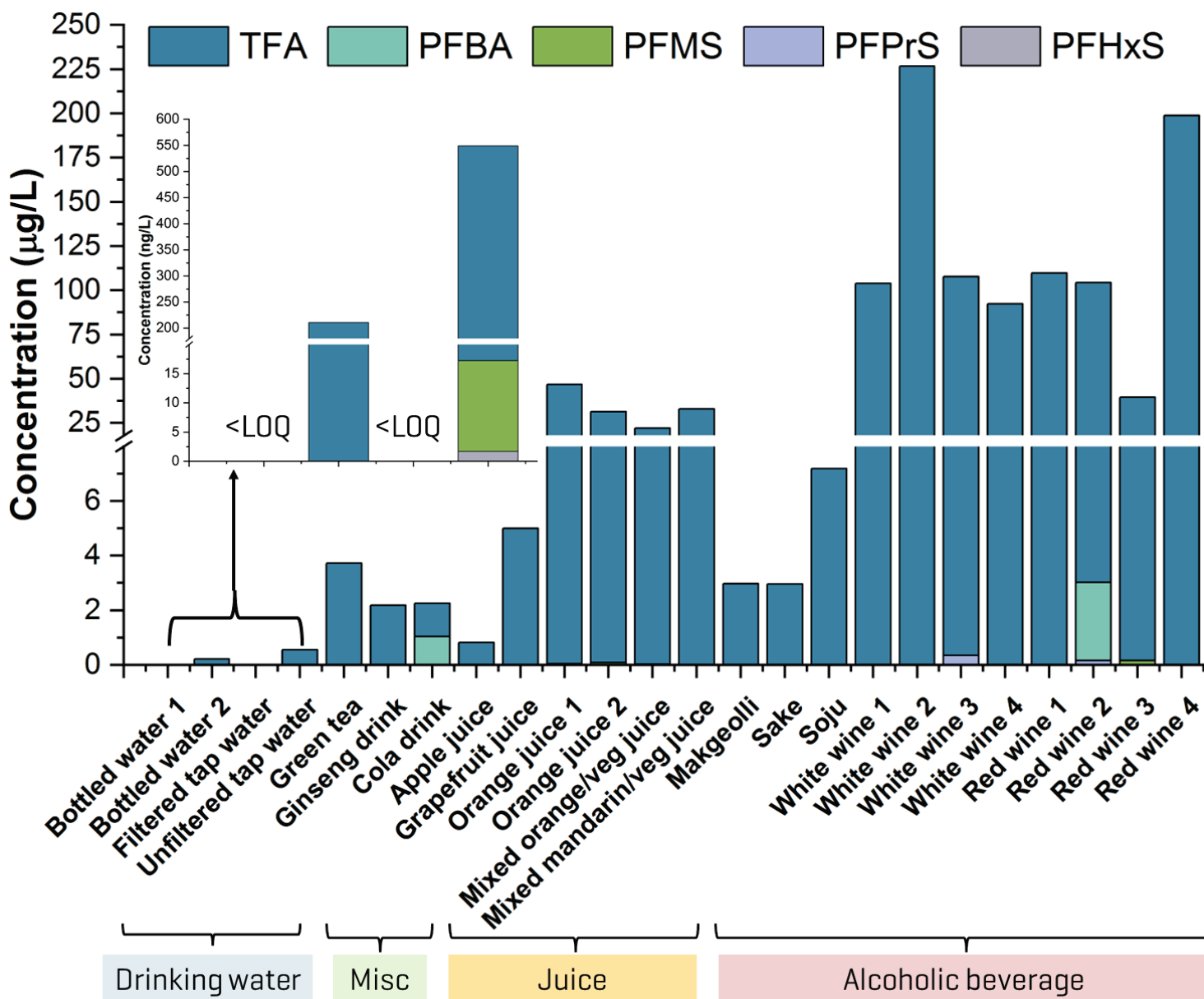


Figure 8. The concentration profiles of 5 PFAs detected at µg/L levels in assorted beverages. Detection was confirmed by the qualifier transition, except when its sensitivity is impacted by the low levels observed in that sample, as was observed for PFPrS and PFHxS in wine and unfiltered tap water. The inset shows an enlarged version of the ng/L concentrations observed in 4 drinking water samples.

Interlaboratory comparison of TFA levels

Table 6 demonstrates the interlaboratory comparison of TFA concentrations measured in 4 samples by the LC-MS/MS method developed here and by an IC-MS method developed at York University.¹⁰ Both methods used the ¹³C₂-TFA internal standard for quantitation. The concentration differences ranged from 8% to 31%, providing a relatively good corroboration of the TFA levels in these 4 beverage samples that were measured by 2 independent techniques.

Table 6: Comparison of TFA concentrations (µg/L) in 4 samples analyzed by SCIEX and York University. The samples were prepared by direct injection in both laboratories, but analyzed by different detection methods, with SCIEX using LC-MS/MS and York University using IC-MS.

