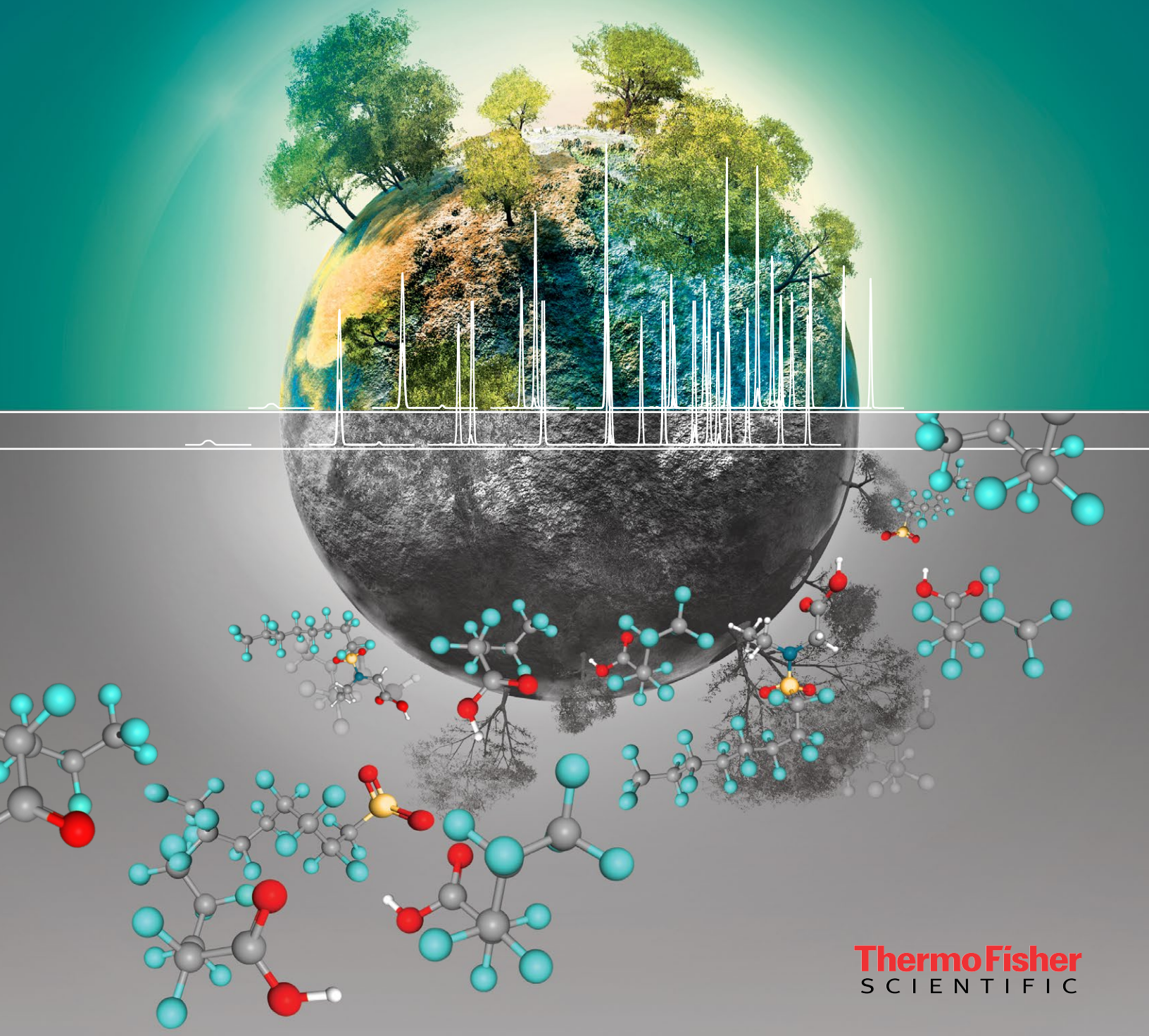
thermo scientific

Setting a new horizon

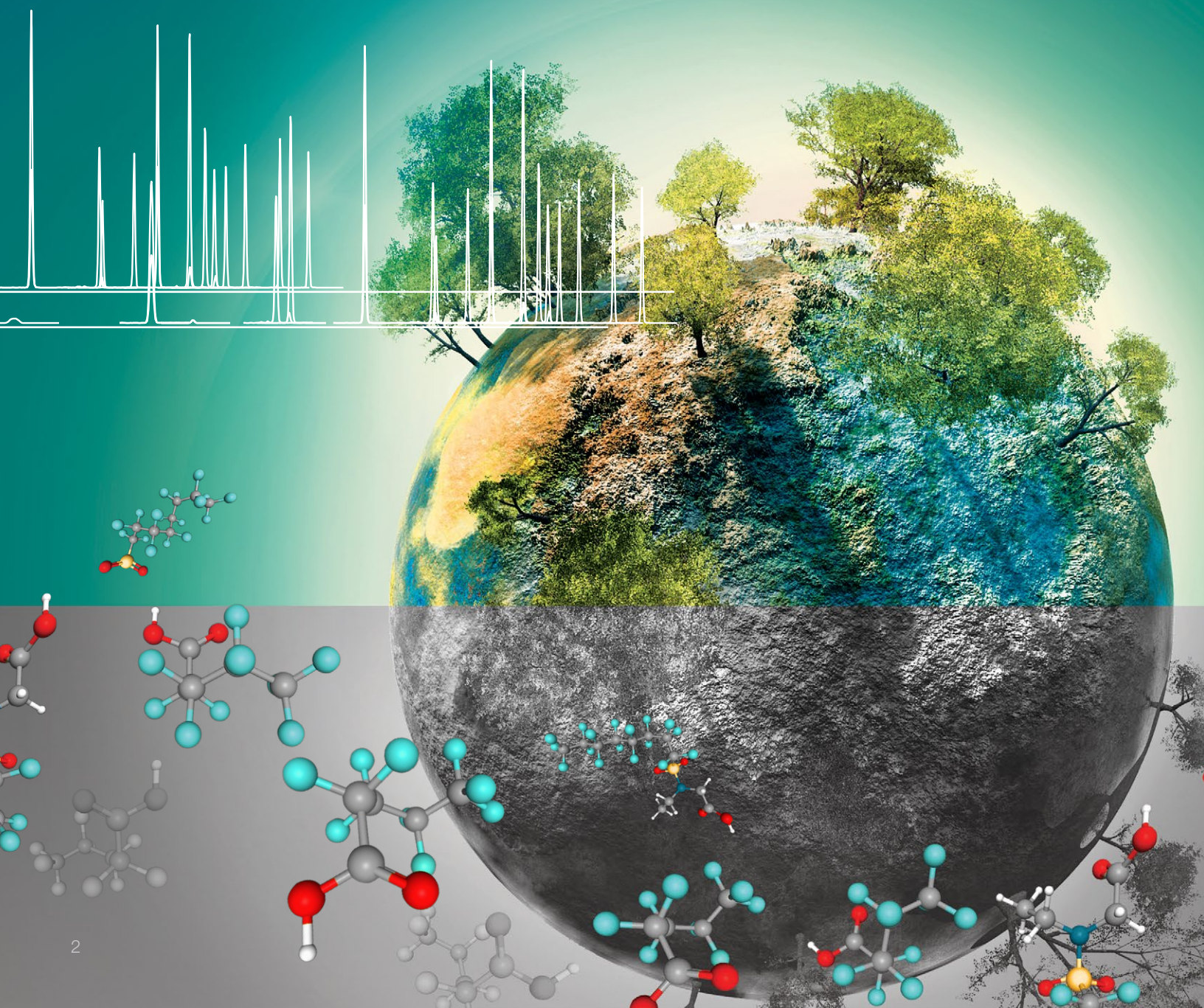
for PFAS workflow applications

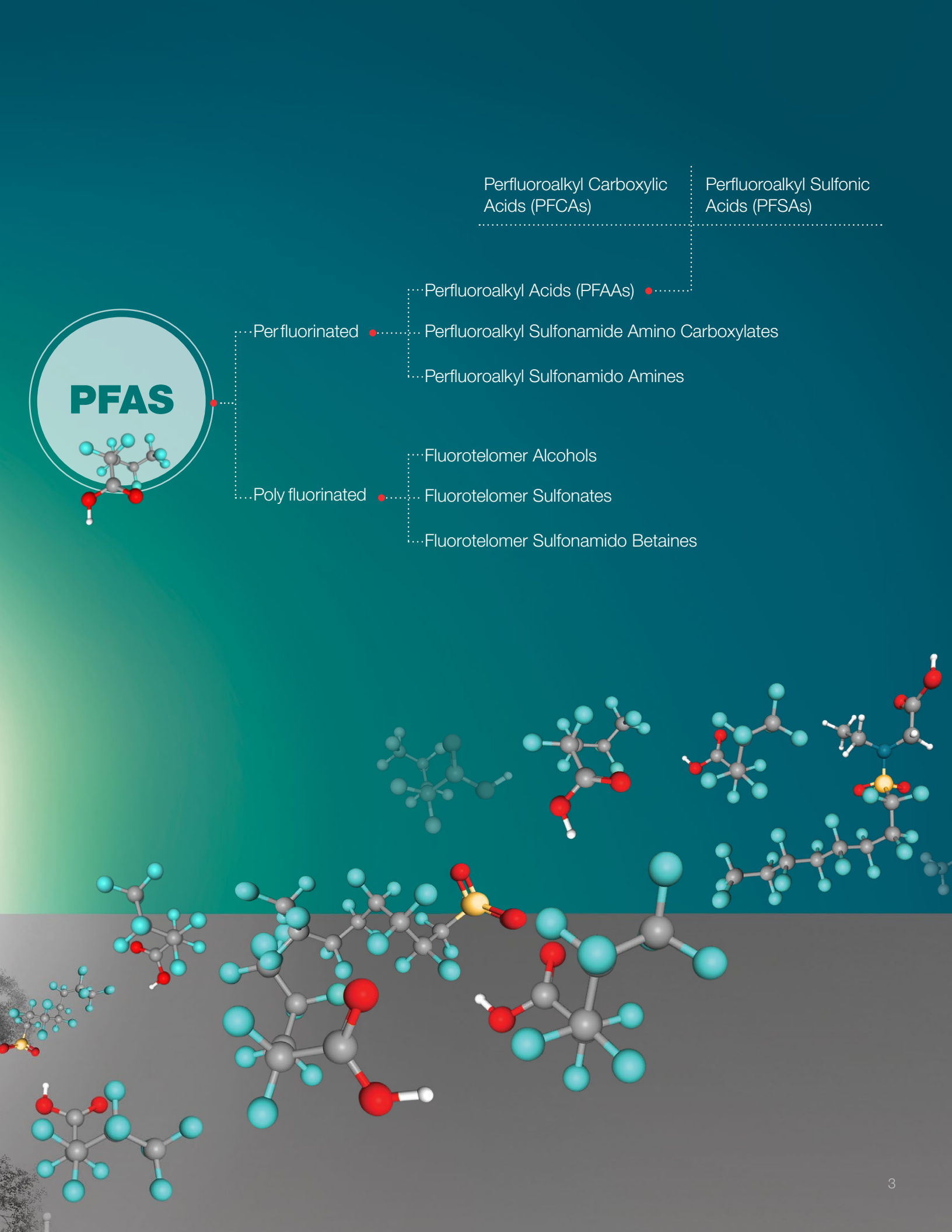


ThermoFisher SCIENTIFIC

PFAS, a global concern

Per- and polyfluoroalkyl substances (PFAS) are among the primary emerging contaminants of concern. The detection and quantification of known PFAS and the discovery of unknown PFAS substances has never been more important. Determining the best workflow for your PFAS analysis can be challenging. Optimal methods will vary depending on the matrix you are working with and goals of your analysis. There are strategies to help you with either targeted analysis of known PFAS compounds or the discovery of unknowns, from a variety of matrices.

