Application Note

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Determination of Per and Polyfluoroalkyl Substances in Soils Using Carbon S SPE by LC/MS/MS

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Abstract

This application note presents the development and evaluation of a multicomponent method for the analysis of per and polyfluoroalkyl substances (PFAS) in soil. The method incorporates a basic methanol extraction followed by a passthrough matrix removal step using an Agilent Bond Elut Carbon S solid phase extraction (SPE) cartridge and quantitative analysis by LC/MS/MS. For the 59 PFAS tested, the average recovery at the low spiking concentration (0.625 ng/g) was 99.9% with a relative standard deviation of 13.5%. Depending upon the soil matrix, the use of the Bond Elut Carbon S cartridges can improve chromatographic peak shape and retention for early eluting compounds such as PFBA.

Introduction

Soil is a complex mixture of organic and inorganic compounds.[1] Many of these organic compounds are co-extracted into the organic solvent along with the target analytes during the extraction process. Without the further removal of these co-extractives, direct injection of extracts can result in multiple matrix effects upon analysis, including matrix ion suppression or enhancement on LC/MS/MS, and accumulation of matrix deposits in the sample flow path and MS ion source. Therefore, it is important to apply a cleanup step to remove matrix co-extractives prior to instrument analysis, without affecting the recovery of the target compounds.

Graphitized carbon black (GCB) has been used widely in sample preparation for efficient removal of pigments and other matrix interferences. However, GCB may cause the loss of some analytes. Carbon S is an advanced hybrid carbon material with optimized carbon content and pore structure. Compared to GCB, Carbon S provides equivalent or better pigment removal from sample matrices, while significantly improving recovery for some GCB-selective analytes (such as planar pesticides). As a result, Carbon S sorbent provides a better balance between analyte recovery and matrix removal efficiency than traditional GCB sorbent.[2] The Carbon S sorbent is applied in the same SPE cartridge format with the same bed mass as GCB SPE. The Carbon S SPE cartridges can be used as a replacement for the GCB cartridges for applications where SPE methodology is used.

This study investigates the postextraction matrix cleanup of 59 PFAS from loamy sand, reed sedge peat, and topsoil using the Bond Elut Carbon S 250 mg, 6 mL cartridges followed by LC/MS/MS analysis.

Experimental

Chemicals and reagents

Native PFAS standards and isotopically labeled analogues were purchased as individual standards from Wellington Laboratories, Inc. (Guelph, ON, Canada). HPLC grade methanol (MeOH) was from Honeywell (Muskegon, MI, USA). Reagent grade acetic acid, ammonium acetate, and ammonium hydroxide were from Sigma-Aldrich (St Louis, MO, USA).

Solutions and standards

The 59 target compounds investigated in this study are listed in Appendix A. A target spiking solution was prepared in methanol at a concentration of 250 ng/mL for all compounds except N-MeFOSA, N-EtFOSA, 6:2/8:2 diPAP, 8:8 PFPi, and 8:2 diPAP, with concentrations of 500 ng/mL, MeFOSE, EtFOSE, PFHxDA, PFODA, and diSAMPAP, with concentrations of 1,000 ng/mL, and 6:2 FTCA, 8:2 FTCA, and 10:2 FTCA, with concentrations of 2,500 ng/mL.

An isotope dilution analogue spiking solution was prepared in methanol with the compounds listed in Appendix A. The concentrations for all the isotopes were 250 ng/mL except for d_7-MeFOSE and d_9-EtFOSE at 1,000 ng/mL, and $^{13}C_2$-6:2 FTCA, $^{13}C_2$-8:2 FTCA, and $^{13}C_2$-10:2 FTCA at 2,000 ng/mL.

An isotope performance standard was prepared in methanol containing $^{13}C_3$-PFBA, $^{13}C_2$-PFOA, and $^{13}C_4$-PFOS at concentrations of 500, 500, and 1,500 ng/mL, respectively.

Calibration standards were prepared in an 80/20 (v/v) mixture of methanol and water. Six standard levels were used for calibration ranging from 0.25 to 2.5 ng/mL for all the target compounds listed in Appendix A, except for the fluorotelomer carboxylic acids and sufonamido ethanols. The concentrations of 6:2 FTCA, 8:2 FTCA, and 10:2 FTCA ranged from 0.25 to 25 ng/mL. The concentrations of EtFOSE and MeFOSE ranged from 0.1 to 10 ng/mL. The concentration of the isotope dilution analogues in the standards was 0.5 ng/mL for all the analogues in Appendix A except for the labeled fluorotelomer carboxylic acids and sufonamido ethanols. The concentrations of $^{13}C_2$-6:2 FTCA, $^{13}C_2$-8:2 FTCA, and $^{13}C_2$-10:2 FTCA were 4 ng/mL. The concentrations of d_9-EtFOSE and d_7-MeFOSE were 2 ng/mL. The concentrations of the isotope performance standards $^{13}C_3$-PFBA, $^{13}C_2$-PFOA, and $^{13}C_4$-PFOS were 5, 5, and 15 ng/mL, respectively.

A solution of 1% ammonia in methanol (v/v) was prepared the same day as the extractions.

Equipment and materials

Sample analysis was performed using an Agilent 1290 Infinity II LC system consisting of an Agilent 1290 Infinity II high speed pump (G7120A), an Agilent 1290 Infinity II multisampler (G7167B), and an Agilent 1290 Infinity II multicolumn thermostat (G7167B). The LC system was modified for PFAS analysis using the Agilent InfinityLab PFC-free HPLC conversion kit (part number 5004-0006). The LC system was coupled to an Agilent 6470B triple quadrupole LC/MS equipped with an Agilent Jet Stream electrospray ion source. Agilent MassHunter workstation software was used for data acquisition and analysis. The Agilent PFAS MRM database (G1736AA) was used for optimized MRM settings.

The PFAS-suitable consumables used for the PFAS extraction and analysis are listed in Table 1.[3,4] Three sample matrices were used for evaluation: clean sandy loam (Supelco part number CLNSOIL3), dark reed sedge peat, and organic topsoil. A multipurpose rotator model 150 (Scientific Industries, Springfield, MA) tube rotator was used to fully invert the sample tubes during extraction.

