Application Note

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Analysis of PFAS and Other Environmental Contaminants in Soil and Oat Plants Using High-Resolution GC/Q-TOF

Authors

Luann Wong, Gabrielle Black, and Thomas Young
Department of Civil and Environmental Engineering, University of California, Davis

Sofia Nieto, Matthew Giardina, Matthew Curtis, and Tarun Anumol
Agilent Technologies, Inc.

Abstract

Soil is one of the major environmental repositories of per- and polyfluoroalkyl substances (PFAS)[1], and the presence of PFAS in soil can potentially lead to ground water and food contamination. Current PFAS methods typically only cover 40 to 80 PFAS and vastly underestimate their presence in many environmental samples based on mass balance studies.[2,3] Further, liquid chromatography/mass spectrometry (LC/MS) has significant limitations with respect to the analysis of some of the volatile classes of PFAS, which is where gas chromatography/mass spectrometry (GC/MS) should be considered as an important complementary technique.

This study describes different approaches for the extraction and analysis of PFAS in soil and plants using an Agilent 7250 gas chromatography/quadrupole time-of-flight mass spectrometer (GC/Q-TOF). PFAS and other environmental contaminants were detected using a target screening methodology based on an accurate mass personal compound database and library (PCDL) of these pollutants. A broader range of contaminants was also identified in the soil and plant samples, including polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs), and flame retardants, using a nontargeted screening and an extensive unit mass NIST23 library.

Introduction

PFAS are persistent synthetic organic pollutants with a potential to bioaccumulate.[4] The list of PFAS substances curated by the Environmental Protection Agency (EPA) currently includes nearly 8,000 PFAS chemicals based on structure[5] ranging from volatile PFAS, such as ubiquitous fluorotelomer alcohols (FTOHs), to long-chain PFAS, including the most commonly detected perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS). While long-chain PFAS are being phased out of production, the manufacturing of shorter chain length PFAS is increasing due to the assumption that more volatile PFAS are less toxic. These shorter chain length PFAS such as 6:2 FTOH are more difficult to detect with LC/MS using established methods, and recent studies have indicated that they are equally toxic.[6,7]

Soil is a significant reservoir of PFAS as well as of many other persistent environmental contaminants, and thus can contribute to contamination of ground water, atmosphere, and biota. Therefore, to better understand the source and transport of these contaminants, both soil and plant extracts have been analyzed using the Agilent 7250 GC/Q-TOF.

To maximize the sensitivity of PFAS detection, a target screening approach based on a PFAS accurate mass library was used. The PFAS PCDL used in this study included over 150 electron ionization (EI) PFAS spectra along with retention times (RTs) and retention indices (RIs), and is described elsewhere.[8]

In addition to PFAS, many persistent pollutants were identified in both soil and plants, where both target and nontarget screening workflows were used. These pollutants included pesticides, polyaromatic hydrocarbons (PAHs), PCBs, PBDEs, and flame retardants.

Experimental

Sample collection

Soil and oat plants were sampled from two fields in California (F1 and F2) that have historically received biosolids. The soil samples were collected prior to the application of biosolids (labeled PreA for preapplication). A certified USDA organic (Org) field was also sampled prior to treating the subplots with compost (Comp) and compost and lime (C&L). The compost was collected as well. The soil was also sampled at harvest time (Hvst). Plants were collected in the same regions as the soil samples.

Sample preparation

The soil and plant samples were either extracted with methylene chloride (DCM) for liquid injections or subjected to headspace solid-phase microextraction (HS-SPME). For DCM extraction, 2 g of soil was weighed into a 50 mL glass centrifuge tube and 5 mL of DCM was added. The 50 mL centrifuge tubes containing the samples were vortexed using a Heidolph Multi Reax Vibrating Test Tube Shaker at speed 5 for 5 minutes and centrifuged at 3,000 rpm for 5 minutes. Approximately 0.5 mL of supernatant extract was transferred into 2 mL autosampler vials. Whole plant samples that included stems, leaves, seeds, and seed pods were cut into 2 to 5 mm sections. Then, 2 g of plant samples were extracted with methylene chloride the same way as the soil. Method blank samples for each set were also generated.

For HS-SPME, the soil (2 g) and finely chopped plant material (1 g) were transferred into a 20 mL headspace vial, and either 2 or 3 mL of DI water were added, respectively.

SPME conditions

The HS-SPME was performed using an Agilent PAL 3 CTC autosampler. Four different fibers were tested (Agilent 100 µm PDMS, 95 µm CWR/PDMS, 65 µm DVB/PDMS, and 80 µm DVB/CWR/PDMS, part number 5191-5878), and the SPME conditions were optimized. The fiber conditioning was carried out at 300 °C for 5 minutes. The samples were equilibrated for 10 minutes, and the SPME fiber was inserted into the vial headspace. Extraction was carried out at 50 °C for 35 minutes at 300 rpm (programmed for 10 seconds on, 2 seconds off cycle), with the desorption into the GC inlet at 250 °C for 7 minutes. The GC injection port was equipped with the 0.75 mm id liner for SPME analysis and the resistant to wear Merlin Microseal septa.

Data acquisition

The GC/MS analysis was performed using an Agilent 7250 GC/Q-TOF system. All the data were acquired in full spectrum acquisition mode. Two different GC columns were used to acquire the data. The DB-624 is a midpolar GC column and provided the best retention and separation for GC-amenable PFAS compounds. This column was used for PFAS screening using the PFAS PCDL. The nonpolar DB-5ms column was also used to take advantage of RI information available for all the compounds with EI spectra in the NIST23 library. The data acquisition parameters are described in Table 1.

Table 1. Data acquisition parameters.

	Agilent DB-5ms	Agilent DB-624
MS	Agilent 7250 GC/Q-TOF	
GC	Agilent 8890 GC	
Inlet	Multimode inlet, Agilent Ultra Inert 4-mm liner single taper with wool	
Inlet Temperature	70 °C for 0.01 min, 300 °C/min to 250 °C	
Injection Volume	1 µL	
Column	Agilent J&W DB-5ms Ultra Inert (UI), 30 m × 0.25 mm, 0.25 µm	Agilent DB-624 Ultra Inert, 30 m × 0.25 mm, 1.4 µm
Oven Temperature Program	35 °C for 2 min, 7 °C/min to 210 °C, 20 °C/min to 300 °C, 4 min hold	30 °C for 2 min, 3 °C/min to 75 °C, 2 °C/min to 110 °C, 10 °C/min to 210 °C, 20 °C/min to 240 °C, 2 min hold
Column Flow	1.2 mL/min constant flow	1 mL/min constant flow
Carrier Gas	Helium	
Transfer Line Temperature	250 °C	
Quadrupole Temperature	150 °C	
Source Temperature	200 °C	
Electron Energy	70 eV	
Emission Current	Variable by time segment, 0.01 to 5 µA	
Spectral Acquisition Rate	5 Hz	
Mass Range (Tune)	50 to 1,200 *m/z*	

Data processing

The nontargeted workflow was performed in Agilent MassHunter Unknowns Analysis software (version 12.1) and involved the SureMass chromatographic deconvolution and the NIST23 EI library search. RIs and accurate mass information were used to confirm the compound identification. The suspect screening was performed using the GC/Q-TOF Screener tool of MassHunter Quantitative Analysis software (version 12.1) and accurate mass libraries for pesticides and PFAS.