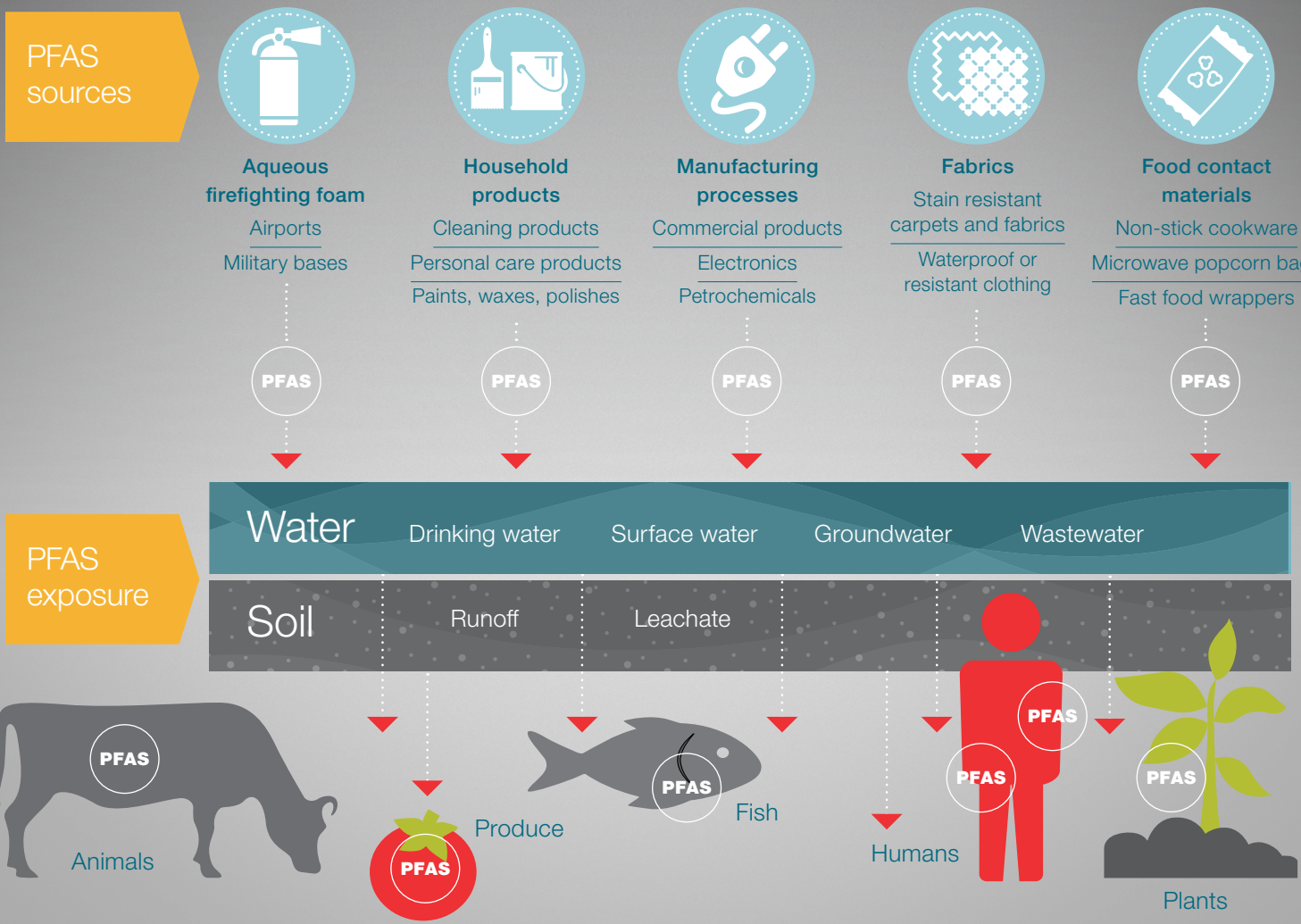



Perfluoroalkyl Carboxylic Acids (PFCAs)
Perfluoroalkyl Sulfonic Acids (PFSAs)
Perfluoroalkyl Acids (PFAAs)
Perfluorinated
Perfluoroalkyl Sulfonamide Amino Carboxylates
Perfluoroalkyl Sulfonamido Amines
PFAS
Fluorotelomer Alcohols
Poly fluorinated
Fluorotelomer Sulfonates
Fluorotelomer Sulfonamido Betaines

PFAS transport through the environment and analysis strategies

The vast uses of PFAS compounds has resulted in a great number of sources for these substances to enter the environment. Common modes of transport are runoff, especially with firefighting foams into water, or leachate from landfills, discharge from manufacturing processes or improper disposal. Once in the ecosystem, plants, animals and humans are all exposed to PFAS. The C-F bonds in the PFAS molecule are very strong, which make metabolism of these compounds very difficult. Therefore, PFAS bioaccumulates over time and causes various health concerns.

The workflow for analyzing PFAS will depend on the goals of your analysis. Many labs are doing targeted analysis where a specific list of PFAS molecules are analyzed and quantified. It is estimated there are over 5000 different types of PFAS compounds; some labs will want to discover and identify unknown PFAS through untargeted screening.



Workflow strategies

Sample collection → Sample preparation → Analysis → Data processing

Targeted analysis

- Identification and quantitation based on a known candidate list of compounds
- Established or regulated methods available
- Confirms presence of a compound based on limit of detection

Unknown screening

- Discover new or unexpected compounds
- Detection is independent of a candidate list
- Find new compounds of interest in previously run samples by retrospective data analysis

