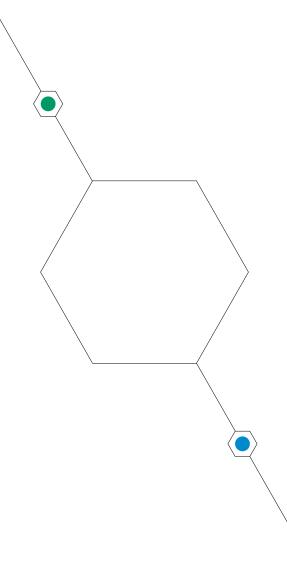


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Per- and polyfluoroalkyl substances (PFAS), formerly called perfluorinated compounds (PFCs), are a class of synthetic chemicals that pose significant environmental and health challenges due to their persistence and bioaccumulation.

Commonly found in a wide array of products, from non-stick pans to firefighting foams, PFAS are valued for their resistance to heat, water, and oil. However, these same properties contribute to their stability in the environment, making them resistant to natural degradation processes and allowing them to accumulate in the food chain. The widespread presence of PFAS has raised global concerns, as these substances have been linked to various health issues including liver damage, immune system dysfunction, and cancer.

Given the complexities associated with PFAS analysis, there is a need for robust, precise, and scalable solutions that can support ongoing monitoring and research initiatives. Detecting and managing PFAS effectively requires sophisticated analytical tools capable of identifying these compounds at very low concentrations across various environmental matrices. Technologies such as Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/ MS) and High-Resolution Mass Spectrometry (HRMS) can be essential for assessing PFAS contamination accurately. These advanced methods offer the sensitivity and selectivity necessary for tracing PFAS in complex samples, making them invaluable for both environmental monitoring and regulatory compliance.

#### Strengthen Your Analytical Game Plan with Waters Corporation

In this eBook, we delve into how advanced LC-MS/MS and HRMS technologies are helping scientists and regulators worldwide to tackle PFAS challenges head-on. From sample preparation to data analysis, Waters Corporation stands ready to advance public health and environmental safety by providing the tools needed to measure, manage, and mitigate the impact of PFAS.

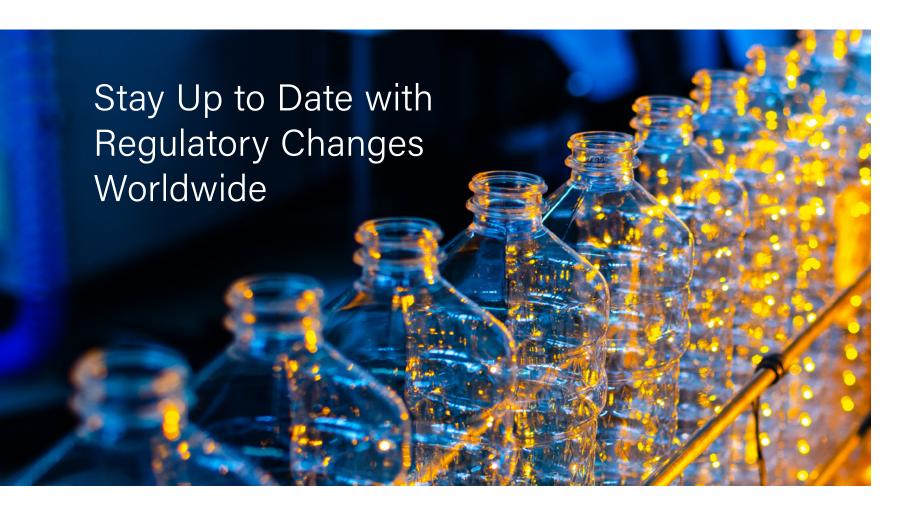
Join us as we explore the cutting-edge solutions that make Waters Corporation a leader in PFAS analysis, driving scientific progress and regulatory compliance.



Streamline Your

and Support





The rising concern for human exposure and the associated health effects, along with the accumulation of PFAS in the environment has led to the tightening of restrictions for the manufacture, import, sale, and use of PFAS. A growing number of regulations exist in many countries that place limits on the presence of selected PFAS compounds in various products and materials, including food, water, and consumer products. In addition, some primary PFAS manufacturers

have started withdrawing from the marketplace and retail chains have committed to eliminating or reducing PFAS in food packaging, textiles and/or other products. This chapter will explore the regulatory landscape of PFAS and address the two categories of regulations for a variety of geographic locations. PFAS are controlled by production, use, sale, and trade regulations as well as water and food safety regulations.

Streamline Your

Laboratory Operations

with Waters' Services

and Support

# Evolving Regulations and Industry Responses to PFAS Concerns

There is a growing international effort to manage PFAS use by balancing environmental health with practical and economic considerations.

- Global Actions: Countries are moving to phase out the production and use of PFAS due to environmental and health concerns.
- International Agreements: Many nations have joined the Basel, Rotterdam, and Stockholm Conventions to limit PFAS use.
- Challenges: Immediate bans are difficult due to the absence of alternatives and potential economic impacts.
- **EU Measures:** The EU has seen proposals to ban PFAS in non-essential uses under REACH regulations.
- US Federal and State Regulations: The EPA's PFAS Strategic Roadmap guides federal action, while states like Maine, Minnesota, and Washington have more aggressive bans.
- China's Stance: As a significant PFAS producer, China is beginning to implement more stringent regulations on these chemicals.
- Variability: While some countries have strict regulations, including prohibitions in consumer goods, others have less stringent or poorly enforced PFAS regulations.



#### PFAS in Drinking Water

Efforts to regulate PFAS in drinking water often reflect a compromise between health concerns and practical measurement capabilities.

- **Ingestion Focus:** Control of PFAS in drinking water is prioritized due to the primary exposure pathway being ingestion.
- International Limits: Regulatory limits for PFAS in drinking water vary internationally, with most countries regulating each PFAS chemical individually.
- EU Approach: The EU regulates PFAS as a class, setting a standard based on total PFAS concentration, although enforceability is challenged by the lack of a standardized methodology for measuring total PFAS.
- EU Directive: Directive (EU) 2020/2184 controls PFAS in drinking water, setting a parametric value of 100 ng/L for 20 individual PFAS and 500 ng/L for total PFAS, with member states needing to comply by January 2026.
- US Standards: The EPA's National Primary Drinking Water Regulation (NPDWR) sets enforceable Maximum Contaminant Levels (MCLs) for several PFAS compounds, with public water systems required to monitor and act if levels exceed these limits by 2029.
- Others: Health Canada proposes a 30 ng/L limit for all PFAS, Japan has a provisional 50 ng/L limit for the sum of PFOS and PFOA, while England and Wales have a guidance of 100 ng/L for any PFAS in final water.

#### **PFAS in Surface Waters** and Groundwater

The following reflects the EU's comprehensive approach to safeguarding the environment from the harmful effects of PFAS, with ongoing efforts to enhance regulatory measures.

