

Lower Regulatory Limits Prompt Innovation in PFAS Testing

SGS INSTITUT FRESENIUS adapts to evolving standards for PFAS testing with investments in Waters Instrumentation, Software, and Consumables, particularly the Waters Xevo TQ Absolute Mass Spectrometer and waters_connect for Quantitation Software.

PFAS TESTING AT SGS INSTITUT FRESENIUS

As the world's leading testing, inspection and certification company, SGS prides itself on establishing the global benchmark for sustainability, quality, and integrity. With 98,000 employees and a network of over 2,650 offices and laboratories around the globe, the company works to enable a better, safer, and more connected world. SGS INSTITUT FRESENIUS is part of the SGS Group in Germany and a leading provider of non-medical laboratory analysis in Europe.

SGS INSTITUT FRESENIUS has over 175 years of experience in the field of analytics. This outstanding knowledge is the basis of the company's excellent reputation among manufacturers, retailers, service providers and consumers – both in Germany and internationally. SGS INSTITUT FRESENIUS' Taunusstein site employs about 750 people, with about 120 chemical specialists working on the analysis of about 100 different substance classes, particularly those requiring low limits of quantification (LOQ).

One such area of expertise is per- and polyfluoroalkyl substances (PFAS), a diverse group of chemicals that represent a significant threat to the ecosystem and human health. PFAS are the focus of continuous media coverage and the subject of current regulatory changes due to their persistence in the environment.



SGS INSTITUT FRESENIUS is a leading provider of non-medical laboratory analysis in Europe.

WORKING WITH WATERS

While the technical capabilities of instrumentation and software always play a vital role in its decision-making process, SGS INSTITUT FRESENIUS finds the support and service they receive from Waters™ as particularly valuable to attain the analytical capabilities the company strives to achieve. Mr. Stephan Lebertz, Operational Laboratory Manager of Connectivity & Products NonFood, SGS INSTITUT FRESENIUS, explains:

"While the instrumentation certainly demonstrates the performance we need, a crucial factor is the excellent support we receive from Waters. Our collaboration with Waters has been beneficial, especially in terms of technical support, which was effective in getting the system running smoothly. Our colleagues in other SGS facilities with the same products have also reported positive experiences with the cooperation between Waters and their teams, resolving issues through good communication. This relationship is crucial for optimal functionality."

"Like non-target screening, PFAS analysis requires specialists dedicated to the task to ensure the development of robust, valid methods and the generation of trustworthy data. Our PFAS testing services help protect the environment and human health, and our customers rely on our expertise related to analysis, legislation and prevention. Precise measurement requires the use of highly sensitive methods. Developing new methods becomes essential, as existing ones may not meet the stringent requirements set by new regulations."

MR. STEPHAN LEBERTZ

Operational Laboratory Manager of Connectivity & Products NonFood, SGS INSTITUT FRESENIUS

To stay ahead of evolving regulatory standards for PFAS, SGS INSTITUT FRESENIUS has invested in the latest liquid chromatography coupled with tandem mass spectrometry (LC-MS/MS) technology from Waters to achieve proposed regulatory LOQs down to 0.001 µg/kg.

EVOLVING REGULATORY STANDARDS FOR PFAS ANALYSIS

There are more than 4,000 individual PFAS compounds, a large portion of which exhibit exceptional stability leading to a lack of degradation in the environment. They enter ecosystems through diverse pathways where they are not naturally present, accumulating over time in soil and waterways. If the chemicals get into the groundwater or drinking water, plant-based agricultural products and fish cultures are also contaminated. Furthermore, animal foodstuffs such as milk and meat can be contaminated by PFAS-contaminated animal feed.

Due to their effective water-repellent characteristics, these industrial chemicals are used in multiple industries, such as textiles, paper packaging for food, printing inks for magazines, metal, photography, fire-fighting foams, and refrigerants. As industries turn to the use of recycled materials, PFAS migration from packaging materials into foodstuffs is increasingly being discussed. The wide range of usage is reflected in the customer base of SGS INSTITUT FRESENIUS.

The company's client base is described by Mr. Lebertz:

"We have a diverse range of customers, both large and small, who specifically request capabilities at the level of precision we aim to achieve. We collaborate with governmental agencies, major beverage and food producers, and prominent retailers. Additionally, we engage with smaller companies focusing on recycling processes, tapping into the emerging market driven by startups and larger recyclers."

While historically only perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) received significant attention, there is a growing awareness of other substances within the PFAS group, such as perfluorononanoic acid (PFNA) and perfluorohexane sulfonic acid (PFHxS). As a result, regulatory frameworks continue to adapt to address emerging challenges and protect both the environment and human health.