Instrument conditions

The HPLC conditions are listed in Table 2 and the MS conditions are listed in Table 3. The MRM transitions for the targets and isotopes dilution analogues are listed in Appendix A. Figure 1 shows a typical chromatogram constructed from extracted target product ions for standard at 2 ng/mL.

Table 1. PFAS suitable consumables and supplies.

Agilent Consumables and Supplies	Part Number
Carbon S cartridge, 250 mg, 6 mL	5610-2082
Polypropylene autosampler screw top vials, 2 mL, and caps	5191-8151 and 5191-8150
Centrifuge tubes and caps, 15 mL	5610-2039
InfinityLab PFC delay column, 4.6 × 30 mm	5062-8100
ZORBAX RRHD Eclipse Plus C18 column, 2.1 × 100 mm, 1.8 µm	959758-902
Vac Elut SPS 24 manifold with collection rack for 10 × 75 mm test tubes	12234003
Collection rack and funnel set for 12 or 15 mL conical tubes, for Vac Elut SPS 24 manifold	12234027

Table 2. HPLC conditions.

Parameter	Value
Mobile Phase	A) 5 mM ammonium acetate in water B) Methanol
Injection Volume	5 µL
Column Temperature	30 °C
Flow Rate	0.400 mL/min
Gradient	Time (min) % A % B 0 85 15 1.00 85 15 1.50 45 55 5.50 30 70 7.00 20 80 12.00 0 100 14.40 0 100 14.50 85 15

Table 3. MS conditions.

Parameter	Value
MS/MS	6470B triple quadrupole LC/MS
Polarity	Negative
Drying Gas	230 °C, 4 L/min
Sheath Gas	250 °C, 12 L/min
Nebulizer Gas	15 psi
Capillary Voltage	2,500 V
Nozzle Voltage	0 V

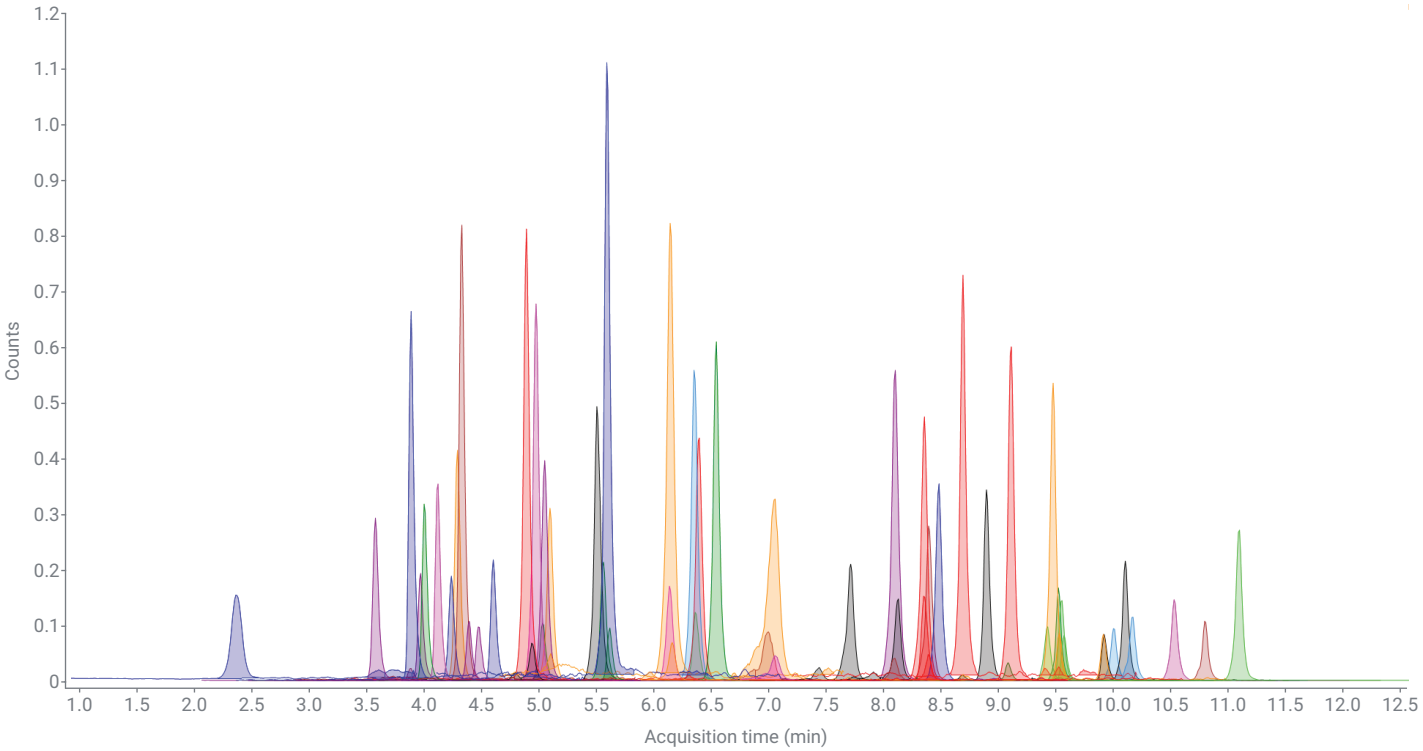

Figure 1. Target quant ion chromatogram for a calibration standard at 2 ng/mL for most compounds (compounds listed in Appendix A).

Calibration and quantitation

Stable-isotope dilution methodology was used for quantitation where the responses and concentrations of the targets are measured relative to the responses and concentrations of the isotope dilution analogues.[5] The corresponding isotope dilution analogue for each target compound is listed in Appendix A. Response curves were fitted using 1/x weighted linear least squares regression model and included the origin (0,0). The concentration for PFAS standards supplied as salts were corrected to the acid concentration in solution.

Sample preparation

The sample preparation closely followed the extraction procedure in ASTM D7968-17a except for replacing the syringe filtration step with a passthrough cleanup using the Carbon S cartridge. The steps in the extraction process are listed in Figure 2.