Results and discussion

Characteristic EI fragmentation of PFAS

One of the approaches that could be beneficial for PFAS screening in complex matrices is a suspect screening approach since it allows for high sensitivity and specificity of detection. When using a high-resolution accurate mass GC/MS, this approach can be greatly facilitated by using accurate mass libraries to screen for a large number of target compounds that could, in theory, be unlimited. Thus, the accurate mass GC/MS PCDL for over 100 volatile and semivolatile PFAS compounds that was previously created[6] was used in this work for PFAS screening in soil and plant samples. The PFAS compound classes in the PCDL included perfluoroalkyl iodides (PFAIs), fluorotelomer iodides (FTIs), fluorotelomer alcohols (FTOHs), fluorotelomer olefins (FTOs), fluorotelomer acrylates (FTACs), fluorotelomer methacrylates (FTMACs), fluorotelomer carboxylic acids (FTCA), fluorotelomer unsaturated carboxylic acids (FTUCA), perfluoroalkane sulfonamides (FASA), among others, many of which are uniquely amenable to GC/MS analysis. The electron ionization (EI) mode was chosen for the PFAS PCDL as a more universal technique compared to chemical ionization. EI covers a broader range of PFAS compound classes and allows users to easily screen for other contaminants in the same data file. While many PFAS compounds can highly fragment in EI, most of them nevertheless have specific fragment ions that could be selected by the GC/Q-TOF suspect screening algorithm or manually, as target or qualifier ions. Some of the most typical and specific fragments for the different PFAS compound classes are shown in Table 2.

Table 2. Characteristic fragments of volatile PFAS in EI.

Characteristic Fragments	Neutral Loss (*m/z*)	PFAS Class; % of Base Ion, as Maximum Observed for a Given PFAS Class							
		FTOH	PFAI	FTI	FTAC	FTMAC	FTO	PFAL	FASA
[M]+	0	–	40	100	30	90	–	–	–
[M-I]+	126.9045	–	100	–	–	–	–	–	–
[M-H_2O-HF]+	38.0168	100	–	–	–	–	–	–	–
[M-CHO-F]+	48.011	–	–	–	–	–	–	90	–
[M-H_2O-F-HF-C_2H_2]+	83.0308	80	–	–	–	–	–	–	–
[M-H_2O-2F]+	56.0074	70	–	–	–	–	–	–	–
[M-C_2F_5]+	118.992	–	–	50	–	–	–	–	–
[M-HF-I]+	146.9107	–	–	50	–	–	–	–	–
[M-H_2O-CF_3]+	87.0058	30	–	–	–	–	–	–	–
[M-H_2O-2F-CF_3]+	126.0026	30	–	–	–	–	–	–	–
[M-F]+	18.9984	6	–	–	10	5	5	–	1
[M-CHO-2F]+	66.9995	–	–	–	–	–	–	25	
[M-SO_2-CH_3]+	78.9854	–	–	–	–	–	–	–	25
[M-H_2O-CF_2]+	68.0074	25	–	–	–	–	–	–	–
[M-HF]+	20.0062	20	–	–	–	–	–	–	–
[M-2F-CF_3]+	106.992	–	–	–	–	–	20	–	–
[M-H]+	1.0078	15	–	1	–	–	–	–	–
[M-CH_3]+	15.0235	–	–	–	–	10	–	–	5
[M-H-HF]+	21.0141	15	–	–	–	–	–	–	–
[M-F-2HF]+	59.0109	15	–	–	–	–	–	–	–
[M-H_2O-F]+	37.009	15	–	–	–	–	–	–	–
[M-CF_3-HF]+	89.0014	–	–	10	–	–	5	–	–
[M-F-HF]+	39.0046	–	–	–	–	–	10	–	–
[M-NH_2SO_2]+	79.9806	–	–	–	–	–	–	–	10
[M-C_2H_3-2F]+	65.0203	–	–	–	–	–	10	–	–
[M-CHO]+	29.0027	–	–	–	–	–	–	5	–
[M-SO_2-H]+	64.9697	–	–	–	–	–	–	–	5
[M-SO_2-F]+	82.9603	–	–	–	–	–	–	–	5
[M-SO_2-CF_3-HF]+	152.9633	–	–	–	–	–	–	–	5

Selection of SPME fiber for soil analysis

Four different SPME fibers were evaluated for the ability to extract volatile compounds (including PFAS) from soil: PDMS, CWR/PDMS, DVB/PDMS, and DVB/CWR/PDMS. The test was performed using soil (2 g) sampled from the same location, mixed with 2 mL of water, and run under the same SPME conditions. Total ion chromatograms (TIC) generated by each fiber tested are shown in Figure 1. Both DVB/PDMS and DVB/CWR/PDMS fibers produced a significant number of peaks and showed the ability to extract a wide range of compounds.

The number of the identifiable peaks was also evaluated for each of the fibers (Table 3). DVB/PDMS and DVB/CWR/PDMS had a comparable number of library hits that was slightly higher for DVB/CWR/PDMS. Therefore, it was selected for further analysis.

Table 3. SPME fibers performance. The number of components generated by the SureMass deconvolution algorithm as well as number of NIST23 library hits (Library Match Score cutoff 75) are shown.

Fiber Type	Number of Components	Number of Hits
PDMS	422	228
CWR-PDMS	514	419
DVB-PDMS	687	560
DVB-CWR-PDMS	683	570