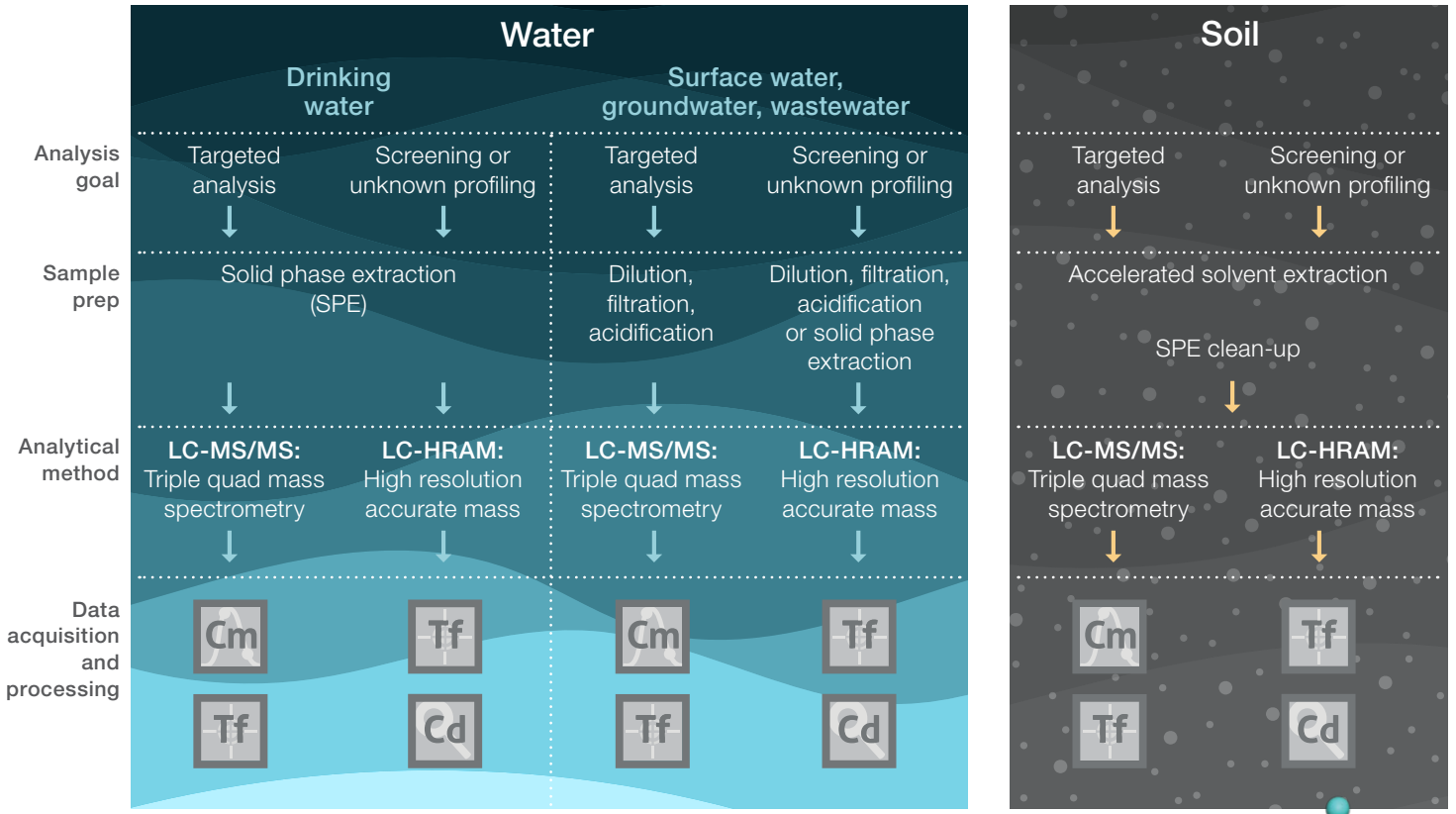
PFAS sampling

Careful sampling is important in PFAS analysis. A representative sample must be obtained without introducing any background PFAS into the sample. PFAS can be found in many sources while sampling and in the laboratory. Items to avoid when sampling are waterproof clothing, adhesives, sampling device and materials coming into contact with vehicle upholstery, and common blue ice packs used in shipping. In the lab, avoid items such as aluminum foil, sticky notes and some materials used in the flow path of analytical instruments. It is important to use instruments with minimal fluoropolymers. Polypropylene sampling vessels must be used for water and soil samples as well as the devices used to collect the sample.

PFAS workflow

PFAS workflows will be different based on the matrix you are working with and the goals of your analysis, either targeted analysis or unknown screening. Each matrix uses a different sample preparation method. For water, solid phase extraction (SPE) will be used for drinking water while other water types will use dilution, filtration and/or acidification. For soils, accelerated solvent extraction (ASE) is the optimal method. All the PFAS workflows use liquid chromatography (LC) for separation, but the best mass spectrometer is determined by the analysis type, targeted or unknown screening.

The data processing software will depend on the type of workflow. Both Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software or Thermo Scientific™ TraceFinder™ software are designed for targeted analysis and quantification. Thermo Scientific™ Compound Discoverer™ software streamlines compound identification and structural elucidation.



Everyday PFAS analysis in drinking water

Established methods:
U.S. EPA 537.1
U.S. EPA 533

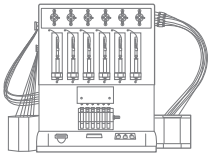
SPE sample preparation to mass spectrometry analysis

Thermo Fisher Scientific can supply and support everything you need to detect and quantify PFAS in drinking water. Many established methods, including regulatory, require collection into polypropylene bottles, followed by sample preparation by SPE and analysis using triple quad mass spectrometry.

Thermo Scientific™ Dionex™ AutoTrace™ 280 PFAS solid-phase extraction instrument

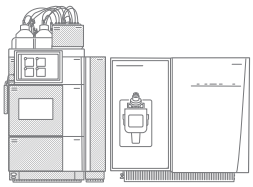
- Improves recovery and reproducibility
- Significantly reduces risk of background PFAS
- Improves lab efficiency

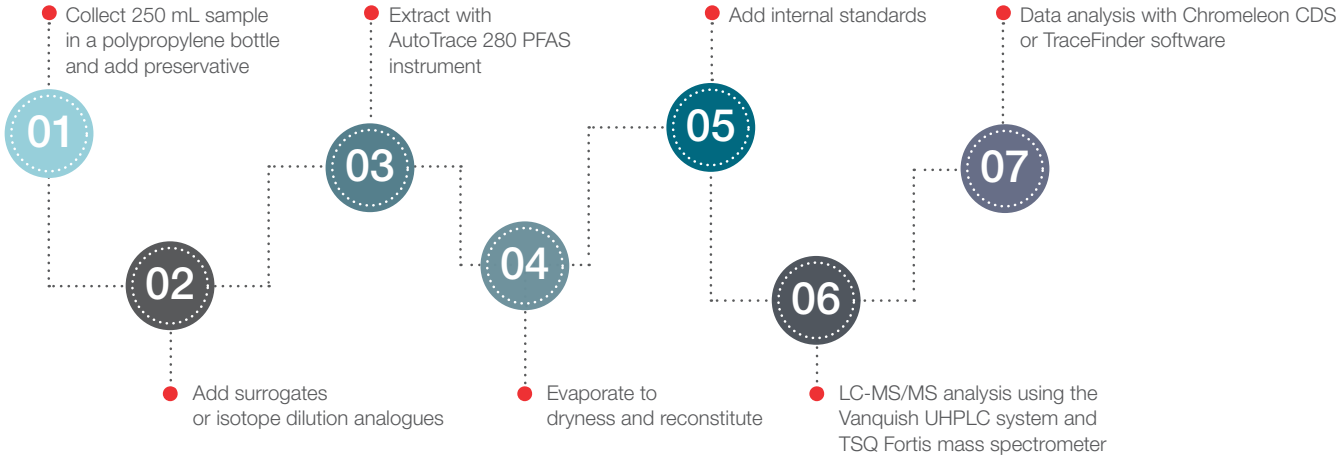
The AutoTrace 280 PFAS system ensures inertness and prevents PFAS contamination into samples during extraction, while at the same time delivering consistent and reliable performance.