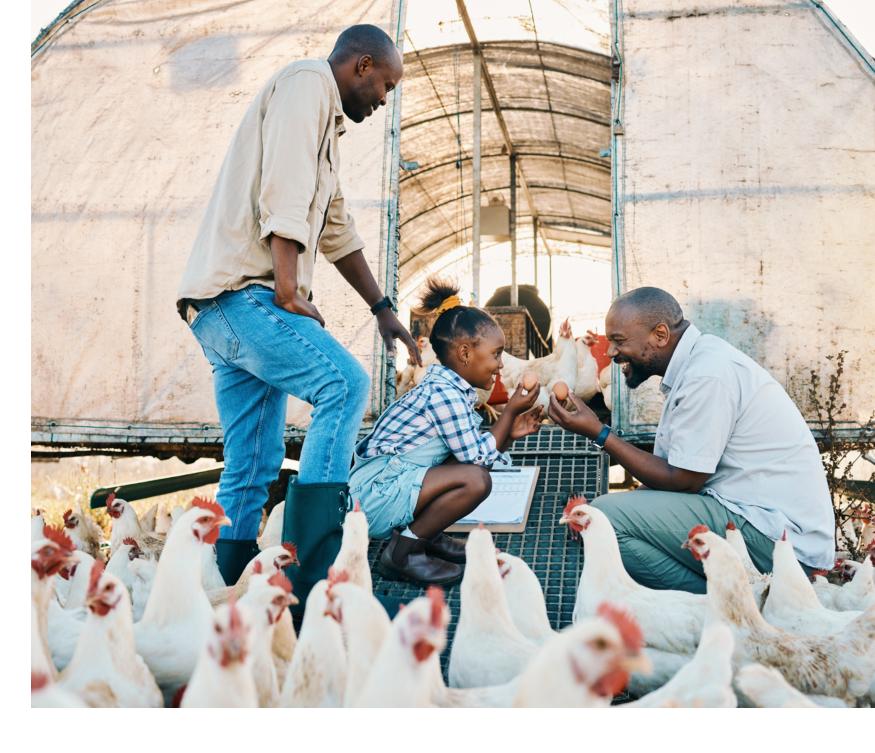
- **Regulatory Focus:** Few countries have regulations for PFAS in non-portable water, which is crucial for environmental protection.
- **EU Legislation:** The EU's Water Framework Directive and its daughter directives aim to protect water bodies from pollutants, including PFAS.
- Current EU Standards: Presently, only PFOS is listed as a priority pollutant with stringent Environmental Quality Standards (EQS) for water and biota.
- Proposed Changes in EU: An amendment is under consideration to expand the list of PFAS classified as priority pollutants and to assess ecotoxicological risks based on a sum of 24 PFAS, using PFOA-equivalents.



#### PFAS in Food

Key points regarding the regulation and monitoring of PFAS in foods and food packaging in different parts of the world are listed here.

- **Europe:** The only region with enforceable limits for PFAS in food, specifically in animal-derived foods, as per EU regulations.
- EU: Maximum levels have been set for four priority PFAS compounds, which, if exceeded, require the removal of the food product from the market. Member States are advised to collect data on a broader range of PFAS and foods to monitor contamination levels. A provisional agreement is in place to ban PFAS in food packaging, and Denmark has already implemented such a ban since July 1, 2020.
- Switzerland: Aligns with EU regulations on PFAS levels in certain foods.
- UK: Currently has no specific PFAS restrictions in food or food contact materials.
- Others: Some countries, like Australia and New Zealand, have non-regulatory 'trigger points' to guide further investigation if PFAS are detected in food.
- US: The US FDA announced a voluntary phase-out of PFAS in food packaging by manufacturers starting February 28, 2024.





#### Regulation of PFAS in Chemical Materials

Regulating PFAS in chemical materials is critical due to their widespread use and potential environmental and health hazards. This chapter explores how various regions address the regulation of PFAS in chemical products, focusing on compliance and safety measures across alobal markets.

#### Balancing Industrial and Environmental Needs

Efforts to manage PFAS in chemical materials must strike a balance between industrial requirements and environmental health concerns, involving specific limits for PFAS to ensure product safety. Different industries encounter unique regulations tailored to the distinct risks associated with various product types. There is significant international variation in PFAS regulation, with some countries focusing on individual chemicals and others adopting broader frameworks.

#### US and APAC/Greater China Regulations

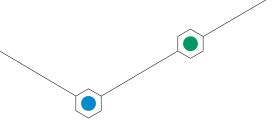
 United States: The US regulates PFAS primarily through the Environmental Protection Agency (EPA) under the Toxic Substances Control Act (TSCA). Recent legislative updates have mandated stricter PFAS evaluations and limits. The EPA's PFAS Strategic Roadmap outlines steps for reducing environmental contamination, including enforceable Maximum Contaminant Levels (MCLs) for specific PFAS compounds in consumer products.

#### APAC/Greater China:

China: PFAS regulation is part of China's broader environmental protection efforts. China regulates PFAS under its Environmental Protection Law and includes them in its priority pollutants list, requiring pollution controls and promoting safer alternatives.

Japan and South Korea: Both countries regulate PFAS through comprehensive chemical management laws—Japan under the Chemical Substances Control Law and South Korea under K-REACH. These regulations enforce strict PFAS monitoring and control measures, particularly concerning water pollution and product safety.

Contamination



#### **EU Regulations: Comprehensive Measures** for PFAS Control

The EU's approach to PFAS in chemical materials involves comprehensive restrictions under the Stockholm Convention, which prioritizes over REACH for certain substances:

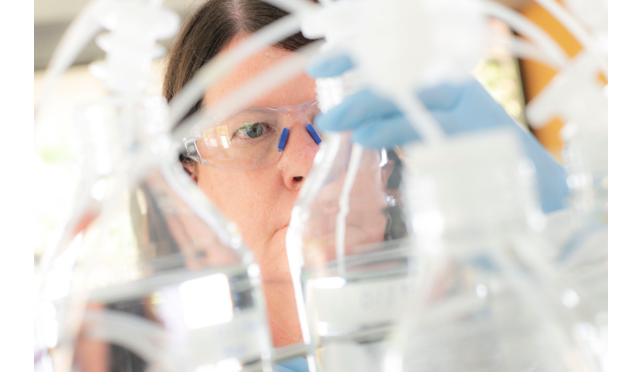
■ Stockholm Convention on POPs: Under the Stockholm Convention, PFAS such as PFOA, PFOS, and PFHxS have been moved to Annexes A and B, signifying their status as substances that are banned from manufacture, use, and international trade except under specific, controlled circumstances. This supersedes previous regulations under **REACH** for these substances.

#### Regulation Limits for PFAS Under Stockholm Convention

Here are the current regulation limits under the Stockholm Convention for PFAS classified in Annexes A and B:

Compound	Regulation Limit
PFOS, its salts and related substances	Below 25 ppb for PFOS and its salts; 1000 ppb for sum of related substances
PFOA, its salts and related substances	Below 25 ppb for PFOA and its salts; 1000 ppb for sum of related substances
PFHxS, its salts and related substances	Below 25 ppb for PFHxS and its salts; 1000 ppb for sum of related substances

These stringent limits are part of a broader effort to mitigate the environmental and health impacts of these persistent chemicals.