Method performance evaluation

The method performance was first evaluated by measuring recovery accuracy and precision of five replicate extractions at two spiking levels in the loamy sand matrix. Next, sedge peat and topsoil samples were tested for residual PFAS. The improvement of method performance was evaluated by comparing the results of samples extracts with and without the use of the Carbon S cleanup.

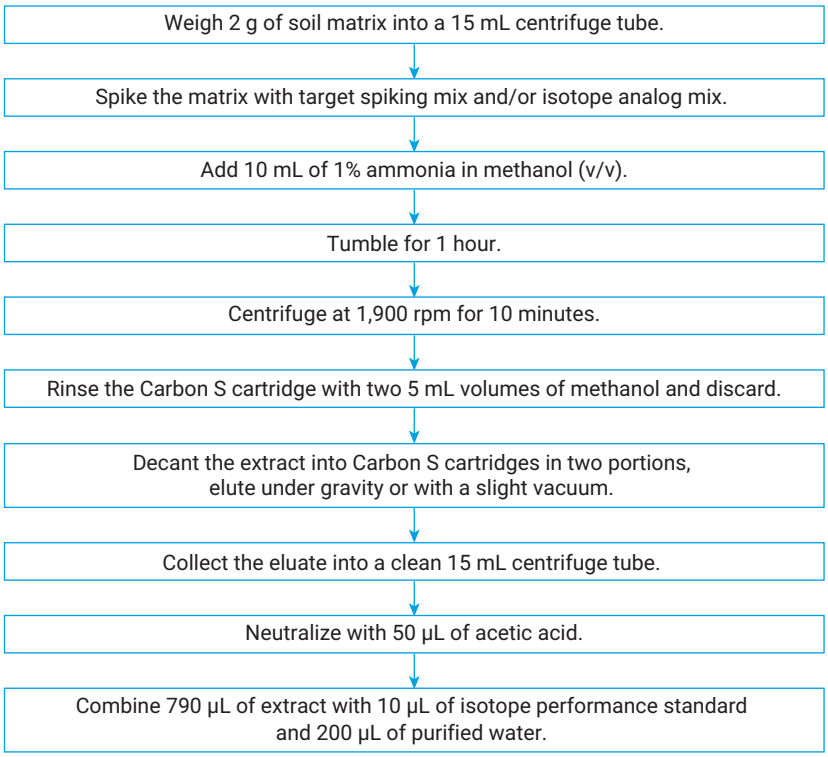

Figure 2. Soil extraction protocol followed in this study.

Loamy sand samples were spiked with either 5 µL (low-level spike) or 50 µL (high-level spike) of the target spiking solution and 20 µL of the isotope dilution analogue spiking solution. For the low-level spike, the concentration of PFAS targets in 2 g of soil was 0.625 ng/g for most target compounds except N-MeFOSA, N-EtFOSA, 6:2/8:2 diPAP, 8:8 PFPi, and 8:2 diPAP at 1.25 ng/g, EtFOSE, N-MeFOSE, PFHxDA, PFODA, and diSAmPAP at 2.5 ng/g, and 6:2 FTCA, 8:2 FTCA, and 10:2 FTCA at 6.25 ng/g. The soil concentrations for the high-level spike were 10-fold greater.

Method blanks were also included in the sample set. Cartridge blanks (rinsate collected from the methanol rinse) and matrix blanks were also analyzed to ensure the system and cartridges were free from PFAS contamination before sample analysis.

Results and discussion

Calibration

To evaluate the method calibration quality, the calculated concentration of each target at each calibration level was calculated based upon the response curve (Figure 3). For levels 2 to 6, the accuracy ranged from 75.1 to 100.0% with an average of 95.4%. For level 1, the accuracy ranged from 66.3 to 99.9% with an average of 89.5%. A quality control standard[5] was prepared from the target spiking solution independent of the calibration solutions at a concentration of 2 ng/mL for most compounds. The accuracy of the quality control standard ranged from 74.7 to 99.7% with an average of 94.1% These results are plotted in Figure 4 and demonstrate good calibration accuracy over the concentration range implemented in the study.

Figure 3. Calculated concentration accuracy for calibration levels 1 to 6.

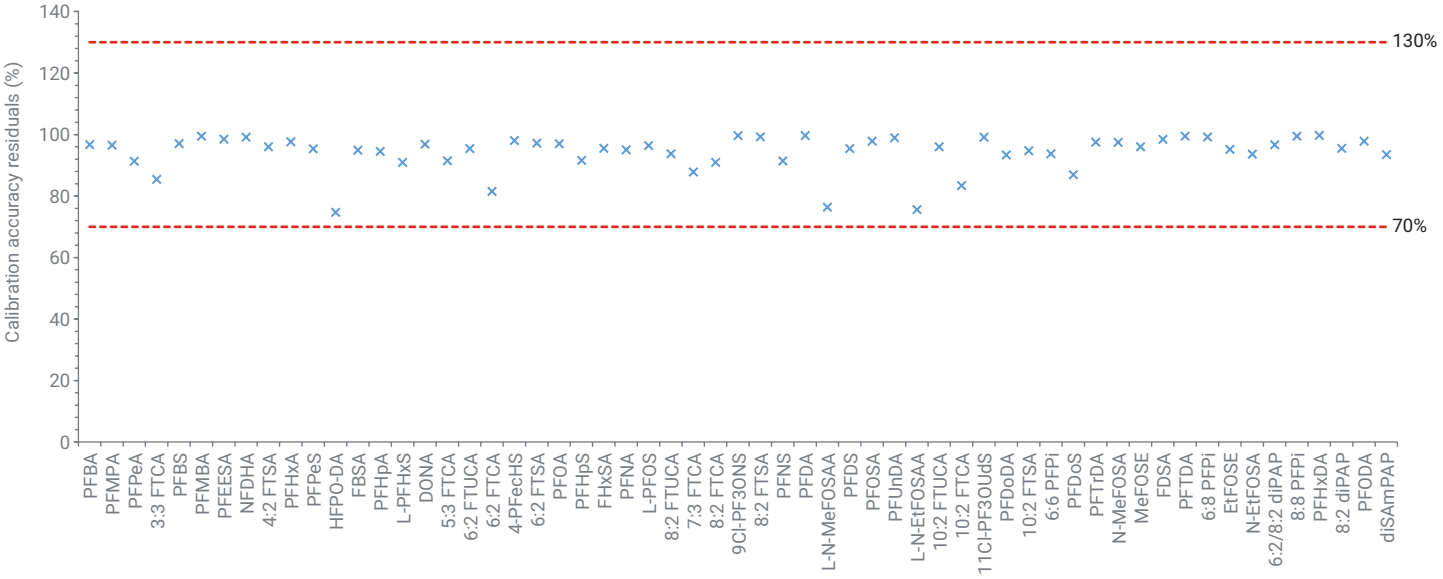

Figure 4. Calculated concentration accuracy for the quality control standard at 2 ng/mL for most compounds.