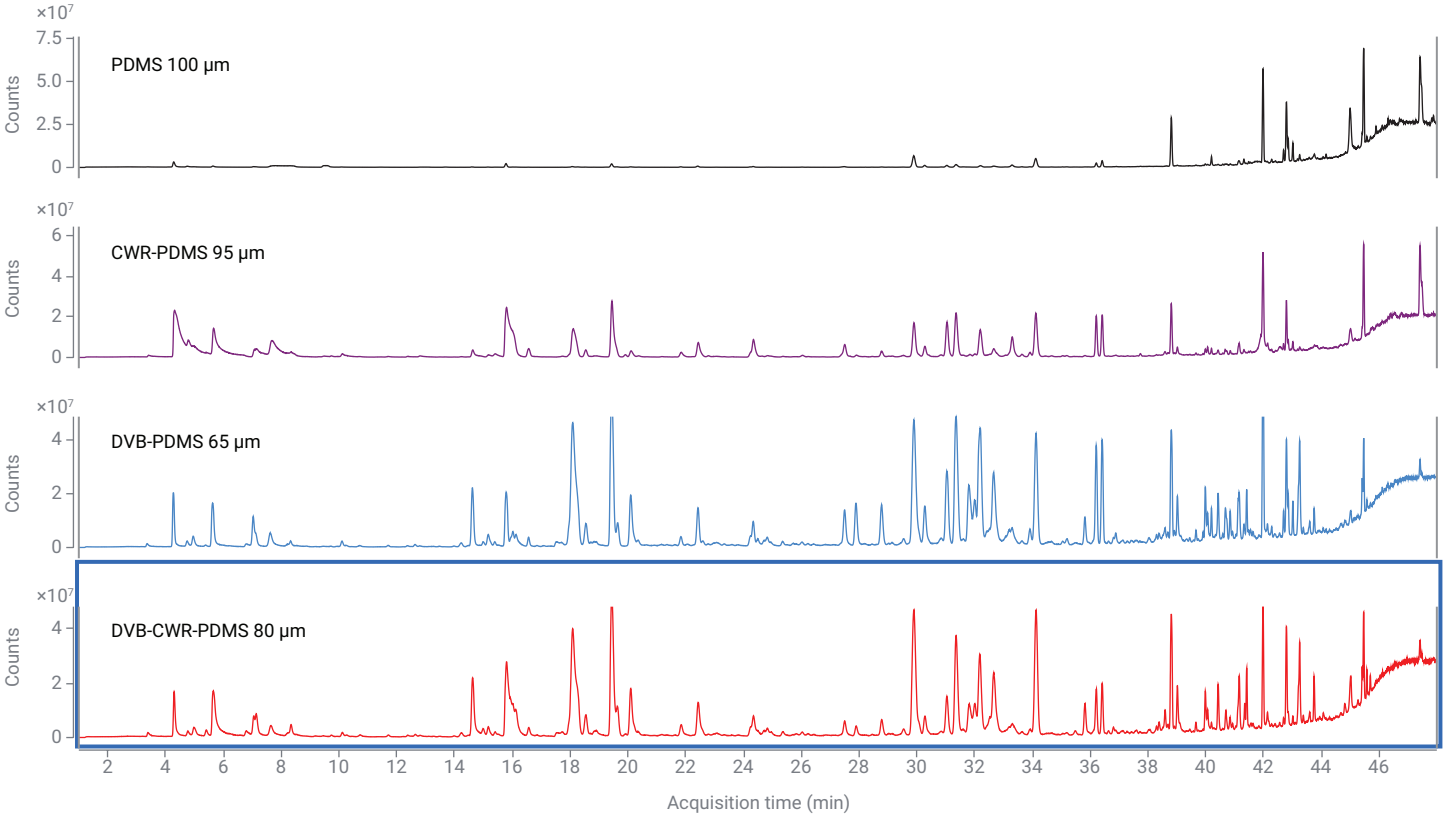


Figure 1. SPME fiber performance on soil samples.

Detection of volatile PFAS in soil and plant samples using accurate mass PFAS library

For PFAS detection using the accurate mass PFAS PCDL for GC/Q-TOF, the midpolar DB-624 GC column (for more detail, see Table 1) was used.

Both targeted and nontargeted methodologies that involved the GC/Q-TOF Screener and the Unknowns Analysis software, respectively, were used to identify PFAS in soil and plant samples. An advantage of using the nontargeted analysis is that both accurate mass libraries, as well as large comprehensive public libraries such as NIST, could be used to screen for the contaminants simultaneously without reinjection.

There are several benefits of the targeted, PCDL-based suspect screening approach, which is performed entirely in MassHunter Quantitative Analysis software and has been described in detail previously.[9,10] Some of the main advantages of this approach include high sensitivity and a high degree of flexibility and automation of the data analysis method setup and results validation. The validation requires minimal human involvement prior to the reporting. Together this provides a user with a highly effective and time-saving tool for targeted analysis.

A few PFAS compounds were detected when analyzing the data from SPME. An example of a compound identified in a few soil and plant samples using the GC/Q-TOF Screener is shown in Figure 2. This compound is a volatile 6:2 fluorotelomer alcohol, frequently detected in environmental matrices. Due to the trace amount of this compound, it was not found in a nontargeted approach.