#### Global Impact and Industry Adaptation:

- Compliance Requirements: Industries worldwide must adapt to these stringent standards, requiring rigorous testing and documentation for PFAS content in products.
- Impact on Global Trade: These regulations affect not only the EU market but also have far-reaching implications for international trade, as global manufacturers must comply with these standards to maintain access to the EU market.

Regulating PFAS in chemical materials involves a complex interplay of health, environmental, and industrial factors. By setting and enforcing stringent PFAS limits under the Stockholm Convention, regulatory bodies aim to minimize the adverse effects of these chemicals on human health and the environment, fostering safer use and disposal practices across industries. This chapter underscores the importance of continued vigilance and adaptation in regulatory strategies to effectively manage the challenges posed by PFAS in chemical materials.

Quality Control

"Waters is committed to unlocking the potential of science to improve the world."



## Waters Corporation's Pioneering Role in **PFAS Analysis**



Waters Corporation has long recognized the critical need for sophisticated analytical approaches to PFAS detection. Leveraging years of experience and substantial investments in research and development, Waters has developed a state-of-the-art solution for PFAS analysis, encompassing every step from sample preparation to data processing and proficiency testing. Our commitment is reflected in our comprehensive suite of tools designed for accurate PFAS detection and quantification across various matrices including drinking water, groundwater, soil, and food.



Read Waters first PFCs application note from 2006 published in collaboration with Örebro University, Sweden: Analysis of Perfluorinated compounds (PFCs) on the ACQUITY™ UPLC™ System & the Quattro Premier XE IN ES-MS/MS

#### **Advanced Analytical Tools** and Customer Support

At the heart of our PFAS analysis solution is the advanced Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) technology. LC-MS/MS is renowned for its high sensitivity and selectivity, which are crucial for accurately analyzing samples with low PFAS concentrations. This capability ensures that our instruments can deliver reliable and precise measurements, crucial for meeting regulatory compliance and safeguarding public health.

Waters Corporation's LC-MS/MS systems are not only designed for performance but also for efficiency, enabling high-throughput analysis that saves time and enhances productivity. This efficiency is vital for laboratories tasked with processing large volumes of samples under tight regulatory deadlines.



Streamline Your

and Support



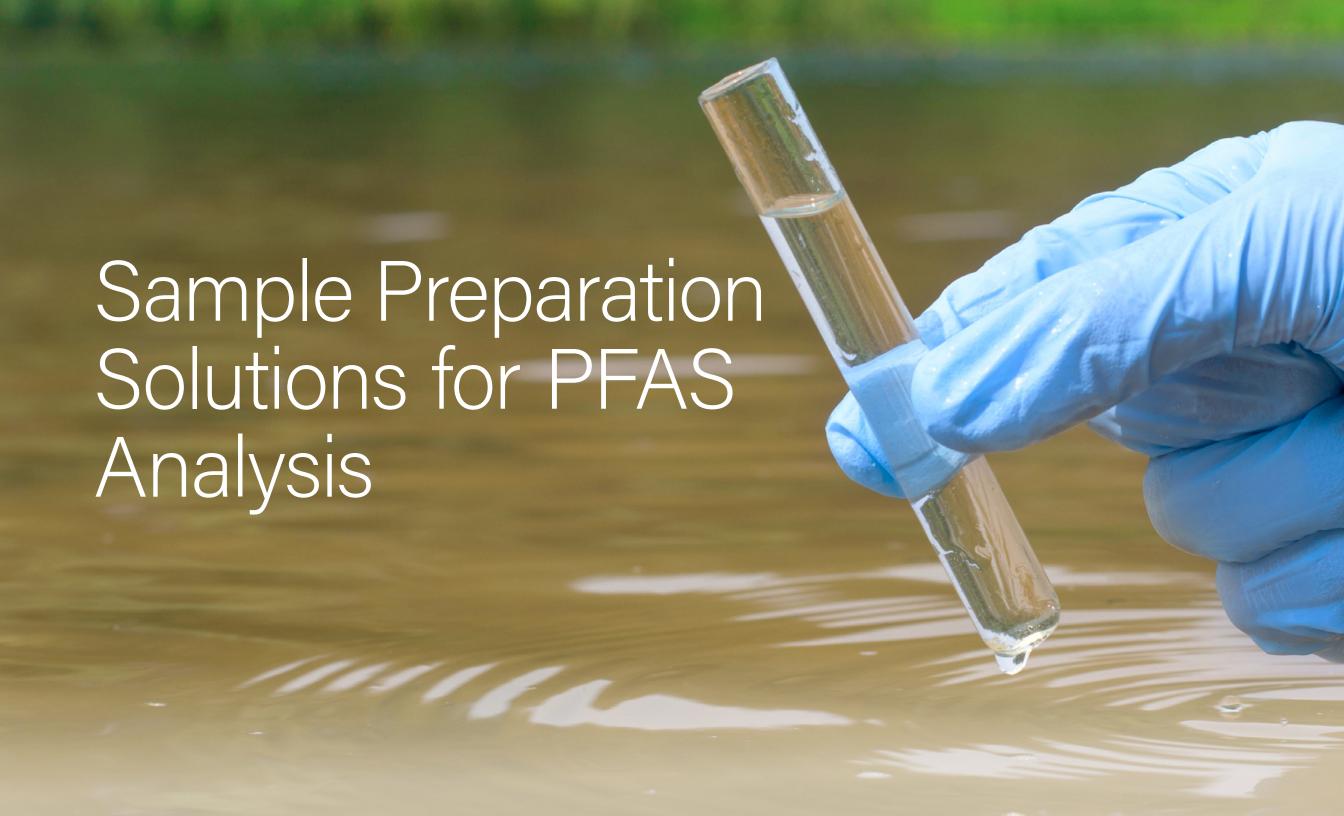
#### **Ensuring Compliance and Supporting Public Health**

Our commitment extends beyond providing advanced analytical instruments. Waters Corporation offers end-to-end support to our customers through the entire testing process from initial sample collection to the final steps of data analysis. Our team of experts works closely with laboratories to ensure that every phase of the testing process is aligned with current regulatory standards, thereby delivering results that are both accurate and legally defensible. Read more about our Analytical Professional Services Online here.

This comprehensive support helps laboratories not just to meet but to exceed regulatory requirements for PFAS testing, ensuring that all data generated is robust and reliable. By doing so, Waters Corporation plays a pivotal role in supporting the development of policies and regulations that effectively manage and control PFAS contamination.

#### Waters Corporation: A Trusted Partner in PFAS Analysis

Waters Corporation stands at the forefront of PFAS analysis, offering powerful and reliable LC-MS/MS solutions that ensure low limits of detection and high confidence in results. With our advanced technology, comprehensive support, and commitment to innovation, Waters Corporation is the ideal partner for laboratories worldwide, helping them navigate the complexities of PFAS testing and compliance, while contributing to the broader goal of enhancing human health and environmental safety.



Sample preparation is a critical initial step in the analysis of Per- and Polyfluoroalkyl Substances (PFAS), setting the stage for accurate detection and quantification. This section outlines the essential procedures and technologies used to minimize contamination and ensure the integrity of PFAS testing across various matrices.

