

# PFAS Analysis in Food Packaging Using an Agilent 6495D Triple Quadrupole LC/MS



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1290 Infinity III LC

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## Abstract

The increasing concern over per- and polyfluoroalkyl substances (PFAS) in food packaging materials, and their potential migration into food, requires accurate and reliable characterization methods. This study quantified 110 PFAS, including 73 native and 37 labeled compounds from food plastic bag material using an Agilent 6495D triple quadrupole liquid chromatography/mass spectrometry (LC/TQ) system. The method detection limit was within 0.2  $\mu\text{g}/\text{kg}$  for all 73 target analytes. Most analytes demonstrated excellent linearity with  $R^2$  values exceeding 0.99. Quality control (QC) samples, matrix spiked at 10  $\mu\text{g}/\text{kg}$ , showed recovery rates ranging from 65 to 135% for 95% of the analytes, with precision (%RSD)  $\leq$  20%. These performance attributes highlight the sensitivity and reliability of the 6495D LC/TQ system for PFAS screening in food plastic bags.

## Introduction

PFAS are a class of highly persistent chemicals that are accumulating in the food chain, raising significant health and environmental concerns. These substances are increasingly regulated at various levels nationally, regionally, and globally. Numerous guidelines have identified many PFAS targets for restriction and elimination, including their salts and related compounds.<sup>1-4</sup> PFAS are commonly found in food packaging and other food contact materials (FCMs), where they can migrate into food, leading to consumer exposure.<sup>3,4</sup> In response to tightening regulations on long-chain PFAS, industries are shifting towards short-chain PFAS alternatives. While these substitutes are less prone to bioaccumulation, they pose significant concerns due to their widespread environmental presence, even in remote locations. Short-chain PFAS are more persistent and mobile in water compared to their long-chain counterparts, potentially posing greater environmental and health risks.<sup>4</sup> The U.S. Food and Drug Administration (FDA) has taken significant steps to eliminate the use of PFAS in food packaging. As of February 2024, the FDA announced that grease-proofing substances containing PFAS are no longer being sold by manufacturers for food contact use in the U.S. market.<sup>5</sup> These banned PFAS include long-chain compounds such as PFOA and PFOS, as well as short-chain compounds such as 6:2 FTOH.

A sensitive method for precisely quantitating PFAS in food packaging materials is crucial for implementing stricter regulations in consumer products. Such a method helps manufacturers comply with these regulations, thereby avoiding legal penalties. This application note proposes a sensitive method for quantifying PFAS in plastic food packaging materials. The method aims to support the global discussion on effectively managing PFAS and mitigating their adverse effects.

## Experimental details

### Chemicals and reagents

All the chemicals and solvents used for this study were LC/MS grade and purchased from Sigma-Aldrich (St. Louis, MO, USA). Ultrapure LC/MS grade water was from Agilent (part number 5191-4498).

### Consumables

All consumables used in this study were sourced from Agilent and rigorously tested to ensure their suitability for PFAS analysis, delivering ultralow PFAS background levels.<sup>6</sup> The list of these consumables is provided in Table 1.

**Table 1.** Consumables list for the experimental work.

Item Description	Part Number
Agilent 15 mL Falcon tubes	5610-2039
Agilent Captiva 5 mL polypropylene (PP) syringe	9301-6476
Agilent Captiva Premium syringe filter, nylon membrane	5190-5092
Agilent 2 mL polyfluorinated compound (PFC)-free PP vials	5191-8150
Agilent 250 µL PP vials and caps	5190-2242, 5191-8151

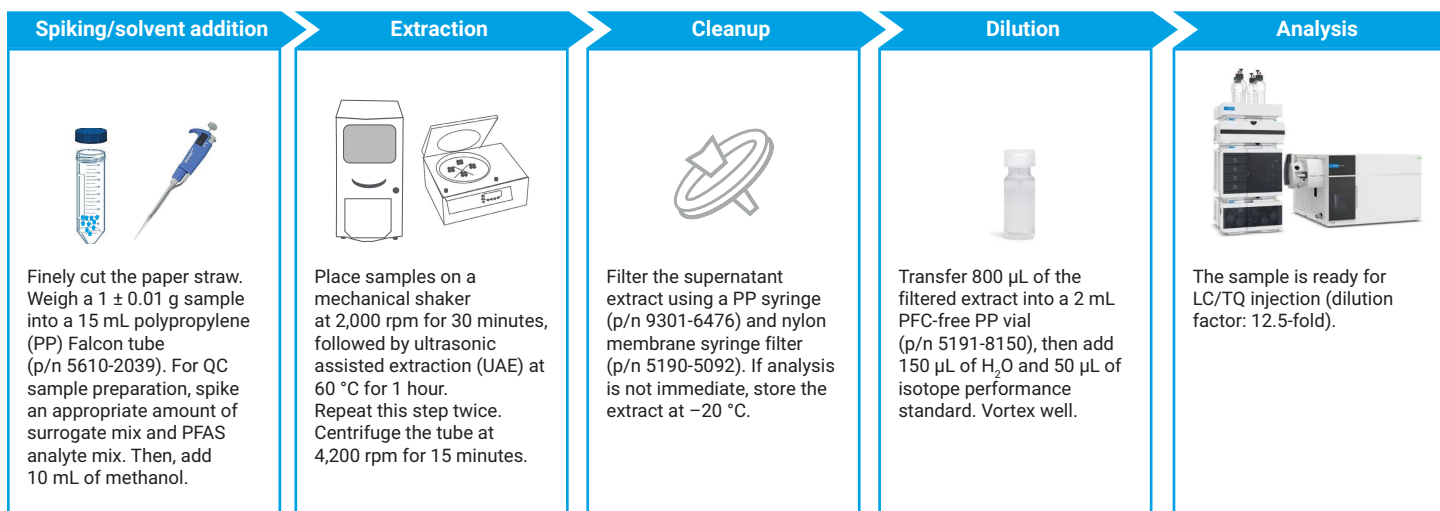
### Standards and calibration preparation