Sample: soil, F1

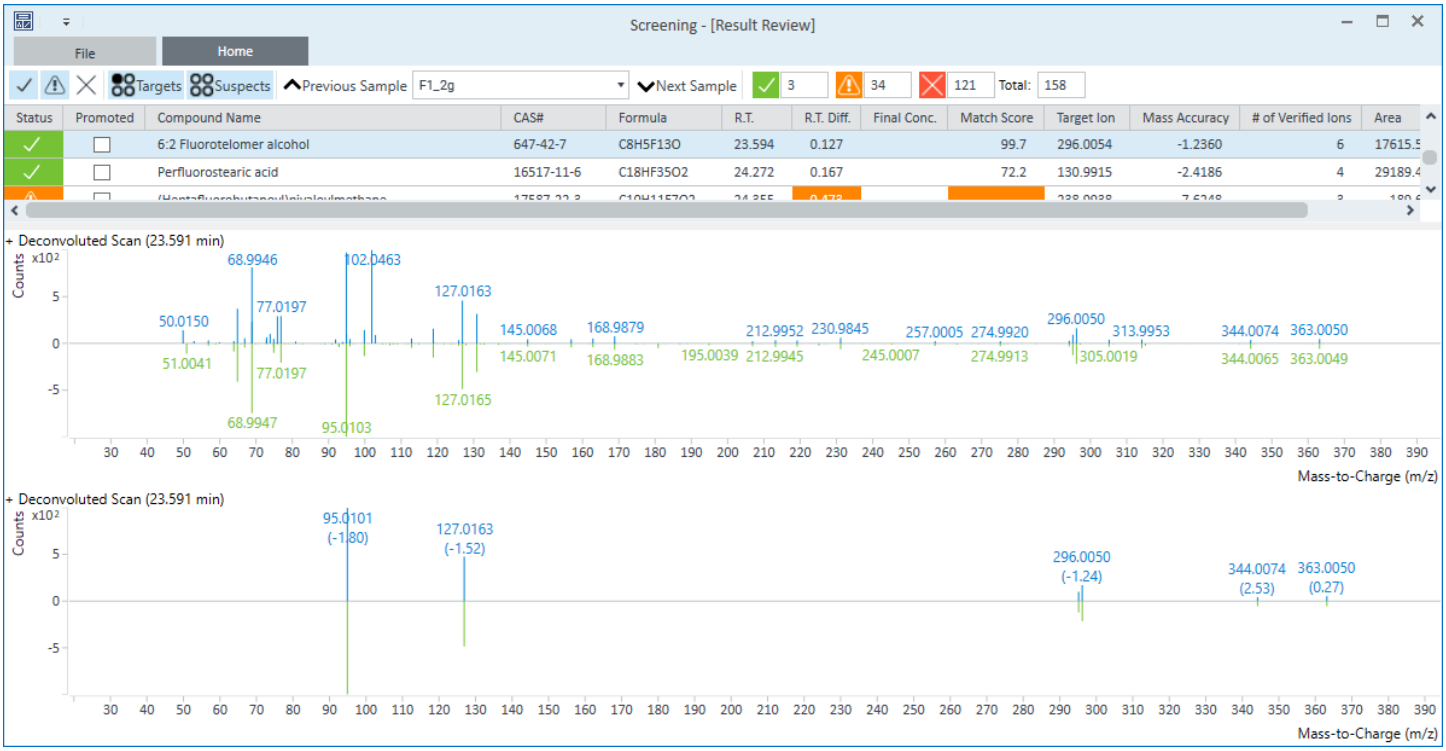
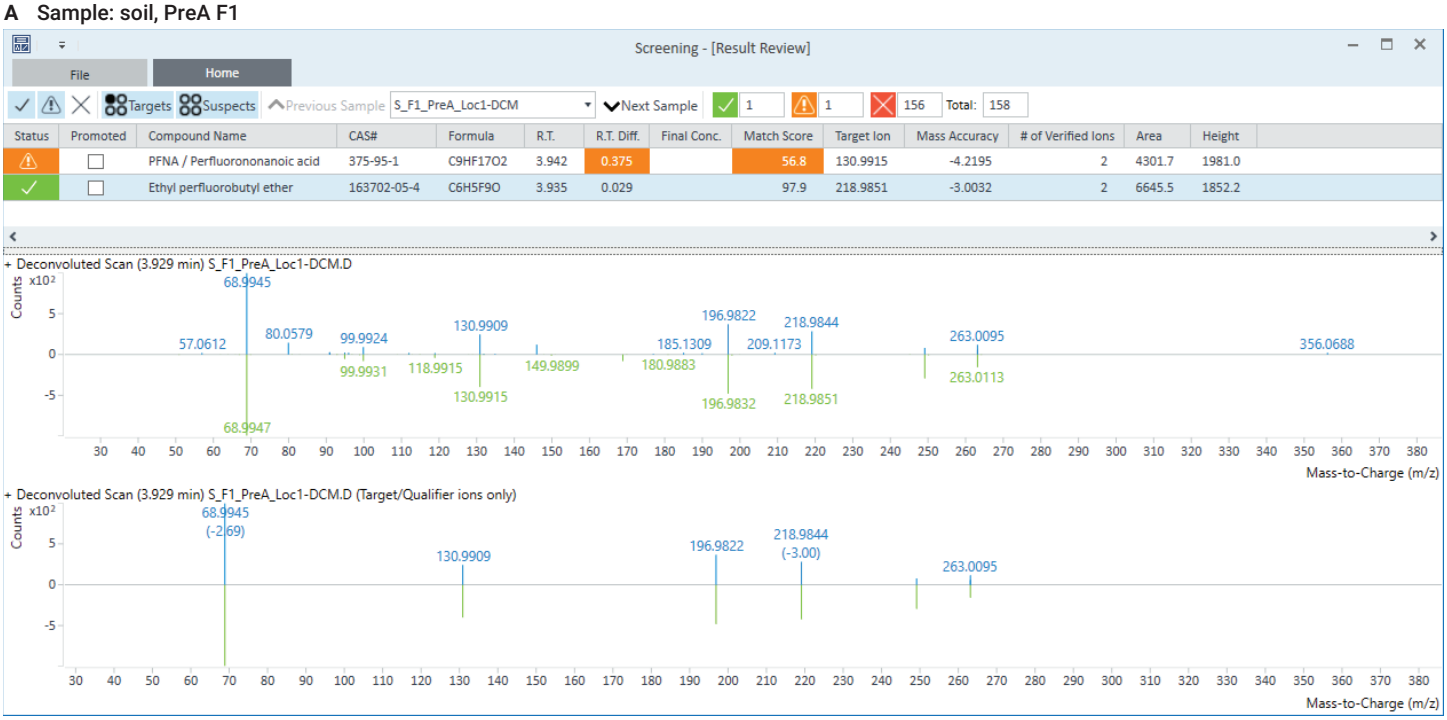


Figure 2. 6:2 FTOH detected in soil using SPME and PFAS PCDL-based screening approach. The mirror plot at the top shows the deconvoluted compound spectrum versus the spectrum from the PFAS PCDL. The mirror plot at bottom displays only target and qualifier ions.

When performing nontarget analysis, the chromatographic deconvolution uses the SureMass algorithm, which is specifically optimized for high-resolution EI data to ensure high speed, sensitivity, and integrity of spectral extraction. While the suspect screening approach provided the highest degree of sensitivity and was able to detect more PFAS compounds, one of the more abundant PFAS was detected in both approaches (Figures 3A and 3B).

All the PFAS compounds identified in soil and plant samples were detected by matching the PFAS PCDL.

