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secrets of science
magazine

02/2026

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How a process engineer and a new online TOC analyzer keep microscopic defects off semiconductor wafers

Saving lives, money and reputation with a fast, new method of bacterial testing in food
Genome-guided MALDI TOF offers clear identification of *Bacillus cereus* group dangers

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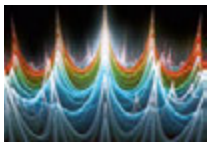


Resolve coeluting confusion with GC-MS deconvolution software

Streamlined workflow improves identification accuracy in complex mixtures

A bit like lasagna: Proper slicing and analysis show what packaging film is really made of

Microtome sections reveal their secrets with the AIRsight™ infrared and Raman microscope

Using electrochemistry-mass spectrometry to reveal tomorrow's contaminants, today

Sparking innovation in the prediction of chemical transformation products (TPs)

A security check for samples

How to protect your instruments and data – always?

Saving lives, money and reputation with a fast, new method of bacterial testing in food

Genome-guided MALDI TOF offers clear identification of *Bacillus cereus* group dangers

How do hospitals and clinical labs keep track of all their data?

LabGateway brings together complex information streams for better quality, traceability and productivity

Patrick Ducoroy, Sibylle Collard,
Shimadzu Chemistry & Diagnostics

Hospitals and laboratories face increasing pressure to improve productivity, reduce errors, ensure traceability and optimize workflows. Furthermore, they have to efficiently manage the information flows between instrumentation and the Laboratory Information System (LIS), including analytical processing and results. For this reason, it is essential to possess flexible, robust digital technology designed to meet this need: with a seamless interoperability across a range of individual software, reinforcing quality as well as traceability of analyses within the laboratory. High-quality middleware provides the answer – and delivers improvements in quality, traceability and productivity. This is precisely where LabGateway comes in.

In clinical laboratories and hospitals, the volume of data to manage has never been greater. Every sample generates a chain of information: sampling parameters, instrument data, consumables used, intermediate results, validation steps. Added to this are regulatory requirements, deadlines and the need to ensure flawless traceability. In this environment, the challenge is no longer simply a matter of producing reliable analyses, but of tracking and directing an ever-increasing flow of progressively dense and complex information.

LabGateway middleware was designed specifically to address these challenges. Conceived as a true bridge between instruments, information systems and laboratory teams, it offers a structured, fluid and secure approach to clinical data management. Its objective is clear: to enable professionals to focus on their biological expertise while providing them with a tool capable of orchestrating all technical data flows.

Because this issue is such a growing concern for the hospitals and clinical laboratories we all depend on, Shimadzu decided to act. The company was already intimately familiar with the digital complexity and data parameters of their own instruments, so they had a head start on developing a solution.

Here is what Patrick Ducoroy, Managing Director of the Clinical Department at Shimadzu Chemistry & Diagnostics, says: *"This software has been developed based on close observation of the field. Our design team, composed of software engineers with over fifteen years of experience working alongside biologists, understands the realities of technical platforms, the constraints of instruments and automats, traceability requirements and productivity challenges. We identified the key issues, including manual multiple re-entries, dispersed data, lack of visibility and complex integrations. And we decided to create a solution able to collect and structure all of that, in order to truly simplify daily operations for everyone involved."*

A plug-and-play software solution that connects the dots

Customizable and scalable

LabGateway middleware offers an automated, customizable and scalable solution for managing and monitoring the entire data and workflows within hospitals and clinical laboratories. It has been developed in such a way that it enables efficient integration into the existing environment. The solution is installed on a server and, thanks to its settings, connections are created between the various systems linked to the laboratory and its activities, and modules are activated in order to provide the necessary functionalities for performing and monitoring analyses. →

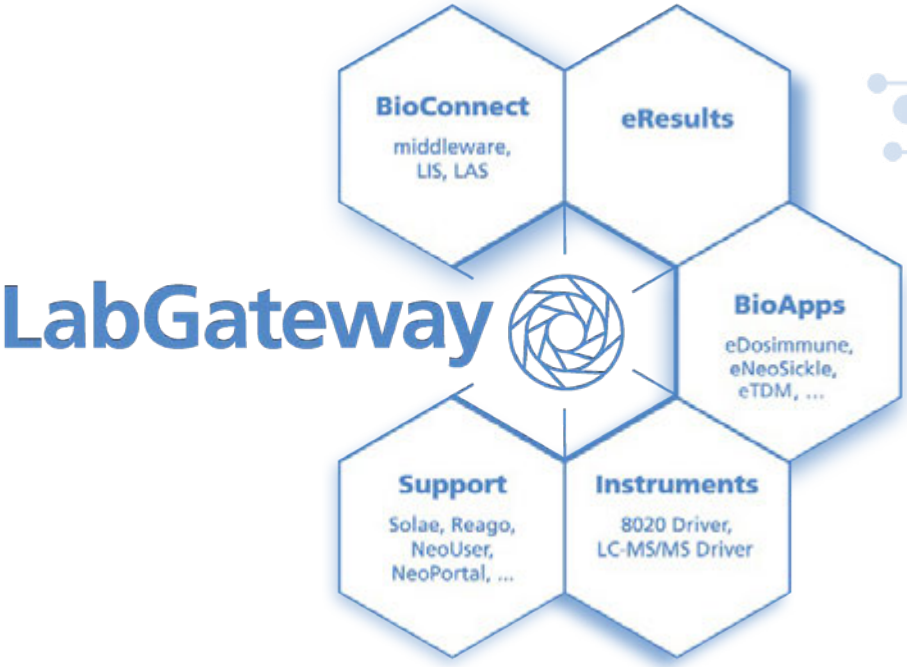


Figure 1: The middleware is composed of five main components, each with a targeted function. Depending on customer needs and the environment, LabGateway can be adapted to deploy the specific required components.

LabGateway's modularity makes it a tool that can be adapted to specific needs and allows users to add to or complete existing processes within the laboratory.

- **BioConnect module:** LabGateway can integrate with LIS or LAS systems through HL7 connectivity (a bi-directional communication protocol), ensuring communication and data integrity.
- **eResults module:** supports data interpretation while reducing the risks of manual errors.
- **BioApps module:** focuses on specific bio-applications (pathologies such as immunodeficiencies, sickle cell disease, etc.), improving the automated processing of raw data and facilitating the monitoring of pathological sample results.
- **Instruments module:** facilitates interconnectivity with laboratory instruments (e.g. LC-MS/MS, MADLI) and automation of analysis workflows through drivers.
- **Support module:** delivers a range of modules to configure and parameterize the middleware, ensuring the traceability of data from sample to results, including quality control data.

Metaphorically spoken, thanks to a user-friendly interface and easy configuration management (interface, connection, profiles, etc.), LabGateway transcends the term tool and becomes a real partner for hard-working laboratory teams.

Interpretation of multiple pathologies

Moreover, LabGateway allows the management of multiple pathologies within a single laboratory or hospital. Thanks to its BioApps module, the middleware can be used for various biological applications. It adapts and evolves according to laboratory needs and analytical applications, such as sickle cell disease screening or immunosuppressants.

The middleware collects all the information at each stage of the analytical process, and thanks to its optimized interface, the results of the analyses are contextualized and centralized while providing easy access to any data at any time, whether sample results, control quality results or the stability of instrumentation.

Connection with LIS

LabGateway establishes the link between the middleware and laboratory instruments; thus, the LabGateway solution enables the connection with the instrumentation and LIS using the HL7 protocol. This functionality provides strong connectivity between the laboratory systems and the LIS, allowing better traceability, automatized transfer of data, decreased manual errors and time savings, ensuring better quality of data.

An optimized traceability at every stage of your clinical analyses

LabGateway also centralizes and organizes all the data collected at every stage of analysis, improving laboratory operation management from samples, quality control and reagents, through instruments and automats, to the analysis and visualization of result data.

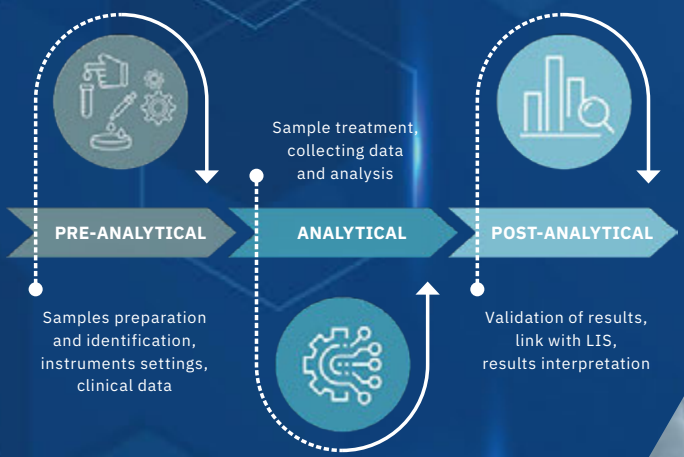


Figure 2: The traceability of the data is guaranteed at every analytical stage, from samples to results

Of particular interest in this context is that LabGateway collects, mostly **automatically,** the data generated by the instruments, automated equipment and peripheral systems. This reduces or eliminates the need to juggle between multiple interfaces or to manually check for consistency in data. All raw data collected is structured and integrated into a single, consistent flow. ⟶

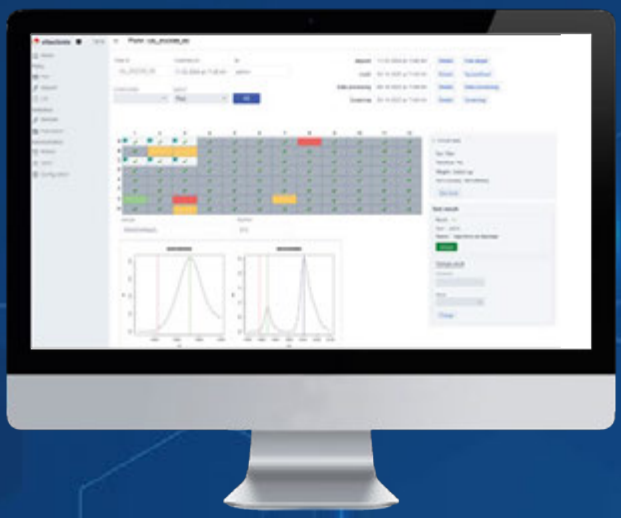


Figure 3: LabGateway enables the tracking and monitoring of all data and parameters, which are contextualized to facilitate the analysis and interpretation of results

LabGateway ensures the centralized management of all laboratory information. Sample data, results, technical parameters, consumables used, instrument events, etc. are organized in a clear, accessible and usable manner. This centralization reduces errors, improves analytical consistency and strengthens overall process quality.

Focused on traceability and compliance

Traceability is one of LabGateway's core strengths. Every step, every action, every interaction with an instrument, sample or consumable can be recorded.

Moreover, LabGateway middleware provides secure storage of all collected data. Information is stored reliably, can be accessed at any time and is organized to facilitate checks, verifications and retrospective analyses.

Beyond all of these functionalities, LabGateway delivers a built-in ability to adapt to any laboratory's organization, instruments and workflows. LabGateway quickly becomes a valued co-worker, helping laboratories streamline operations, reduce repetitive tasks and free up time for higher value activities.

In a sector where every minute matters and where data quality directly impacts patient care, having a reliable, robust and profession focused middleware makes a real difference. LabGateway solution offers a clever and concrete response to the current challenges facing laboratories: managing complexity, increasing efficiency and ensuring seamless traceability.

More than a technical tool, LabGateway is a partner designed to support laboratory teams, strengthen their expertise and enhance overall performance. It is an innovation designed to serve those who work hard to improve science and health every day.

Note

For more information and references, please refer to the digital version of this edition.

How green is your solvent – and how do you know?

GreenSOL is the first in-depth solvent greenness guide for analytical chemists

Elia Psillakis, Technical University of Crete, Greece

Eugenio Alladio, University of Torino, Italy

Alice Mondello, University of Messina, Italy

Paolo Oliveri, University of Genova, Italy

Francisco Pena-Pereira, University of Vigo, Spain

Analytical laboratories are shifting toward greener practices. As a result, solvents are often assessed and selected for their lower toxicity and safer profiles during laboratory handling. However, this narrow lens of assessment can create an illusion of greenness, where risks are simply relocated to another stage of the solvent's life cycle. A "greener" solvent may, in fact, be highly energy-intensive to manufacture or present a major challenge for waste treatment. True progress in green analytical chemistry requires looking deeper into the complete life cycle of solvents.

Solvents and the move toward more sustainable practices

Solvents are indispensable in analytical chemistry, directly impacting the outcome and reliability of the analytical results. While their consumption in analytical sciences is a fraction of industrial use, the cumulative volumes are still staggering: Liquid chromatography alone uses an estimated 150 million liters annually. Current trends, aligned with the principles of green analytical chemistry and green sample preparation, advocate the use of solvents that minimize environmental, health and safety (EHS) impacts as a critical strategy for mitigating the environmental footprint of analytical procedures and safeguarding laboratory personnel. In addition, initiatives to reduce solvent consumption (e.g., through miniaturization and the implementation of recovery, reuse and recycling strategies) support the broader goals of circular analytical chemistry and advance sustainability in the field. These developments are further propelled by increasingly stringent regulations on solvent usage and disposal, alongside a growing emphasis on greener laboratory practices.

The GreenSOL solvent life cycle story

For decades, solvent selection in analytical chemistry has lacked a clear, evidence-based guide tailored to its distinct needs. While solvent guides existed, they were designed primarily for industrial synthesis rather than analytical applications. To address this gap, a European team of researchers – guided by the principles of green and circular analytical chemistry – has developed GreenSOL, the first comprehensive solvent selection guide designed specifically for analytical applications.

To assess greenness, GreenSOL adopts a life cycle approach and evaluates each solvent across its production, laboratory use and waste phases. First published in TrAC-Trends in Analytical Chemistry GreenSOL is more than a high-impact scientific paper, it's a practical guide, accompanied by a free, interactive, web-based tool empowering analysts to make informed solvent choices. GreenSOL evaluates 49 common and niche solvents, selected to ensure broad coverage of chemical classes and physicochemical properties relevant to analytical workflows. In addition, nine deuterated solvents are included: These have previously been overlooked in solvent guides.

GreenSOL
supported by SHIMADZU

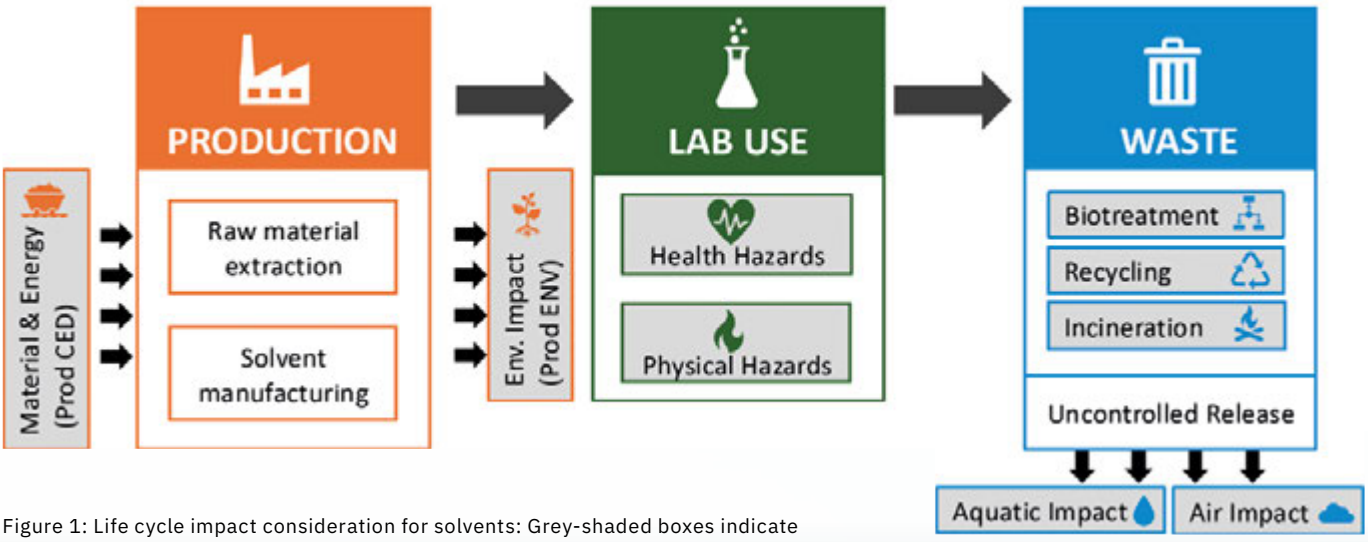


Figure 1: Life cycle impact consideration for solvents: Grey-shaded boxes indicate the impact categories considered for solvent assessment

The three phases of assessment: Production, use and waste

A large part of GreenSOL's uniqueness lies in its three-phase life cycle evaluation system (Figure 1). Each of the three phases depends on multiple attributes and has subcategories. GreenSOL ensures that a single solvent characteristic (e.g., high volatility) is appropriately accounted for within each phase while preventing multiple penalties for the same characteristic.