However, the extensive variety of PFAS compounds poses a challenge in regulating and establishing limits. Each compound is characterized by distinct structures, making it challenging to develop effective methods for their identification and quantification. Environmental samples, such as water and soil, may contain substances that can disrupt PFAS measurements, introducing inaccuracies. Additionally, the extraction of PFAS from complex samples requires meticulous preparation to mitigate interference or incomplete extraction, which could compromise result reliability and potentially lead to false positives or negatives.

Mr. Lebertz describes these challenges:

"You must be well-versed in various chemical analysis techniques because PFAS analysis involves a broad chemical structure. It's not just about the four specific PFAS; there are numerous others to consider. This complexity makes PFAS analysis one of the most challenging tasks in the field of chemical analysis."



Mr. Lebertz (right) works at the Taunusstein site to provide impurities testing services for clients.

In Europe, Commission Regulation (EU) 2023/915 lists maximum limits for perfluoroalkyl substances in animal-based foods. In addition, Commission Recommendation (EU) 2022/1431 advises to monitor PFAS substances in a wider range of foodstuffs to collect representative data with expected LOQs down to 0.001 µg/kg. The European Commission holds overall responsibility for planning the monitoring of PFAS in food for official control, but it is the competent authorities and food companies in each member state that are obliged to carry out analyses to check regulatory compliance.

"Detecting PFAS is challenging due to their low concentrations. Current and potential future regulations are driving us to conduct PFAS analysis with very low detection limits. This push, both from regulators and our customers, motivates us to improve our lab processes. The challenge lies in aligning regulations with available technology."

MR. STEPHAN LEBERTZ

Operational Laboratory Manager of Connectivity & Products NonFood, SGS INSTITUT FRESENIUS

ACHIEVING THE LOWER LOQ FOR PFAS

Staying abreast of regulatory changes requires SGS INSTITUT FRESENIUS to invest in the latest analytical technology. Ahead of the regulatory changes, Mr. Lebertz identified only two instrument vendors that offered systems with the sensitivity needed to reach the lower LOQs for challenging compounds like PFAS. After an extensive testing process, he explains why SGS INSTITUT FRESENIUS chose the Waters Xevo™ TQ Absolute Mass Spectrometer, which was installed in December 2022:

"For this project, the low LOQ was a major focus. Leading up to the installation, we engaged in extensive R&D work focused on low LOQ methodologies, procedures, and extraction processes. Subsequently, we took advantage of the opportunity to use demo labs to understand the capabilities of the newly available instrumentation. Each system undergoes rigorous testing within the framework of this project's procedures. This approach helps us gather comparable data sets, allowing us to make an informed decision based on both technical capabilities and performance. We started measurements with the new instrument in February 2023."



SGS INSTITUT FRESENIUS added the Waters Xevo TQ Absolute Mass Spectrometer to an existing suite of instruments used for PFAS analysis.

The new system adds to the existing suite of instruments that SGS INSTITUT FRESENIUS uses for PFAS analysis, and will be used specifically for the lower LOQ analyses on food matrices, to avoid contamination.

In addition to obtaining new instrumentation, SGS INSTITUT FRESENIUS also simultaneously worked on developing new methods to achieve the LOQ that would be eventually required by regulatory agencies. Mr. Lebertz describes this extensive process:

"Our method encompassed three major stages: extraction, cleanup, and preconcentration. Additionally, we addressed the complexity of different matrices, with foodstuffs being one of the most intricate. During the early stages, we worked on method development to gain a thorough understanding of the various options for developing methods applicable to fats, fish, potato products, eggs, and other complex matrices. The goal was to achieve effective results for various matrices in an efficient and robust manner. We aimed for a streamlined approach that minimizes the number of different extraction and other procedures needed, ensuring versatility and efficiency across a range of matrices."



SGS INSTITUT FRESENIUS started measurements with the Waters Xevo TQ Absolute Mass Spectrometer in February 2023.

Mr. Lebertz emphasizes the importance of acknowledging the widespread presence of PFAS, and how this impacts the testing laboratory itself:

"If there is an issue with PFAS, low-level measurements will reveal it. However, addressing the blank value challenge is key, and having procedures in place to handle it is essential. If low-level PFAS occur in the instrument blank, it is impossible to report an accurate value for the sample. Method development is therefore an ongoing process. For example, we currently test every single material in our laboratory to reduce the possibility of PFAS contamination. Testing two pipette tips from the same box might yield different results — one clean and the next one not. While this approach can be expensive, it is necessary to ensure the validity and reliability of our data. It's also a worrying scenario because the more we test, the more instances of contamination we identify."

In addition to instrumentation, the company has been using waters_connect™ for quantitation to reduce time spent on data review and processing large sample batches. The benefits of the software include built-in data integrity tools and an intuitive user interface designed to reduce training burden, so a laboratory like SGS INSTITUT FRESENIUS can generate high-quality LC-MS/MS data and report results easily on the Waters Xevo TQ Absolute. Again, support from Waters played a key role in the successful integration of the software, helped by regular meetings with SGS INSTITUT FRESENIUS.