Native and isotopically labeled PFAS standards were sourced from Wellington Laboratories Inc. (Guelph, ON, Canada) and Toronto Research Chemicals (Toronto, ON, Canada) as stock solutions, solution mixes, or powdered standards. Twelve calibration standards were prepared with concentrations of 1, 2, 5, 10, 50, 100, 500, 1,000, 5,000, 10,000, 25,000 and 50,000 ng/L (ppt) in a methanol:water mixture (80:20, v:v). Each calibration level included a constant amount of surrogate mix used as an extracted internal standard (EIS), and an isotope performance standard mix (EPA 533IS) used as a nonextracted internal standard (NIS).

### Sample extraction procedure

A plastic bag used for seafood packaging was purchased from a local grocery store. The bag was cut into pieces smaller than 5 × 5 mm<sup>2</sup> to increase the surface area that was exposed to the extraction solvent. The pieces were tested as samples in this study.

A simple and rapid sample preparation method was developed, based on solvent extraction, to leach PFAS from plastic bag samples.<sup>7,8</sup> The detailed extraction workflow is illustrated in Figure 1. Three levels of fortified plastic bag samples for quality control (QC) were prepared, with native PFAS spiking concentrations at 1.0 µg/kg for low spike QC (LSQ), 10 µg/kg for medium spike QC (MSQ), and 50 µg/kg for high spike QC (HSQ). A surrogate mix was used as an EIS and spiked into the sample tube before extraction. EPA 533IS was used as an NIS and was added to the LC vial before LC/TQ analysis.<sup>9</sup> A matrix blank was prepared without the native PFAS standard mix. After adding the solvent, the test samples underwent mechanical shaking, cleanup, and dilution before being injected into the LC/TQ system, as shown in Figure 1. The entire extraction process involved a total dilution factor of 12.5-fold.



**Figure1.** Workflow to extract PFAS from a plastic bag matrix.

## Instrumentation

An Agilent 1290 Infinity II LC system was used for chromatographic separation. To minimize PFAS contamination, the standard LC system fluid path was replaced with the Agilent InfinityLab PFC-free HPLC conversion kit (part number 5004-0006), which includes a bottle head assembly, pump head adapter assembly, inline filter, multiwash tubing kit, and a PFC delay column. The delay column was used to maximize the removal of the PFAS background caused by mobile phases.

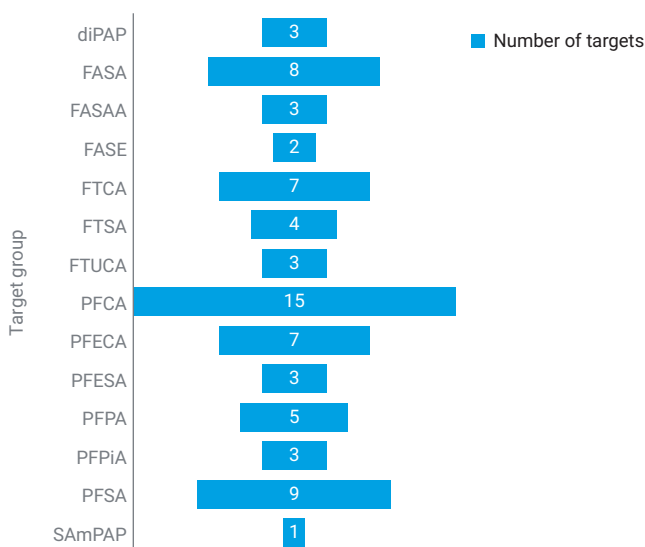
For chromatographic separation, an Agilent ZORBAX RRHD Eclipse Plus C18 column (2.1  $\times$  100 mm, 1.8  $\mu$ m, part number 959758-902) was employed. A gradient method was used with an elution time of less than 15 minutes, as outlined in the Agilent PFAS MRM Database (part number G1736AA). This method involved 5 mM ammonium acetate in water (mobile phase A) and 100% methanol (mobile phase B) at a flow rate of 0.4 mL/min. The total run cycle time from injection to injection was approximately 18 minutes.