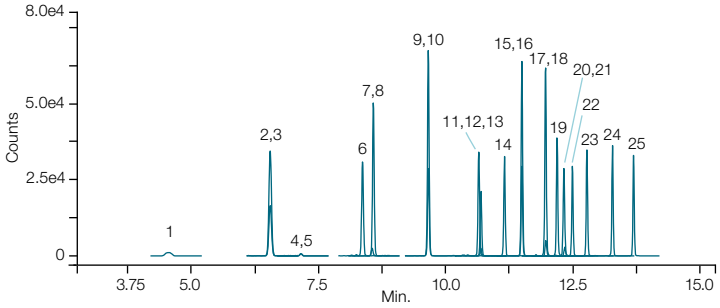
Thermo Scientific™ TSQ™ Fortis triple quadrupole mass spectrometer with the Thermo Scientific™ Vanquish™ UHPLC system fitted with the PFC free kit

- Excellent quantitative performance at low dwell times
- Enhanced confidence in data and outstanding robustness that prolongs instrument uptime
- Simplicity and ease-of-use for users of all expertise levels





General targeted PFAS analysis workflow in drinking water samples based on either US EPA Method 537.1 or US EPA Method 533.



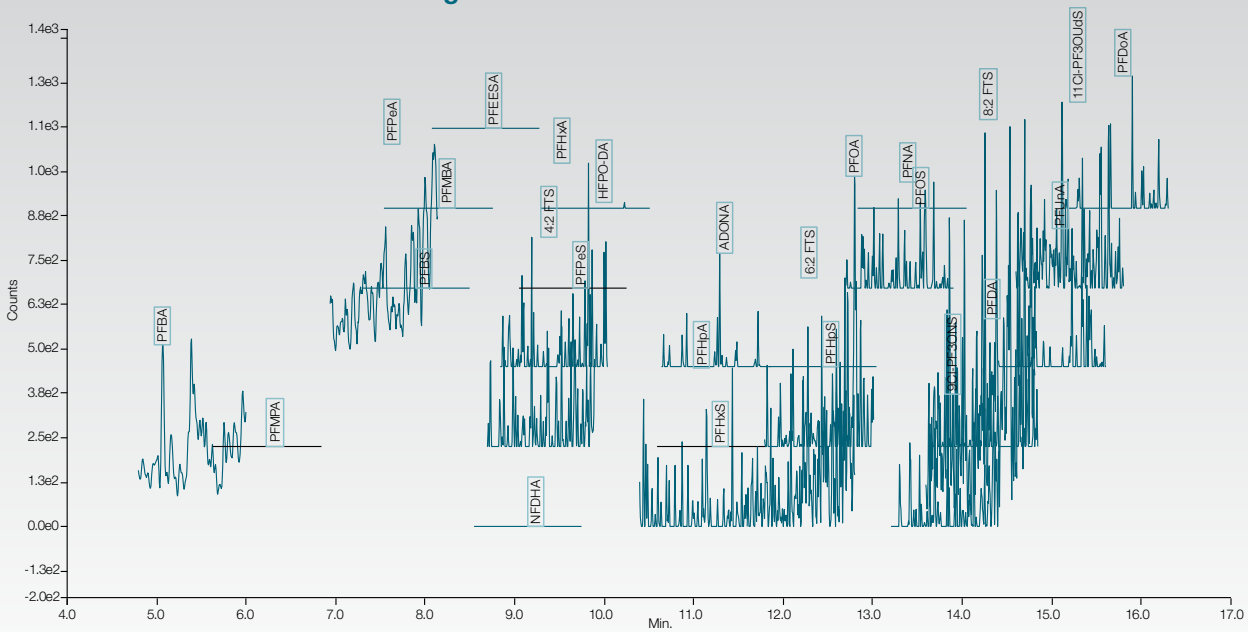
Excellent separation of all 18 PFAS compounds and isotropically labeled standards in under 15 minutes.

Peak number	Analyte	Fortified conc. (ng/L)	Mean recovery (%)	RSD	Fortified conc. (ng/L)	Mean recovery (%)	RSD
1	PFBS	16.0	107	3.3	80.0	98.3	3.6
2,3*	PFHxA	16.0	108	2.3	80.0	106	2.6
4,5*	HFPO-DA	16.0	84.1	7.5	80.0	88.6	6.3
6	PFHpA	16.0	113	2.7	80.0	117	1.3
7	PFHxS	16.0	120	3.4	80.0	123	2.1
8	ADONA	16.0	117	2.5	80.0	121	1.1
9,10*	PFOA	16.0	113	2.5	80.0	119	1.6
11	PFNA	16.0	114	2.9	80.0	118	2.1
12,13*	PFOS	16.0	113	4.5	80.0	117	2.9
14	9Cl-PF3ONS	16.0	96.1	4.1	80.0	103	2.6
15*,16	PFDA	16.0	105	3.2	80.0	111	2.1
17*,18	NMeFOSAA	16.0	103	5.2	80.0	110	5.2
19	PFUnA	16.0	96.8	5.0	80.0	103	3.1
20*21	NEtFOSAA	16.0	100	9.9	80.0	104	2.3
22	11Cl-PF3OUdS	16.0	88.5	5.5	80.0	97.1	4.8
23	PFDoA	16.0	89.8	4.4	80.0	97.3	3.4
24	PFTrA	16.0	89.6	3.8	80.0	95.8	3.7
25	PFTA	16.0	89.0	4.8	80.0	98.1	3.3

* Designates the isotope labeled internal standard or surrogate.

All 18 target compounds spiked at 2 levels, show recoveries well within the method limits of 70–130% and reproducibility is under the required 20%.

PFAS blank LC-MS/MS chromatograms



Preparing PFAS water samples with the AutoTrace 280 PFAS shows negligible background.

Direct inject targeted PFAS methods

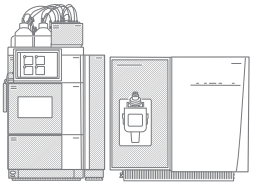
PFAS

Established methods:
U.S. EPA 8327
ASTM D7979

These alternative methods are sometimes preferred for groundwater, surface water and especially for wastewater. Direct injection methods, like U.S. EPA 8327 or ASTM D7979 are based on sample dilution, filtration and acidification followed by LC-MS/MS analysis. This direct analysis method is for 24 diverse types of PFAS compounds in a wide variety of non-drinking water matrices.