#### **Minimizing Contamination**

Understanding and mitigating sources of contamination is crucial in PFAS analysis due to the widespread use of PFAS in various products and laboratory supplies. To prevent contamination:

- Containers: Use high-density polyethylene (HDPE) containers pre-washed with methanol for sample collection.
- Avoid Contaminative Materials: Steer clear of items such as aluminum foil, glass transfer pipettes, glass autosampler vials, vial caps with Teflon® seals, and low-retention pipette tips.
- Recommended Consumables: Utilize polypropylene vials with polyethylene caps for sample analysis to minimize background contamination. Test each consumable for PFAS background levels prior to use.
- Solvents and Water: Be vigilant about the potential PFAS contamination in LC-MS grade solvents and water purification systems. Testing these for PFAS before use is advised.

#### Implementing LC-MS/MS Systems with a Waters PFAS Installation Kit

To combat contamination from the analytical equipment itself, employing a PFAS Installation Kit is critical:

- PEEK Solvent Tubing: Replace Teflon-coated tubing with PEEK tubing to eliminate PFAS leaching from mobile phase and wash lines.
- Isolator Column: Install a 50 mm column, included in the kit, after the solvent mixer and before the analytical column to delay any potential system contaminants from co-eluting with PFAS analytes.
- Stainless Steel Coil and 50 μL Extension Loop: A stainless steel (SS) coil installed between the solvent mixer and the isolator column and a SS 50 µL extension loop after the injector further enhance system performance and improve PFAS chromatographic peak shape.





Read this whitepaper that includes full procedures and best practices for testing, controlling, and mitigating PFAS contamination in typical laboratory environments.



#### Solid-Phase Extraction for PFAS Analysis

Solid-phase extraction (SPE) plays a crucial role in PFAS analysis due to the complex nature of PFAS. SPE allows selective extraction and concentration of PFAS from various matrices, which can improve sensitivity and accuracy of analytical methods. Typically, a weak-anion exchange (WAX) sorbent is used for PFAS extraction by SPE. This is because WAX contains both reversed-phase retention beneficial for fluoroalkyl chains and anion-exchange retention for commonly acidic PFAS head groups. Also, some US EPA methods document the use of specific SPE types for extraction.

#### Sep-Pak PS-2 Cartridges for EPA Method 537.1 for Drinking Water

EPA method 537.1 requires a specific cartridge, Sep-Pak™ PS-2 (styrene-divinyl benzene copolymer), for the extraction of PFAS in drinking water that cannot be modified. This cartridge has been used and demonstrates all necessary analytical requirements for the method.



For more information, please refer to the following application note: Perfluorinated Alkyl Substances (PFAS) in Drinking Water: Extraction Using the PS2 Cartridge in Accordance with EPA 537.1.

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#### Oasis™ WAX, WAX/GCB and GCB/WAX for PFAS Analysis

Outside of EPA method 537.1, most PFAS extraction is performed using WAX sorbents as it is more selective for PFAS. It is used across various matrices including drinking water, non-potable water, food, soils, tissue, and more. Since SPE is a critical step for PFAS analysis, contamination from the cartridges can cause false positives and require time and labor for laboratories to rerun samples. Due to the need for cleanliness, Waters offers SPE cartridges that have undergone a quality control pre-screening test for low levels of 32 PFAS. This test is completed by a third-party accredited PFAS laboratory.



Oasis WAX, WAX/GCB, and GCB/WAX for PFAS Analysis.

#### Oasis WAX for PFAS Analysis

Oasis WAX for PFAS Analysis are SPE cartridges that are QC-tested by an accredited third-party laboratory for low-residual PFAS, and designed for environmental and food testing applications for PFAS. The WAX sorbent chemistry is used for various methods such as EPA 533, EU 2022/2388, ISO 25101, ISO 21675, and EPA 1633 (EPA 1633 also requires a carbon cleanup) for matrices including potable and non-potable aqueous, soil, tissue, and food. Waters offers five different parts for Oasis WAX for PFAS Analysis to align with existing methods. Additionally, outside of using for specific methods, across laboratories performing PFAS determination for food and environmental samples, WAX cartridges are the industry standard.

For more information about the use of Oasis WAX for PFAS Analysis in specific methods, please reference the application notes below:



Oasis WAX for Extraction for Per- and Polyfluorinated Alkyl Substances (PFAS) from Drinking Water in Accordance with EPA Method 533

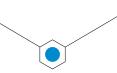


The Waters Start Up Guide: Guidelines and Recommendations for the Analysis of PFAS in Environmental Samples



Analysis of Legacy and Emerging Perfuorinated Alkyl Substances (PFAS) in Environmental Water Samples Using Solid Phase Extraction (SPE) and LC-MS/MS





Dual-Phase Oasis WAX/GCB and GCB/WAX for PFAS Analysis for Complex Matrices

The complexity of PFAS analysis, especially in challenging matrices like non-potable water, soils, and biosolids, demands efficient sample preparation methods. With the release of EPA Method 1633, these types of complex matrices require the use of both a WAX concentration/ cleanup step plus additional cleanup step using graphitized carbon black (GCB). Oasis WAX/GCB and GCB/WAX for PFAS Analysis are dual-phase bi-layer cartridges containing both sorbents in one device. They also undergo the same QC-testing ensuring low-residual PFAS as Oasis WAX for PFAS Analysis cartridges. These dual-phase SPE cartridges integrate Weak Anion Exchange (WAX) and Graphitized Carbon Black (GCB) layers, significantly streamlining the sample preparation process by reducing the handling of

loose carbon powder and combining multiple steps into one. To align with EPA Method 1633 and the order of the clean-up steps, for aqueous samples the WAX/GCB orientation should be selected, where for soils, tissues, and other solid samples, the GCB/WAX orientation should be used, EPA Method 1633 is performance-based and allows for dual-phase cartridges if the acceptance criteria for the method are met. The demonstration of the cartridges' suitability for water and soil and tissue samples for EPA 1633 can be examined further in the application notes listed below. Additionally, when working with PFAS determination of complex matrices outside of EPA 1633 such as food, or non US-environmental samples, the addition of carbon adds an extra layer of cleanup which may be beneficial for challenging matrices.

Read these application notes that use the new WAX/GCB GCB/WAX SPE cartridges:



EPA 1633 Application Note: Establishing and Assessing the Method



in Water Samples **EPA 1633 Application Note: Analyzing PFAS** 



**EPA 1633 Application Note: Analyzing PFAS** in Soil and Tissue Samples



Analysis of 28 EU Regulated and Recommended PFAS in Food via LC-MS/MS - Part 1: Vegetable, Fruit and Baby Food

#### Features and Benefits:

- Quality Control: Rigorous testing from an accredited third-party organization ensures low residual levels of PFAS, reducing background contamination and false positives.
- **Simplified Workflow:** The design of these cartridges removes four manual steps (weighing, vortexing, centrifugation, and filtering) from the EPA Method 1633 sample preparation workflows, enhancing throughput and reproducibility.
- Increased Efficiency: The cartridges decrease extraction times by up to 20%, allowing faster processing without sacrificing accuracy.
- **Expanded Applications:** These cartridges are not only effective in water and soil samples but also show increased recovery rates for neutral PFAS in food matrices, demonstrating their versatility.