For targeted quantification, the study used the 6495D LC/TQ system equipped with an Agilent Jet Stream (AJS) ion source operating in negative ionization mode, using Agilent MassHunter LC/MS Acquisition software version 12.1 Update 3. Autotuning was performed in standard quadrupole mode to optimize instrument parameters. The acquisition method was based on the Agilent PFAS MRM Database for 108 compounds and two additional analytes (PFUnDS and PFTrDS). This method covers the four regulated PFAS in EU 2023/915, 40 PFAS in EPA 1633, and the recommended targets under EURL POPs for PFAS in food and feed, AOAC SMPR 2023.003, US FDA C-010.03, and USDA CLG-PFAS 2.04 for PFAS in food.

## Results and discussion

### Method sensitivity and linearity

The 6495D LC/TQ system, equipped with the latest innovative iFunnel technology, demonstrated excellent sensitivity for 73 native PFAS across 14 target groups (Figure 2). The abbreviations for these 14 target groups are defined in Table 2. The MRM overlay of nine PFSA targets in LSQ (Figure 3) illustrates the symmetric separation and superior sensitivity of the 6495D LC/TQ system for determining PFAS in plastic bags. Isomers such as linear and branched perfluorooctane sulfonate (L-PFOS and br-PFOS) were successfully separated and quantified in the matrix extract.

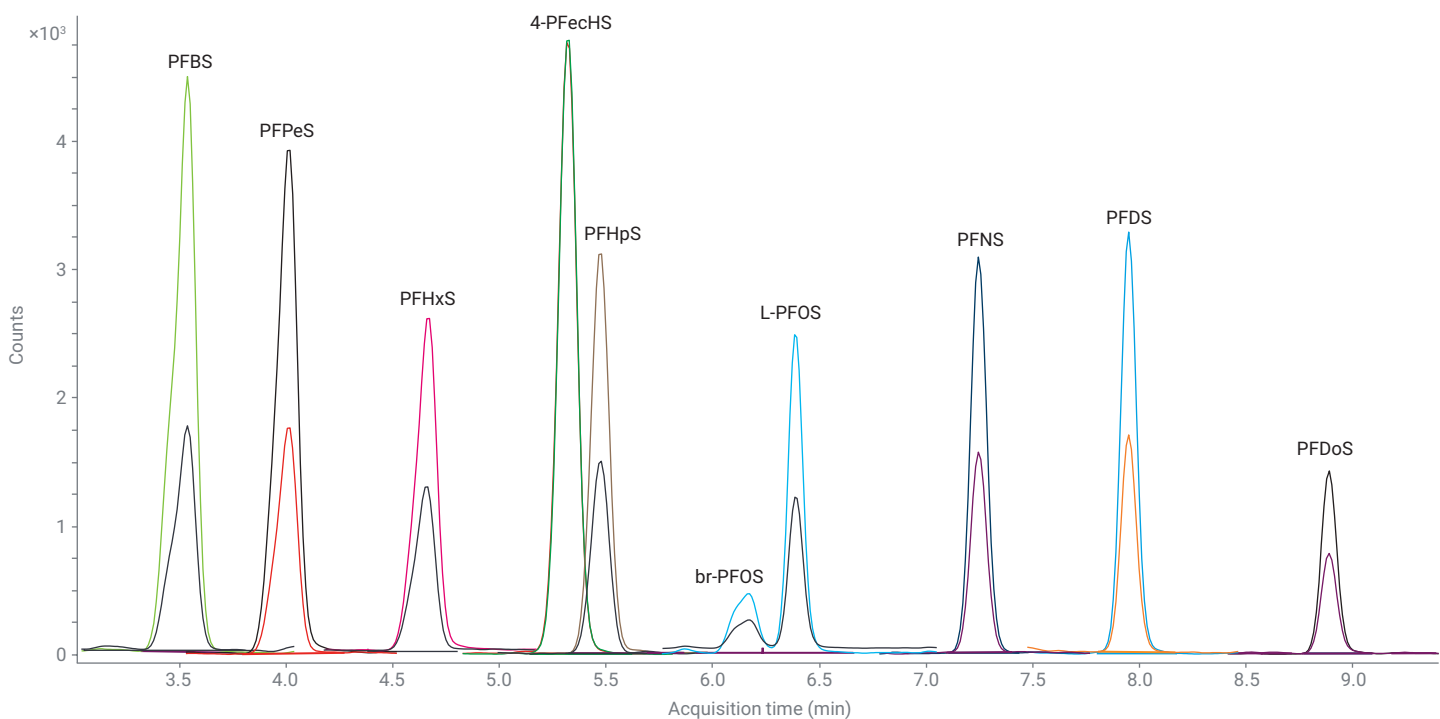


**Figure 2.** Distribution of 73 native PFAS across different groups.

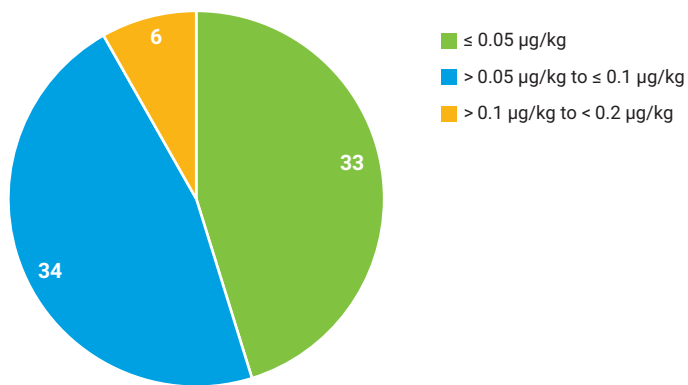
**Table 2.** Abbreviations for 14 PFAS groups.