Blank analysis

To ensure that the extraction and analysis consumables, extraction procedure, and LC/MS/MS system were free from PFAS contamination, an extraction blank was performed along with each extraction set. In addition, the methanol rinsate from duplicate cartridges (Figure 2) was collected and analyzed to ensure that the Carbon S sorbent and cartridges were free from PFAS residue. Confirmation of the extraction and cartridge blanks was used to establish the low-level spike as the minimum reporting limit by setting the background limit to 1/3 of the minimum reporting limit (MRL).[5] Figure 5 shows the quantitative results of the blank analyses. The orange bars are the average residual PFAS measured in the cartridge rinsates, and the blue bars are the average residual PFAS measured in two extraction blanks of sandy loam. The hashed green line is the concentration of the low-level spike in 2 g of soil which was 0.625 ng/g for most target compounds except: N-MeFOSA, N-EtFOSA, 6:2/8:2 diPAP, 8:8 PFPi, and 8:2 diPAP at 1.25 ng/g, EtFOSE, N-MeFOSE, PFHxDA, PFODA, and diSAmPAP at 2.5 ng/g, and 6:2 FTCA, 8:2 FTCA, and 10:2 FTCA at 6.25 ng/g. The hashed red line in Figure 5 shows the background limit. The background concentrations of PFAS in the blanks were well below the 1/3 MRL threshold for all target PFAS confirming the low-level spike as the MRL.

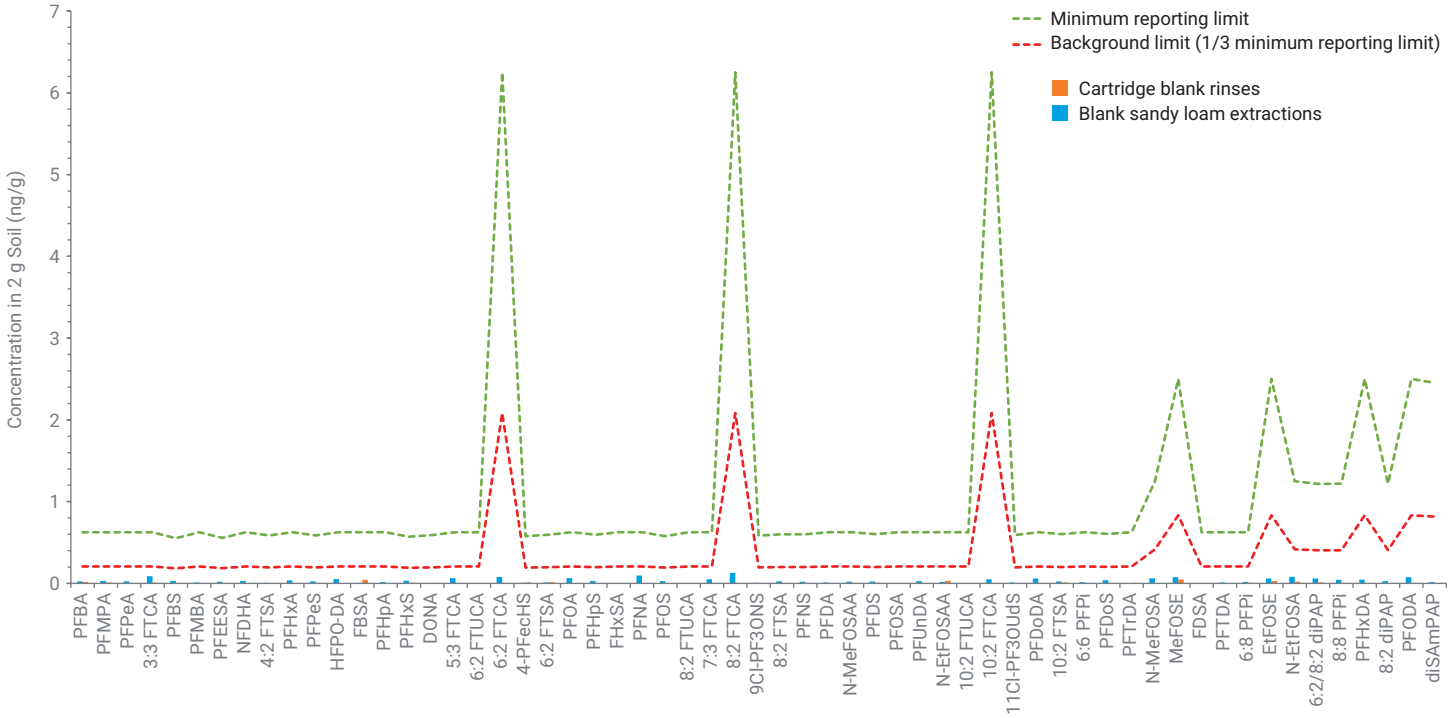

Figure 5. Averages for two replicate cartridge blank rinses and two replicate blank sandy loam extractions. The hashed green line represents the concentration of the low-level spike and minimum reporting limit. The hashed red line indicates the background limit.

Figure 6 shows a total MRM chromatogram for the target compounds for a blank cartridge rinse. These results demonstrate no reportable PFAS above the low-level spike, thus confirming that no PFAS contamination is being introduced during the sample preparation.