In GreenSOL, individual subcategories are assessed on a scale of 1–10 (1 = least favorable, 10 = most recommended) and then combined to generate a composite score for each phase. Composite phase scores are helpful for a quick overview, but the real strength of the guide lies in the detailed subcategory breakdown. GreenSOL presents this comprehensive perspective, empowering analysts to prioritize criteria based on their specific application and operational context.

The detailed results of the solvent assessments are presented in Table 1. A color-coding scheme is applied to scores within each category and subcategory to facilitate the visual comparison of solvent performance. The colors used are: red (1 ≤ score ≤ 3), yellow (4 ≤ score ≤ 7) and green (8 ≤ score ≤ 10).

In many ways, GreenSOL is full of surprises, precisely because it exposes an uncomfortable reality: Solvent greenness is a complex, multi-layered compromise rather than a simple label. Our results powerfully reinforce the need to evaluate the entire life cycle. For instance, hexane's lab use score was, as expected, very poor. However, its proposed "greener" replacements reveal their own trade-offs. While pentane reduces laboratory risks, it has a substantial environmental impact in the event of an uncontrolled release. Meanwhile, heptane lowers health risks but retains high physical hazards and poses a greater risk to aquatic species. →

GreenSOL		PRODUCTION		USE		WASTE						
Solvent	CAS Number	Prod CED	Prod ENV	Physical Hazards	Health Hazards	Aquatic Impact	Air Impact	Waste ENV	Biotreat.	Recycling	Incineration	Waste Treat.
Acetone	67-64-1	6	9	7	5	10	4	6	6	2	2	3
Acetonitrile	75-05-8	3	8	7	3	10	4	6	9	2	3	4
Benzene	71-43-2	7	9	4	1	6	5	5	9	4	6	6
Benzyl alcohol	100-51-6	3	7	10	6	10	8	9	10	6	4	6
Butan-1-ol	71-36-3	6	9	9	4	10	8	9	10	7	6	7
Butan-2-ol	78-92-2	3	8	9	4	10	8	9	10	6	4	6
N-butyl acetate	123-86-4	4	8	7	5	7	8	7	10	7	6	7
N-Butylpyrrolidinone	3470-98-2	1	6	9	6	8	8	8	6	5	1	3
Carbon disulphide	75-15-0	7	8	2	1	5	4	4	5	4	4	4
Carbon tetrachloride	56-23-5	7	8	5	1	4	1	2	2	7	6	5
Chlorobenzene	108-90-7	4	7	8	3	3	8	4	6	9	6	7
Chloroform	67-66-3	7	1	9	1	9	4	6	2	7	5	4
Cumene	98-82-8	5	9	9	2	2	9	4	10	8	7	8
Cyclohexane	110-82-7	5	9	3	4	2	8	4	8	3	6	6
1,2-Dichlorobenzene	95-50-1	4	6	9	5	1	4	2	6	8	4	6
Dichloromethane	75-09-2	7	7	9	3	9	3	5	1	7	6	4
Diethanolamine	111-42-2	4	8	9	6	8	8	8	10	5	2	4
Diethyl ether	60-29-7	2	8	1	2	5	4	4	1	1	4	2
Diisopropyl ether	108-20-3	7	9	4	4	10	6	8	6	3	6	5
Dimethyl sulfoxide	67-68-5	7	5	9	10	10	8	9	10	5	2	5
N,N-Dimethylacetamide	127-19-5	4	8	10	3	10	8	9	10	6	3	6
N,N-Dimethylformamide	68-12-2	5	9	9	2	10	8	9	10	5	3	6
1,4-Dioxane	123-91-1	1	8	3	2	10	8	9	3	4	3	3
Ethane-1,2-diol	107-21-1	7	9	10	8	10	9	9	10	4	1	4
Ethanol	64-17-5	9	9	7	9	7	9	8	9	2	3	4
Ethyl acetate	141-78-6	5	8	7	4	9	8	8	8	2	3	4
Ethyl tertiary butyl ether	637-92-3	7	9	4	3	10	6	8	6	2	4	4
Heptane	142-82-5	9	10	3	5	1	7	3	10	5	6	7
Hexane	110-54-3	10	10	3	1	4	6	5	7	3	6	5
Isobutyl acetate	110-19-0	5	8	7	7	7	7	7	10	6	6	7
Isopropyl acetate	108-21-4	5	8	7	4	10	7	8	9	3	4	5
Methanol	67-56-1	9	10	7	3	10	5	7	8	2	3	3
Methyl acetate	79-20-9	7	9	7	4	9	3	6	5	1	1	2
4-Methylpentan-2-one	108-10-1	4	8	7	3	9	6	7	10	6	3	6
2-Methylpentane	107-83-5	8	9	3	4	2	6	4	6	3	6	5
N-Methylpyrrolidone	872-50-4	1	6	9	3	10	8	9	10	4	2	4
Octan-1-ol	111-87-5	1	9	9	6	2	8	4	10	8	6	8
Pentane	109-66-0	7	9	7	5	3	2	2	3	6	10	6
Pentan-1-ol	71-41-0	4	8	9	6	10	8	9	10	7	5	7
Propan-1-ol	71-23-8	5	8	7	5	10	7	8	10	4	3	5
Propan-2-ol	67-63-0	8	9	7	5	10	10	10	10	2	4	4
Propane-1,2-diol	57-55-6	4	7	10	10	10	8	9	10	5	2	4
Propyl acetate	109-60-4	2	7	7	5	8	8	8	10	7	6	7
Pyridine	110-86-1	1	4	7	4	8	8	8	8	5	4	5
Tetrachloroethylene	127-18-4	7	6	10	4	2	6	4	3	10	5	6
Tetrahydrofuran	109-99-9	1	7	7	3	10	5	7	2	2	4	3
Toluene	108-88-3	7	9	4	2	5	7	6	10	6	7	8
Triethanolamine	102-71-6	4	8	9	10	10	8	9	10	5	2	4
Water	7732-18-5	10	10	10	10	10	10	10	10	4	3	5

Table 1: ▲ ► Individual category scores of solvents, including composite scores for the waste phase subcategories of environmental impact (Waste ENV) and treatment potential (Waste Treat.)

GreenSOL		PRODUCTION		USE		WASTE						
Solvent	CAS Number	Prod CED	Prod ENV	Physical Hazards	Health Hazards	Aquatic Impact	Air Impact	Waste ENV	Biotreat.	Recycling	Incineration	Waste Treat.
Acetone-d6	666-52-4	6	9	7	4	10	3	6	4	1	2	2
Acetonitrile-d3	2206-26-0	3	8	7	4	10	3	6	9	2	3	4
Benzene-d6	1076-43-3	6	9	4	1	5	5	5	8	3	6	5
Chloroform-d	865-49-6	8	1	8	2	9	4	6	1	6	5	3
Deuterium oxide	7789-20-0	10	10	10	10	10	10	10	10	4	3	5
Dichloromethane-d2	1665-00-5	7	7	9	2	9	3	5	1	7	6	4
Dimethyl sulfoxide-d6	2206-27-1	7	5	9	10	10	8	9	10	6	3	6
Methanol-d4	811-98-3	9	10	7	3	10	3	5	3	2	3	3
Toluene-d8	2037-26-5	7	9	4	4	5	7	6	10	6	7	8

A digital tool for evidence-based decision-making

Understanding that a static table in a paper has limited daily utility, the team developed an interactive, free web application with the assistance of Shimadzu (https://greensol.tuc.gr/). This is where GreenSOL really comes to life, transforming it from an academic exercise into a decision-support system for routine lab work, method development and educational training. Analysts can filter solvents based on the physicochemical properties they need (e.g., boiling point, polarity or water solubility) and instantly see how the candidates rank in terms of greenness. They can also compare solvents within the same chemical family, find viable alternatives or create custom 2D and 3D plots to visualize trade-offs between production, use and waste scores.

Another actionable step labs can take to reduce their impact is to set and enforce green procurement and safety standards using GreenSOL's scores. This can be achieved by excluding any solvent with a critically poor score in a non-negotiable category, such as health hazards. For commonly used solvents that are difficult to replace, analysts can use subcategory scores to select the option with the lowest overall burden, making informed trade-offs between, for example, production energy demand and waste treatment viability.

GreenSOL aligns with a powerful shift in the field: the move toward circular analytical chemistry. This philosophy emphasizes minimizing waste, recovering resources and designing inherently sustainable processes. By highlighting the waste phase, labs are encouraged to think about solvent recovery and reuse. A waste treatment strategy can be built by using waste-phase data. For solvents with high recycling scores, implementing even simple on-site recovery can turn a costly lab into a circular asset.

Using the truth constructively

GreenSOL highlights that true solvent greenness is not about finding a perfect choice but about navigating inevitable trade-offs with responsibility and insight. Transparency is essential to prevent burden-shifting from one life cycle stage to another. A reliable guide must reveal these compromises rather than conceal them: Focusing solely on toxicity may ignore a high energy burden, while optimizing only for production could create a downstream waste problem. This holistic approach raises the question: Are we solving one issue by creating another elsewhere in the solvent's life? This shift to life-cycle thinking is the fundamental lesson.

The search for a perfectly "green" solvent is like chasing a myth. No single solvent satisfies all criteria across its entire life cycle. Instead, our practical goal should be to make informed choices that minimize overall environmental and health impacts. In fact, the biggest gains from our considerable efforts to reduce solvent impacts are achieved through reductions in solvent use and method optimization.

The ultimate message is clear: The greenest solvent is the one you do not use. But when a solvent is necessary, selecting the greenest option is now a guided, evidence-based decision. GreenSOL provides the missing map for this journey, marking the path to more sustainable laboratories and a better future.

Note

For more information and references, please refer to the digital version of this edition.

Trust algorithms over eyeballing

Fast, reliable color analysis according to European Pharmacopoeia using Multi Data Report

Dr. Benjamin Thomas, Shimadzu Europa GmbH

Color intensity is an important quality criterion for pharmaceutical products. Color plays a crucial role in how we judge a liquid's quality, freshness and safety. Even a slight brownish tint in clear water can signal dangerous contamination. For this reason, the color intensity of liquids is fully tested in pharmacopoeias such as the European Pharmacopoeia (Ph. Eur.).

In many laboratories, this assessment is still carried out visually, with specialists repeatedly comparing samples to reference standards. It works – but it's time-consuming, strains the eyes and highly depends on lighting conditions and the individual's color perception. It's about time for a better solution!

Let the technology do the work – you put the kettle on

Iro has a headache. Day after day, the pharmacy technician has to analyze samples according to Ph. Eur. Time for a break! She makes herself a cup of tea to relax, and as she looks into the cup, a thought occurs to her: Why not automate the tedious process?

A made-up scenario – but one that reflects reality in many laboratories and inspired an intuitive software solution designed to make life easier for many professionals: LabSolutions Multi Data Report (MDR). Independent of lighting and human perception, it's almost as easy as making tea.

Capturing every shade: Ph. Eur. color grades and CIELAB coordinates

The European Pharmacopoeia differentiates between 37 color grades of brown, yellow and red in varying intensities. Since the qualified medicinal products are clear liquids, the specified colors are very faint, with only very subtle differences between the individual standards. Relying solely on visual comparison can therefore be difficult, particularly under poor lighting conditions or with impaired vision.

To address this, a revision of Ph. Eur., chapter 2.2.2, introduced instrumental assessment using CIELAB color values as an alternative approach. The CIELAB color space describes every color using a three-dimensional coordinate system, as shown in Figure 1.

The L* axis represents lightness: Pure grayscale values have an L* value between 0 (black) and 100 (white), while all other coordinates are 0. The perceived color of a colored sample can be defined in two ways:

- Polar coordinates (C* and h°)
- Cartesian coordinates (a* and b*)

L* is referred to as the "lightness index," regardless of whether Polar or Cartesian coordinates are used. In Polar coordinates, C* is referred to as "chroma" and h° as the "hue angle." The hue angle h° describes the angle relative to the a* axis, ranging from red (0°) through yellow (90°), green (180°) and blue (270°). The perceived color becomes more intense with increasing chroma, i.e., with greater distance from the L* axis. →

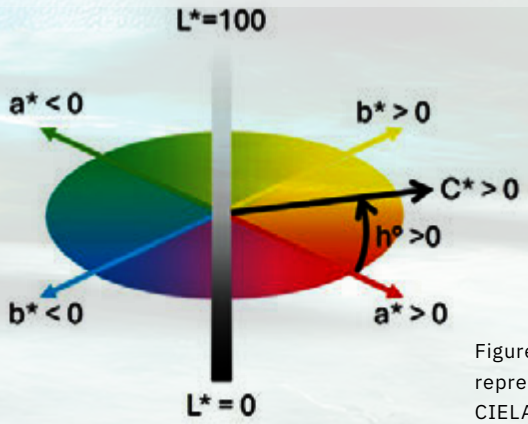


Figure 1: Schematic representation of CIELAB coordinate system including color wheel

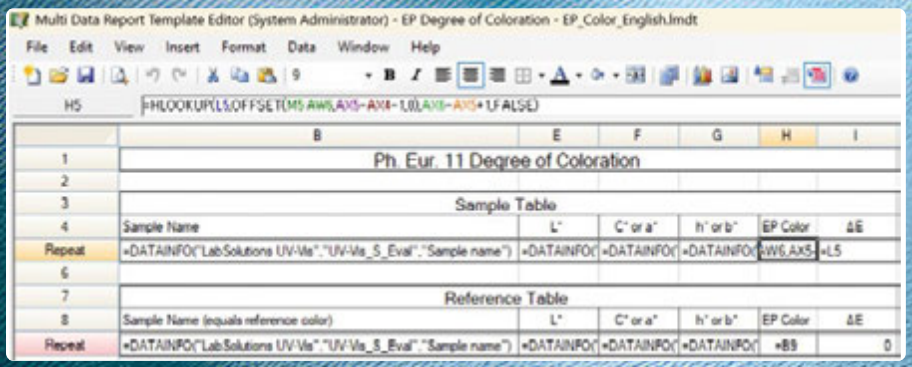


Figure 2: LabSolutions Multi Data Report Template Editor for editing report templates with formulas

Template: EP Degree of Coloration - EP_Color_English.lmdt (Template Signature: 1/23/2026 10:56:52 AM(+01:00) : Confirm[System Administrator])

EP 11 Degree of Coloration

Sample Table						Raw Data Signature		
Sample Name	L*	Chroma	Hue	Color	ΔE	Status	Date	Name
Mint	71.481	75.994	86.867	GY1	32.23	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Italian Lemon	84.588	31.081	91.620	B1	7.54	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Apple	72.449	59.239	82.521	GY2	36.89	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Herbal Tea	61.786	91.511	73.776	GY1	51.22	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Blueberry	55.890	56.977	44.373	R1	56.18	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Forest Berry	55.908	59.808	49.565	R1	56.34	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor
Chamomile	92.707	26.302	99.977	BY1	4.34	Confirmed	1/23/2026 10:39:40 AM(+01:00)	Viktor

Figure 3: Print preview of the LabSolutions Multi Data Report showing chroma and hue analysis

The Cartesian coordinates were defined to be as intuitive as possible: a* describes the red (positive values) or green (negative values) color component, while b* describes the yellow (positive values) or blue (negative values) color component.

Automated analysis

Calculating color differences in the CIELAB system reduces the influence of lighting and individual color perception, as the spectrometer measures under reproducible conditions without stray light.

The UV-1900i Plus with LabSolutions DB software has been optimized for use in pharmaceutical laboratories and allows reliable measurement and analysis in full compliance with data integrity requirements. However, since each sample still has to be compared with 37 standards, the final analysis continues to be time-consuming. The optional Multi Data Report within LabSolutions Manager offers an effective solution here.

The template for analysis according to Ph. Eur., chapter 2.2.2, is shown in edit mode in Figure 2 and is described in detail in Application Note SCA-100-28. The advantage is that formulas and raw data placeholders are built into a template that can only be edited by designated individuals, depending on assigned user rights. Only when the final report is generated from the MDR template and the raw data sets, the predefined placeholders are populated with data and a PDF document is created.

Both the templates and the raw data, as well as the final reports, can be digitally signed and protected against unauthorized modification. Manually modifying formulas or individual values in the report is not permitted. Every step of the analysis is fully documented in the audit trail.