Abbreviation	Description
diPAP	Polyfluoroalkyl phosphoric diester
SAmPAP	Perfluorooctane sulfonamido-ethanol-based phosphate diester
FASA	Perfluoroalkane sulfonamides
FASAA	Perfluoroalkane sulfonamido acetic acid
FASE	Perfluoroalkane sulfonamido ethanol
FTCA	Fluorotelomer carboxylic acid
FTSA	Fluorotelomer sulfonic acid
FTUCA	Fluorotelomer unsaturated carboxylic acid
PFCA	Perfluoroalkyl carboxylic acid
PFECA	Perfluoroether carboxylic acid
PFESA	Perfluoroether sulfonic acid
PFFPA	Perfluoroalkyl phosphonic acid
PFPIA	Perfluoroalkyl phosphinic acid
PFSA	Perfluoroalkyl sulfonic acid

The method detection limit (MDL) was evaluated using the multi-injection statistical methodology commonly applied in trace analysis of complex matrices.<sup>10,11</sup> In this study, nine continuous injections from two technical replicates of LSQ samples were performed, followed by an MDL calculation using MassHunter Quantitative Analysis software 12.1. The MDL values (based on sample weight) for each target are summarized in Table 3. Figure 4 illustrates the MDL distribution for all targets. All 73 analytes achieved an MDL of  $\leq 0.2 \mu\text{g}/\text{kg}$ . Among these results, 33 analytes exhibited an MDL of  $\leq 0.05 \mu\text{g}/\text{kg}$ , while 34 targets fell within the MDL range of 0.05 to 0.1  $\mu\text{g}/\text{kg}$ . Additionally, superior low MDLs were achieved for critical PFAS, such as 0.02  $\mu\text{g}/\text{kg}$  for PFHxS and 0.03  $\mu\text{g}/\text{kg}$  for PFOA, PFOS, and PFNA. These results highlight the exceptional sensitivity of the PFAS analysis in food plastic bag material using a 6495D LC/TQ system with the PFC-free conversion kit, ensuring accurate PFAS quantitation without false positives.



**Figure 3.** Overlaid MRM chromatogram of nine PFSA targets in the plastic bag LSQ at a spiking level of 1  $\mu\text{g}/\text{kg}$  (the target concentration in the ready-to-inject sample vial was 80  $\text{ng}/\text{L}$ ).



**Figure 4.** MDL distribution of all 73 target analytes.

LOQ is the lowest concentration of the analyte in the test material that has been validated with acceptable recovery and repeatability, by applying the entire workflow and identification criteria.<sup>12</sup>

In this work, prespiked sample QCs (LSQ, MSQ, and HSQ) were used to establish the method LOQ, following these identification criteria:

- Recovery between 65 and 135% with %RSD  $\leq 20\%$
- Intraday retention time (RT) tolerance 1%
- Signal to noise ratio (S/N)  $\geq 3:1$
- Ion ratio of quantifier and qualifier within  $\pm 30\%$

Table 3 summarizes the LOQ values for each analyte. Sixty-nine analytes achieved an LOQ of  $\leq 10 \mu\text{g}/\text{kg}$ , demonstrating the outstanding performance of the developed workflow for quantifying PFAS in plastic bag samples. For short-chain PFAS, including PFBS and PFPeS from the PFSA group, and PFBA and PFPeA from the PFCA group, an LOQ of 1  $\mu\text{g}/\text{kg}$  was achieved. LOQ was not determined for analytes 6:8 PFPI, 8:8 PFPI, and diSAM-PAP due to poor recovery and not meeting performance criteria.

The method linearity range for each target was established with a minimum of five calibration levels. All target analytes exhibited excellent  $R^2$  values exceeding 0.99. Additionally, the accuracy of each calibration standard fell within the typical acceptable limits of 70 to 130%.

Table 3. Analytical results summary (continued on next page).