Sandy loam spikes

Five replicate extractions of sandy loam at the low-level spike and high-level spike were carried out. In Figure 7, the blue bars represent the average recoveries and the yellow line represents the percent relative standard deviations (RSD) for the low-level spike. Recoveries were within the 50 to 150% for all compounds and RSDs were below 30% for all compounds except 3:3 FTCA and PFDoS. The average recovery for all compounds was 99.3% with an RSD of 13.5%. Figure 8 shows the average recoveries and RSDs for the high-level spikes. Recoveries were within 70 to 130% for all compounds except for 3:3 FTCA, 5:3 FTCA, 6:2 FTUCA, and 8:2 FTUCA. The RSD for all the high-level spikes were below 30%. The average recovery for all compounds was 99.2% with an RSD of 8.5%. These results demonstrate good spike recoveries at both spike level concentrations.

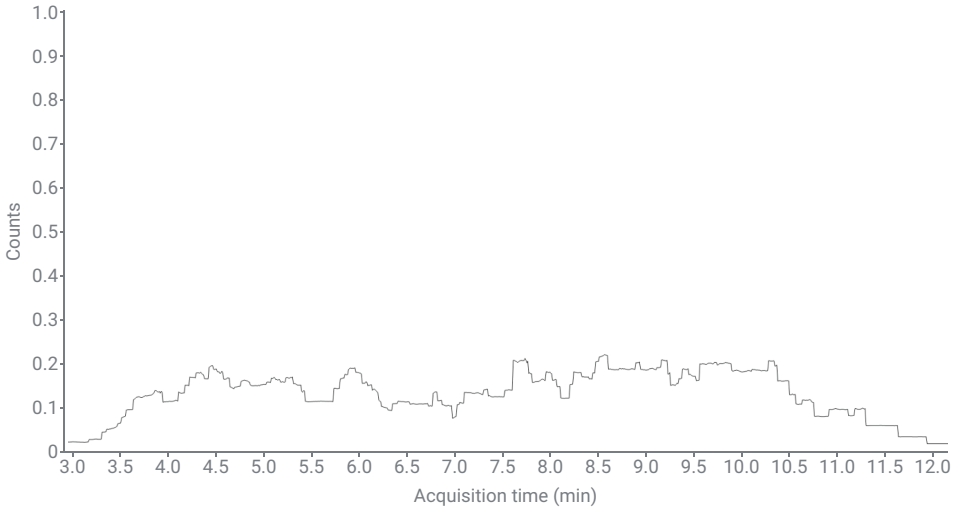

Figure 6. Total MRM chromatogram for cartridge blank rinse.

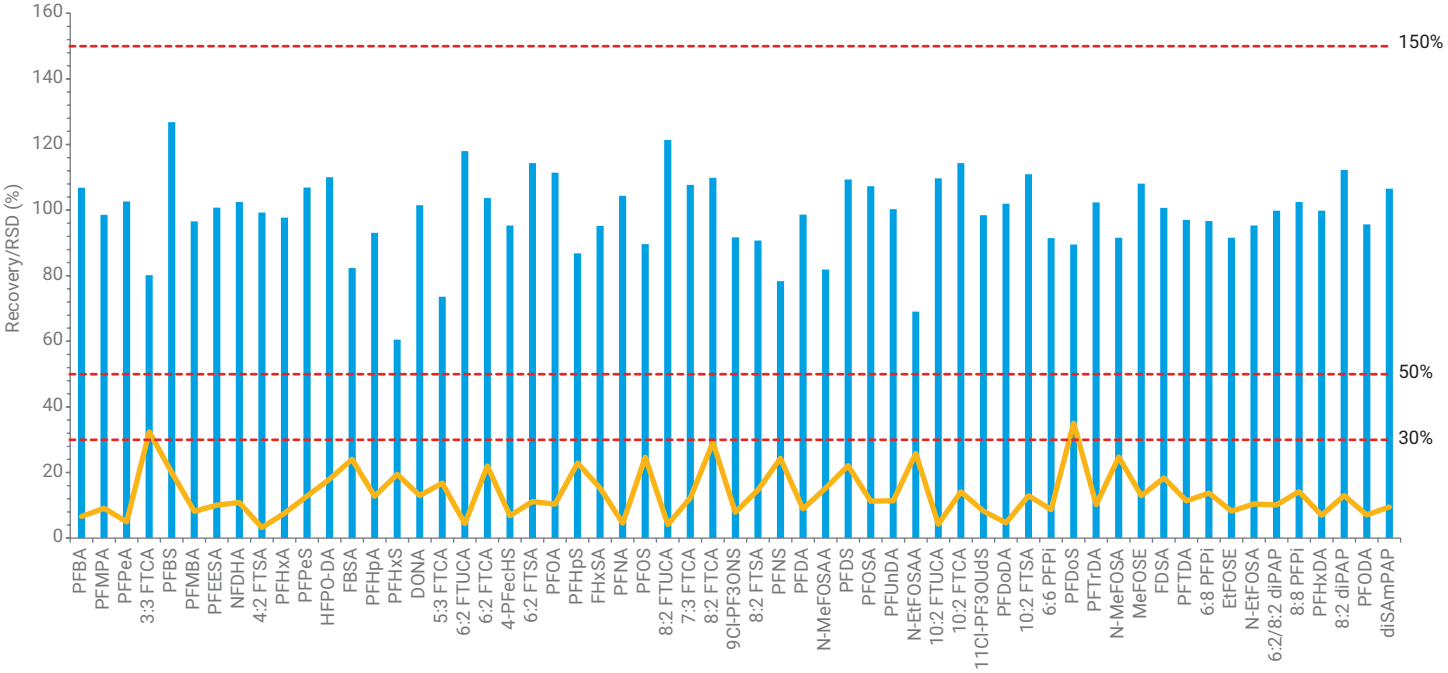

Figure 7. Average recovery for 5 replicate extractions for sandy loam at the low-level spike (blue bars) and RSDs (yellow line).