A Sample: soil, PreA F1



B Sample: soil, PreA F1

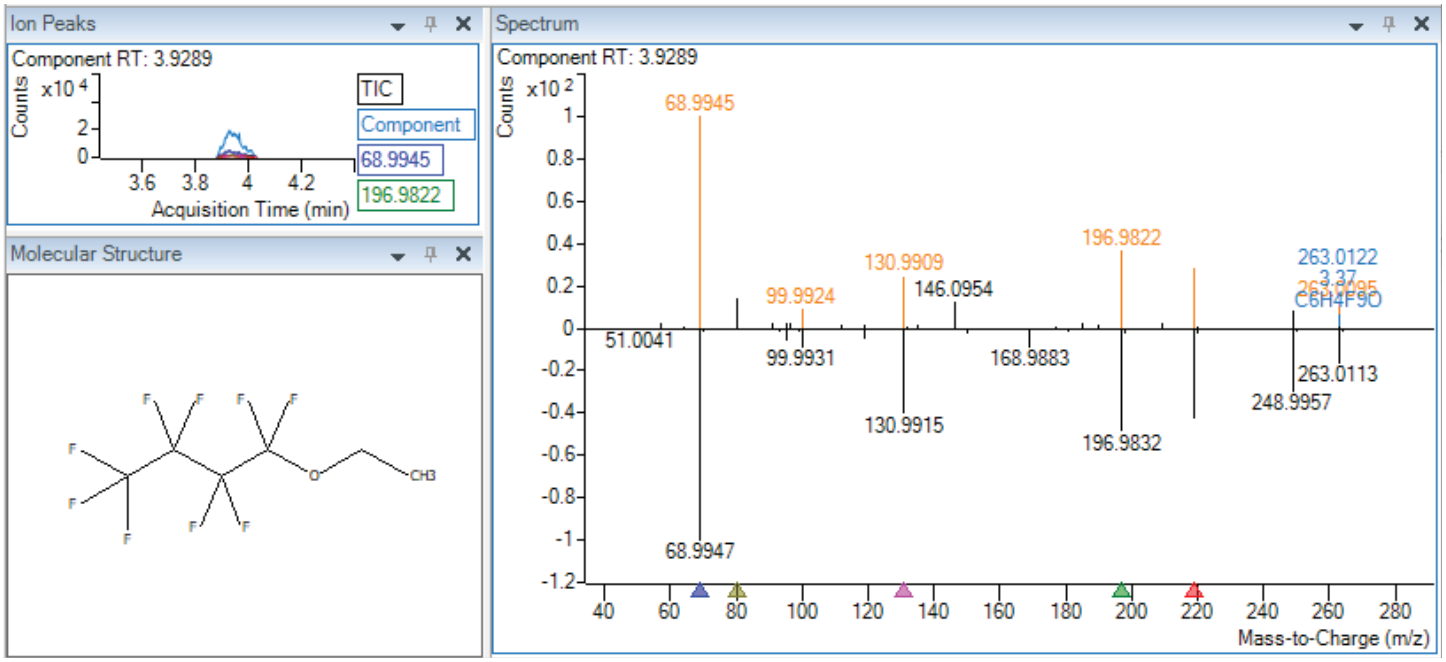


Figure 3. PFAS (ethyl perfluorobutyl ether) identified in DCM soil extracts using PFAS PCDL in both target screening (A) and an untargeted, deconvolution-based approach in the Unknowns Analysis software (B).

Overall, the HS-SPME approach for PFAS extraction worked best and provided a higher number of identified volatile PFAS compounds. The amounts of PFAS detected (summarized in Table 4) were estimated based on the standard injections where the actual concentrations in soil and plant samples have not been determined.

Identification of other contaminants in soil and oat plants

The identification of the additional contaminants in soil and plant samples was performed for both DCM extracts and SPME. However, while SPME allowed better detection of volatile compounds, a higher number of the environmental contaminants that included PCBs, PBDEs, pesticides, PAHs, and flame retardants, were detected in DCM extracts and will thus be the focus of the further discussion.

The separation was carried out using the DB-5ms UI column to be able to use the RI values from the extensive NIST23 library, and thus increase confidence in compound identification by using the RI penalty function for library hits. This column phase is also compatible with the GC/Q-TOF Pesticide PCDL, which could be considered for screening GC/Q-TOF accurate mass EI data for pesticides and PAHs. After a quick prescreening, the identified pollutants were grouped by contaminant classes and approached separately.

PCBs and PBDEs were identified in the nontargeted approach using the Unknowns Analysis and NIST23 library. To eliminate false positives based on the accurate mass EI data while searching a unit mass library, the Unknowns Analysis ExactMass tool was used. This tool is described in further detail in Figure 4A, which shows an example of one of the BDEs detected in a soil extract.

There were 20 different PCBs and PBDEs detected in the soil extracts (Figure 4B). The only oat plant extract where this group of contaminants (BDE-47) was detected was grown in field F2.

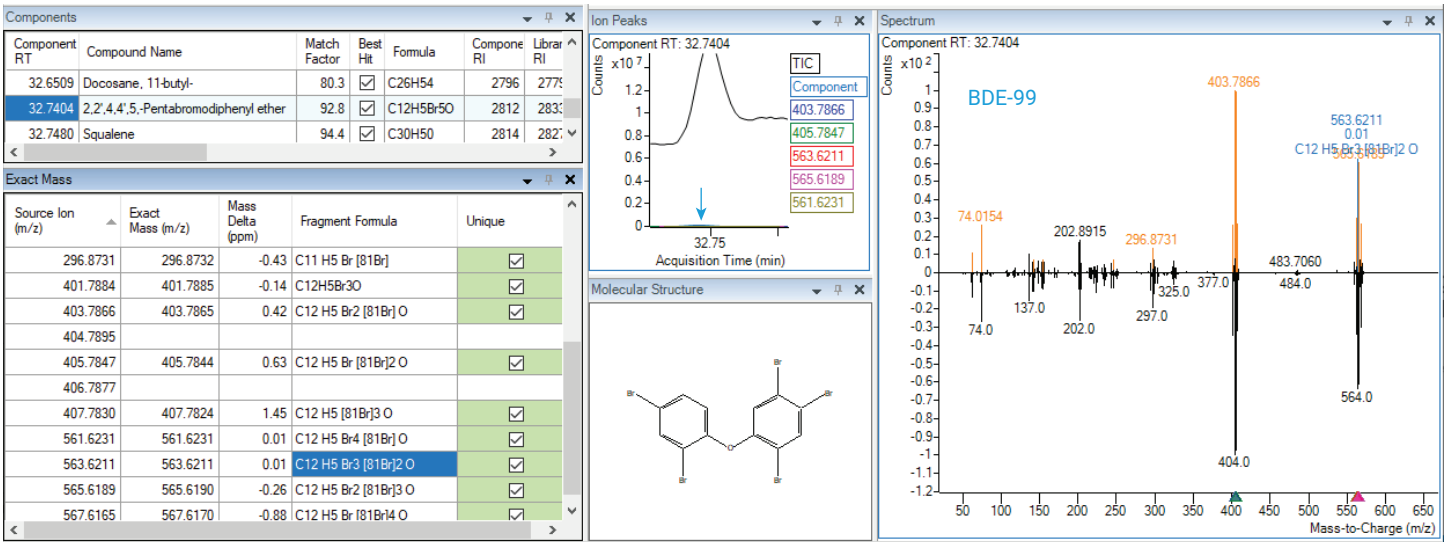
Note that PCBs and PBDEs were not detected by SPME due to their high boiling point.

Another prominent group of contaminants identified in soil extracts was pesticides, and the GC/Q-TOF Screener workflow with Pesticide PCDL was used for quick and streamlined detection of these pollutants. The original version of the Pesticide PCDL, which is RT-based, was supplemented with RIs to be able to use the PCDL in the screener workflow together with the data acquired using a different chromatographic method. The GC/Q-TOF Screener method was set up in agreement with the SANTE guidelines. However, RT windows were expanded to allow for an additional RT error introduced using a different chromatographic method.

Table 4. PFAS detected in soil and plants by HS-SPME using the accurate mass PFAS PCDL and suspect screening approach. The estimated amounts (in pg on column) are shown.