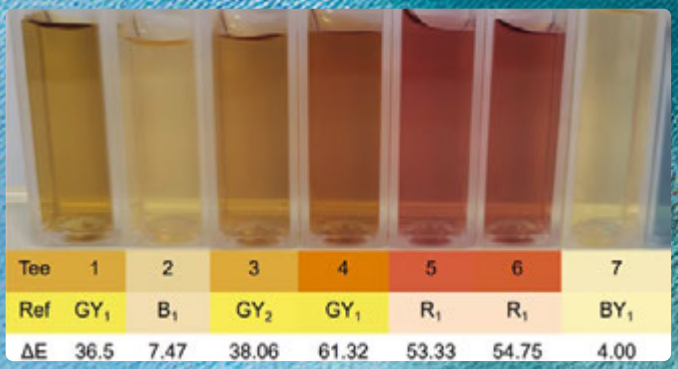


Figure 4: Tea samples and their corresponding Ph. Eur. color grades: Mint (GY_1), Italian Lemon (B_1), Apple (GY_2), Herbal Tea (GY_1), Blueberry (R_1), Forest Berry (R_1) and Chamomile (BY_1) (from left to right)

Time for a tea break: Example measurement from Mint to Chamomile

Various tea varieties were analyzed as a practical example of color analysis. The print preview of the resulting Multi Data Report is shown in Figure 3.

The status of the electronic signature for each raw data set is clearly visible in these reports. The specific assignments of samples to reference solutions are identical, regardless of which type of color coordinates is used.

Figure 4 shows the analyzed tea samples and their assigned Ph. Eur. color grades. The calculated CIELAB colors of each sample and its corresponding reference solution are shown below the image to facilitate clearer visualization. The analyzed tea varieties (from left to right in Figure 4) are Mint (GY_1), Italian Lemon (B_1), Apple (GY_2), Herbal Tea (GY_1), Blueberry (R_1), Forest Berry (R_1) and Chamomile (BY_1), each prepared according to the instructions.

For practical use in a quality control laboratory, the Multi Data Report template can be expanded with pass/fail judgements in just a few clicks by defining the expected color grade of each sample prior to measurement. For clearer presentation of the results, conditional cell formatting can be applied, similar to that used in standard spreadsheet software.

The formerly visual analysis of Ph. Eur. color grades is now handled automatically thanks to LabSolutions Multi Data Report. To illustrate the approach, tea samples were analyzed, and their color classification meets expectations. Automation via LabSolutions not only simplifies the analysis for users, but also enables verifiability via digital signatures and plausibility checks that can be implemented quickly and without specialized expertise. That means less hassle and more time for relaxing with a cup of tea.

Note
For more information and references, please refer to the digital version of this edition.

How to diagnose and fix retention time fluctuations

Dr. Anna Cooper, Shimadzu UK

Expert troubleshooting: Tips for stable HPLC retention times and reliable results

If retention times in high-performance liquid chromatography (HPLC) drift or fluctuate, even selective detectors cannot guarantee correct identification. Controlling and understanding retention time is therefore essential for robust HPLC methods. This article – the second in a series on troubleshooting for users of lab instrumentation – introduces the major factors that cause retention time fluctuations and offers practical ways to diagnose and correct them.

Troubleshooting HPLC retention time fluctuations

Retention time is one of the most important parameters in HPLC. It is used to identify analytes, to check system suitability and to judge method robustness. Modern HPLC systems typically use UV-Vis, fluorescence or refractive index (RI) detection. While optical detectors such as UV-Vis and fluorescence are often highly selective for compounds with chromophores or fluorophores, they all rely on one fundamental assumption: that the chromatographic system produces reproducible retention times.

Figure 1: Example of chromatogram with retention time shift

If retention times drift or fluctuate, even selective detectors cannot guarantee correct identification. Peaks may fall outside the predefined time window or even swap elution order, leading to ambiguous or incorrect results. Controlling and understanding retention time is therefore essential for robust HPLC methods.

What are the main causes of retention time fluctuations, and how can they be identified, fixed or even prevented? ⟶

1. Temperature – a silent but powerful parameter

Temperature has a direct influence on retention in both reversed-phase and normal-phase HPLC. As temperature increases:

- the viscosity of the mobile phase decreases;
- column backpressure falls;
- the interaction between analyte and stationary phase is altered.

A common rule of thumb is that **a change of 1 °C can shift retention time by about 1–2 %**, with late eluting analytes usually being affected more strongly than early ones. In practice, this means that a seemingly minor fluctuation of 3–5 °C can noticeably change total runtime and elution order.

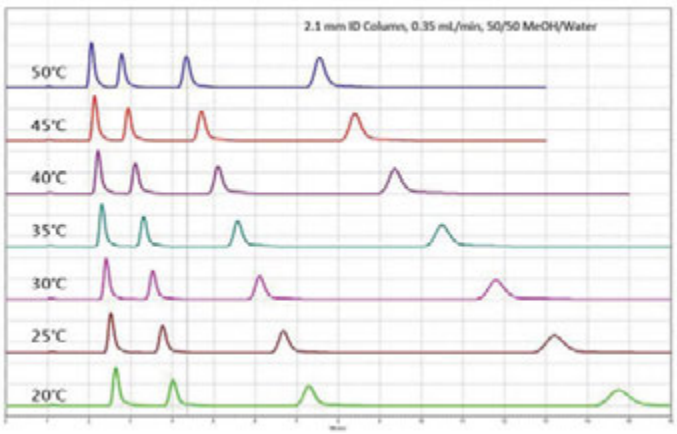


Figure 2: Retention time shifts for four parabens measured at different temperatures

Temperature changes do not affect all analytes equally. For example, sorbic acid and benzoic acid might be baseline-separated at 20 °C but coelute at 30 °C, and further temperature increases may even reverse their elution order. If such effects are not noticed, samples can be misidentified or reported incorrectly.

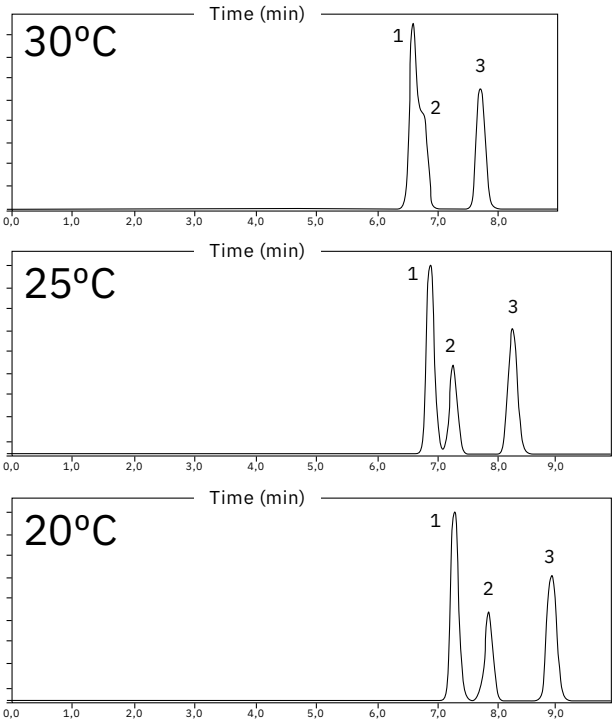


Figure 3: Separation of sorbic acid (1), benzoic acid (2) and methylparaben (3) at 20 °C, 25 °C and 30 °C

For larger analytes, temperature can also induce conformational changes (e.g., partial unfolding or rearrangement of secondary/tertiary structure), exposing or masking interaction sites and thereby affecting retention, selectivity and peak shape.

Shorter run times are not always advantageous
Chromatograms of paraben mixtures measured at 20 °C and 50 °C typically show that the overall analysis time at 50 °C is almost halved. This can be useful when wishing to speed up a method, provided the column's maximum temperature is respected. However, higher temperatures can reduce column lifetime by creating a harsh environment for the silica backbone, particularly with acidic or neutral pH conditions.

2. Flow rate – diagnosing pump-related retention drift

The second major factor controlling retention time is the flow rate. In both gradient and isocratic runs, the retention factor and the gradient profile are expressed relative to the flow rate. Any deviation from the programmed flow has a direct effect on retention time.

Wear and tear in the pump
HPLC pumps contain consumable parts such as:

- Piston seals
- Check valves
- Pump heads and pistons

Over time, these components wear and may become leaky or fail to seal properly. The result is a flow rate that is lower or unstable compared to the set value. Retention times begin to drift or scatter, often accompanied by pressure fluctuations.

Simple pump check
The easiest way to check the pump performance is by calibrating it. Use a graduated cylinder and connect a backpressure capillary directly to the pump, setting a defined flow rate. Then compare the time it takes to deliver a specified volume against the expected flow rate to check for discrepancies.

Significant deviations indicate that seals, check valves or other pump components may require maintenance or replacement. It's important to regularly inspect the consumables in your HPLC system and keep spare parts on hand to quickly replace any faulty components.

Practical tips:
- Establish a **regular pump calibration routine** and document results.
- Replace piston seals, check valves and other consumables at defined intervals or when flow problems are suspected.
- Monitor system pressure and flow-integrated readouts; unstable baselines or erratic pressure are often early warning signs.

3. Eluent effects – the mobile phase as a source of drift

In many laboratories, retention time fluctuations can be traced back to the mobile phase. Even small changes in composition, density or preparation procedure can significantly alter elution strength.

3.1. Inadequate re-equilibration in gradient runs
Reversed-phase-methods often use gradients and a strong organic wash step to remove strongly retained analytes. After such a step, the column must be fully re-equilibrated to the initial conditions before the next injection.

If the equilibration time is too short:
- the column will contain a significant fraction of the strong solvent;
- the effective starting composition will be more organic than intended;
- retention times will shorten from run to run or show oscillating patterns.

A common guideline is to allow **at least 10 column volumes** for equilibration in reversed-phase chromatography and significantly more for normal-phase, Hydrophilic Interaction Liquid Chromatography or ion-pair methods.

If the equilibration is too short, it can lead to retention time fluctuations or, as shown in Figure 5, progressively shorter retention times from measurement to measurement due to the strong solvent still on the column. In this case, the column is no longer in equilibrium. →

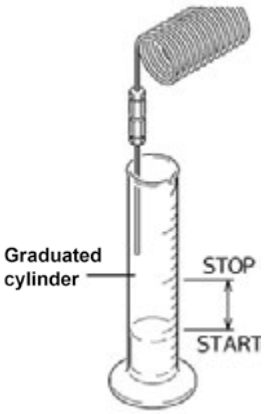


Figure 4: Pump check using a graduated cylinder and backpressure capillary

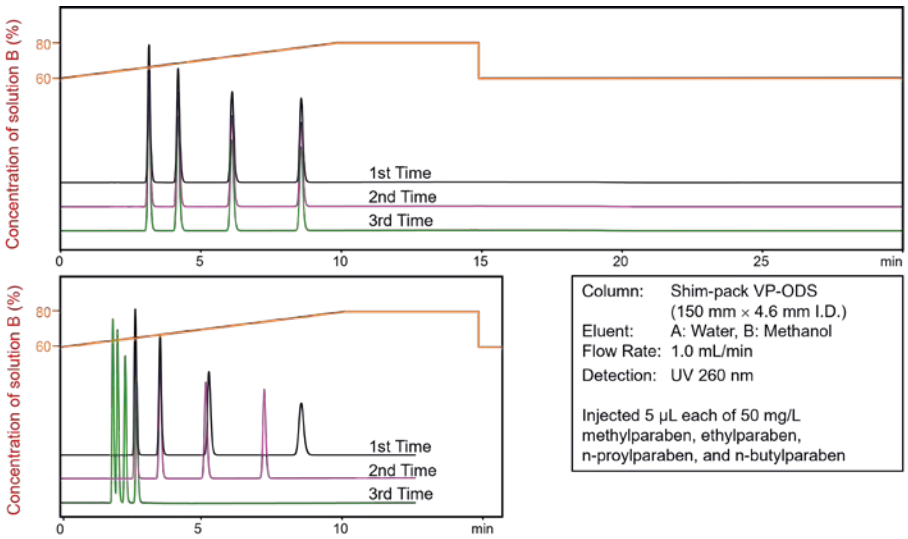


Figure 5: Effect of insufficient column equilibration

3.2. Changes in eluent composition during storage

Mobile phases must be protected from evaporation and contamination. If bottles are left open or inadequately sealed:

- organic solvent content can change (e.g., acetonitrile evaporating from a water/acetonitrile mixture);
- the elution strength decreases over time, leading to progressively **longer retention times**;
- oxygen uptake or CO_2 absorption can alter pH, especially in unbuffered aqueous phases;
- bacterial growth can also form in aqueous mobile phases which can impact on the performance of the instrument.

Practical tips:

- Use **properly sealed, chemically compatible bottles**.
- Label eluents with **preparation date, composition and preparer's initials**.
- Avoid exposing eluents to direct sunlight or to the cold airflow of air conditioners.
- Use carbon filters on the solvent bottles to limit solvent evaporation and improve the health and safety in the laboratory.

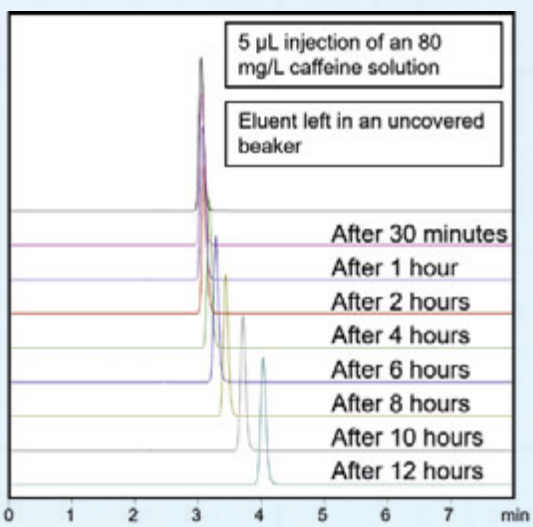


Figure 6: Effect of eluent evaporation from an unsealed eluent bottle

3.3. Inconsistent eluent preparation

Even when the correct solvents are used, preparation mistakes can lead to differences in elution strength.
A classic example is the preparation of a “50 % methanol in water” mobile phase:

Tech 1:

- **Water/methanol = 1/1 (v/v)**
- Measure 500 mL of water and 500 mL of methanol separately, then mix them together.
- The total volume created is not 1 L but 0.94 L.

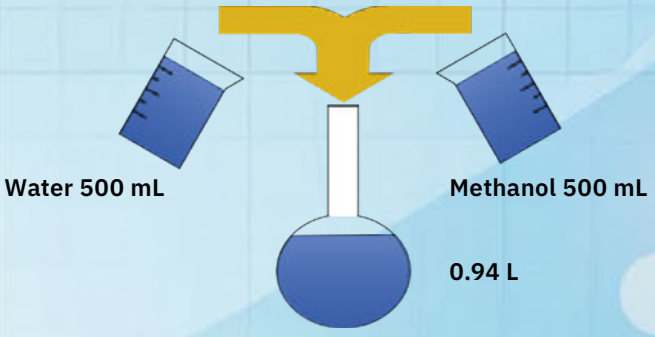


Figure 7: Example eluent preparation: water/methanol = 1/1 (v/v)

Tech 2:

- **50 % (v/v) methanol-water solution**
- Add 500 mL of methanol to a 1-L volumetric flask and fill up to 1 L with water.
- The total volume created is 1 L, with a higher proportion of water when compared with the previous example.

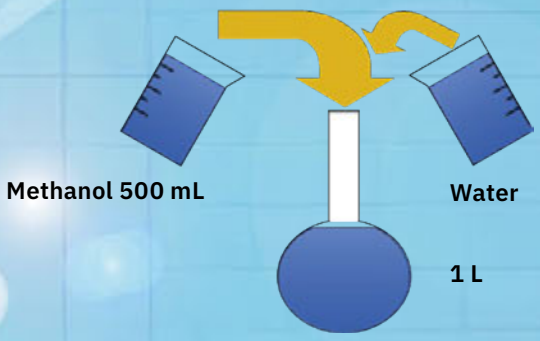


Figure 8: Example eluent preparation: 50 % (v/v) methanol-water solution

Both analysts might call their solution “50 % MeOH,” but in practice these two solutions have different elution strengths, as seen in the following example with a phosphate buffer and acetonitrile. The retention times of the individual analytes fluctuate significantly and, in the worst case, can fall outside the identification time window. ⟶

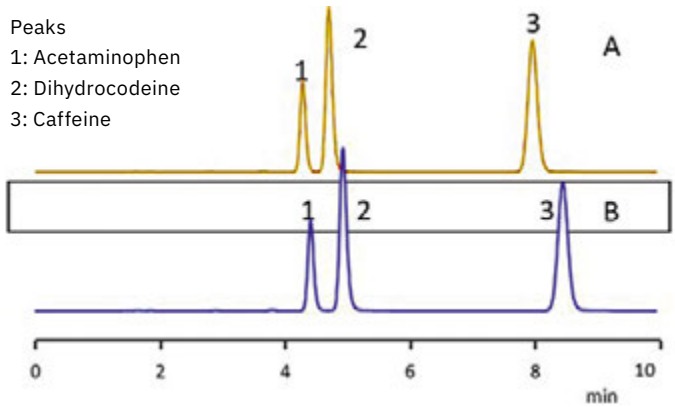


Figure 9: Retention time shifts caused by differences in mobile phase preparation methods

Mobile phase A:
20 mmol/L sodium(phosphate) buffer
<pH 2.5>/acetonitrile = 9:1 (v/v)

Mobile phase B:
20 mmol/L sodium(phosphate) buffer
<pH 2.5> containing 10 % (v/v) acetonitrile

Practical tips to avoid this:
- Always define whether concentrations are **% (v/v), % (w/w) or % (w/v)**.
- Use **volumetric glassware** and written SOPs for eluent preparation.
- Whenever possible, have mobile phases prepared from **concentrated stock solutions** or directly by the instrument's proportioning system.
- For critical applications, consider using **commercially premixed mobile phases** to eliminate operator variability.