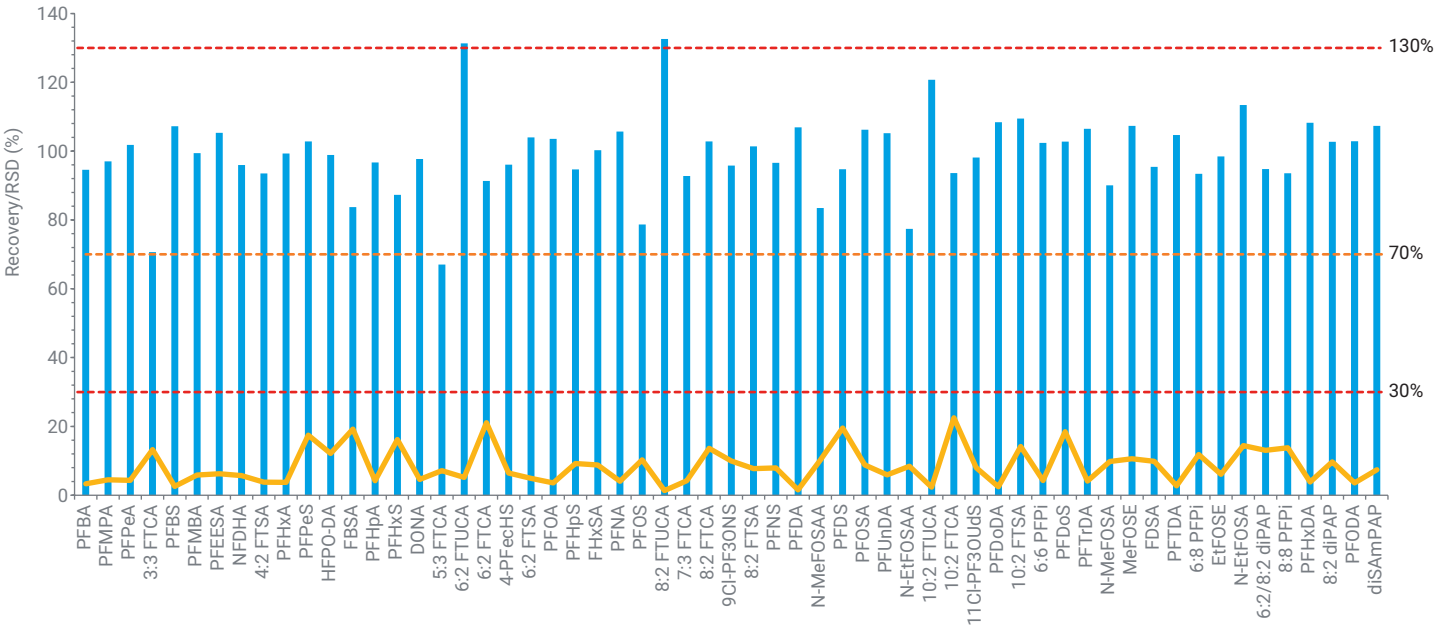

Figure 8. Average recovery for five replicate extractions for sandy loam at the high-level spike (blue bars) and RSDs (yellow line).

Reed sedge peat and topsoil analysis

Two soils were selected for PFAS residue analysis: sedge reed peat and topsoil from two commercial suppliers. Peat was chosen because it consists mainly of organic matter with a high concentration of organic acids and low mineral content. Topsoil was selected for its higher bulk density and inorganic mineral content compared to peat.

Three extractions were performed on each soil type. Table 4 shows the results of the analyses. PFAS levels exceeding the MRL were only found in the peat sample. The concentration of PFBA,

Table 4. Average concentrations of PFAS measured in soil samples.

Acronym	Reed Sedge Peat	Topsoil
10:2 FTCA	<MRL	<MRL
10:2 FTSA	<MRL	<MRL
10:2 FTUCA	<MRL	<MRL
11Cl-PF3OUdS	<MRL	<MRL
3:3 FTCA	<MRL	<MRL
4:2 FTSA	<MRL	<MRL
4-PFecHS	<MRL	<MRL
5:3 FTCA	<MRL	<MRL
6:2 FTCA	<MRL	<MRL
6:2 FTSA	<MRL	<MRL
6:2 FTUCA	<MRL	<MRL
6:2/8:2 diPAP	<MRL	<MRL
6:6 PFPi	<MRL	<MRL
6:8 PFPi	<MRL	<MRL
7:3 FTCA	<MRL	<MRL
8:2 diPAP	<MRL	<MRL
8:2 FTCA	<MRL	<MRL
8:2 FTSA	<MRL	<MRL
8:2 FTUCA	<MRL	<MRL
8:8 PFPi	<MRL	<MRL

Acronym	Reed Sedge Peat	Topsoil
9Cl-PF3ONS	<MRL	<MRL
diSAmPAP	<MRL	<MRL
DONA	<MRL	<MRL
EtFOSE	<MRL	<MRL
FBSA	<MRL	<MRL
FDSA	<MRL	<MRL
FHxSA	<MRL	<MRL
HFPO-DA	<MRL	<MRL
MeFOSE	<MRL	<MRL
N-EtFOSA	<MRL	<MRL
N-EtFOSAA	<MRL	<MRL
NFDHA	<MRL	<MRL
N-MeFOSA	<MRL	<MRL
N-MeFOSAA	<MRL	<MRL
PFBA	4.5 ng/g	<MRL
PFBS	<MRL	<MRL
PFDA	<MRL	<MRL
PFDoDA	<MRL	<MRL
PFDoS	<MRL	<MRL
PFDS	<MRL	<MRL

Acronym	Reed Sedge Peat	Topsoil
PFEESA	<MRL	<MRL
PFHpA	0.83 ng/g	<MRL
PFHpS	<MRL	<MRL
PFHxA	<MRL	<MRL
PFHxDA	<MRL	<MRL
PFHxS	<MRL	<MRL
PFMBA	<MRL	<MRL
PFMPA	<MRL	<MRL
PFNA	<MRL	<MRL
PFNS	<MRL	<MRL
PFOA	<MRL	<MRL
PFODA	<MRL	<MRL
PFOS	<MRL	<MRL
PFOSA	<MRL	<MRL
PFPeA	2.98 ng/g	<MRL
PFPeS	<MRL	<MRL
PFTDA	<MRL	<MRL
PFTrDA	<MRL	<MRL
PFUnDA	<MRL	<MRL

PFPeA, and PFHpA measured in the peat sample were 4.51, 2.98, and 0.83 ng/g, respectively. The concentration of PFAS residue measured in the topsoil were all below the MRL.

