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The Impact of Automation on Sample Introduction for Trace Contaminant Analysis

Yoshiro Hiramatsu discusses how automated GC–MS/MS workflows simplify PFAS testing, improve safety, and boost productivity in routine labs.

2025-10-23 (UTC)

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The analysis of trace contaminants has long presented a challenge to laboratories due to the complexity of sample preparation steps, lengthy workflows, and the need for high sensitivity. Recent advances in automation, particularly for GC–MS/MS workflows, are transforming the way

laboratories handle contaminants, such as per- and polyfluoroalkyl substances (PFAS).

At the 2025 North American Chemical Residue Workshop (NACRW), Shimadzu's GC-MS Product Specialist, Yoshiro Hiramatsu, presented on the automated sample introduction approaches developed by his team. Their work specifically addresses the analytical complexities of neutral PFAS compounds, demonstrating the significant operational advantages of automation in this field.

Why Are Neutral PFAS a Focus in Trace Contaminant Analysis?

PFAS are widely monitored using LC–MS/MS, especially non-volatile species such as perfluorocarboxylic acids (PFCAs). However, neutral PFAS present unique issues. As Hiramatsu explains:

“Some neutral PFAS compounds are known to act as precursors to other substances. For example, fluorotelomer alcohols (FTOHs) have been used in food packaging due to their grease-proof properties; however, they are being phased out as they are precursors. Monitoring these neutral PFAS alongside toxic PFAS using LC–MS/MS contributes to safer human health.”

The problem is that neutral PFAS compounds, including iodinated analogs, often ionize poorly in electrospray ionization (ESI) and are more volatile, making GC-based approaches preferable.

How Does Automation Simplify Sample Preparation?

Traditional workflows for PFAS analysis involve time-consuming extraction using solvents such as ethyl acetate, followed by centrifugation or solid-phase extraction. Automation changes the game.

"With some techniques, it takes several hours for PFAS to be extracted from samples, " says Hiramatsu. “By using headspace techniques such as solid-phase microextraction (SPME) and dynamic headspace (DHS), we can skip the extraction step. With these approaches, sample preparation is minimal; simply place the sample in a vial, and it’s ready for analysis.”

This streamlined approach not only saves time but also reduces the risk of solvent exposure for chemists.

What Benefits Can Labs Expect from Automated Workflows?

Automated sample introduction delivers tangible improvements in day-to-day lab operations:

- Higher throughput: “Laboratories can achieve higher throughput from sample preparation to reporting,” Hiramatsu notes.
- Improved safety: Reduced solvent handling means less exposure for chemists.
- Reproducibility: Automation minimizes human error and improves consistency across analyses.

These gains are particularly valuable for routine testing labs, where simplified standard operating procedures (SOPs) can directly translate into productivity boosts. “Automation allows laboratories to increase the number of samples analyzed per day with limited human resources. The GC–MS/MS technique also simplifies data processing, further reducing errors and speeding up workflows,” Hiramatsu adds.

Can Automation Extend Beyond PFAS Testing?

While neutral PFAS served as the proving ground, the benefits of automation extend far beyond. Headspace-based extraction is already a standard method in GC–MS, and its applications are growing.

“In the pharmaceutical field, nitrosamine analysis using DHS–GC–MS/MS is becoming more widespread,” says Hiramatsu."Another example is the analysis of moldy odors, which is also performed using automated sample preparation techniques. These approaches eliminate complex steps and increase laboratory capacity across many workflows.”

What Should Labs Consider Before Transitioning to

Automation?

For laboratories evaluating the move from manual to automated workflows, Hiramatsu offers practical advice:

“GC–MS systems offer a variety of automated sample injection options. If you are considering updating your sample preparation procedures or expanding your laboratory’s capabilities, consult with your instrument vendor to discuss which system would best suit your project. Automation will accelerate your laboratory’s output and enhance its capabilities.”

How Will Automation Shape the Future of Trace Contaminant Analysis?

As regulations and public concern over contaminants like PFAS increase, laboratories must enhance efficiency, throughput, and accuracy while maintaining safety. Automated sample introduction is crucial for this, as it streamlines workflows, reduces solvent use, and expands analytical capabilities in trace contaminant analysis. This trend reflects a broader industry shift, with labs adopting robotics, AI, and integrated systems across sectors. The focus is now on where automation can have the most significant impact. Hiramatsu's work demonstrates how targeted automation addresses current analytical challenges and paves the way for smarter, faster, and safer labs.