4. Other causes of retention time drift

Beyond temperature, flow and eluents, several additional factors can cause retention time fluctuations:
- **Insufficient buffer capacity** or incorrect buffer pH
- Poor online mixing in low-pressure gradient systems
- A **partially dried-out or contaminated column**, especially after storage in pure organic solvent or 100 % aqueous phase in reversed-phase systems
- Column aging or damage (loss of bonded phase, voids)

Practical tips if fluctuating retention times occur:
- Verify **temperature control**.
- Check the **pump** and **flow calibration**.
- Prepare **fresh eluents** using a validated procedure and compare retention times for reference standards.
- If problems persist, test with a **new column** to distinguish between column-related and system-related causes.

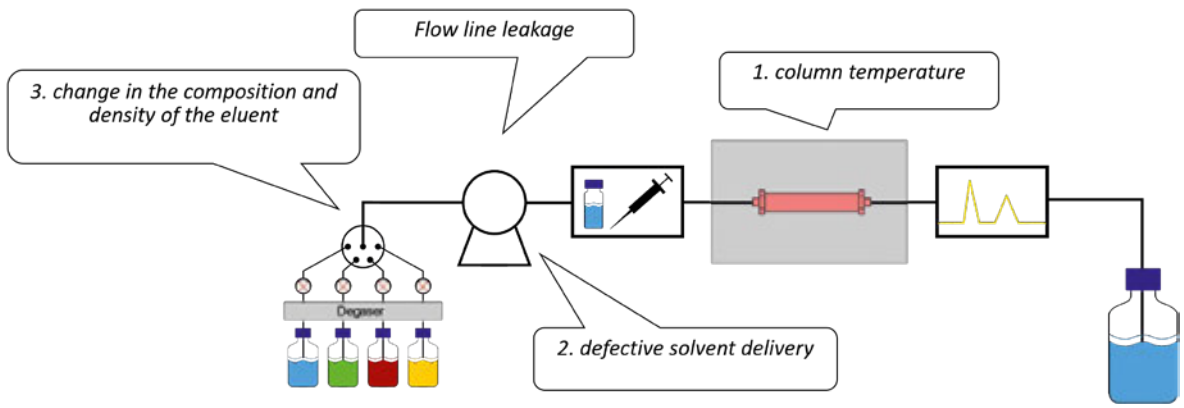


Figure 10: Common causes of retention time drift in HPLC: column temperature, solvent delivery issues and changes in eluent composition or density

5. Practical checklist – keeping retention times under control

General
- ☐ Run system suitability tests with reference solutions and document retention times and resolution.
- ☐ Keep a **column diary** (number of injections, mobile phase used, storage conditions) and a **maintenance log** for the instrument.

Temperature
- ☐ Always use a **column oven** when retention time stability is important.
- ☐ Avoid large changes in laboratory temperature and air drafts around the column compartment.

Flow/Pump
- ☐ Perform regular **pump performance checks** and replace consumables on schedule.
- ☐ Monitor system pressure for unusual fluctuations or gradual changes.

Eluents
- ☐ Develop and follow **SOPs for eluent preparation**.
- ☐ Store eluents in sealed containers, correctly labeled and away from heat or direct sunlight.
- ☐ Allow adequate **re-equilibration time** after gradient runs or solvent changes, especially for:
  - Normal-phase methods
  - Reversed-phase methods with ion-pair reagents
  - Methods using 100 % aqueous mobile phases

Problematic conditions to watch
- ☐ Reversed-phase runs with **100 % aqueous eluent**
- ☐ Highly acidic or moderately to strongly alkaline eluents (typically pH > 7) on silica-based columns
- ☐ Long idle times without flow, especially with buffered or saline mobile phases

Final thoughts

Fluctuations in retention time are more than an annoyance: They directly affect the reliability of qualitative and quantitative results. Often small and easily overlooked issues – like a slightly warm laboratory, a worn pump seal or a loosely capped eluent bottle – are enough to destabilize retention and invalidate results.

By systematically considering temperature, flow rate, eluent preparation and column condition, most retention time problems can be diagnosed and solved quickly. Careful documentation, robust methods and a few simple daily checks go a long way toward ensuring that retention times remain stable – and that your HPLC data remains trustworthy.

Note
For more information and references, please refer to the digital version of this edition.

Hungry water: Ultrapure water monitoring in the nanometer fab

How a process engineer and a new online TOC analyzer keep microscopic defects off semiconductor wafers

Markus Janssen, Shimadzu Europa GmbH

In a modern semiconductor fab, yield – the percentage of working chips produced on a single silicon wafer – decides whether a new process is profitable. Yet even in spotless cleanrooms, invisible contaminants in the rinse water can undermine months of optimization. This story follows process engineer Lena as she traces an unexpected rise in wafer defects back to the "hungry water" that washes every layer, and how online total organic carbon monitoring helps her see what the water has been hiding.

Red alert: A silicon wafer map exposes a threat

On a night shift in a modern semiconductor fabrication plant, or fab, process engineer Lena stands at an inspection station inside the cleanroom, wrapped head to toe in a "bunny suit" that hides everything but her eyes. In front of her, a monitor shows a wafer map: a neat grid of fields, each representing one future chip. On a stable production line, most of those fields light up green; a few red spots are normal. Tonight, as the inspection finishes, far more red dots than usual begin to blossom across the screen.

Those colors summarize what the fab calls “yield”: the percentage of chips on a wafer that pass all tests. When a new process is ramped up, yield can begin at only about every second chip working and then climbs toward well above 90 % as engineers identify and remove sources of defects. Every percentage point gained means more working chips from the same expensive wafer. A map with too much red therefore makes Lena’s stomach tighten. The air is filtered, the machines are humming along, and the chemicals are all within specification. Yet, some wafers keep failing. Somewhere in the process, something is slipping through – something microscopic – and sabotaging production and, ultimately, profit.

How a silicon wafer becomes a chip

Integrated circuit – chip – production starts with a thin, mirror-shiny disc of ultrapure silicon. On this single wafer, dozens or even hundreds of identical chips are manufactured in parallel. Layer by layer, tiny “wires,” transistors and insulating structures are built up on the surface. It is a bit like constructing a city with sewers, streets, bridges and high-rises, only that everything is measured in nanometers, one-billionth of a meter.

The layers are created in a repeating rhythm. First, the wafer is covered with an extremely thin film of material, for example an insulator or a metal. Then a light-sensitive coating of photosensitive resins – the photoresist – is applied. Using a high-precision optical system, patterns are exposed into this photoresist with ultraviolet light. The exposed parts are developed and washed away, and the underlying film is etched or “doped” only where structures should remain. Afterwards, everything is cleaned, sometimes polished, and the sequence starts again for the next layer. This cycle is repeated hundreds of times until billions of transistors are in place and the wafer is ready to be diced into individual chips.

Figure 1:
TOC-1000e S

Hungry water and huge volumes

Every layer added to the wafer is washed and cleaned before the next one can be applied. The water doing this quiet but crucial job is not tap water but ultrapure water. It is so clean that engineers sometimes call it “hungry water,” and the name sticks.

Stripped of almost all dissolved minerals, ions and particles, it is chemically unbalanced and behaves as a very effective solvent. It “grabs” anything it touches, from traces of process chemicals to tiny amounts of material from pipes and tanks. This is ideal for cleaning surfaces, because at the nanometer scale even a few particles or molecules introduced by the rinse can cause trouble. ⟶

From total organic carbon to killer particles

In the world of chip production, water-borne contamination causes trouble in two main ways. Larger particles, including tiny bits of material and occasional microbial cells or fragments, behave like miniature boulders in a landscape of nanometer-scale lines. They can locally block the light or physically bridge neighboring structures during patterning. Even when living microorganisms are removed or inactivated by filtration, UV or other sanitization steps, their remains still count as organic carbon and show up in the “total organic carbon” that engineers work hard to minimize.

Engineers bundle all these organic molecules together under one practical number: total organic carbon, or TOC. In an online TOC analyzer, a small volume of water is briefly held in a measurement cell after being exposed to intense ultraviolet light. This oxidizes the organics to inorganic carbon species such as bicarbonate, which change the electrical conductivity of the water. From that change, the instrument calculates the TOC value in the low microgram-per-liter range. TOC is not only a cleanliness indicator, it is also a measure of how much “food” is available for any microbes that manage to enter the system. If TOC rises, biofilms can grow more easily in pipes and tanks, and those microbial colonies in turn shed cells and fragments that behave as killer particles on the wafer surface.

Seeing what the water knows

Lena knows that her fab already monitors the water, but the existing online TOC analyzer was installed in a different technology era. It is not optimized for the very low organic levels and the particularly persistent compounds that matter so decisively in today’s nanometer production. So her team decides to look more closely at one critical use point in the ultrapure water loop and installs a latest-generation online TOC analyzer designed specifically for ultrapure water monitoring in semiconductor manufacturing: Shimadzu’s new TOC-1000e S (Figure 1).

The instrument itself seems inconspicuous, about the size of a small desktop printer and light enough to be carried to different measurement points or mounted on the wall next to the water line. What interests Lena is the view it gives into the water’s “inner life.” On the bright touchscreen, she sees a live TOC trend, updating every few minutes. Because the sample flows continuously through a short measurement line, the analyzer reacts quickly when the organic load changes. Small spikes now appear where the old TOC system showed only a flat line.

Over several weeks, Lena and her colleagues overlay these TOC curves with tool logs and maintenance records. They notice that organic peaks always follow certain process sequences and are strongest at one branch of the distribution system. The analyzer cannot say which molecule is present, and it does not remove contamination. It does, however, tell the team when the water quality changes and where in the system this change first becomes visible.

With that information, the fab can work systematically instead of guessing. Engineers focus their inspections on a limited section of piping, adjust resin replacement intervals and tighten rinsing recipes around sensitive lithography steps. As these measures take effect, the TOC excursions at the use point become smaller and less frequent (Diagram 1). On Lena’s wafer maps, the once persistent defect pattern gradually fades into the background noise of everyday production.

From clean water to everyday electronics

Lena has not “solved” the grand challenge of contamination in semiconductor fabs. No single tool can do that. But in her corner of the factory, one concrete and critical goal has been achieved. A stubborn defect pattern has been traced to its source and brought under control, and the process ramp now moves a step closer to the high yields the fab needs. Every avoided defect means fewer wafers scrapped, less energy and water wasted, lower costs incurred and more reliable chips reaching customers.

Those chips will quietly power everyday life: in smartphones and laptops, in cars and trains, in medical devices and communication networks. As future technology nodes shrink further to sub-3 nm, the water that rinses each layer will only become more critical. Giving that “hungry water” a clear, quantitative voice through state-of-the-art TOC monitoring helps fabs manage invisible risks today and lays the foundation for the electronics that will shape tomorrow.

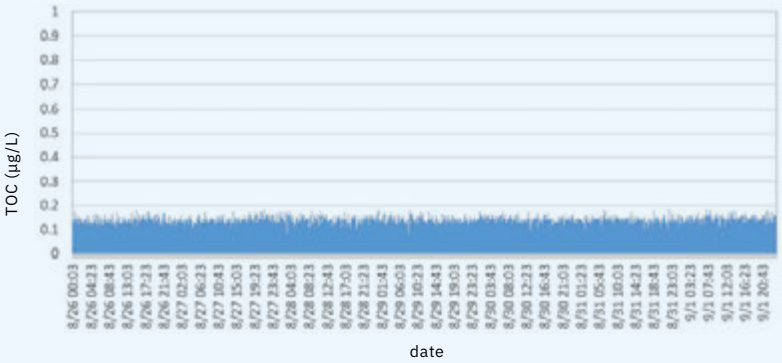
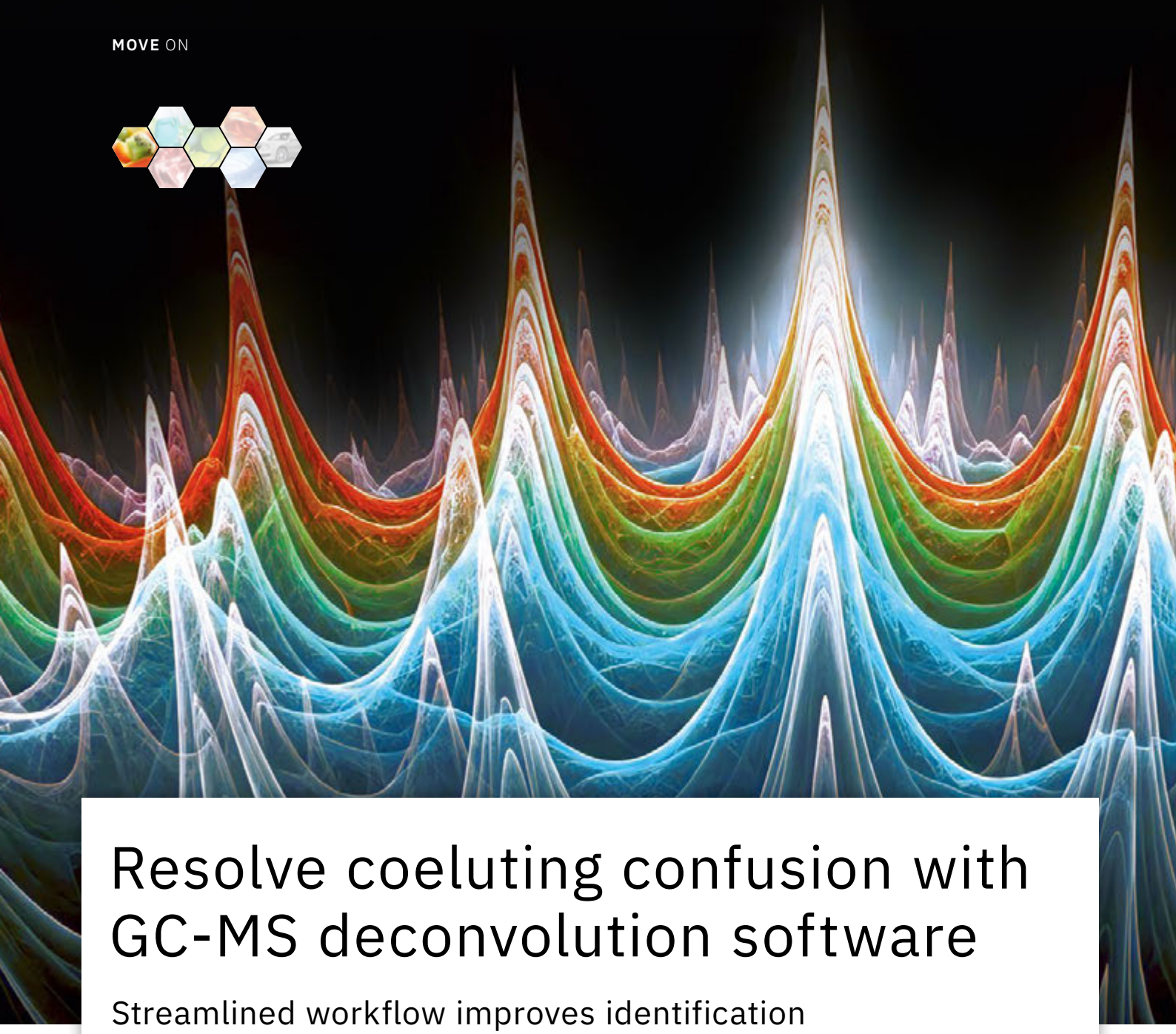


Diagram 1: TOC trend graph of semiconductor-grade ultrapure water

Note

For more information and references, please refer to the digital version of this edition.