Matrix removal efficiency

The efficiency of matrix removal was qualitatively assessed by visually inspecting the sample extract pigment before and after passthrough Carbon S cleanup for the peat and topsoil samples (Figure 9). Significant pigment removal was achieved for both matrix extracts. For the peat (Figure 9A), the extract color was orange/brown before Carbon S cleanup and became a barely perceptible yellow after passing through the sorbent. For topsoil (Figure 9B), the extract was a slight yellow before cleanup and turned completely clear after cleanup.

Total ion chromatograms were compared between matrix extracts with and without Carbon S cleanup. For peat extracts without Carbon S cleanup, it was found that the earliest eluting peak (PFBA) had a distorted peak shape and shifted retention time compared to extracts that underwent Carbon S cleanup. Figure 10 shows an examples of extracted MRM quant ion chromatograms for $^{13}C_3$-PFBA with and without Carbon S cleanup. The chromatographic peak shape for $^{13}C_3$-PFBA in the peat extract without Carbon S cleanup appears wide and partially split (Figure 10A) compared to the $^{13}C_3$-PFBA peak in the extract than underwent Carbon S cleanup (Figure 10B). Also, the retention time shifted half a minute earlier in the peat extract. These results demonstrate that the efficient matrix cleanliness provided by Carbon S passthrough cleanup can reduce the matrix effects for some targets and improve data quality and consistency.

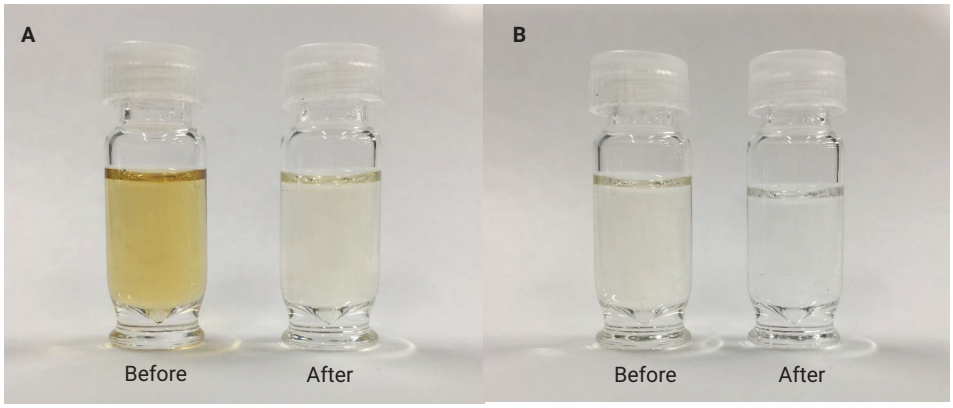

Figure 9. Qualitative pigment removal comparison before and after Carbon S passthrough cleanup for (A) peat and (B) topsoil.

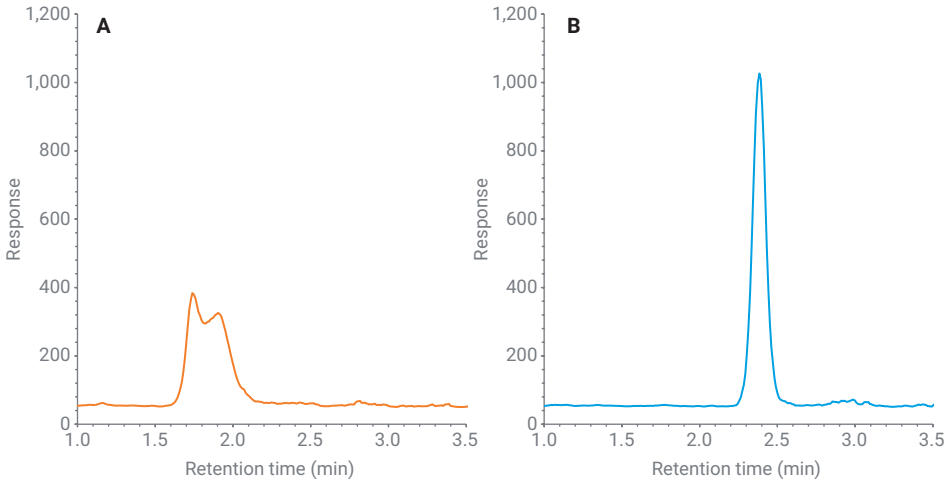

Figure 10. Comparison of $^{13}C_3$-PFBA quant ion chromatographic peak shape and retention time differences between peat matrix without Carbon S cleanup (A) and with Carbon S cleanup (B).

Conclusion

The results show that use of the Agilent Bond Elut Carbon S SPE cartridge provided efficient passthrough matrix cleanup for PFAS analysis in soil samples. Average recoveries for the 59 PFAS studied were in the 99% range with RSDs for most compounds less than 30%. For reed sedge peat extract, the use of Carbon S improved the peak shape integrity and retention consistency of PFBA compared to extracts without the use of Carbon S cleanup.

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5. Method 533: Determination of Perand Polyfluoroalkyl Substances in Drinking Water by Isotope Dilution Anion Exchange Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry. United States Environmental Protection Agency, **2019**.

Appendix A

Table A1. Target spiking solution and target concentration in matrix.