Thermo Scientific™ TSQ™ Altis triple quadrupole mass spectrometer with the Vanquish UHPLC system fitted with the PFC free kit

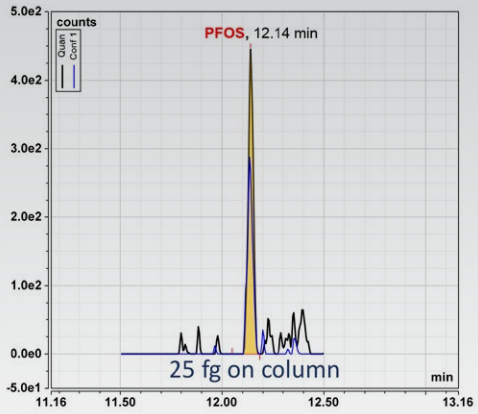
- Ultimate sensitivity in matrices ranging from simple to complex
- Outstanding instrument robustness enables increased confidence with no loss of instrument uptime
- Ultrafast selected reaction monitoring (SRM) increases the number of molecular quantifications in less time



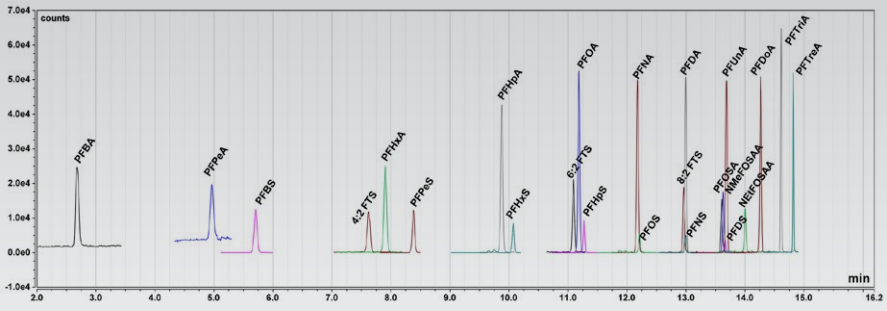
Compound	Recoveries %							
	Reagent water		Ground water		Surface water		Waste water	
	Low level	High level	Low level	High level	Low level	High level	Low level	High level
PFBA	77%	78%	71%	75%	74%	74%	58%	75%
PFPeA	84%	80%	104%	80%	115%	81%	88%	78%
PFBS	87%	81%	95%	81%	95%	79%	72%	77%
PFHxA	82%	81%	83%	79%	86%	80%	77%	74%
4:2 FTS	81%	82%	90%	78%	87%	79%	76%	91%
PFPeS	80%	80%	82%	79%	85%	78%	80%	83%
PFHpA	84%	81%	88%	80%	89%	80%	74%	81%
PFHxS	81%	81%	87%	78%	94%	81%	85%	85%
6:2 FTS	84%	82%	85%	80%	87%	94%	78%	79%
PFOA	83%	80%	88%	82%	123%	83%	83%	86%
PFHpS	81%	81%	84%	76%	83%	78%	79%	86%
PFNA	79%	81%	84%	80%	86%	80%	79%	82%
PFOS	91%	82%	91%	78%	93%	81%	79%	90%
8:2 FTS	85%	80%	81%	75%	76%	79%	78%	83%
PFNS	85%	75%	89%	79%	81%	76%	72%	78%
PFDA	80%	81%	86%	78%	85%	79%	74%	83%
NMeFOSAA	77%	81%	80%	77%	86%	81%	82%	84%
PFOSA	76%	76%	87%	75%	91%	75%	79%	81%
PFDS	82%	78%	89%	77%	85%	79%	72%	81%
PFUnA	76%	76%	80%	81%	75%	78%	75%	83%
NEtFOSAA	82%	79%	89%	77%	89%	81%	80%	85%
PFDoA	79%	82%	83%	78%	85%	82%	79%	85%
PFTriA	87%	86%	89%	79%	92%	91%	87%	89%
PFTreA	109%	103%	112%	91%	113%	119%	100%	110%

Most recoveries in different water matrices at 60 and 200 ng/L are within the 70% to 130% range.

Excellent quantitative results for PFAS direct analysis in the low ng/L range in non-drinking water matrices using dilution and filtration for sample preparation.



PFOS chromatogram of an injection of 1 ng/L, which is five times lower than the reporting limit of quantitation.



Overlaid chromatograms of all PFAS compounds included in this method.

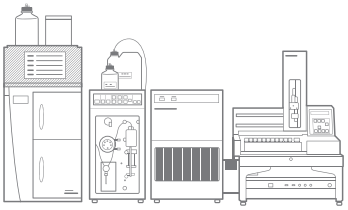
AOF by combustion ion chromatography

Could other PFAS molecules be present?

Automated combustion ion chromatography (CIC) provides a complimentary screening method indicate the possible presence of non-targeted PFAS or other fluorine containing compounds.

Thermo Scientific™ combustion ion chromatography system

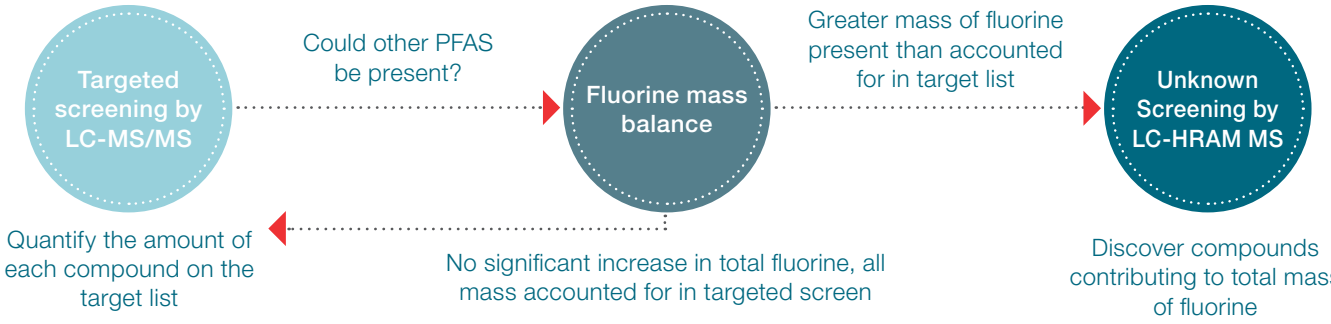
- Eliminates complex sample preparation steps using an automated method
- Produces fewer environmental contaminants
- Highly sensitive
- Easy-to-use and saves time