Target Number	Compound Name	CAS Number	Surrogate	RT (min)	MDL (µg/kg)	LOQ (Validated) (µg/kg)	% Recovery LSQ (1 µg/kg)	% Recovery MSQ (10 µg/kg)	% Recovery HSQ (50 µg/kg)
1	PFBPA	52299-24-8	Cl-PFOPA	1.2	0.02	1	95	103	119
2	PFBA	375-22-4	<sup>13</sup> C <sub>4</sub> -PFBA	3.1	0.03	1	87	103	91
3	PFMPA	377-73-1	<sup>13</sup> C <sub>4</sub> -PFBA	3.2	0.02	1	79	81	82
4	PFPeA	2706-90-3	<sup>13</sup> C <sub>5</sub> -PFPeA	3.5	0.03	1	76	81	81
5	3:3 FTCA	356-02-5	<sup>13</sup> C <sub>5</sub> -PFPeA	3.5	0.10	1	95	93	94
6	PFBS	375-73-5	<sup>13</sup> C <sub>3</sub> -PFBS	3.5	0.04	1	81	83	82
7	PFHxPA	40143-76-8	Cl-PFOPA	3.6	0.10	1	81	121	109
8	PFMBA	863090-89-5	<sup>13</sup> C <sub>5</sub> -PFPeA	3.6	0.03	1	75	77	78
9	Cl-PFHxPA	N/A	Cl-PFOPA	3.7	0.04	10	50	103	100
10	PFEESA	113507-82-7	<sup>13</sup> C <sub>3</sub> -PFBS	3.7	0.04	1	85	88	86
11	NFDHA	151772-58-6	<sup>13</sup> C <sub>5</sub> -PFHxA	3.9	0.04	1	76	78	78
12	4:2 FTSA	757124-72-4	<sup>13</sup> C <sub>2</sub> -4:2 FTSA	3.9	0.05	1	89	89	76
13	PFHxA	307-24-4	<sup>13</sup> C <sub>5</sub> -PFHxA	4	0.03	10	58	76	77
14	PFPeS	2706-91-4	<sup>13</sup> C <sub>5</sub> -PFHxS	4	0.05	1	75	78	78
15	HFPO-DA	13252-13-6	<sup>13</sup> C <sub>3</sub> -HFPO-DA	4.1	0.03	1	94	95	97
16	FBSA	30334-69-1	<sup>13</sup> C <sub>3</sub> -PFHxS	4.2	0.03	1	84	88	84
17	P5MeODIOXOAc	1190931-41-9	<sup>13</sup> C <sub>3</sub> -HFPO-DA	4.4	0.12	1	105	93	92
18	PFHpA	375-85-9	<sup>13</sup> C <sub>4</sub> -PFHpA	4.6	0.04	10	ND	72	77
19	PFHxS	355-46-4	<sup>13</sup> C <sub>3</sub> -PFHxS	4.7	0.02	1	83	90	83
20	DONA	919005-14-4	<sup>13</sup> C <sub>4</sub> -PFHpA	4.7	0.03	1	71	73	76
21	PFOPA	40143-78-0	Cl-PFOPA	4.8	0.04	10	26	90	98
22	5:3 FTCA	914637-49-3	<sup>13</sup> C <sub>2</sub> -6:2 FTUCA	4.8	0.05	1	81	87	88
23	6:2 FTUCA	70887-88-6	<sup>13</sup> C <sub>2</sub> -6:2 FTUCA	4.8	0.03	1	84	88	92
24	6:2 FTCA	53826-12-3	<sup>13</sup> C <sub>2</sub> -6:2 FTCA	5	0.05	10	ND	104	102
25	4-PFecHS	646-83-3	<sup>13</sup> C <sub>8</sub> -PFOS	5.3	0.07	1	78	83	83
26	6:2 FTSA	27619-97-2	<sup>13</sup> C <sub>2</sub> -6:2 FTSA	5.4	0.07	1	91	89	73
27	PFOA	335-67-1	<sup>13</sup> C <sub>8</sub> -PFOA	5.4	0.03	10	ND	68	75
28	PFHpS	375-92-8	<sup>13</sup> C <sub>8</sub> -PFOS	5.5	0.07	1	74	76	77
29	MeFBSA	68298-12-4	<sup>13</sup> C <sub>8</sub> -PFOSA	5.7	0.08	1	74	75	78
30	FHxSA	41997-13-1	<sup>13</sup> C <sub>8</sub> -PFOS	6	0.04	1	78	80	78
31	PFNA	375-95-1	<sup>13</sup> C <sub>9</sub> -PFNA	6.3	0.03	1	65	78	80
32	PFOS	1763-23-1	<sup>13</sup> C <sub>8</sub> -PFOS	6.4	0.03	1	75	78	78
33	8:2 FTUCA	70887-84-2	<sup>13</sup> C <sub>2</sub> -8:2 FTUCA	6.6	0.05	10	46	78	82
34	PFDPa	52299-26-0	Cl-PFOPA	6.6	0.08	10	ND	94	109
35	7:3 FTCA	812-70-4	<sup>13</sup> C <sub>2</sub> -8:2 FTUCA	6.7	0.06	1	86	91	92
36	HFPO-TA	13252-14-7	<sup>13</sup> C <sub>9</sub> -PFNA	6.7	0.06	1	71	73	75
37	8:2 FTCA	27854-31-5	<sup>13</sup> C <sub>2</sub> -8:2 FTCA	6.7	0.09	10	ND	76	95
38	9Cl-PF3ONS	756426-58-1	<sup>13</sup> C <sub>8</sub> -PFOS	6.9	0.06	1	67	70	70
39	FOSAA	2806-24-8	<sup>2</sup> H <sub>3</sub> -N-MeFOSAA	7.1	0.09	1	91	94	93
40	8:2 FTSA	39108-34-4	<sup>13</sup> C <sub>2</sub> -8:2 FTSA	7.2	0.06	1	89	89	75
41	PFNS	68259-12-1	<sup>13</sup> C <sub>8</sub> -PFOS	7.2	0.05	1	79	83	85
42	PFDA	335-76-2	<sup>13</sup> C <sub>6</sub> -PFDA	7.2	0.08	1	71	78	76
43	8:3 FTCA	34598-33-9	<sup>13</sup> C <sub>6</sub> -PFDA	7.6	0.07	1	92	95	93
44	N-MeFOSAA	2355-31-9	<sup>2</sup> H <sub>3</sub> -N-MeFOSAA	7.6	0.10	1	80	84	83
45	MeFHxSA	68259-15-4	<sup>13</sup> C <sub>8</sub> -PFOSA	7.8	0.10	1	77	74	77