#### **QuEChERS Method Integration**

For fresh food produce and simple agricultural commodities, the QuEChERS method offers a quick and effective alternative to alkaline digestion and extraction with methanol. The QuEChERS Approach involves shaking the sample with a mixture of salts and solvents followed by a phase separation and cleanup using d-SPE. However, it is advisable to check with regional requirements as the QuEChERS method alone may not be suitable for reaching required regulatory limits.



Waters QuEChERS kits streamline d-SPE sample prep for efficient multi-residue food and agricultural analysis.

- Waters QuEChERS Kits: These kits provide all necessary materials, including pre-weighed extraction buffer salts and a selection of d-SPE materials, tailored to different matrix-specific challenges.
- Advantages: QuEChERS is known for its ease of use, speed, and effectiveness in reducing contamination risks, making it particularly suitable for high-throughput environments.

The sample preparation phase is foundational in ensuring the reliability and accuracy of PFAS analysis. By effectively managing potential contamination sources, employing advanced tools like the PFAS Kit and Oasis WAX, WAX/ GCB, and GCB/WAX for PFAS analysis and Sep-Pak PS-2 cartridges, and integrating versatile methods such as QuEChERS where applicable, laboratories can achieve precise and dependable analytical results. These strategies streamline the sample preparation process and enhance the efficiency and capability of laboratories to handle diverse sample matrices in PFAS analysis. This comprehensive approach ensures that labs are well-equipped to meet regulatory standards and contribute to environmental safety monitoring.



Total Workflow for the Sensitive Analysis of Per- and Polyfuoroalkyl Substances (PFAS) in Fish, Meat, Edible Offal, and Eggs





## Advanced Liquid Chromatography (LC) for Reliable Separation

As lab managers and analytical chemists well know, PFAS contamination is a pervasive challenge, particularly given its ubiquity in laboratory environments. In PFAS analysis, the separation stage is critical and is adeptly handled by the ACQUITY Premier System, which is equipped with MaxPeak™ High Performance Surfaces (HPS) Technology. This technology enhances sensitivity, analyte recovery, and reproducibility by minimizing analyte/surface interactions, which is crucial for achieving reliable detection levels required by regulatory standards. The ACQUITY Premier BEH™ C<sub>10</sub> (recommended for legacy methods) and Atlantis™ Premier BEH C<sub>10</sub> AX (recommended for methods that include short and ultra-short chain PFAS) columns, provide superior peak shapes and stable retention times, even at large injection volumes. These features make the ACQUITY Premier System an ideal choice for labs seeking to maintain high throughput without compromising on quality and

accuracy. The system's robustness and configuration flexibility, combined with a PFAS Solution Installation Kit, ensure that the risk of contamination from mobile phases or system components is minimized, thus enhancing lab efficiency and reducing false detections.

For more information, please reference the application notes listed below:



Expanding the Range of PFAS in a Single Injection to Include Ultra Short Chains Using the Atlantis Premier BEH C, AX Mixed Mode Column



Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Accordance with EPA 1633 Part 1: Establishing and Assessing the Method



Revolutionize your separations and enhance your lab efficiency with the ACQUITY Premier System.





#### Mass Spectrometry (MS) Detection with Unmatched Sensitivity

Meeting lower detection limits for PFAS consistently is one of the most pressing issues labs face, driven by evolving regulatory requirements across different regions. The Waters Xevo<sup>™</sup> TO Absolute Mass Spectrometer excels here. As the most sensitive tandem quadrupole MS available, the Xevo TQ Absolute allows laboratories to achieve the lowest limits of quantitation for PFAS compounds in complex matrices. This instrument is particularly valuable in environments where reaching challenging regulatory levels is crucial. Its design incorporates reduced energy consumption, aligning with the environmental responsibilities of labs performing PFAS analysis. Additionally, the Xevo TQ Absolute supports a direct injection approach, which facilitates high-throughput analysis by reducing sample preparation steps and minimizing potential contamination sources.

For more information, please reference the application notes listed below:



Improved Sensitivity for the Detection of Per- and Polyfluorinated Alkyl Substances in Environmental Water Samples Using a Direct Injection Approach on Xevo TO Absolute



Ultra-Trace Detection of Per-and Polyfluoroalkyl Substances (PFAS) in Drinking Water to Meet New **US EPA Interim Health Advisory Levels** 

#### **Efficient Data Management and** Processing with waters\_connect for Quantitation

Harness the unmatched sensitivity of the Xevo TQ Absolute with the most modern, intuitive, efficient quantitation software solution established on the market.

The MS Quan App included with the waters connect™ for Quantitation Software focusses your attention where it is most needed by providing a simple, insightful, visual user experience that saves time and reduces error.

Discover seamless workflows with one click from acquisition to processing methods as well as a radical commitment to ease of use and simplicity; enabling users of different experience levels to produce highly accurate, reliable and sensitive results.

Data review is accelerated by using rulesets tailored to regulations as well as saving 50% of time spent on data review with Exception Focused Review (XFR).



#### **Enhancing PFAS Analysis** with waters connect System **Monitoring Software**

PFAS testing demands high sensitivity and accuracy due to complex environmental matrices and strict regulatory standards from agencies like the EPA. Traditional lab management methods often fall short in handling the rigorous requirements of PFAS analysis. The integration of waters connect System Monitoring Software with LC-MS systems provides a modern solution that significantly boosts lab productivity and instrument uptime, crucial for effective PFAS testing.

- Real-Time Instrument Monitoring: waters connect System Monitoring enables continuous, real-time monitoring of LC-MS systems. This feature is vital for labs to dynamically scale their operations in response to fluctuating PFAS analysis demands, ensuring optimal instrument usage and efficiency.
- Rapid Troubleshooting and Issue Resolution: The software promptly notifies lab personnel of any system errors or status changes, allowing for quick troubleshooting. This capability is essential to minimize downtime and maintain continuous operation, which is particularly important in high-throughput environments focused on PFAS detection.

- **Detailed Performance Insights:** Offering a comprehensive view of instrument performance and historical data, waters connect System Monitoring helps lab managers make informed decisions about system maintenance and management. This proactive approach prevents unexpected system failures and optimizes longterm operational efficiency.
- Remote System Scheduling: The real-time system scheduling functionality within System Monitoring streamlines this process by allowing users to reserve systems for multiple purposes (regular sample runs, calibration and maintenance, etc.). This functionality is vital for optimal system performance and management, particularly in fast-paced laboratories.

Pairing waters connect System Monitoring with high sensitivity Xevo Tandem Quadrupole Systems enables laboratories to manage their PFAS testing workload more effectively. By providing remote system status viewing, efficient system usage, rapid response to issues, detailed tracking of system history, and easy scheduling of instrument runs and maintenance, this software solution enhances laboratory efficiency, productivity, and data integrity.



For more information, please refer to the following white paper: Improving the Efficiency of PFAS and Other High Profile Analysis Using LC-MS Systems With waters\_connect System Monitoring Software



and Support

#### **Integrating Technology** and Sustainability

The Xevo TQ Absolute not only meets analytical and operational demands but also addresses the environmental impact of laboratory practices. Awarded the ACT label for its sustainable features, the Xevo TQ Absolute is designed with a smaller footprint and lower resource consumption, reflecting the commitment Waters has to sustainability. The instrument's efficient design and operational excellence ensure that labs can maintain high performance while supporting their environmental and sustainability goals.