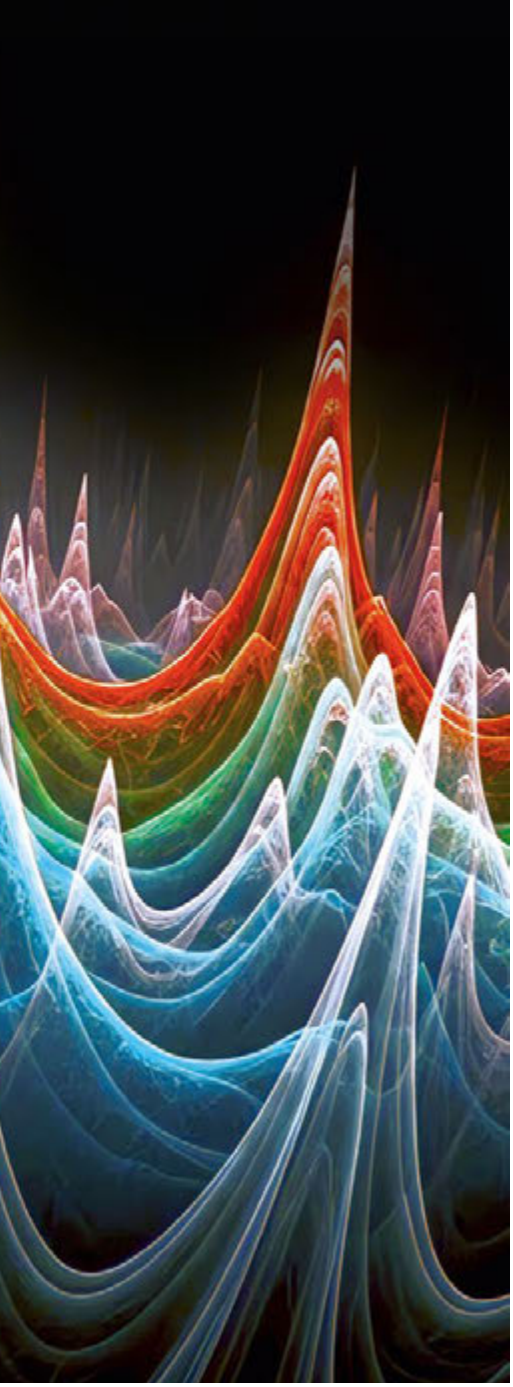


Resolve coeluting confusion with GC-MS deconvolution software

Streamlined workflow improves identification accuracy in complex mixtures

Waldemar Weber, Shimadzu Europa GmbH

Complex GC-MS samples often contain multiple compounds that coelute and merge into a single chromatographic peak. These mixed spectra make identification uncertain, and conventional peak integration can easily misinterpret the data. Advanced deconvolution software addresses this challenge. That's good news for labs dealing with complex matrices, especially in the food industry.



A clearer view of hidden peaks

Labs working with aroma components in food or attempting to identify hidden trace-level peaks in complex, high-matrix samples using GC-MS (gas chromatography-mass spectrometry) often need an additional tool to separate coeluting peaks.

The most sophisticated and efficient tool for this purpose is deconvolution software. It addresses the challenge by modeling the measured signal as a superposition of individual elution profiles. The result is a resolved deconvolution chromatogram aligned with the total ion chromatogram (TIC), the separation of hidden component peaks and the reconstruction of cleaner MS spectra for each compound. Altogether, this increases confidence in the qualitative analysis of impurities and trace components masked by abundant analytes.

With resolved spectra per component, analysts can verify identities more transparently through objective spectral matching and review multiple candidate fits with clear similarity in the deconvolution software library. Deconvolution also streamlines and supports targeted workflows: Known compounds can be screened quickly to narrow the search space, while unknowns are explored using spectral libraries.

A practical example

To illustrate the advantages of deconvolution software in GC-MS analyzes, we examined a combined mixture of pesticide standards (Mix 64, Mix 13 and Mix 7), encompassing 50 compounds in total. Data was acquired using a low pressure GC method that reduces flow resistance to achieve fast run times but sacrifices chromatographic resolution, intentionally generating coelutions. Below, you can see how deconvolution reliably separated these coeluting peaks, reconstructing clean spectra for individual pesticides. →

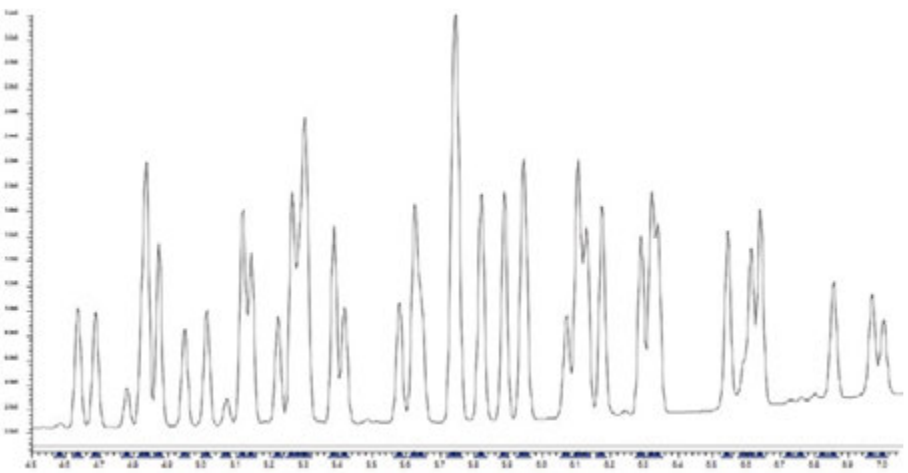


Figure 1: Shimadzu GC-2030 + QP2050 with AOC-30i

Original TIC and deconvolution chromatograms, together with representative spectra and practical settings, demonstrate how accelerated GC workflows can deliver highly accurate qualitative results.

The analytical hardware and software:

Main unit: Nexis GC-2030 with QP2050 mass spectrometer

Accessory: AOC-30i liquid sampler

Main consumables: SH-5MS LPGC column (5 m × 0.18 mm × 0.01 µm)

Software: LabSolutions GCMS and LabSolutions Insight Explore

Achieving the clarity required

The results obtained for the measured pesticide mixture are shown in Figure 2. The chromatogram presents the total ion current for the pesticide mixture used. The blue triangle on the x-axis indicates coelutions recognized by the deconvolution software. The low-pressure GC approach offers the advantage of creating very fast measurements, in this case of around 7.5 minutes. A common disadvantage of that approach is often insufficient separation performance. Although the mixture of 50 pesticide compounds is less complex than typical screening mixture applied at pesticide screening, the number of coelutions is high, making a clear identification of compounds difficult and unreliable.

However, for a qualitative screening of targeted compounds, a combination of low-pressure GC-MS methods with subsequent deconvolution provides both speed and accuracy. For example, a chromatogram peak at 5.74 minutes RT is demonstrated in Figure 3.

Figure 2 shows that three peaks coelute at the peak of 5.74 minutes: p,p'-dde, 2,2',3,4,4'-pentachlorobiphenyl and trans-chlordane. The upper part of Figure 2 illustrates how the peak was deconvoluted. Two specific m/z values are presented for each compound: p,p'-dde with m/z 246 and 248, pentachlorobiphenyl with m/z 373 and 375 and trans-chlordane with m/z 326 and 328.

Deconvolution using the Labsolutions Insight Explore module effectively separated all three components, enabling reliable identification. A standard background spectrum

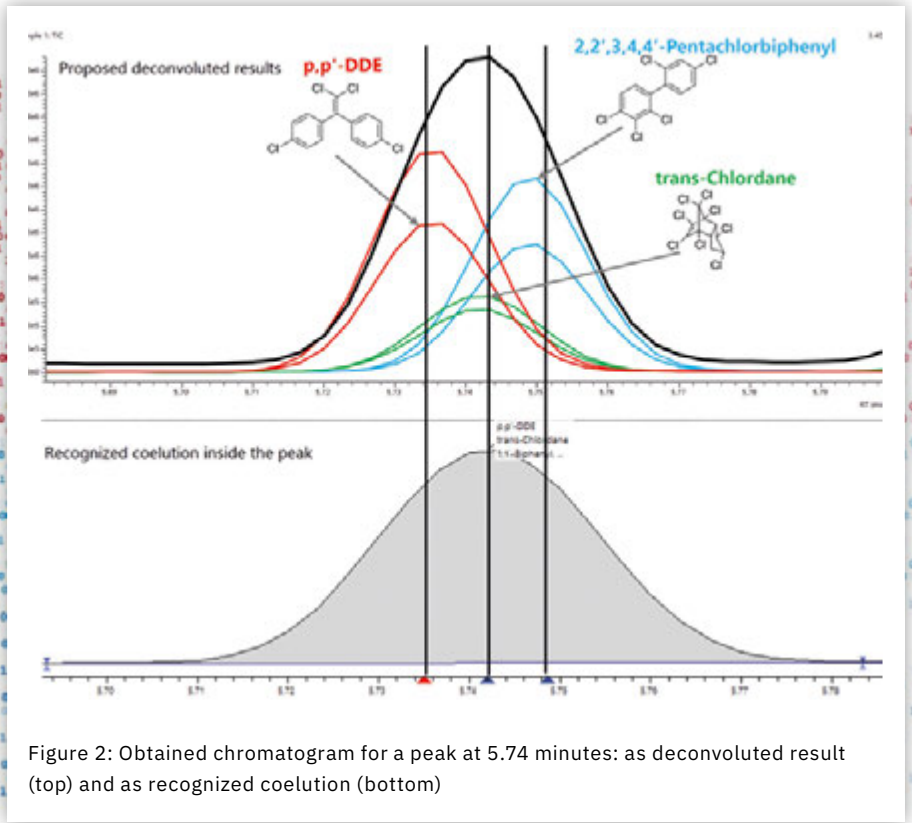


Figure 2: Obtained chromatogram for a peak at 5.74 minutes: as deconvoluted result (top) and as recognized coelution (bottom)

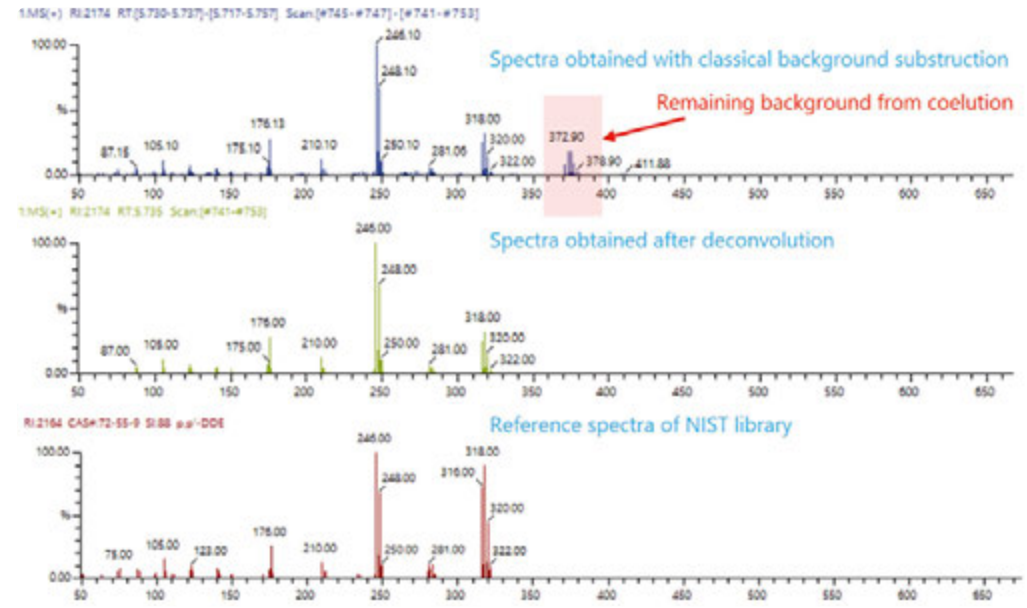


Figure 3: Obtained MS spectra for p,p'-dde: after background correction (top), after deconvolution (middle) and NIST reference spectra (bottom)

correction often only partially removes incorrect mass fragments from the spectrum, which can result in more false positives and negatives. Using the peak at 5.74 minutes as an example, Figure 3 demonstrates that a simple background correction of the p,p'-dde spectrum shows incorrect mass fragments at m/z 372–373, which clearly originate from trans-chlordane. In contrast, the deconvoluted spectrum corresponds closely to the reference spectrum. Therefore, a library search after deconvolution would be significantly more accurate.

In this application, we showed that deconvolution substantially enhances qualitative GC-MS analysis of complex, fast run chromatograms by separating coeluting compounds and reconstructing clean mass spectra for each component.

Using a low pressure GC method intentionally optimized for speed, deconvolution reliably resolves overlapping pesticide signals that conventional integration and simple background correction cannot, improving library match scores and reducing false positives and negatives. This approach enables rapid, confident screening workflows, allowing targeted compounds to be analyzed quickly while unknowns are explored with greater certainty.

Note

For more information and references, please refer to the digital version of this edition.

A bit like lasagna: Proper slicing and analysis show what packaging film is really made of

Microtome sections reveal their secrets with the AIRsight™ infrared and Raman microscope

Dr. Kai Klein, Dr. Aikaterini Karatzia, Shimadzu Europe

Modern plastic film packaging used in the food and pharmaceutical industries keeps products fresh and protected. This packaging typically consists of multiple layers bonded together, and analyzing these layers is important for quality control, recycling and more. However, doing that can be quite complicated. How do you measure multiple layers of a film that itself is only a few micrometers thick? One new way to do that is to apply the advantages of distinct instruments in a novel way.

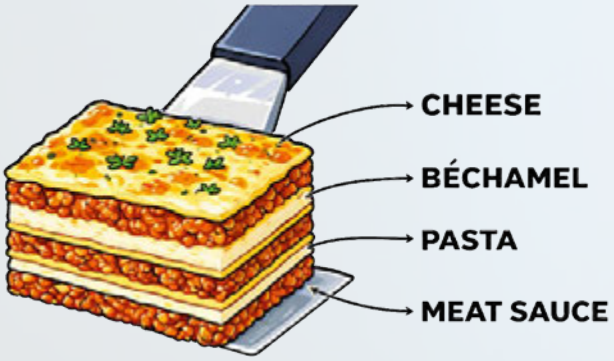


Figure 1: Lasagna “cross-section”

Consider lasagna

It’s time for dinner, and you’re hungry. Tonight, you’re looking forward to one of your favorite dishes: lasagna. Suddenly, it’s there on your plate. You have a good overview of what it looks like, and it does look good! Maybe you are so hungry or so eager to enjoy the experience of lasagna in your mouth that you immediately start eating. Or, perhaps, you pause for a moment to further inspect the finer points of your dinner. You gently slice through your little piece of heaven and inspect its inner workings. The cross-section reveals all: layers of meat sauce, béchamel, pasta and cheese which together create a culinary sensation (Figure 1).

In a similar way, it takes many different layers of plastic film to create a fully functional piece of modern packaging. Commonly, there is a surface layer acting as a barrier against oxygen and/or moisture, a carrier layer providing stability and a printed layer designed to appear attractive to the customer. In rarer cases, an additional layer may be included to protect against odor or light.

Analyzing these layers is of great importance for a number of reasons: for scientific research, material development, quality control, in waste management and recycling. For disposal and recycling, for example, it is essential to know exactly which material is to be recycled. And, from a scientific perspective, this knowledge makes it possible to continuously improve and refine packaging.

Slicing: The first challenge of analyzing plastic film packaging

However, analyzing these layers can sometimes be quite complicated. How do you measure multiple layers of a film that itself is only a few micrometers thick? To understand why packaging works so well, it is worth taking a look into this microscopic world. That's where the microtome cutting tool comes into play.

With the help of a microtome, extremely thin and smooth slices of these materials can be produced. The cross-section obtained with the microtome provides insights into the number, sequence and thickness of individual layers, the material transitions and adhesive layers, as well as any irregularities or defects that could lead to reduced shelf life. Therefore, regular analysis of packaging materials in the food and pharmaceutical sectors is of great importance for quality assurance. →

After selecting a suitable piece of the sample, it is clamped into the microtome holder. For multilayer films, it is recommended to position the sample perpendicular to the cutting direction to ensure a clean cross-section (Figure 2).

The choice of blade and the thickness of the cut layer often depend on the planned analysis. For transmission measurements with an infrared microscope, thinner sections are cut using harder blades compared to, for example, reflection measurements. For transmission measurements, the sections can be lightly fixed at the ends with adhesive tape so that the area to be examined remains exposed. For reflection measurements, the sections can be placed on a metal-coated surface or, if sufficiently thick, on a standard glass microscope slide.