**Table 3.** Analytical results summary (continued).

Target Number	Compound Name	CAS Number	Surrogate	RT (min)	MDL (µg/kg)	LOQ (Validated) (µg/kg)	% Recovery LSQ (1 µg/kg)	% Recovery MSQ (10 µg/kg)	% Recovery HSQ (50 µg/kg)
46	PFDS	335-77-3	<sup>13</sup> C <sub>8</sub> -PFOS	7.9	0.09	1	78	82	83
47	PFUnDA	2058-94-8	<sup>13</sup> C <sub>7</sub> -PFUnDA	8	0.06	1	68	70	71
48	N-EtFOSAA	2991-50-6	<sup>2</sup> H <sub>5</sub> -N-EtFOSAA	8	0.09	1	75	77	82
49	PFOSA	754-91-6	<sup>13</sup> C <sub>8</sub> -PFOSA	8	0.04	1	78	79	81
50	10:2 FTUCA	70887-94-4	<sup>13</sup> C <sub>2</sub> -10:2 FTUCA	8.2	0.06	1	76	79	83
51	11Cl-PF3OUdS	763051-92-9	<sup>13</sup> C <sub>8</sub> -PFOS	8.3	0.09	1	65	67	68
52	PFUnDS	749786-16-1	<sup>13</sup> C <sub>7</sub> -PFUnDA	8.5	0.06	1	69	69	75
53	PFDoDA	307-55-1	<sup>13</sup> C <sub>2</sub> -PFDoDA	8.5	0.13	10	63	72	73
54	10:2 FTSA	120226-60-0	<sup>13</sup> C <sub>2</sub> -8:2 FTSA	8.5	0.07	1	125	128	108
55	10:2 FTCA	53826-13-4	<sup>13</sup> C <sub>2</sub> -10:2 FTCA	8.5	0.05	50	25	14	88
56	6:6 PFPI	40143-77-9	<sup>13</sup> C <sub>2</sub> -PFDoDA	8.7	0.08	1	78	83	82
57	PFDoS	79780-39-5	<sup>13</sup> C <sub>8</sub> -PFOS	8.9	0.09	1	67	72	72
58	PFTTrDA	72629-94-8	<sup>13</sup> C <sub>2</sub> -PFDoDA	8.9	0.09	10	63	71	67
59	N-MeFOSA	31506-32-8	<sup>2</sup> H <sub>3</sub> -N-MeFOSA	9.2	0.10	1	98	98	99
60	FDSA	N/A	<sup>13</sup> C <sub>8</sub> -PFOSA	9.2	0.06	1	67	70	71
61	MeFOSE	24448-09-7	<sup>2</sup> H <sub>7</sub> -MeFOSE	9.2	0.12	1	76	82	84
62	PFTTrDS	791563-89-8	<sup>13</sup> C <sub>2</sub> -PFTDA	9.3	0.08	1	70	72	78
63	6:2 diPAP	57677-95-9	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -6:2 diPAP	9.3	0.07	1	82	87	88
64	PFTDA	376-06-7	<sup>13</sup> C <sub>2</sub> -PFTDA	9.3	0.15	1	70	75	75
65	6:8 PFPI	610800-34-5	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -6:2 diPAP	9.4	0.11	ND	26	29	30
66	N-EtFOSA	4151-50-2	<sup>2</sup> H <sub>5</sub> -N-EtFOSA	9.6	0.12	1	80	83	86
67	EtFOSE	1691-99-2	<sup>2</sup> H <sub>9</sub> -EtFOSE	9.6	0.09	1	92	94	98
68	6:2/8:2 diPAP	943913-15-3	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -6:2 diPAP	9.9	0.04	10	60	65	71
69	8:8 PFPI	40143-79-1	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -6:2 diPAP	10	0.05	ND	26	29	31
70	PFHxDA	67905-19-5	<sup>13</sup> C <sub>2</sub> -PFHxDA	10.1	0.07	1	82	79	83
71	8:2 diPAP	678-41-1	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -8:2 diPAP	10.4	0.03	1	73	76	80
72	PFODA	16517-11-6	<sup>13</sup> C <sub>2</sub> -PFHxDA	10.7	0.06	1	76	79	84
73	diSAmPAP	2965-52-8	( <sup>13</sup> C <sub>2</sub> ) <sub>2</sub> -8:2 diPAP	11	0.05	ND	50	53	58