The combination of advanced LC separation using the ACQUITY Premier System and precise detection with the Xevo TQ Absolute provides a comprehensive solution for PFAS analysis. For laboratories engaged in PFAS analysis, staying ahead of regulatory changes while managing operational efficiency and costs is a continual challenge. The Waters' integrated LC-MS/MS solutions not only rise to meet these challenges but also drive your lab towards greater scientific and operational excellence. By choosing Waters, you're not just upgrading your technology—you're enhancing your lab's capability to deliver reliable, timely, and costeffective results that make a difference, paving the way for more sustainable and responsible scientific practices.



# Advanced HRMS Solutions for Comprehensive PFAS Analysis





#### **Empowering Advanced Scientific Discovery with HRMS Solutions** for PFAS Analysis.

For labs tasked with the demanding and dynamic field of PFAS analysis, the Waters high resolution MS (HRMS) solutions offer a comprehensive suite of tools that not only meet current analytical needs but also provide the flexibility to adapt to emerging challenges. Non-target screening (NTS) or advanced structural characterization with HRMS is a powerful complementary technique for the discovery and identification of known or novel PFAS. If your focus is going beyond quantitative analyses, these HRMS technologies empower your lab to deliver precise, reliable results, and drive scientific discovery forward.

#### Benefits for Your Lab:

The advanced HRMS solutions address critical customer pain points such as the need for higher selectivity, the ability to handle complex samples, and the requirement for robust data management and analysis tools. Labs can expect:

- Increased sensitivity and specificity in PFAS detection.
- Enhanced capability to identify and quantify both known and unknown PFAS compounds.
- Streamlined workflows that reduce sample handling and increase throughput.
- Sophisticated structural characterization tools that aid in distinguishing closely related PFAS compounds.

#### Research and Non-Targeted Screening (NTS) Capabilities with Xevo G3 QTof

As lab managers and analytical chemists well know, the pervasive nature of PFAS presents significant challenges in environmental and health safety testing. The Xevo G3 QTof Mass Spectrometer offers an unparalleled solution, delivering the high sensitivity needed for the complexities of PFAS analysis along with the specificity of accurate mass measurements (less than 3 ppm). Its data independent acquisition mode (MS<sup>E</sup>) offers functionality for both screening and quantitative analysis. The Xevo G3 QTof demonstrated a high sensitivity, in the order of ng/L. The platform also supports NTS and the identification of unknown PFAS with accurate mass accurate mass precursor and fragment measurements.

This dual qual/quan capability, along with a comprehensive accurate mass PFAS Library, is essential for labs tasked with

QUANTOF **DUAL STAGE** QUADRUPOLE pore Lens ........... X5 CEL STEP WAVE XS TRANSFER HIGH FIELD ION DETECTION PUSHER

monitoring a wide array of PFAS compounds, including those not yet regulated or fully studied. The Waters PFAS Library is based on experimental data acquired on analytical standards of PFAS that includes accurate mass precursor ions, retention time, and accurate mass fragment ions.

The integration of the powerful waters connect Software platform with the Xevo G3 QTof simplifies complex screening or discovery workflows. This system allows labs to rapidly transition between exploring unknown compounds in their samples to targeted quantification, ensuring comprehensive coverage and confident characterization. By maximizing sample information from detailed characterization to accurate quantitation, Xevo G3 QTof empowers labs to validate their findings with complete confidence.

For more information, please reference the application notes listed below:



Direct Injection Screening Method for Per- and Polyfluoroalkyl Substances (PFAS) in Drinking Water Using the High Resolution Time of Flight Mass Spectrometer, the Xevo G3 QTof



Non-target Screening Workflow (NTS) for the Analysis of Per and Polyfluoroalkyl Substances (PFAS) in Animal **Products Using Xevo G3 QTof** 

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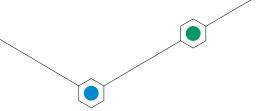
and Support



Improve your qualitative and quantitative capabilities with outstanding sensitivity using the Xevo G3 QTof.

Caption?

Contamination



#### Enhanced Separation and Detection with SELECT SERIES™ Cyclic™ IMS

For labs pushing the boundaries of research and requiring detailed structural characterization, the <u>SELECT SERIES</u> <u>Cyclic IMS</u> adds a vital dimension to PFAS analysis. Ion mobility provides an additional dimension of separation and increased system peak capacity without adding analysis time. This innovative system combines Cyclic Ion Mobility (cIM) with high-resolution time-of-flight mass spectrometry, effectively distinguishing PFAS from other compounds in complex matrices and even resolving isomeric forms like linear and branched PFAS.

The SELECT SERIES Cyclic Ion Mobility Spectrometry (IMS) System represents a groundbreaking advance in PFAS analytical techniques. By integrating liquid chromatography with cyclic ion mobility separation, this system markedly enhances the detection of PFAS compounds in complex environmental matrices.



For more information, read the application note: The Application of Cyclic Ion Mobility to Non-Targeted Analysis of Per- and Polyfluoroalkyl substances (PFAS) in Environmental Samples

#### Key Benefits of Cyclic Ion Mobility in PFAS Analysis:

#### 1. Enhanced Detection and Identification:

- The SELECT SERIES Cyclic IMS System facilitates the confident identification of known PFAS through the precise measurement of mass, retention times, expected fragment ions, and <u>collision cross-section</u> (CCS) data.
- This method significantly improves the detection of both known and novel PFAS compounds in complex environmental samples, such as water from contaminated sites.

#### 2. Discovery of Novel PFAS:

- Adding ion mobility separation is advantageous for discovering new PFAS as the compounds have a distinct behavior compared to other compound classes of similar m/z.
- An IMS-based filtering approach is instrumental in discovering previously undetected PFAS molecules, thereby expanding the scope of contaminants that can be monitored and remediated.
- Common fragment ion searches can potentially yield new compounds or break down products previously undetected.

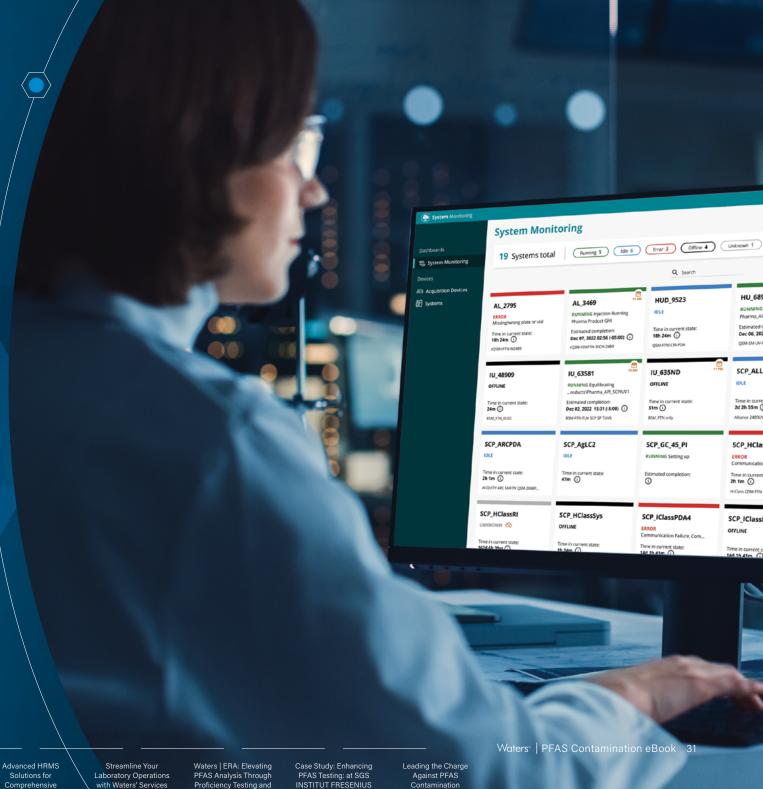
#### 3. Advanced Structural Elucidation:

- The use of ion mobility separation enhances the structural elucidation of known and unknown PFAS compounds. By aligning additional spectral data, researchers can achieve a deeper insight into the molecular structures and behaviors of PFAS, facilitating more effective identification and analysis.
- As authentic standards of new PFAS are limited, the certainty of proposed structures can be supported by the data rich approach of LC-IMS-HRMS

#### Streamlining Workflow with waters connect

Both the Xevo G3 QTof and the SELECT SERIES Cyclic IMS are supported by the comprehensive waters\_connect Software environment. This platform harmonizes workflow management from research and discovery to regulatory quantitative analyses. For labs analyzing PFAS, waters\_connect provides tools for mass defect filtering, online database and comprehensive PFAS library searches, and data set management, which are essential for the efficient processing and analysis of large and complex data sets.

The software's UNIFI™ Application, particularly when coupled with the Xevo G3 QTof and SELECT SERIES Cyclic Ion Mobility, streamlines PFAS screening workflows using direct injection approaches. This method significantly enhances laboratory throughput, enabling confident PFAS identification.



and Support





### Customized Training and Application Support

At Waters, we are committed to enhancing laboratory proficiency, especially in the complex field of PFAS analysis. Our dedicated Global Services Team provides comprehensive training and application-specific support to ensure your lab personnel are well-equipped to handle sophisticated analytical tools and methodologies. Through our extensive training, dedicated support, and services, Waters empowers your lab to exceed regulatory requirements and achieve operational excellence.

Our PFAS outcome-based method application training is specifically designed to expedite the learning curve for region-specific LC-MS methods. Through detailed user guides, on-site solution Success Guides, and training checklists, we focus on speeding up implementation so that labs can quickly move to mastering optimization, troubleshooting, and ultimately achieving analytical success.

We continuously refine our training programs on a global basis to cover a wide array of methods, keeping pace with regulatory updates and expanding your laboratory's capabilities in PFAS analysis.

#### **Optimizing Instrument Productivity** and Analytical Services

Waters helps maintain your instruments at peak productivity, minimizing downtime and enhancing lab performance. Our services include the latest technology upgrades, method transfer, validation, and stringent compliance support to ensure your instruments deliver reliable and consistent results. It is recommended, for example, that Waters provide professional installation of the UPLC PFAS Kit with no major modifications to the UPLC and benchmark the system to be "PFAS-Ready."

#### **Professional and Compliance Services**

Our Compliance Services Team offers a comprehensive suite of services to ensure your laboratory meets all regulatory standards without disruption. From instrument to software qualification, we help you establish and maintain quality standards that meet regulatory requirements, protecting your lab from potential non-compliance consequences.

Our Software Compliance Services provide scalable, expert solutions to maintain control over your laboratory systems from installation onwards, ensuring they are fit for intended use and aligned with regulatory demands.

Compliance

"The Waters Team have been instrumental in the development of a custom solution for streamlining the analysis of short-chain PFAS in our lab. [...]

Their proactive approach and expertise have greatly enhanced our capabilities."

Victoria Erdely - Head of Department Method and Instrument Support - Eurofins GfA Lab Services





Waters | ERA™, a leader in the field of certified reference materials (CRMs) and proficiency testing (PT) products, serves as an indispensable partner for laboratories across the globe. Recognized in over 80 countries, Waters | ERA is committed to enhancing the accuracy and reliability of laboratory data through comprehensive testing support and services.

Waters | ERA provides essential support to laboratories across industries such as environment, food safety, and pharmaceuticals, helping them meet stringent quality and accreditation standards while maintaining high performance.

#### **Key Services:**

- Proficiency Testing (PT): Waters | ERA's PT services validate analytical results, ensure testing reliability, and enable comparison against peer benchmarks, highlighting areas for improvement.
- eDATA™ Informatics: This platform equips QA managers with tools for performance analysis and risk management, improving operational visibility and fostering process enhancements across laboratory networks.

Streamline Your

Laboratory Operations

with Waters' Services

and Support

 Custom Reporting and Support: Tailored support from Waters | ERA ensures laboratories meet specific quality objectives and maintain a competitive edge.

These streamlined services simplify laboratory management, enhance proficiency testing, and improve overall analysis quality, allowing laboratories to focus on core operations.

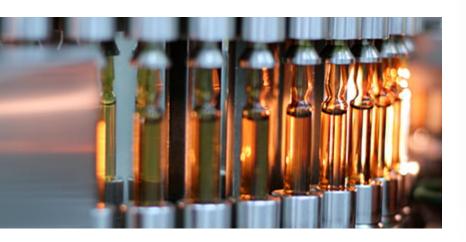


#### The Importance of Proficiency Testing in PFAS Analysis

This support extends significantly into the critical and increasingly regulated area of Per- and Polyfluoroalkyl Substances (PFAS) analysis.

Proficiency testing is crucial in PFAS analysis for several reasons:

- Regulatory Compliance: It helps laboratories meet stringent quality standards required by regulatory agencies.
- Performance Benchmarking: It enables labs to compare their results with those of peers, providing an external validation of their analytical capabilities.
- **Quality Improvement:** PT results can highlight areas for improvement, helping laboratories refine their analytical processes.



#### Key Products for PFAS Analysis

#### **PFAS Secondary Source Standard Products:**

Recognizing the scarcity of reliable PFAS standard suppliers, Waters | ERA offers a vital resource—PFAS Secondary Source Standards. These standards are meticulously designed to serve as a dependable secondary source for routine quality control. By furnishing a straightforward solution for verification without the necessity for additional dilutions, these standards simplify the process for laboratories, enabling them to maintain accuracy in PFAS quantification. The standards include a comprehensive list of EPA Method 1633 and 533/537 analytes, precisely calibrated to match PFAS method calibration curves, thus facilitating thorough verification.

#### **Proficiency Testing (PT) Products:**

Waters | ERA's PT products are integral to validating the accuracy of laboratory results and ensuring consistency across tests. The PT programs help labs verify the reliability and reproducibility of their testing parameters, identify areas for corrective action, and benchmark their performance against peers. This is especially critical in PFAS analysis, where precision and reliability are paramount due to the health and environmental implications of these substances.