Compound	RT	Quantifier Ion	Soil Samples							Plant Samples				
			F1 PreA	F1 Hvst	F2 Hvst	C&L Hvst	Compost Hvst	Organic Hvst	Organic Compost	F1	F2	Compost	C&L	Org
Ethyl Perfluorobutyl Ether	4.4	218.9851	150.2	–	–	–	–	–	–	–	–	–	–	–
6:1 Fluorotelomer Alcohol	20.94	130.9915	–	2	–	–	–	–	–	2.2	–	–	–	–
6:2 Fluorotelomer Alcohol	23.59	296.0054	–	7.5	0.3	–	–	–	6.9	2.5	–	–	–	–
N-Methylperfluorooctanesulfonamide	43.1	93.9957	0.3	3.4	0.9	2.1	0.4	1.2	0.9	0.2	–	–	–	–

A **Sample: soil, F1**



B

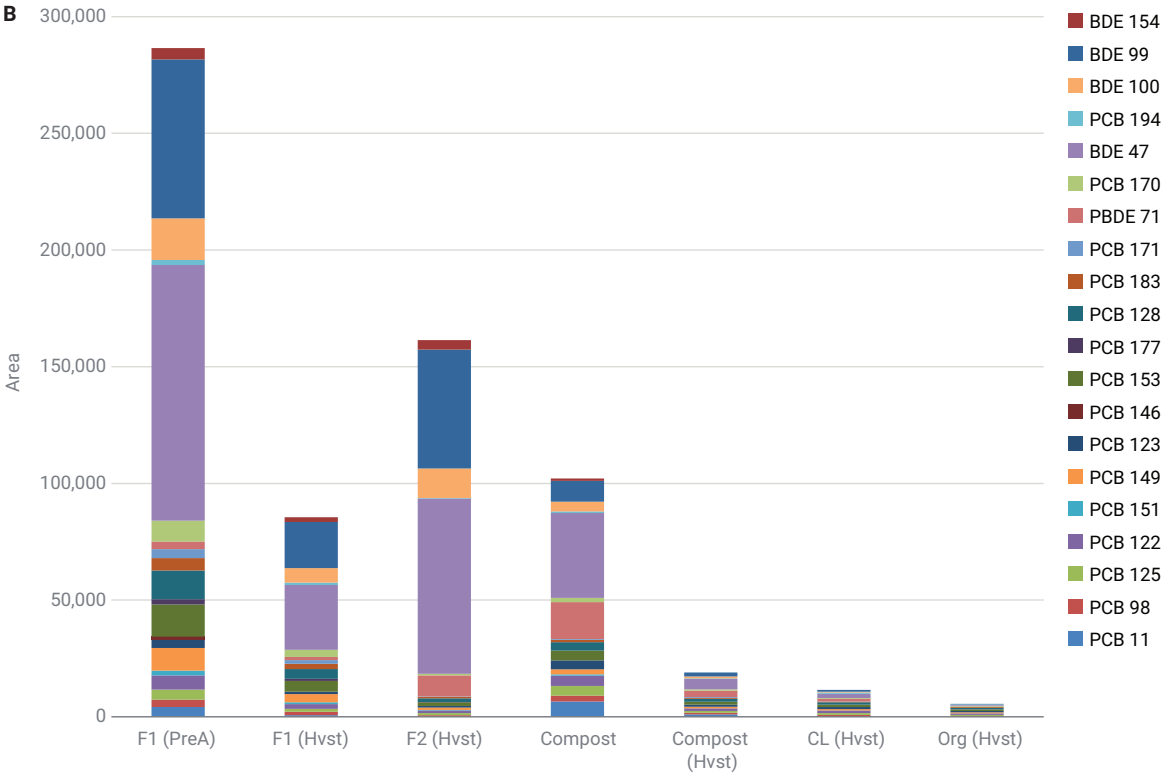


Figure 4. PCBs and PBDEs in soil DCM extracts using NIST23. (A) An example of BDE detected in soil sample collected from F1 at the time of harvesting. ExactMass table (bottom-left panel) shows how well the accurate mass fragment ions matched the unit mass library hit and thus provides the additional confirmation of compound ID. The most selective and abundant ions are highlighted in the mirror plot when *m/z* corresponds to the library hit formula. The arrow in the component chromatogram points to the identified component EICs. (B) Bar graph showing responses of PCB and PBDE for all the soil samples where they have been identified.

Since the DCM extraction method was not optimized specifically for pesticide recovery from plant matrices, only soil samples were processed. In total, over 50 pesticides were detected in soil extracts (Figure 5 and Table 5).

A large number of pesticides were detected in compost and compost-treated soils, and a few pesticides were also identified in organic soil extracts. Another interesting observation was that the insecticides fipronil sulfide and fipronil sulfone were consistently found in the same soil samples. Also, conazole fungicides such as propiconazoles, myclobutanil and difenconazole were mostly detected in compost and compost-treated soils.