How a microtome works

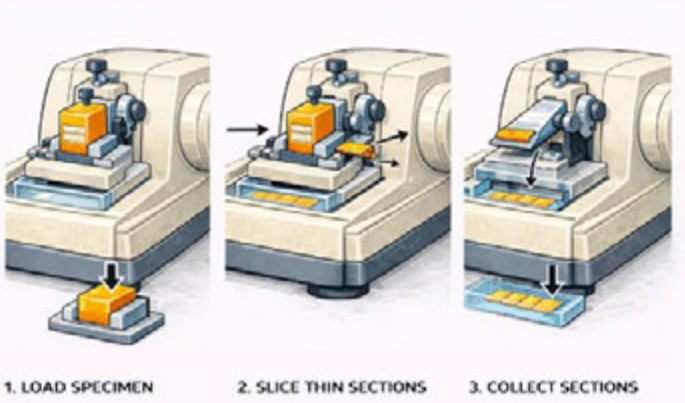


Figure 2: Schematic representation of microtome sectioning for thin sample preparation

FTIR vibration

Raman scattering

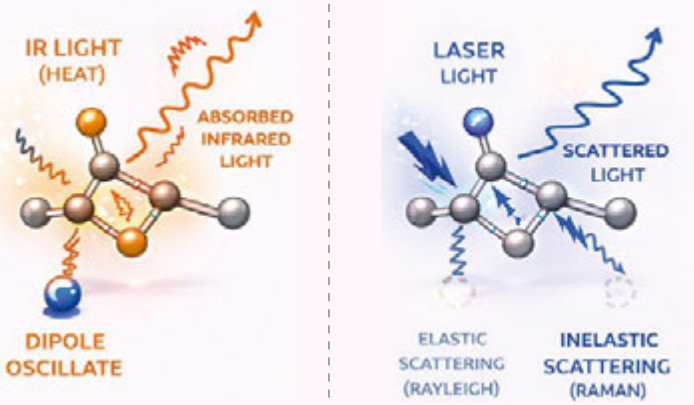


Figure 3: Comparison of infrared absorption and Raman scattering mechanisms at the molecular level

Analyzing: The second challenge of analyzing plastic film packaging

Infrared microscopy enables the acquisition of infrared spectra at defined locations on a sample surface. The AIMsight™ and AIRsight™ microscope systems are equipped with a wide-field camera and a 15× infrared objective for spectroscopic measurements. In addition, the AIRsight™ system provides Raman spectroscopic capabilities using 50× and 100× objectives with visible laser excitation.

Infrared spectroscopy is based on the absorption of infrared radiation by molecular vibrations associated with a change in dipole moment, resulting in variations in bond lengths and bond angles. Raman spectroscopy, by contrast, probes molecular vibrations through inelastic scattering of incident laser light arising from changes in molecular polarizability (Figure 3). The combination of these two methods delivers complementary information on the chemical composition of materials, yielding a more accurate and complete analysis of the sample.

It is important to note that Raman and Infrared (IR) do exhibit complementarity for the same functional groups. Sometimes, a functional group does not show a signal in one method, underscoring the importance of applying both methods. Because most substances and functional groups are either active for Raman or infrared, AIRsight™ enables measurements with both methods – on the same spot, without moving the sample. Being active for both methods usually requires different functional groups in one molecule.

Figure 4 shows the layout of the IR beam path in the AIMsight™ and AIRsight™ microscopes. The sample is placed in the center, at the position enclosed by the red cones. The beam path from below enables transmission measurements, while the one from above allows reflection measurements. The wide-field camera is used to provide an overview of the area of interest. Once an interesting spot has been identified, the view can be switched to the 15× infrared objective for detailed magnification and focus adjustment. In this view, measurement points for transmission or reflection can be set with different apertures, along with an additional point for a background measurement of the surrounding air. After the background measurement, which minimizes interfering signals from CO_2 and water, the actual measurement begins with a predefined number of scans until the final spectrum appears. Following this procedure, line scans and mappings of areas of interest can also be created, consisting of multiple measurement points. The spectra obtained for each measurement point can then be compared with a database for identification.

The Raman lasers, on the other hand, are built in at the top of the microscope and can only hit the sample from the top. The 50× and 100× Raman objectives collect the backscattered light from the sample, which is then translated into a difference spectrum compared to the incident wavenumber. Therefore, Raman spectra are not measured in absolute units like Fourier transform infrared spectroscopy (FTIR) but in relation to the laser light. ⟶

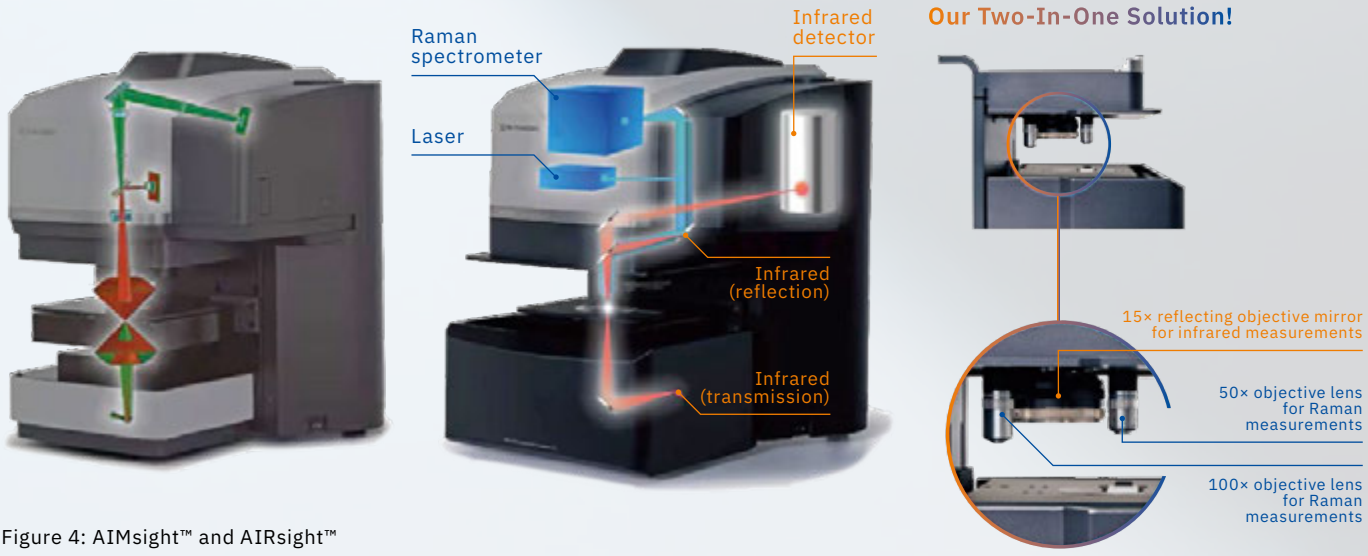


Figure 4: AIMsight™ and AIRsight™

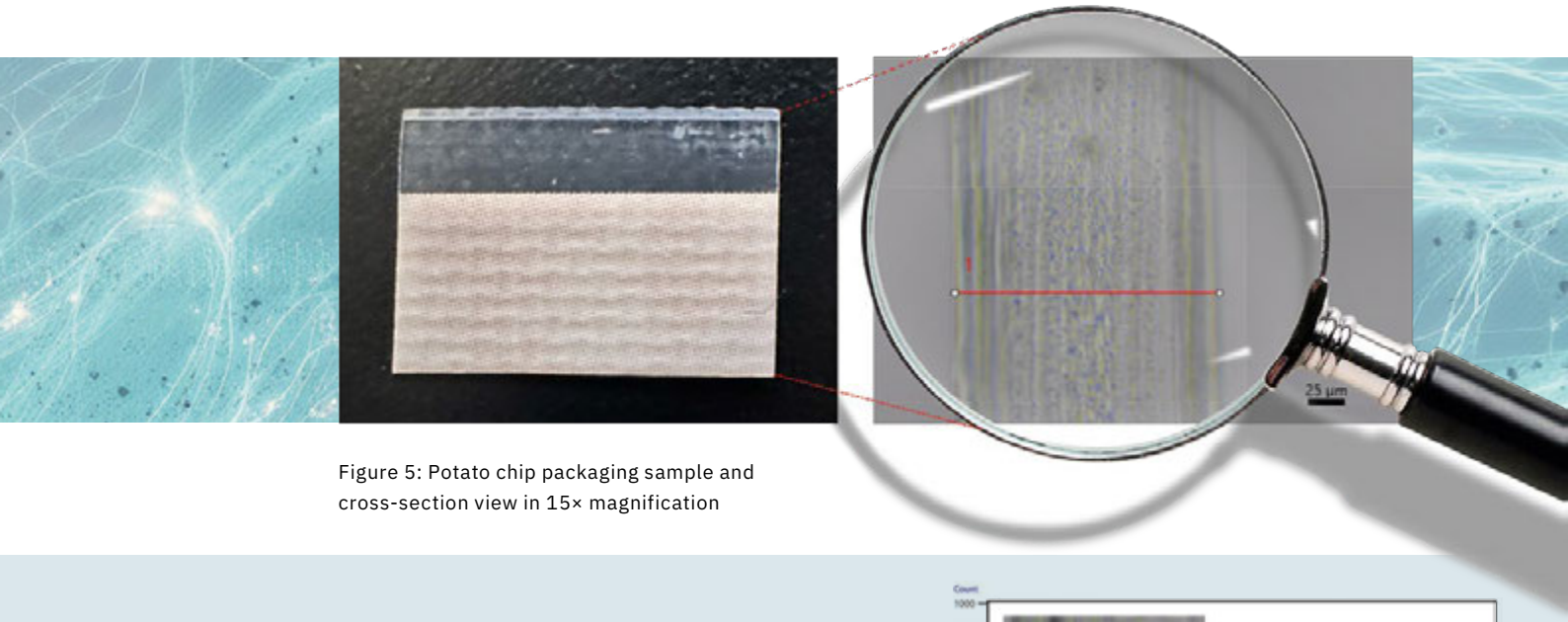


Figure 5: Potato chip packaging sample and cross-section view in 15× magnification

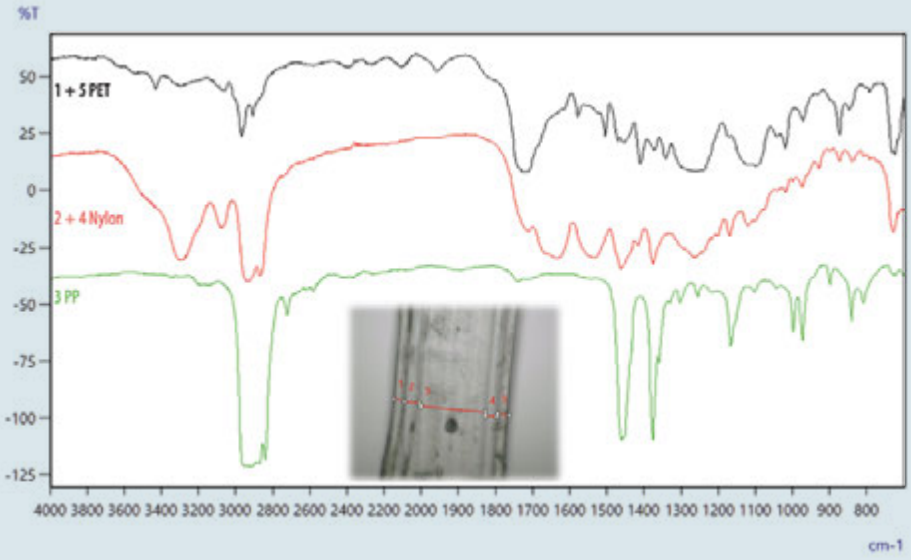


Figure 6: FTIR spectra of the different layers

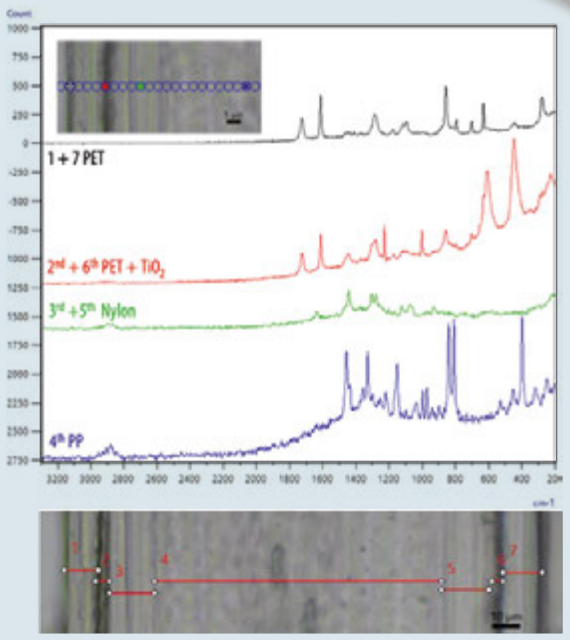


Figure 7: Raman spectra of the different layers and cross-section view in 50× magnification

Putting it all together

The combination of microtome sample preparation with infrared and Raman spectroscopy allows the chemical analysis of individual layers within multilayer packaging films. By preparing thin cross-sections (Figure 5), the internal structure of such films becomes accessible for spatially resolved spectroscopic measurements. This approach is illustrated in the following example using a multilayer film taken from a commercial potato chip packaging.

Optically, five different layers could be distinguished within the cross-section, and infrared spectroscopy was used for their chemical identification. Although five individual layers were detected by FTIR analysis, only three different materials were determined. Starting from the outer surfaces and moving toward the center of the film, the outer layers were found to consist of polyethylene terephthalate (PET), followed by layers of nylon, while the central layer was identified as polypropylene (PP) (Figure 6).

Raman spectroscopy was also employed for the analysis. In addition to the layers identified by FTIR spectroscopy, Raman analysis revealed the presence of two titanium dioxide (TiO_2) layers between the PET and nylon layers, which could not be detected using infrared spectroscopy (Figure 7). This is due to the fact that TiO_2 does not exhibit strong infrared-active vibrational modes but shows a pronounced Raman response as a result of changes in molecular polarizability. This finding highlights the advantage of combining infrared and Raman spectroscopy for the comprehensive characterization of multilayer packaging materials.

A good product requires good ingredients

Although commonly used in biological applications, it is now clear that microtome-prepared cross-sections combined with infrared and Raman microscopy can also be used to enable detailed characterization of multilayer packaging films. While infrared spectroscopy allows reliable identification of polymer layers, Raman spectroscopy offers complementary information, such as the detection of inorganic additives and precise determination of layer boundaries due to higher magnification. The analysis of a commercial chip packaging demonstrates that the AIMsight™ and AIRsight™ microscope systems are well suited for such applications, supporting quality control, material development and recycling processes in the food and pharmaceutical packaging industry. As with lasagna, putting the right things together in the right way makes all the difference.

Note
For more information and references, please refer to the digital version of this edition.

Using electrochemistry-mass spectrometry to reveal tomorrow's contaminants, today

Sparking innovation in the prediction of chemical transformation products (TPs)

Ranil C. T. Temgoua, Helmut-Schmidt-Universität/Universität der Bundeswehr (Hamburg)
& Helmholtz-Zentrum Hereon, Geesthacht, Germany

Every chemical molecule has a story to tell. But what happens to these molecules after they leave the lab and enter the complex reality of nature or the human body? These molecules now embark on a second, secret life: a journey of transformation. They break down, come together with other substances and evolve into new chemical entities. How can we possibly predict their fate?

The few things we know and the many things we don't know about the transformation of our chemicals once they perform their tasks is often called the "iceberg" problem. We know the parent compound and we regulate that, but this is merely the visible tip (Figure 1a). Below the surface, a vast unseen world of new molecules is being created: transformation products (TPs). TPs can be more persistent, more mobile or even more toxic than the original compound, yet they remain largely unknown, undetected and unregulated. Understanding their journey is one of the greatest challenges in modern science.

The question that drives our research is deceptively simple: How do we predict what happens to chemicals in our environment and in our bodies without waiting months or even years for the answer? Conventional methods of studying these pathways are slow, costly and ethically complex. Enzymatic studies using liver microsomes are variable, and environmental fate studies can take months. We have long needed a faster, more controlled and predictive approach.