Target Compound	CAS	Ret Time (min)	Target Quant Ion MRM Transition	Isotope Analog	Isotope MRM Transition
PFBA	375-22-4	2.43	213 → 169	$^{13}C_4$-PFBA	217 → 172
PFMPA	377-73-1	3.57	229 → 85	$^{13}C_5$-PFPeA	268 → 223
3:3 FTCA	356-02-5	3.88	241 → 177	$^{13}C_5$-PFPeA	268 → 223
PFPeA	2706-90-3	3.89	263 → 219	$^{13}C_5$-PFPeA	268 → 223
PFBS	375-73-5	3.97	299 → 80	$^{13}C_3$-PFBS	302 → 80
PFMBA	863090-89-5	4.01	279 → 85	$^{13}C_5$-PFPeA	268 → 223
PFEESA	113507-82-7	4.12	315 → 135	$^{13}C_3$-PFBS	302 → 80
NFDHA	151772-58-6	4.25	295 → 85	$^{13}C_5$-PFHxA	318 → 273
4:2 FTSA	757124-72-4	4.29	327 → 307	$^{13}C_2$-4:2 FTSA	329 → 309
PFHxA	307-24-4	4.33	313 → 269	$^{13}C_5$-PFHxA	318 → 273
PFPeS	2706-91-4	4.39	349 → 80	$^{13}C_3$-PFHxS	402 → 80
HFPO-DA	13252-13-6	4.48	285 → 169	$^{13}C_3$-HFPO-DA	287 → 169
FBSA	30334-69-1	4.58	298 → 78	$^{13}C_3$-PFHxS	402 → 80
PFHpA	375-85-9	4.90	363 → 319	$^{13}C_4$-PFHpA	367 → 322
PFHxS	355-46-4	4.95	399 → 80	$^{13}C_3$-PFHxS	402 → 80
DONA	919005-14-4	4.98	377 → 251	$^{13}C_4$-PFHpA	367 → 322
5:3 FTCA	914637-49-3	5.04	341 → 237	$^{13}C_5$-PFHxA	318 → 273
6:2 FTUCA	70887-88-6	5.06	357 → 293	$^{13}C_2$-6:2 FTUCA	359 → 294
6:2 FTCA	53826-12-3	5.11	377 → 293	$^{13}C_2$-6:2 FTCA	379 → 294
4-PFecHS	646-83-3	5.52	461 → 381	$^{13}C_8$-PFOS	507 → 80
6:2 FTSA	27619-97-2	5.57	427 → 407	$^{13}C_2$-6:2 FTSA	429 → 409
PFOA	335-67-1	5.60	413 → 369	$^{13}C_8$-PFOA	421 → 376
PFHpS	375-92-8	5.63	449 → 80	$^{13}C_8$-PFOS	507 → 80
FHxSA	41997-13-1	6.10	398 → 78	$^{13}C_8$-PFOS	507 → 80
PFNA	375-95-1	6.15	463 → 419	$^{13}C_9$-PFNA	472 → 427
PFOS	1763-23-1	6.17	499 → 80	$^{13}C_8$-PFOS	507 → 80
8:2 FTUCA	70887-84-2	6.36	457 → 393	$^{13}C_2$-8:2 FTUCA	459 → 394
7:3 FTCA	812-70-4	6.37	441 → 337	$^{13}C_5$-PFHxA	318 → 273
8:2 FTCA	27854-31-5	6.40	477 → 393	$^{13}C_2$-8:2 FTCA	479 → 394
9Cl-PF3ONS	756426-58-1	6.55	531 → 351	$^{13}C_8$-PFOS	507 → 80
8:2 FTSA	39108-34-4	7.02	527 → 507	$^{13}C_2$-8:2 FTSA	529 → 509
PFDA	335-76-2	7.07	513 → 469	$^{13}C_6$-PFDA	519 → 474
PFNS	68259-12-1	7.09	549 → 80	$^{13}C_8$-PFOS	507 → 80
N-MeFOSAA	2355-31-9	7.73	570 → 419	d_3-N-MeFOSAA	573 → 419
PFDS	335-77-3	8.10	599 → 80	$^{13}C_8$-PFOS	507 → 80
PFUnDA	2058-94-8	8.11	563 → 519	$^{13}C_7$-PFUnDA	570 → 525
N-EtFOSAA	2991-50-6	8.13	584 → 419	d_5-N-EtFOSAA	589 → 419
PFOSA	754-91-6	8.32	498 → 78	$^{13}C_8$-PFOSA	506 → 78
10:2 FTUCA	70887-94-4	8.36	557 → 493	$^{13}C_2$-10:2 FTUCA	559 → 494
10:2 FTCA	53826-13-4	8.40	577 → 493	$^{13}C_2$-10:2 FTCA	579 → 494
11Cl-PF3OUdS	763051-92-9	8.48	631 → 451	$^{13}C_8$-PFOS	507 → 80
PFDoDA	307-55-1	8.70	613 → 569	$^{13}C_2$-PFDoDA	615 → 570
10:2 FTSA	120226-60-0	8.71	627 → 607	$^{13}C_2$-8:2 FTSA	529 → 509

Target Compound	CAS	Ret Time (min)	Target Quant Ion MRM Transition	Isotope Analog	Isotope MRM Transition
6:6 PFPi	40143-77-9	8.90	701 → 401	$^{13}C_2$-PFDoDA	615 → 570
PFDoS	79780-39-5	9.09	699 → 80	$^{13}C_8$-PFOS	507 → 80
PFTrDA	72629-94-8	9.12	663 → 619	$^{13}C_2$-PFDoDA	615 → 570
PFTDA	376-06-7	9.49	713 → 669	$^{13}C_2$-PFTDA	715 → 670
N-MeFOSA	31506-32-8	9.50	512 → 219	d_3-N-MeFOSA	515 → 169
FDSA	N/A	9.52	598 → 78	$^{13}C_8$-PFOSA	506 → 78
6:8 PFPi	610800-34-5	9.54	801 → 401	$(^{13}C_2)_2$-6:2 diPAP	993 → 97
MeFOSE	24448-09-7	9.54	616 → 59	d_7-MeFOSE	623.1 → 59
N-EtFOSA	4151-50-2	9.88	526 → 219	d_5-N-EtFOSA	531 → 169
EtFOSE	1691-99-2	9.89	630 → 59	d_9-EtFOSE	639.1 → 59
6:2/8:2 diPAP	943913-15-3	10.02	889 → 443	$(^{13}C_2)_2$-6:2 diPAP	793 → 97
8:8 PFPi	40143-79-1	10.11	901 → 501	$(^{13}C_2)_2$-6:2 diPAP	793 → 445
PFHxDA	67905-19-5	10.18	813 → 269	$^{13}C_2$-PFHxDA	815 → 770
8:2 diPAP	678-41-1	10.55	989 → 543	$(^{13}C_2)_2$-8:2 diPAP	993 → 97
PFODA	16517-11-6	10.81	913 → 369	$^{13}C_2$-PFHxDA	815 → 770
diSAmPAP	2965-52-8	11.10	1,203 → 526	$(^{13}C_2)_2$-8:2 diPAP	993 → 97

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