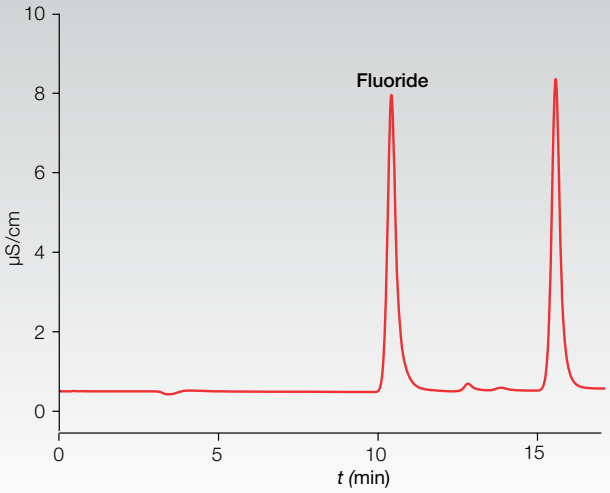
Adsorbable organic fluorine (AOF) by combustion ion chromatography

Analyzing for adsorbable organically-bound fluorine is used to determine if the mass of fluorine present in the sample exceeds that in the targeted screen. If the total amount is higher, then other PFAS may be present in the sample which were not on the target list.

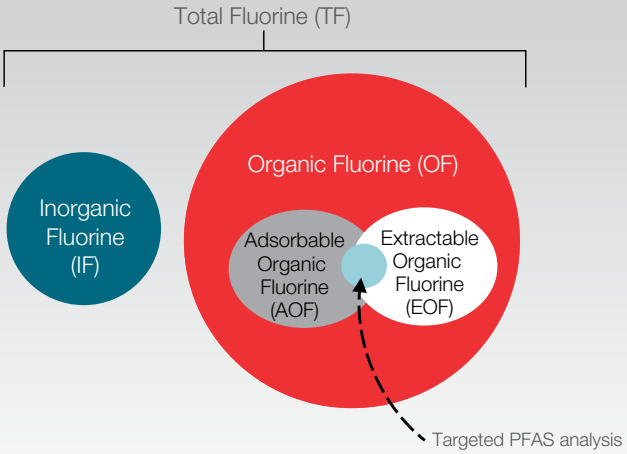
The use of this technique is well documented for the determination of other adsorbable organic halogen-containing components (AOX).



AOF-CIC provides an easy-to-use and economical way to determine if other PFAS molecules might be present in your sample. This technique can help to optimize the utilization of analytical instrumentation by selecting and only analyzing "suspicious" samples.



CIC chromatogram of industrial wastewater, diluted 1:10.



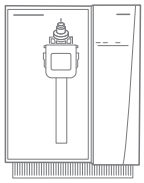
Total fluorine consists of both inorganic and organic components. The organic part contains compounds that are adsorbable (AOF) and extractable (EOF), both of which have a subset of analytes that are typically targeted by LC-MS/MS analysis. There are also organic compounds that are not captured be either of these approaches.

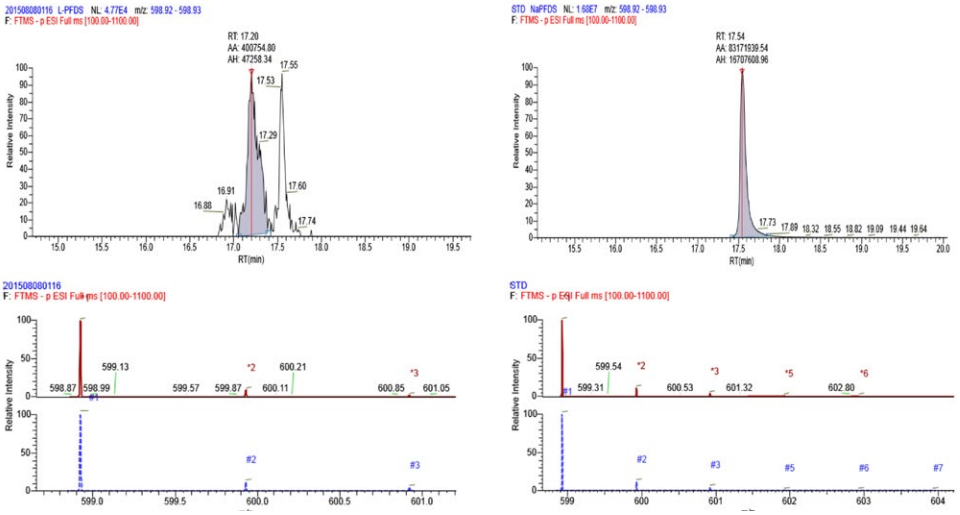
Screening for unknown PFAS

PFAS compounds can be detected and quantitated by using a triple quadrupole mass spectrometer (MS) in targeted analysis. However, the identification and quantitation of unknown PFAS uses LC coupled to high resolution mass spectrometry (HRAM MS). With significant advances in HRAM MS comes can this move to the first column to not only increase the range of potential targets monitored, but to also increase confidence in assignments, access the power of comprehensive tools to identify unknowns and emerging contaminants, and retrospectively analyze data even when the sample no longer exists.

Thermo Scientific™ Orbitrap Exploris™ 120 mass spectrometer

- Ultra high-resolution capability
- Removes concerns over false positives/negatives
- Eliminates matrix interferences
- High mass accuracy to generate reliable results
- Significantly accelerates the path to confident results for both expert and novice MS users





A UCMR3 sample shown having trace hits for a non-targeted compound (PFDS). Post-run identification was performed by looking at the isotopic pattern recognition, accurate mass and retention time for confirmation. Note the real-world water sample chromatogram on the left shows the linear (RT 17.5) and branched isomers (RT 17.2) of PFDS, vs the linear PFDS isomer standard on the right.

Routine quantitative workflows and non-targeted analysis can be performed in a single analysis.