Sample: soil, F1

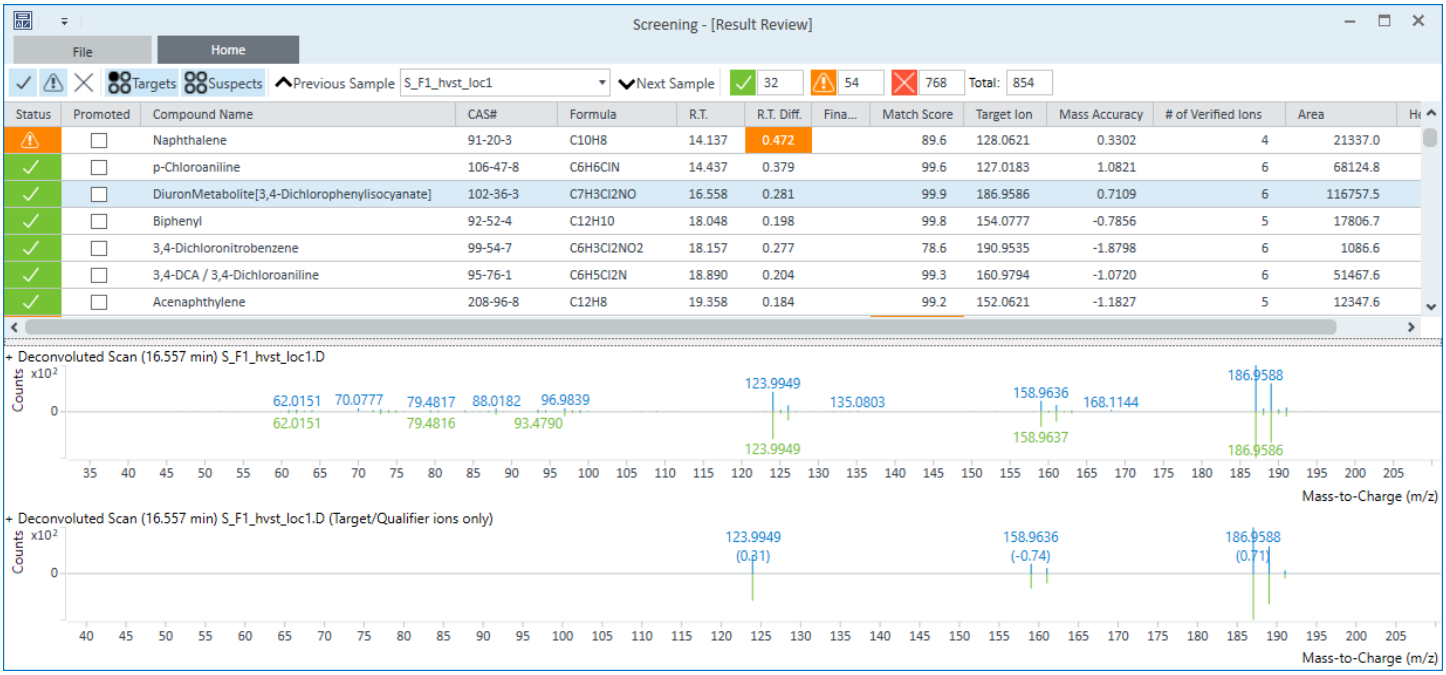


Figure 5. GC/Q-TOF Screener window of MassHunter Quantitative Analysis software when screening for pesticides in soil extracts using the Pesticides PCDL.

Table 5. Pesticides detected in soil extract using the accurate mass Pesticide PCDL and suspect screening approach.

Compound Name	RT	RT Delta*	Library Match Score	F1 PreA	F1 Hvst	F2 Hvst	C&L Hvst	Compost Hvst	Org Hvst	Org Compost
1,2,4-Trichlorobenzene	14.62	0.17	98.1	x						
Diuron Metabolite	16.56	0.28	99.9	x	x	x	x	x		x
1,2,3,5-Tetrachlorobenzene	16.98	0.32	90.7	x						
2,4,6-TCP/2,4,6-Trichlorophenol	17.44	0.25	99.3				x	x	x	Trace
Nicotine	17.56	0.05	97.9							x
Lufenuron	18.71	0.22	99.7			x				x
3,4-DCA/3,4-Dichloroaniline	18.88	0.21	99.9	x	x	x				
Pentachlorobenzene	20.42	0.35	99.4	x	x					x
DEET/Diethyltoluamide	21.46	0.22	82.1	Trace	Trace	Trace	x	x	Trace	x
2,3,4,5-Tetrachloroanisole	22.74	0.32	99.8	x						x
Bromoxynil	23.14	0.09	99.9	Trace			x	x		
HCB/Hexachlorobenzene	23.52	0.36	99.7	x	x	x	Trace	x	x	x
Dichloran (Dicloran)	23.84	0.16	97.8		x	x				x
Swep (MCC)	24.27	0.10	85.6	x	x	x				
PCP/Pentachlorophenol	24.27	0.24	99.7				Trace	x		x

Compound Name	RT	RT Delta*	Library Match Score	F1 PreA	F1 Hvst	F2 Hvst	C&L Hvst	Compost Hvst	Org Hvst	Org Compost
Pyrimethanil	25	0.10	82.5					Trace		x
Chlordene	25.1	0.03	98.5							x
Pentachloroaniline	25.74	0.24	99.7	x	x		x	x		x
Dithiopyr	26.85	0.40	93.7	x	x	x	x	x		x
Anthraquinone	27.59	0.05	99.7	x	x	x	x	x	x	x
4,4'-Dichlorobenzophenone	27.86	0.02	80.3	x						x
Fipronil Sulfide	28.13	0.43	99.7			x	Trace	x		x
Cyprodinil	28.27	0.05	99.1				Trace	x		x
Diuron	28.28	0.31	78.1				Trace	x		Trace
Fluopyram	28.49	0.18	93				x	x		x
Chlorbenside	28.99	0.21	92.2	x	x	x				
Chlordane-*trans* (γ-Chlordan)	28.82	0.03	99.7	x	x	x	x	x	x	x
Triclosan	28.85	0.03	99.3	x	x	x		x		x
Chlordane-*cis* (α-Chlordan)	29.06	0.04	99.9	x	x	x	x	x	x	x
Nonachlor-*trans*	29.11	0.07	99.9	x	x	x	x	x	x	x
Flutolanil	29.23	0.11	85.2					x		x
Fludioxonil	29.27	0.18	99.6							x
Dieldrin	29.5	0.05	84.6	x	Trace	Trace				
p,p'-DDE	29.42	0.04	99.2	x	x	x	x	x	x	x
Oxadiazon	29.43	0.14	97.7				x	x		x
o,p'-DDD (Mitotane)	29.52	0.07	99.9	x	x	x	Trace	x	x	
Fipronil Sulfone	29.34	0.33	98.6	Trace		x	Trace	x		x
Myclobutanil	29.48	0.11	98.8					x		x
p,p'-DDD	30.03	0.02	99.5	x	x	x	x	x	x	Trace
Nonachlor-*cis*	30.03	0.04	99.9	x	x	x	Trace	Trace		x
Carfentrazone-ethyl	30.32	0.13	98.8			x				
Bromoxynil octanoate	30.39	0.06	88.4	x			x	Trace		
Propiconazole I	30.43	0.11	96.4				x	x	Trace	x
Chloridazon (PAC)	30.44	0.06	91.5					x		
Propiconazole II	30.5	0.04	96				x	x	Trace	x
Tebuconazole	30.7	0.03	92.7				x	x		x
Chlorbenside Sulfone	30.7	0.39	89.6		Trace	Trace	x	x		x
Bifenthrin	31.08	0.09	98.6	Trace	x	Trace	x	x	x	x
cis-Permethrin	32.19	0.00	99.1	x	x	x	Trace	x	x	x
trans-Permethrin	32.28	0.01	81			x			Trace	Trace
Difenconazole II	34.09	0.01	88.9					Trace		x

* RT delta is recalculated from RI.
Trace indicates that the Library Match Factor is below 75.

PAHs are included into the Pesticide PCDL and were screened together with pesticides in a single workflow. PAHs were mostly detected in soil extracts. However, phenanthrene and fluoranthene were also identified in most plant samples. This was not unexpected considering that phenanthrene and fluoranthene were the most abundant PAHs detected in the soil.

A prominent group of contaminants identified in soil and oat plants was flame retardants. The accurate mass spectra for most of these compounds are already included in the Pesticide PCDL. For a more comprehensive coverage of this group of pollutants, a couple of flame retardants identified in the Unknowns Analysis with NIST23 library, missing in the Pesticide PCDL, were added to the Quant method directly from the Unknowns Analysis software, and thus were screened together with the rest of the targets. Remarkably similar responses were observed between soil and plant extracts for this group of pollutants (Figure 7).

Among the most abundant flame retardants identified in soil and plant samples were tributyl phosphate, tris(2-chloropropyl) phosphate, and tris(3-chloropropyl) phosphate, the phosphorus flame retardants of frequent use.