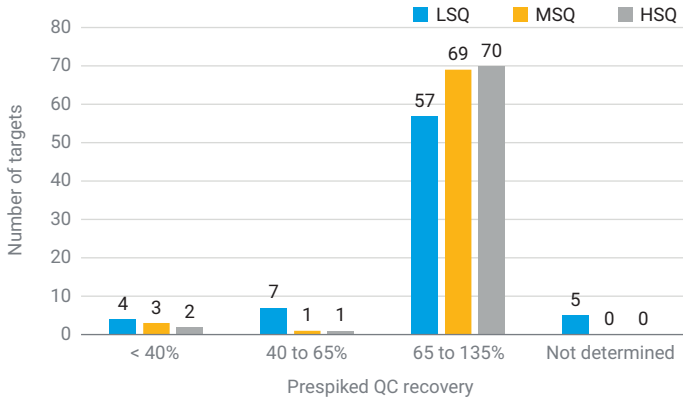
ND: Not determined. The LOQ for three compounds was not determined due to lower recovery. Recovery at LSQ was not determined due to matrix interference.

### Method recovery and precision

The method recovery was calculated based on the mean percent recovery of matrix-spiked QCs, while method precision was assessed using the %RSD of recoveries, calculated from triplicate injections of each technical preparation (n = 6). As described in the sample preparation procedure, three levels of QCs, including LSQ, MSQ, and HSQ samples were prepared. A constant amount of surrogate mix was spiked into each QC sample to serve as an EIS for correcting the target recovery. This method has proven highly accurate by using an EIS to compensate for matrix effects and target loss during sample extraction.<sup>9,12,13</sup> The EPA 533 isotope performance standard mix, containing three labeled PFAS (<sup>13</sup>C<sub>3</sub>-PFBA, <sup>13</sup>C<sub>2</sub>-PFOA, and <sup>13</sup>C<sub>4</sub>-PFOS), was added to the ready-to-inject extract for evaluating surrogate recoveries.

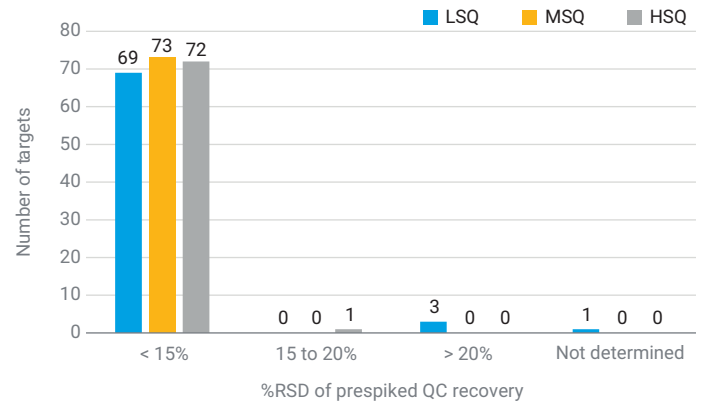
Recoveries of LSQ, MSQ, and HSQ for each analyte are summarized in Table 3. Figure 5 shows the recovery distribution at LSQ, MSQ, and HSQ. Most targets met recovery rates from 65 to 135% across all three levels of QCs, based on the typical acceptable range for PFAS in food matrices from AOAC SMPR 003. Furthermore, ≥ 95% of targets met recovery rates from 65 to 135% at both MSQ and HSQ, with only a few targets falling within the recovery range of 40 to 65% or lower. For the method precision evaluation, ≥ 95% of targets achieved %RSD of recoveries at all QCs within 15%, which is significantly lower than the general 20% requirement. These results confirm the excellent extraction efficiency and reproducibility of the PFAS analysis from plastic bag samples.

Poor recoveries were consistently observed for a few targets in this study, such as 8:8 PFPI and 6:8 PFPI, with recoveries less than 40% across all QCs. However, the %RSD of recoveries for 8:8 PFPI and 6:8 PFPI was within 6%, despite the poor recovery rates. Notably, these targets are currently not listed in any of the discussed regulatory guidelines.