U.S. EPA Method 537 target list

PFAS compound	Critical Level (ng/L)	DL (ng/L)	LCMRL (ng/L)
PFBS	0.15	0.2	<0.5
PFDA	0.15	0.26	<0.5
PFDoA		0.47	0.73
PFHpA	0.09	0.15	<0.5
PFHxA	0.13	0.19	<0.5
PFHxS		1.7	2.4
PFNA	0.11	0.17	<0.5
PFOA		0.22	0.5
PFOS		0.26	0.5
PFTA	0.15	0.2	<0.5
PFTrDA		0.31	0.55
PFuNA		0.38	1

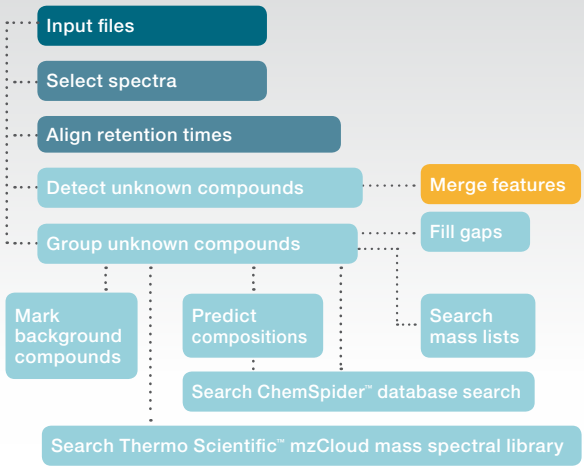
U.S. EPA Method 537 target list

PFAS compound	Critical Level (ng/L)	DL (ng/L)	LCMRL (ng/L)
PFBA		0.19	0.64
PFODA		0.55	1
PFDS	0.13	0.19	<0.5
PFHxDA		0.12	0.5
PFPA	0.18	0.19	<0.5

Using a full scan approach, required detection limits or MRLs can be achieved while interrogating for other untargeted PFAS compounds.

The compounds highlighted in blue are additional analytes that are not part of the original U.S. EPA Method 537 list but were found in processed drinking water from the same UCMR3 water extracts.

For complex samples with unknown amounts of other PFASs, utilization of Compound Discoverer software can reduce the data processing time and quickly show results.

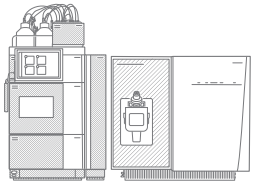


Workflow example in Compound Discoverer software. Flow-chart style elements can be easily dragged and dropped into place for easy customization.

PFAS extraction and analysis in soil

The need to analyze PFAS in soil samples is also extremely important. Soil becomes contaminated with PFAS through runoff and leachate from landfills and other sources. Any produce or vegetation growing in this soil is at risk for accumulating PFAS.

Thermo Scientific™ TSQ Quantis™ triple quadrupole mass spectrometer with the Vanquish UHPLC system fitted with the PFC free kit



- Superb sensitivity, even in complex matrices
- Outstanding robustness; prolonging instrument uptime
- Reliability and reproducibility improve data quality for every run and every sample
- Simplicity and ease-of-use allow users of all expertise levels to acquire high quality data with improved confidence in results

Thermo Scientific™ Dionex™ ASE™ 350 accelerated solvent extractor

- Automates extraction for up to 24 samples
- Saves solvent—Just 50 mL used for PFAS
- Saves time—Only 7 minutes per PFAS extraction

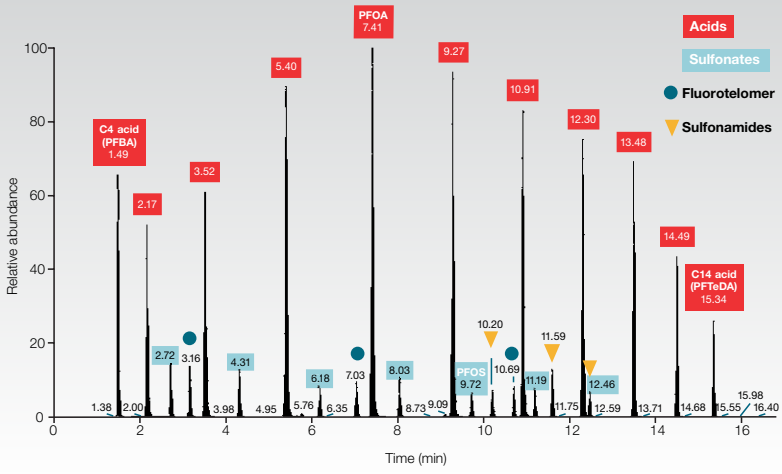
01 2 g of soil extracted using the ASE 350 accelerated solvent extractor

02 SPE clean up of the extract using a styrene divinylbenzene (SDVB)

03 LC-MS/MS analysis using the Vanquish UHPLC system and TSQ Quantis mass spectrometer

04 Data analysis with Chromeleon CDS and TraceFinder software

Accelerated solvent extraction is an effective method for extracting a wide selection of PFAS, from 4-carbon to 14-carbon fluoroalkyl chain lengths and five different polar head-groups, from soil over a wide range of concentrations.



Chromatogram of various PFAS molecules extracted from soil.

Compound	Recovery (%)	Compound	Recovery (%)
$^{13}C_4$-PFBA	71	$^{13}C_3$-PFBS	98
$^{13}C_5$-PFPeA	93	$^{13}C_3$-PFHxS	95
$^{13}C_5$-PFHxA	97	$^{13}C_8$-PFOS	91
$^{13}C_4$-PFHpA	96	$^{13}C_3$-HFPODA	56
$^{13}C_8$-PFOA	94	$^{2}H_3$-NMEFOSAA	93
$^{13}C_9$-PFNA	104	$^{2}H_3$-NETFOSAA	90
$^{13}C_6$-PFDA	99	$^{13}C_8$-FOSA	92
$^{13}C_7$-PFUdA	95	$^{13}C_2$-4:2FTS	110
$^{13}C_2$-PFDoA	97	$^{13}C_2$-6:2FTS	93
$^{13}C_2$-PFTeDA	108	$^{13}C_2$-8:2FTS	98

Recovery of the isotopically labeled PFAS compounds.

Data courtesy of Pacific Rim Labs.

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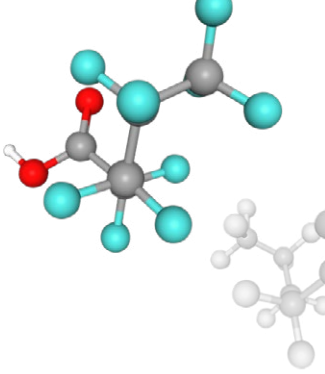

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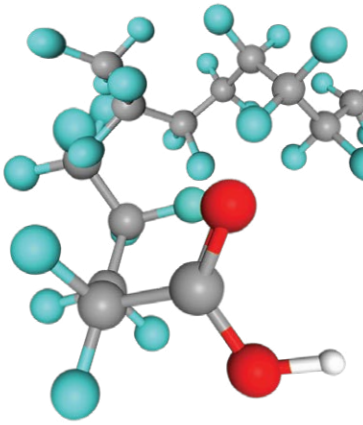

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