The solution lies in a powerful analytical synergy: using electrochemistry to mimic a molecule's fate (similar to living organisms or natural systems conditions) and advanced mass spectrometry to reveal it with stunning clarity. An illustration is given in Figure 1b. →

Figure 1a: The visible tip represents regulated compounds, while the vast underwater mass symbolizes unknown transformation products (TPs)

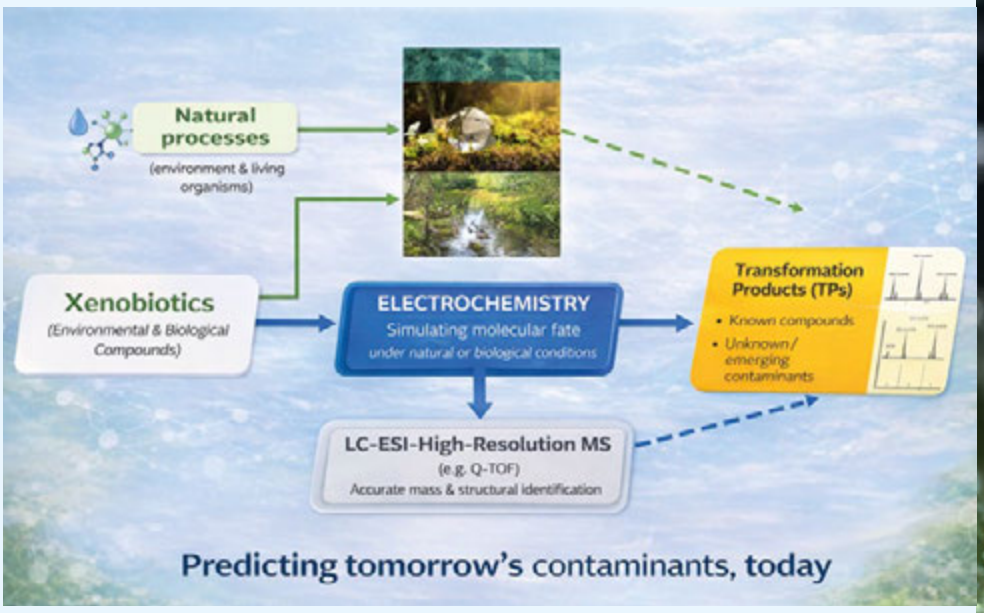


Figure 1b: Analytical workflow using electrochemistry to simulate environmental fate and advanced mass spectrometry for high-clarity identification

Act I: The crystal ball of electrochemistry

The breakthrough lies in a simple, yet profound, realization: Over 90 % of organic compounds are electroactive. This means they can be oxidized or reduced by applying an electrical potential. We can harness this property to simulate metabolic and environmental degradation in a "digital reactor" – an electrochemical cell.

By fine-tuning the potential in this cell, we subject a molecule to controlled redox stress, effectively accelerating its natural aging process. In a matter of minutes, we can generate the very same complex mixture of metabolites and degradation products that would form over weeks or months in nature. It's a clean, reproducible and ethical method that provides a high-fidelity preview of a molecule's future. As illustrated in the diagram below (Figure 2), this electrochemical digital reactor is seamlessly integrated upstream of the mass spectrometer.

But generating these transformation products is only half the story. To truly understand their impact, we must identify them. This is where our predictive vision comes into sharp focus.

Act II: Using the LCMS-9050 Q-TOF as the ultimate decoder

The mixture flowing from our electrochemical reactor is a complex puzzle of unknown compounds. Solving it requires a detector that is not just a sensor but a master detective. This critical partner is the Shimadzu LCMS-9050 Quadrupole Time-of-Flight (Q-TOF) mass spectrometer (see Figure 3).

Its role is to interrogate every product formed with unparalleled precision. Here's how it brings the unseen to light:

1. **It sees everything:** The TPs we generate are often short-lived and in trace concentrations. The outstanding sensitivity of the LCMS-9050 is therefore critical. It ensures that even the lowest-level products are not missed, capturing the most complete profile of all potential TPs.

2. **It provides the "fingerprint":** Seeing is not the same as knowing. To identify a true unknown, we need its "fingerprint." The LCMS-9050 provides stable, ultra-high resolution and highly accurate mass measurements. This isn't just a weight; it's a precise molecular formula, an exact identity card (e.g., $C_{12}H_{15}NO_4S$) and the non-negotiable first step in identifying a molecule from scratch.

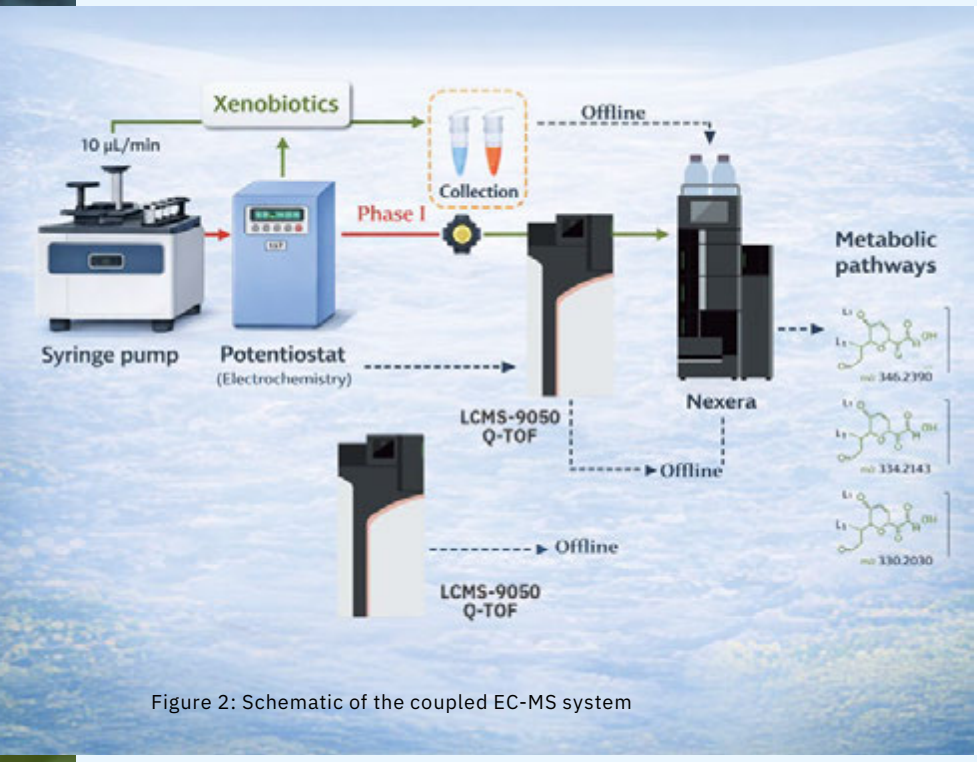


Figure 2: Schematic of the coupled EC-MS system

***Online* EC-MS**

Figure 3: The Shimadzu LCMS-9050 Q-TOF mass spectrometer. Engineered to deliver ultra-high resolution and mass accuracy, it is the ideal tool for the non-targeted identification of unknown compounds.

3. **It unlocks the structure:** With this precise identity, we can use the Q-TOF's MS/MS capability to fragment the molecule. This provides a map of its structure. This high-quality data, combined with Shimadzu's powerful software and extensive spectral libraries, allows us to piece the puzzle together and confidently name these previously hidden compounds.

The synergy: A complete workflow for predictive science

When electrochemistry and the LCMS-9050 Q-TOF are linked in a seamless workflow, we achieve something transformative. We are no longer merely analyzing what something is; we are proactively forecasting what it could be.

In our research, this powerful partnership allowed us to answer critical questions rapidly. A concrete example of the results, presented in Figure 4, perfectly illustrates this power: the real-time monitoring of the electrochemical degradation of two neonicotinoid pesticides (imidacloprid, IMI, and clothianidin, CLO), where the Q-TOF identified principal transformation products in less than an hour.

The results speak for themselves: While the pesticides remained stable at rest, a simple "flick of the switch" triggered their transformation. For imidacloprid, the parent molecule vanished almost instantly at –1.5 V, replaced by a fingerprint of new products. Clothianidin, more resilient, held its ground initially but finally yielded at –1.7 V, revealing its hidden degradation path. This demonstrates the surgical precision of electrochemistry and mass spectrometry (EC-MS): We can tune the energy to break even the most stubborn molecules and map their future in minutes.

From passive observation to active design

This powerful combination of EC-MS marks a paradigm shift. We are moving from being passive observers of chemical fate to active architects of a safer chemical future. By predicting a molecule's journey with electrochemistry and illuminating its path with the unparalleled clarity of the Shimadzu LCMS-9050 Q-TOF, we can design better, safer and more sustainable molecules from the very beginning.

The future of chemical analysis isn't just about measuring what we know; it's about discovering what we don't. And that journey of discovery has never been faster, clearer or more inspiring.

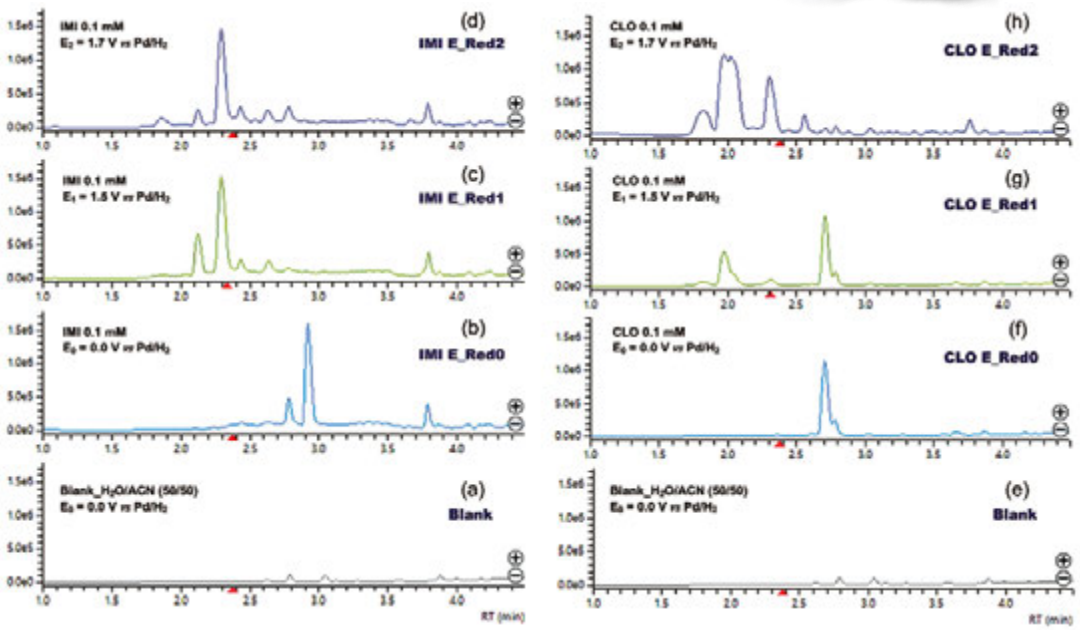
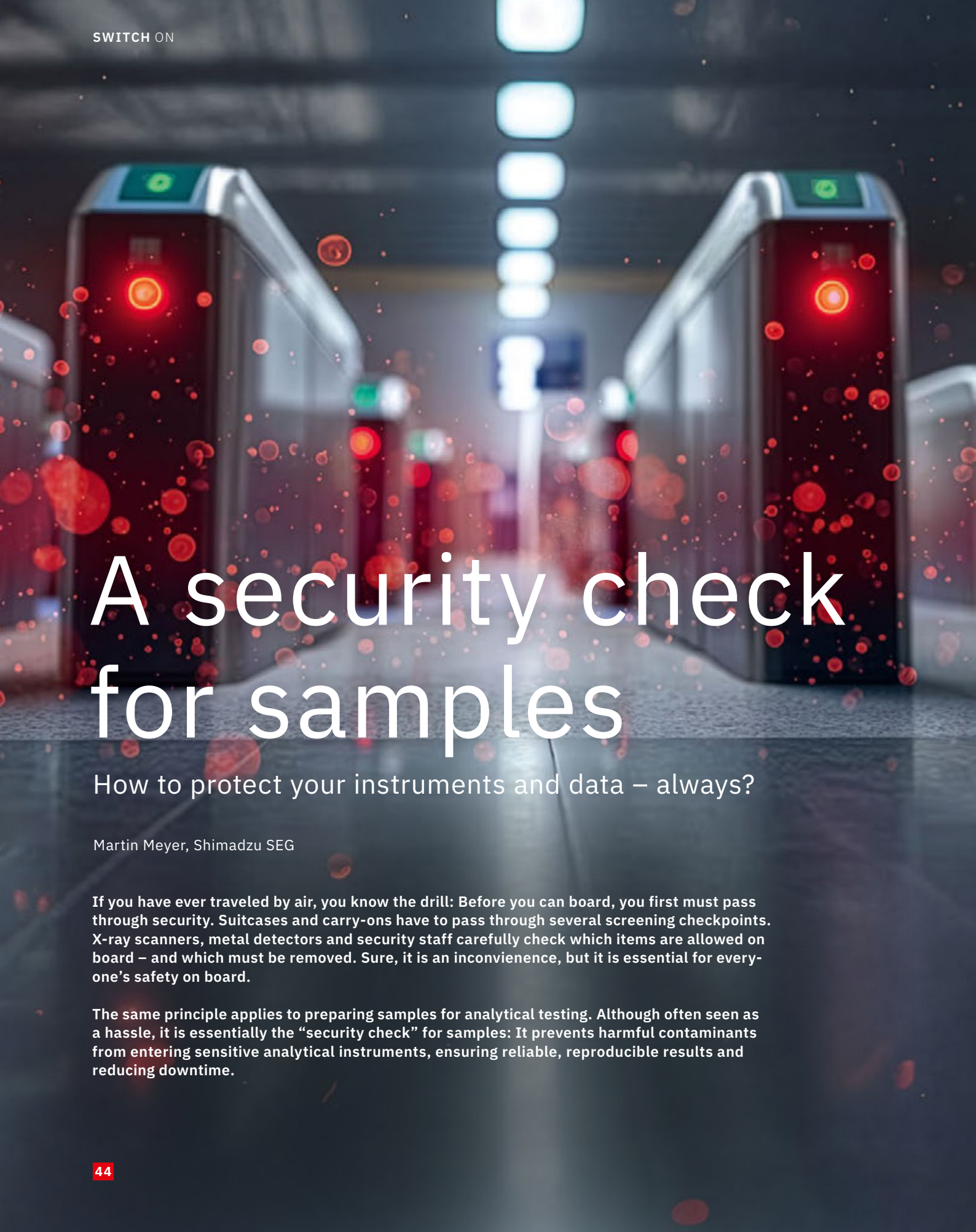


Figure 4: LC-HRMS chromatograms of IMI and CLO (0.1 mM) under different electrochemical conditions: blank, no applied potential (0.0 V) and after application of reduction potentials E_Red1 and E_Red2 in neutral medium (pH 7.4)

Note

For more information and references, please refer to the digital version of this edition.



A security check for samples

How to protect your instruments and data – always?

Martin Meyer, Shimadzu SEG

If you have ever traveled by air, you know the drill: Before you can board, you first must pass through security. Suitcases and carry-ons have to pass through several screening checkpoints. X-ray scanners, metal detectors and security staff carefully check which items are allowed on board – and which must be removed. Sure, it is an inconvienence, but it is essential for everyone's safety on board.

The same principle applies to preparing samples for analytical testing. Although often seen as a hassle, it is essentially the "security check" for samples: It prevents harmful contaminants from entering sensitive analytical instruments, ensuring reliable, reproducible results and reducing downtime.

Figure 1: Shimadzu syringe filter overview

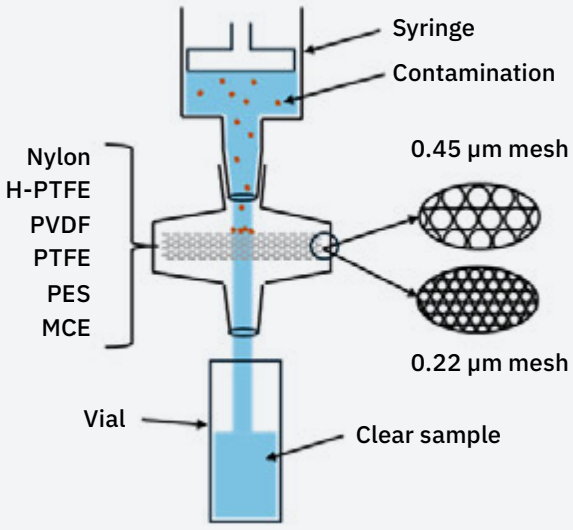
Today, samples and measuring instruments are as diverse as the questions they are designed to help answer. A wide variety of sample matrices – from aqueous solutions and complex biological specimens to organic extracts – can contain a broad range of potential contaminants that may interfere with measurements or damage sensitive instruments. Thoughtful sample preparation (including choosing the right filters) is not just an extra precaution; it is often crucial to producing reliable results and protecting sensitive instruments.

Particles, suspended solids and other undissolved components in samples can cause damage – most often by clogging delicate components such as valves, capillaries and frits. Damage that often shows up as baseline noise, unexpected peaks or an increase in system pressure. Routine filtration can remove these interfering substances before they ever reach the instrument.