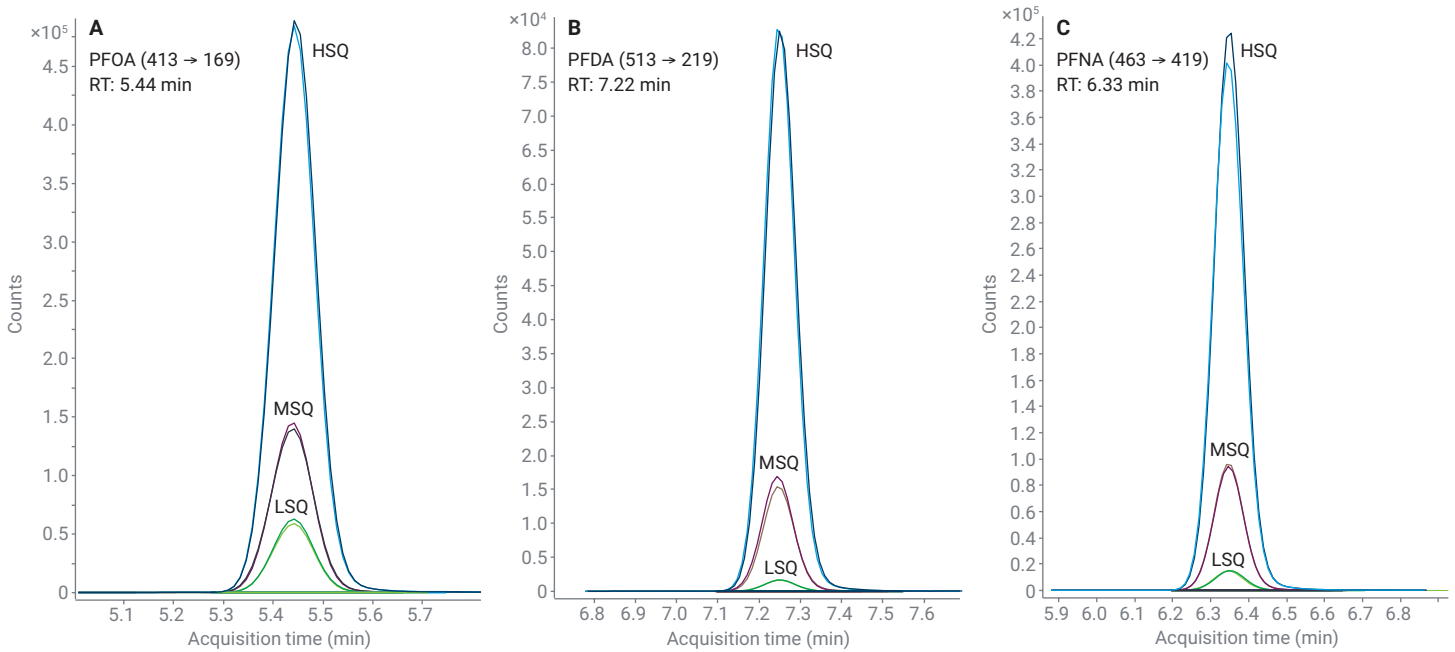


**Figure 5.** Recovery results from prespiked LSQ, MSQ, and HSQ samples.

PFAS compounds from the PFCA group, such as PFOA, PFDA, and PFNA, are critical compounds in various regulations. Figure 7 shows the MRM overlays of duplicate technical preparations of LSQs, MSQs, and HSQs for PFOA, PFDA, and PFNA. These results demonstrate a high reproducibility of target performance and reliability of the developed workflow for routine PFAS analysis in food packaging materials.



**Figure 6.** %RSD of QC recovery distribution at LSQ, MSQ, and HSQ.



**Figure 7.** Overlaid MRM traces of critical targets PFOA (A), PFDA (B), and PFNA (C) from two separate technical preparations of LSQ, MSQ, and HSQ.



### Quantitation of PFAS in food plastic bag

The presence of native PFAS in food plastic bag samples was assessed using the developed analytical workflow. Reagent blanks, prepared without the sample matrix, were analyzed to ensure that no significant background contamination from chemicals, labware, or consumables was present. Separate triplicate preparations of unspiked samples (matrix blank) were conducted following the complete extraction procedure. The LC/TQ quantitative data analysis revealed that several PFAS compounds, including PFOA, 8:2 FTUCA, 10:2 FTCA, 8:2 FTCA, PFHpA, PFHxA, PFOPA, PFDPA, etc., were detected in food plastic bags at concentrations above the MDL.

### Conclusion

This study successfully established a comprehensive workflow for the quantitative analysis of 73 native PFAS in food plastic bag samples. Using a straightforward and efficient solvent extraction method, PFAS compounds were effectively leached from the matrix. The subsequent dilute-and-shoot approach to LC/TQ analysis eliminated the need for drying and reconstitution, streamlining the process. Exceptional chromatographic separation was achieved for all 110 PFAS compounds within the first 12 minutes, demonstrating the capability of the Agilent 1290 Infinity II LC for routine laboratory operations and improved productivity. The Agilent 6495D LC/TQ, equipped with a PFC-free conversion kit, provided outstanding background contamination removal and ppt-level sensitivity, ensuring precise quantitation of PFAS from the food plastic bag matrix. Verification of the method, including sensitivity and recovery, confirmed a suitability for measuring PFAS at lower concentrations in food packaging materials. These robust analytical results empower food plastic bag manufacturers to make informed production decisions, ensuring compliance with future regulatory standards and enhancing consumer safety.

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