#### **Certified Reference Material (CRM) Products:**

Waters | ERA offers Certified Reference Materials (CRMs) essential for maintaining high-quality standards in industries such as environmental, pharmaceutical, and

Streamline Your

and Support

food processing. To deliver confidence, a laboratory needs to maintain a robust and sustainable Quality Control (QC) program. CRMs play a critical role in this as CRMs support laboratories in establishing demonstration of capability, analyst training, root cause analysis, calibration, and developing and validating PFAS methods to meet regulatory compliance.

#### **eDATA and Project Support:**

Waters | ERA provides eDATA, an innovative portal that revolutionizes proficiency testing management. eDATA features include streamlined data entry, on-demand access to PT reports, and tools for tracking and managing compliance activities which are all critical for maintaining PFAS accreditation. To further assist laboratories, Waters | ERA offers custom interlaboratory support. This service is tailored to help laboratories streamline ordering, manage PT compliance, and implement best practices across their networks, enhancing the overall quality of analyses.

As the field of environmental testing, particularly for PFAS, grows in complexity and scrutiny, partnering with Waters | ERA offers laboratories not just data validation and peace of mind, but a comprehensive support system to navigate the challenges of PFAS analysis. By leveraging Waters | ERA's advanced PT products and secondary source standards, labs can ensure compliance with regulations, maintain high analytical standards, and ultimately protect public health and the environment.



# Lower Regulatory Limits Prompt Innovation in PFAS Testing

SGS INSTITUT FRESENIUS, a leader in non-medical laboratory analysis across Europe, has responded proactively to evolving PFAS regulatory standards by incorporating advanced technologies from Waters. This collaboration highlights the integration of the Waters Xevo TQ Absolute Mass Spectrometer and waters\_connect for Quantitation Software significantly enhancing the laboratory's testing capabilities.

The case exemplifies how strategic investments in cutting-edge technologies and strong vendor support can significantly enhance a laboratory's analytical capabilities.

#### **Key Challenges and Solutions**

Facing stringent regulatory demands for lower limits of quantification (LOQ) for PFAS, SGS needed technology capable of achieving ultra-sensitive detection levels. The Waters Xevo TQ Absolute Mass Spectrometer was selected for its precision in measuring low concentrations of PFAS in diverse matrices, including environmental samples and food products.

The laboratory at SGS INSTITUT FRESENIUS, managed by Mr. Stephan Lebertz, has developed new methods to meet these challenges, focusing on robust extraction, cleanup, and preconcentration techniques. This methodological evolution was supported by Waters technologies, which are designed for high efficiency and minimal contamination risk, crucial for reliable PFAS testing.



This partnership not only addresses the technical challenges of PFAS analysis but also positions SGS as a leader in environmental testing, ready to meet the challenges of stringent global standards.

#### **Support and Training**

For Waters, the commitment to supporting SGS extended beyond just providing instruments. The comprehensive customer support and training have been pivotal in smoothly integrating new technologies at SGS, ensuring the lab personnel were well-equipped to utilize the advanced capabilities of the Waters instruments fully. This support has been instrumental in optimizing the lab's operations and enhancing overall productivity.

#### Benefits and Impact

The partnership with Waters has enabled SGS INSTITUT **FRESENIUS to:** 

- Achieve lower LOQs necessary for compliance with current and upcoming regulations.
- Enhance the precision and reliability of PFAS testing, critical for protecting environmental and human health.
- Maintain high throughput and data integrity, which are essential for managing large volumes of samples and complex analyses.
- Gain a strategic advantage in PFAS analysis by expanding the scope to include more PFAS compounds and different matrices.



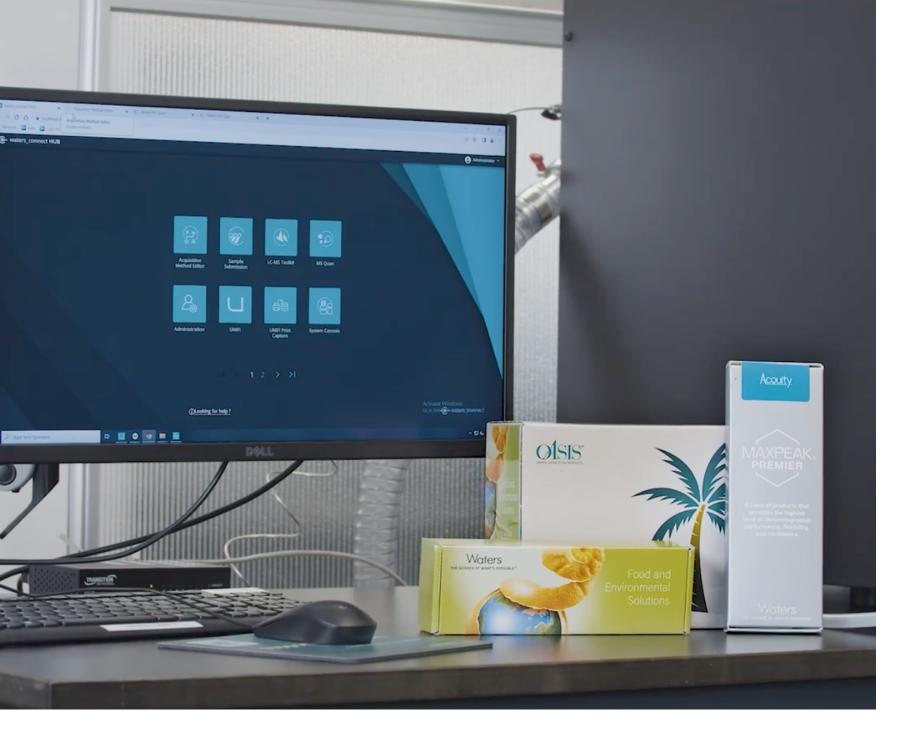
Waters Xevo TQ-S micro mass spectrometer system at SGS INSTITUT FRESENIUS.



Read the whole case study: Discover How SGS Institut Fresenius Is Revolutionizing their PFAS Testing with Waters Technology

and Support





# The Final Word: Collaboratively Advancing the Future of Innovation in PFAS Analysis

Navigating the complexities of PFAS analysis requires more than just robust technology—it demands a partnership that extends beyond the laboratory bench. This eBook has showcased the sophisticated tools and strategic support provided by Waters Corporation and Waters | ERA, equipping labs to tackle the persistent challenges of PFAS with precision and confidence.

Through our advanced LC-MS/MS and HRMS technologies, Waters has redefined the standards of sensitivity and accuracy in PFAS analysis. The addition of Waters | ERA's proficiency testing and certified reference materials further strengthens lab capabilities, ensuring compliance with stringent global regulations and enhancing data reliability.

As we wrap up, remember that managing PFAS isn't just about detecting these compounds; it's about empowering your lab with the right tools and support to ensure your results lead to actionable insights. With Waters and ERA, you gain more than just technological solutions—you gain a reliable ally in your quest to protect public health and the environment.

Together, we're not just responding to the challenge of PFAS—we're leading the way in shaping a safer, healthier future. Thank you for joining us on this critical journey. Let's continue to push the boundaries of what's possible in environmental testing.

Contamination

www.waters.com/PFAS

# Waters™

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