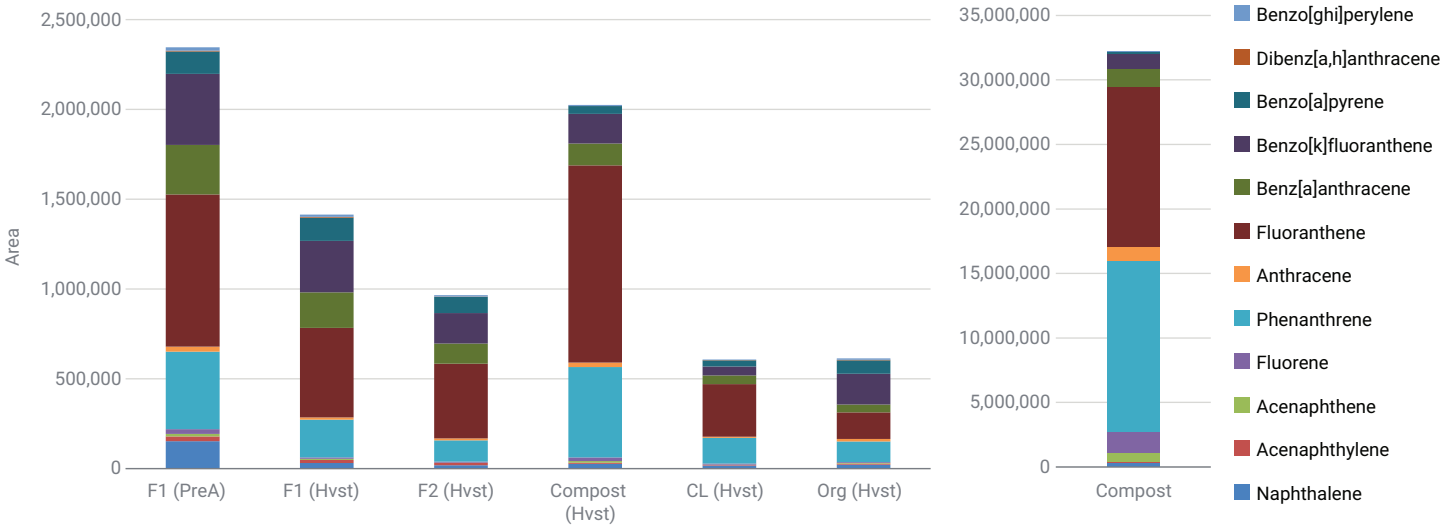


Figure 6. PAHs detected in soil DCM extracts using the accurate mass Pesticide PCDL and suspect screening approach. The bar graph shows the PAH peak area.

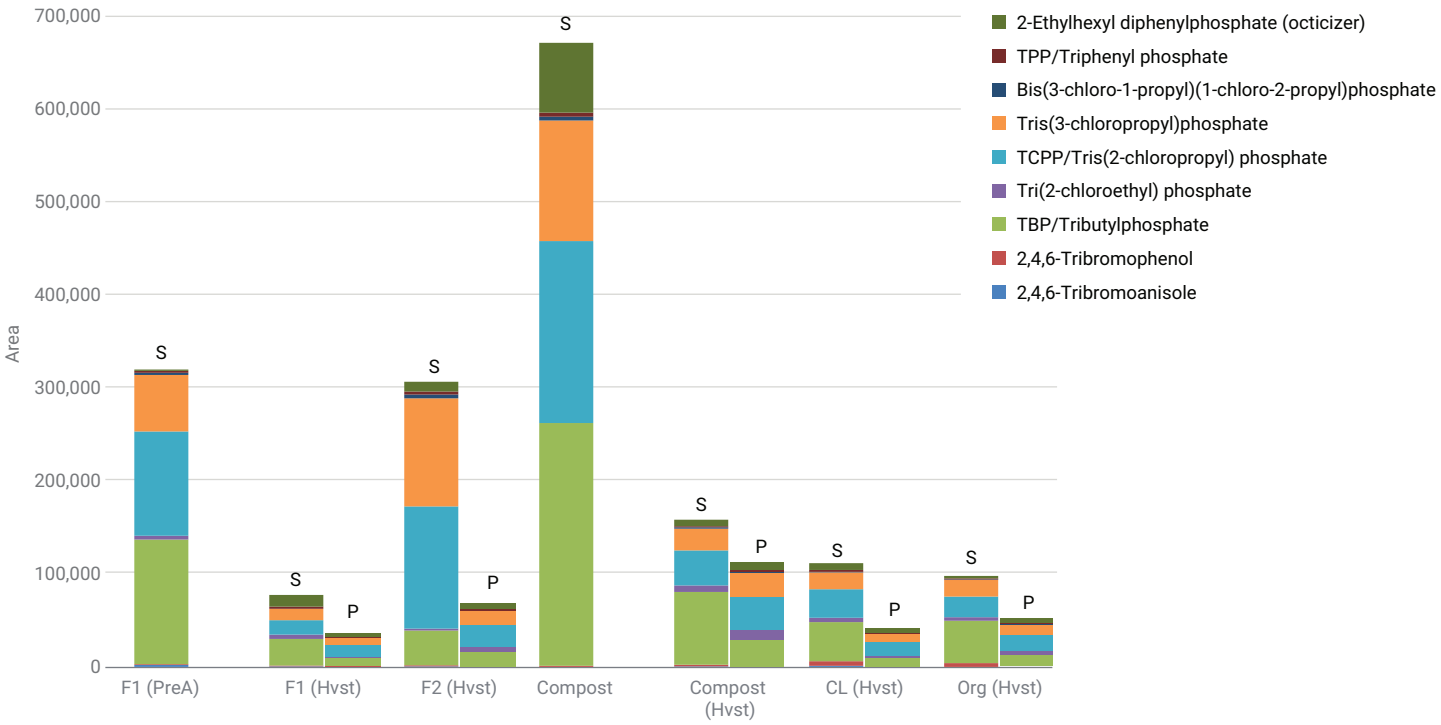


Figure 7. Flame retardants detected in soil and plant DCM extracts using a combined screening approach that included both accurate mass PCDL as well as NIST23 library. The bar graph shows flame retardant response in soil (S) and plant (P) extracts.

Conclusion

PFAS analysis in environmental matrices is a challenging undertaking. In this application note, different approaches for PFAS extraction from soil and plants as well as downstream workflows of data processing have been discussed. The most efficient and sensitive approach for volatile PFAS analysis in soil and plants suggested here is HS-SPME combined with the suspect screening based on the PFAS accurate mass library and high-resolution accurate mass GC/Q-TOF.

In addition, both soil and plant extracts were screened for other contaminants, and various pollutants including PCBs, PBDEs, PAHs, pesticides, and flame retardants were identified using targeted, nontargeted, and combined methodologies.

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