Sample	Concentration (µg/L)		% difference
	LC-MS/MS	IC-MS	
	SCIEX	York	
Unfiltered tap water	0.53	0.43	21
White wine 1	104	121	15
Red wine 2	101	110	8
Red wine 3	39	54	31

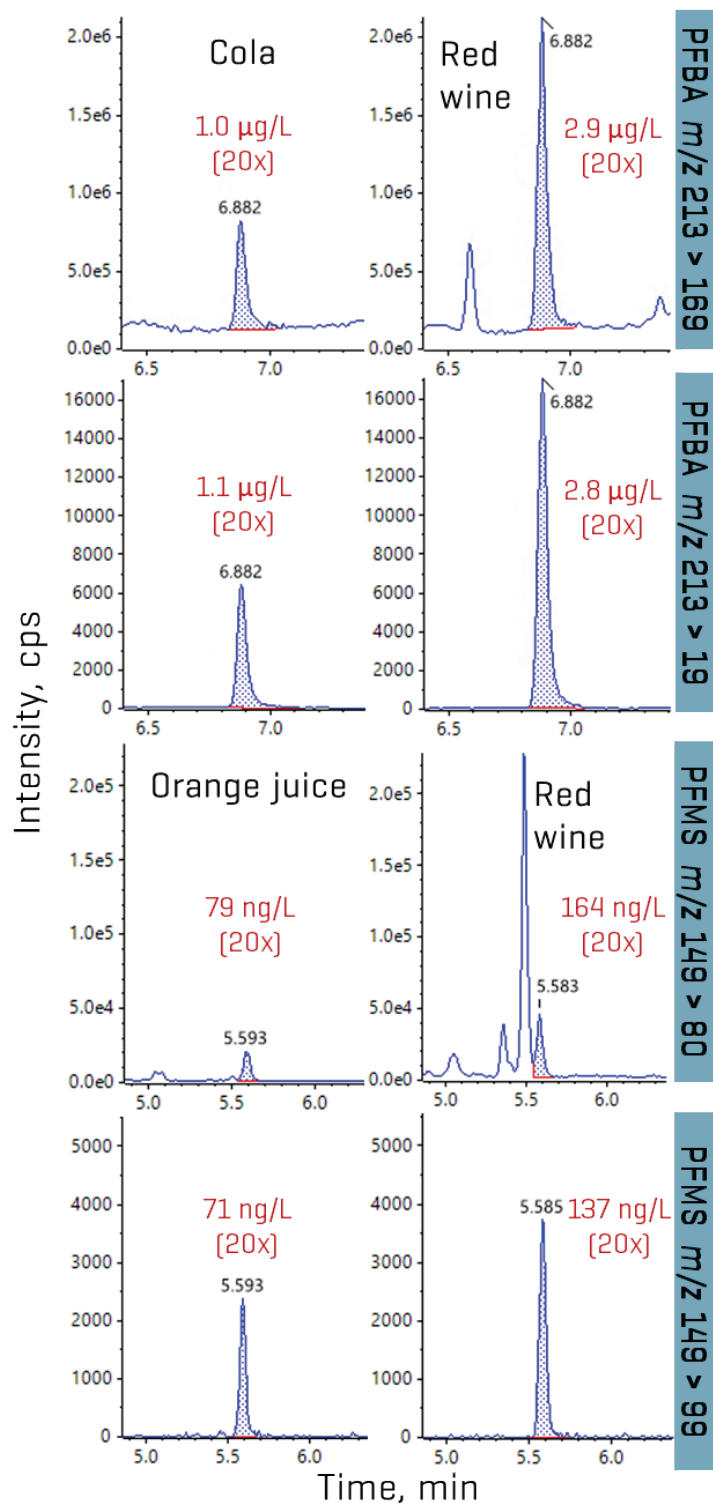


Figure 9. Confirmation of PFBA and PFMS detection using both MRM transitions. The detections of PFBA in cola and red wine and PFMS in orange juice and red wine were confirmed by ion ratio and the qualifier peaks. Similar concentrations (shown in red) were reported between the quantifier and qualifier transitions.

Conclusions

- **Robust retention and separation of ultrashort-chain PFAAs:** Gradient optimization enabled the development of an 11-minute LC run with good retention (>4 min) and RT reproducibility (<1 %CV) for the early-eluting TFA and PFMS.
- **Simple direct injection method:** The wide dynamic range of the SCIEX 7500 system enabled a simple direct injection approach for the quantitation of ultrashort- and short-chain PFAAs in beverages.
- **Good quantitative performance:** Average accuracy ($\pm 30\%$) and precision (%CV <25%) were achieved in solvent standards and beverage spikes prepared at near-LOQ and higher levels for most of the target PFAS.
- **Detection in real-world beverage samples:** Sub-ng/L to µg/L concentrations were detected in a variety of beverage samples, including drinking water, juice, wine and other alcoholic drinks, with TFA present as the dominant PFAA.

References

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