"Software is never perfect, but Waters has been responsive, actively addressing issues, and working collaboratively with us to resolve concerns almost every week. It's a relief that the software issues are being addressed because, when the software is problematic, it can negatively impact the quality of the data and the efficiency of manual work. We've faced challenges with other vendors where the customer service was quite poor. So technical support is a decisive factor when we invest in new software."

MR. STEPHAN LEBERTZ

Operational Laboratory Manager of Connectivity & Products NonFood, SGS INSTITUT FRESENIUS



SGS INSTITUT FRESENIUS has been using waters_connect for quantitation to reduce time spent on data review.

RETURN ON INVESTMENT

SGS INSTITUT FRESENIUS adopts a strategic approach when making decisions regarding capital purchases, with a primary focus on maximizing return on investment (ROI). In this meticulous process, the organization diligently evaluates both the cost and performance aspects of potential instrumentation. This comprehensive analysis serves as a critical foundation for determining the most suitable fit for their specific requirements. Mr. Lebertz explains:

"Our decision is primarily based on our understanding of customer needs and building a solid business case rooted in accurate information from our customers. Our lab processes hundreds of samples, with larger customers typically requiring more significant sample volumes. Preparing for big projects can take several months or even years, and we expect this trend to continue. Our investment returns and capital spending plans match the expected timelines for these projects."

The company's ROI evaluation for this project went beyond the specific PFAS compounds to include other well-known compounds. SGS INSTITUT FRESENIUS requires instruments to serve multiple purposes, creating a double or even triple-fold benefit. Considering the substantial financial investment, Mr. Lebertz explains why it's not prudent for the company to limit its utility to a single business endeavor:

"If the funded project encounters challenges or doesn't succeed, having alternative options allows us to redirect the project for market returns. The Waters Xevo TQ Absolute is capable of handling various substances, extending beyond just food-related matrices. In our PFAS measurements, we cover diverse sample types, including environmental samples and materials like metals, paper, and packaging materials. By evaluating the overall performance of the instrumentation across different compounds, we aim to understand its capabilities thoroughly."

As part of ROI, SGS INSTITUT FRESENIUS also considers software efficiency because it can significantly impact the speed of operations. For example, if software allows for twice the efficiency compared to another option, it translates to substantial cost savings and improved productivity. Another consideration is energy efficiency, as this not only reduces costs but also lessens the environmental impact of the laboratory. The Waters Xevo TQ Absolute presents information about its environmental footprint via the ACT label, certified by My Green Lab, allowing prospective customers to make an informed decision based on environmental impact.

"Certainly, energy efficiency is becoming increasingly important, and we consider factors like energy consumption, heat, noise, and space. I'm very happy with our decision. The instrument is giving us the performance we expected for the LOQs."

MR. STEPHAN LEBERTZ

Operational Laboratory Manager of Connectivity & Products NonFood, SGS INSTITUT FRESENIUS

NEXT STEPS

The SGS INSTITUT FRESENIUS anticipates that the PFAS testing field will continue its evolution due to changes in regulations and testing applications, likely involving both newly identified compounds as well as different materials that require testing. Mr. Lebertz describes what he sees on the near horizon:

"Expanding the scope to include packaging materials, environmental samples, and materials used in products like car interiors is essential. Currently, we are dealing with the four PFAS with low LOQ, but new recommendations are emerging that push for a list of 28 PFAS for foodstuffs and extending the method to cover additional matrices. This expansion will demand additional efforts and will likely be the primary focus of SGS INSTITUT FRESENIUS for the upcoming year."



The Waters Xevo TQ Absolute presents information about its environmental footprint via the ACT label.

In addition, Mr. Lebertz anticipates that the landscape of PFAS testing is poised to undergo a significant expansion in the next three to four years. This projection is underpinned by the work of nongovernment organizations (NGOs) on the potential environmental and health impacts of PFAS compounds. He comments:

"This broader scope considers various chemical structures and aims to capture a range of technical mixtures used in different applications. While the magnitude of the problem is not yet fully understood due to a relatively low number of market samples, ongoing studies and advocacy efforts are pushing for a more comprehensive understanding of PFAS-related issues. The awareness and knowledge of the impact of PFAS are expected to rise, driven by market trends and NGO initiatives in both the U.S. and European markets. As public awareness increases, the demand for more precise measurements will likely grow."

PFAS in the environment – and the challenge of PFAS testing – looks set to remain a focus for a wide range of companies, and in almost all areas of our lives. Mr. Lebertz sees this as perhaps the defining issue of his career at SGS, saying:

"This has been the most difficult and challenging project I have ever had to work on. It's also the most satisfying – solving analytical challenges and getting to robust, reliable methods that can be relied on has required a significant effort, but now, I am confident that whatever comes our way in the future, we are ready."

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