A simple and effective way to remove interfering contaminants is the use of syringe filters (Figure 1). These are attached to a syringe, and the sample is then pushed through the filter using gentle pressure. The key advantage is speed, since applying pressure makes filtration much faster than with traditional paper filters, where the liquid moves through the filter by gravity alone. Syringe filters typically contain a membrane inside, which is enclosed and protected by an outer housing (Figure 2).

Ideally, the membrane should be matched to the individual sample and can have different properties. In most cases, it is important to consider whether the sample is purely aqueous or contains a higher proportion of organic solvents. The membrane should also be able to withstand aggressive chemicals. Table 1 provides guidance on which filters to use for specific types of samples. →

Figure 2: Function and variations of syringe filters



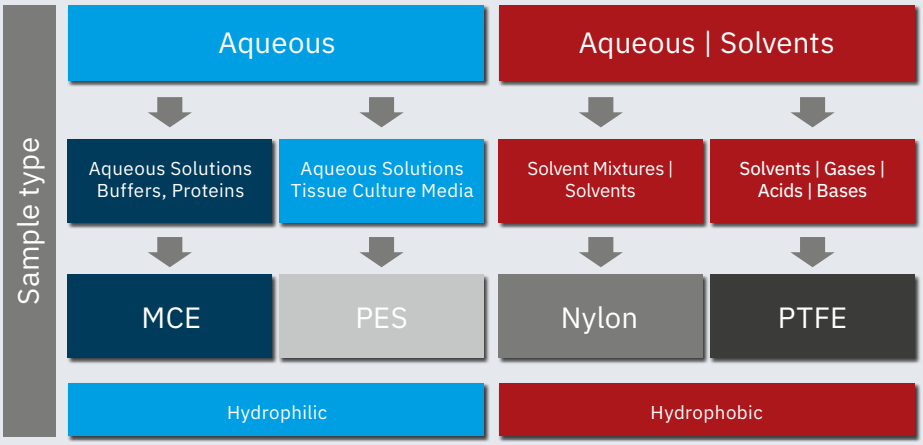


Table 1:
Choosing the right syringe filter

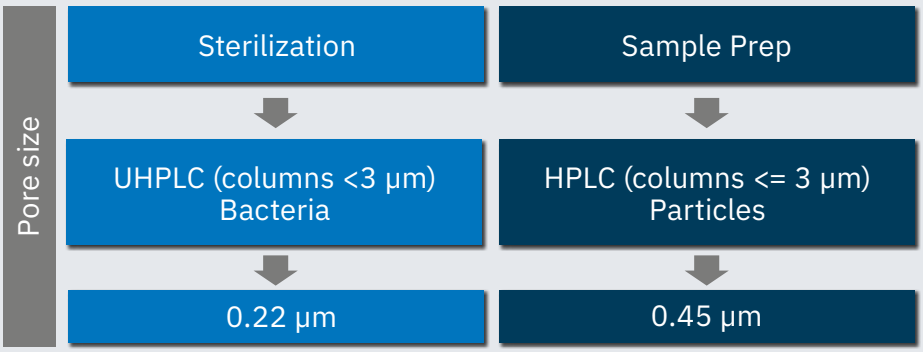


Table 2:
Syringe filter pore sizes

The membrane's pore size also determines which particles are retained by the filter (Table 2). Common pore sizes include:

- 0.2 µm: removes very fine particles and many microorganisms; the standard choice when the highest level of purity is required (e.g., LC-MS)
- 0.45 µm: a commonly used pore size for general HPLC analyses; reliably removes larger particles
- 1–5 µm: prefilter range for the removal of coarse particles

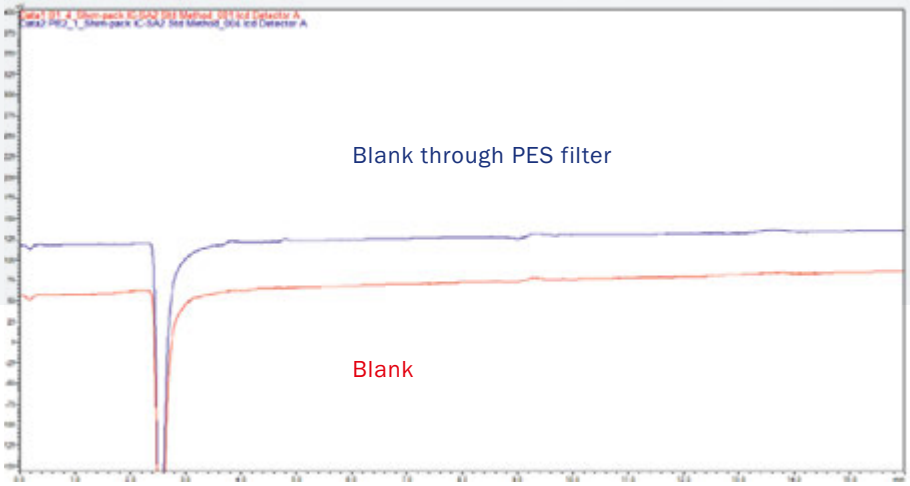
In addition to these standard filters, there are also several specialized solutions available.

For proteins:
PVDF (polyvinylidene fluoride): hydrophilic and low in protein binding – a good choice for protein-containing samples and LC-MS applications. PVDF is more expensive, but has advantageous binding and flow properties.

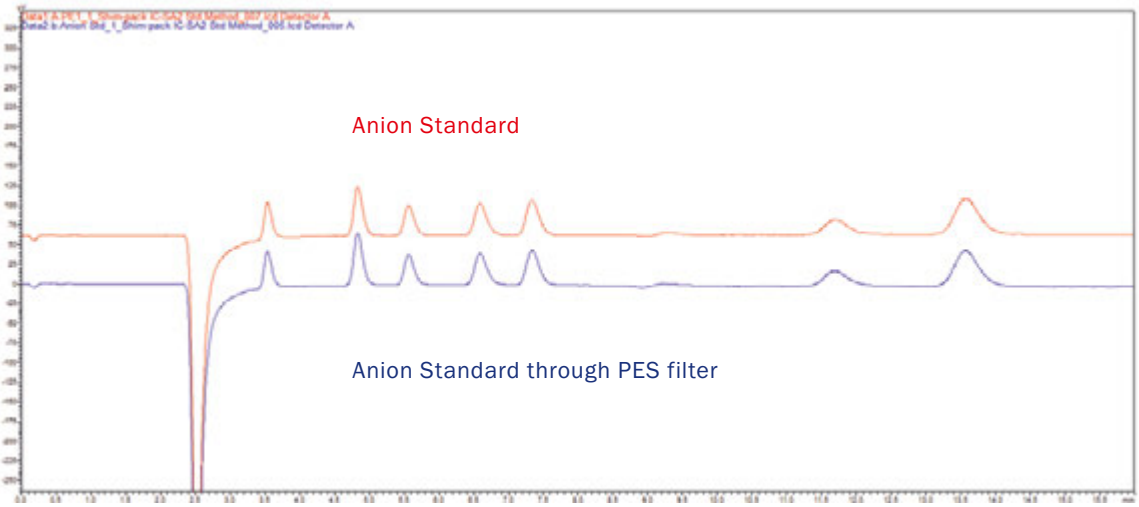
For heavily contaminated samples:
Dual-layer filters: a glass fiber prefilter followed by a PES membrane

In practice, it is important not only that filters remove unwanted substances, but also that they do not alter the sample being analyzed. Two things can happen here: First of all, lower-quality filters may themselves be contaminated and release impurities into the sample. Secondly, filters can also remove substances of interest from the sample or reduce their concentration. If we stick with the airport analogy, it would be just as problematic if the security check caused you to lose your own luggage or if you suddenly found yourself holding someone else's bag.

But let us get back to practical sample work – specifically, experiments involving ion chromatography measurements (Figures 3 and 4). Here, ionized substances such as chloride, fluoride, sulfate and others are identified. Because these substances occur naturally almost everywhere, using clean materials is particularly important. Pure water was measured, as well as water that had been filtered through a PES filter after discarding the first 0.5 mL. The anion standard was measured directly and again after filtration through a PES filter (with the first 0.5 mL discarded). Comparing this with the blank value, you will see that neither the introduction of additional ions nor a loss of the standard analytes could be detected. That is why these filters are particularly well suited for sensitive analytical methods such as ion chromatography. →



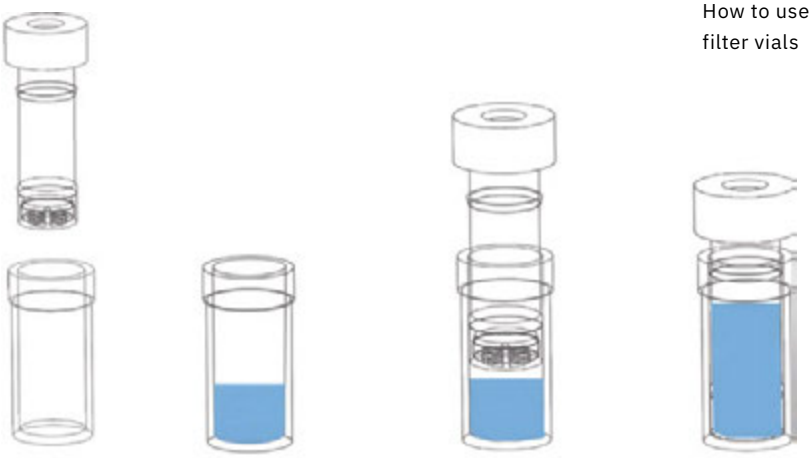
◀ Figure 3:
Emission testing of PES filters using ion chromatography



▼ Figure 4:
Adsorption testing of PES filters using ion chromatography

Figure 5:
Filter vial

Figure 6:
How to use filter vials



Fill
Use a pipette to add sample to the fill line.

Cover
Twist gently to ensure a secure seal.

Plunge
To filter the sample, press the plunger slowly.

In addition to syringe filters, there is an even more convenient filtration method in what are known as filter vials (Figure 5). The sample is placed directly into the vial, and by pressing down the vial cap, the liquid is forced through a membrane built into the bottom. The filtered sample stays in the vial and can then be inserted directly into the analytical instrument (Figure 6).

Filter vials are available in many different versions, with a range of membrane materials, pore sizes and designs (clear or amber). This makes it possible to select the right combination depending on the type of sample and the measuring task.

Ready for take-off with the perfect preparation

Syringe filters and filter vials are simple, cost-effective, yet highly protective measures for modern analytical systems. The right combination of membrane material, pore size and format protects instruments, improves data quality and reproducibility as well as reduces downtime and costs. Making small investments in well-designed “checkpoints” often prevents major unexpected problems. Because whether you are flying or preparing samples, the same rule applies: Safety first.

Note
For more information and references, please refer to the digital version of this edition.

Saving lives, money and reputation with a fast, new method of bacterial testing in food

Genome-guided MALDI-TOF offers clear identification of *Bacillus cereus* group dangers

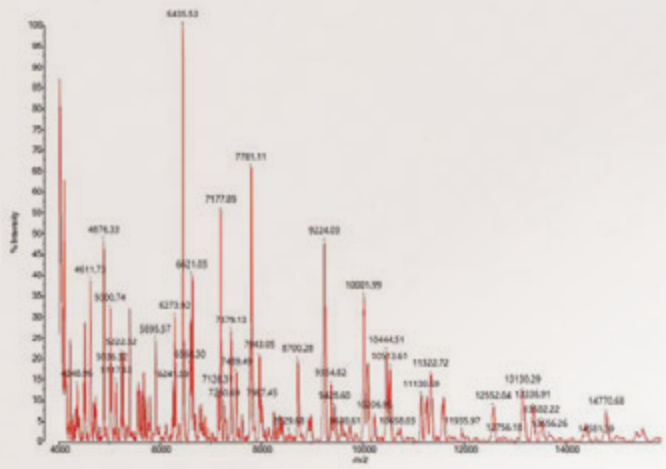
Valentin Pflüger, Mabritec AG

A massive recall of tainted baby formula took place in January 2026. The formula had been tested according to current food safety regulations and found to be in compliance with them. Nonetheless, the testing failed to reveal a toxin which was a member of the *Bacillus cereus* bacteria group. That's because standard testing was simply not precise enough. The good news is that a new, much more precise method had already been developed by a company in Switzerland.

Earlier this year, a number of companies were forced to recall potentially dangerous baby formula. The presence of a toxin called cereulide was suspected and later proven to be present in the formula. The recall cost those companies a lot of money and severely damaged their reputation for quality. But how did that happen? Apparently, the EU-mandated Hazard Analysis and Critical Control Point (HACCP) food safety management program does not properly consider the risk of cereluide contamination in fatty or oily food ingredients.

The *Bacillus cereus* bacteria group

Cereulide is a member of the *Bacillus cereus* bacteria group. This group has major societal relevance because it unites within one highly related bacterial complex: 1. frequent food-poisoning agents, 2. an important biothreat organism and 3. globally used biocontrol strains. →



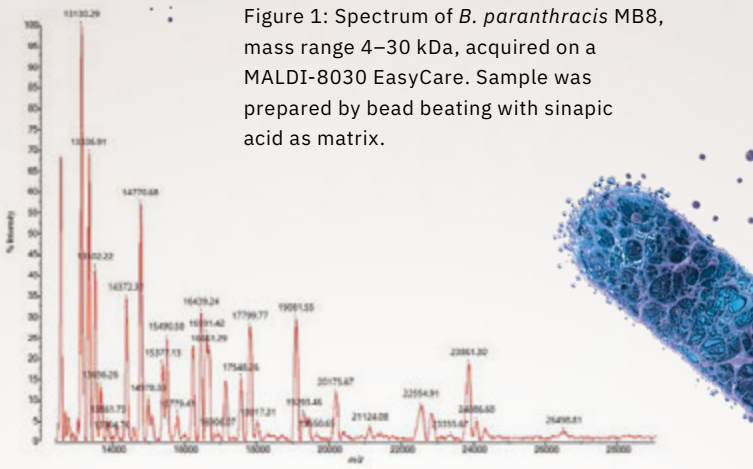


Figure 1: Spectrum of *B. paranthracis* MB8, mass range 4–30 kDa, acquired on a MALDI-8030 EasyCare. Sample was prepared by bead beating with sinapic acid as matrix.

On the public-health side, *B. cereus sensu stricto* and close relatives are among the most common causes of bacterial foodborne disease, while *B. anthracis* causes anthrax and remains central to biosecurity concerns. Meanwhile, *B. thuringiensis* strains are extensively deployed as "biological" insecticides in agriculture, directly supporting food production. In addition, *Bacillus cereus* group species form very resistant spores, which makes them omnipresent and therefore detectable in the majority of all food products.

Traditional testing

Most routine food laboratories see the *Bacillus cereus* group every day, but current standard methods of testing usually stop at a blurred, group-level identification, even though the underlying species range from typical food-poisoning strains to biopesticide residues and rare high-risk lineages. Quantitative criteria (colony forming units: CFU) for the *Bacillus cereus* group in ready-to-eat (RTE) foods typically classify < 10^3 CFU/g as acceptable, ≈ 10^3–10^4 CFU/g as borderline and ≥ 10^4–10^5 CFU/g as unsatisfactory or potentially hazardous, based on assumed cell densities required for toxinogenesis.

Unfortunately, these limits are scientifically unsatisfactory because they neither discriminate emetic (*ces*-positive) from non-emetic strains nor account for strain-specific enterotoxin profiles and matrix-/temperature-dependent toxin production kinetics. That means that the actual hazard is only weakly predicted by total CFU alone.

Improvements have been available, but ...

Whole-genome sequencing is essentially the only method that can, in one step, unambiguously place *Bacillus cereus* group isolates into genomospecies resolved clonal relationships and comprehensively inventory virulence and resistance genes: No combination of phenotypic tests or single/low-plex PCRs can fully achieve that. However, that approach is still not widely used in routine food and clinical laboratories for the simple reason that it requires substantial capital investment, bioinformatics infrastructure and expertise, standardized pipelines and added turnaround time and cost.

Meanwhile, standard Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDI-TOF MS) – widely used in routine microbiology – speeds up the identification process but uses pattern-based matching against clinical-centric libraries that only partially cover the *Bacillus cereus* group.

The background to discovery

Mabritec AG is a company located in the Basel area of Switzerland, specializing in the identification of microorganisms and the characterization of biological systems using MALDI-TOF mass spectrometry. It currently offers the largest MALDI-TOF database for bacteria in the world – MabritecCentral – and it was during the building of this database a few years ago that something else began to develop.

Using a new MALDI-8020 (among others), Mabritec discovered that separating the *Bacillus cereus* group based on ribosomal protein masses using MALDI-TOF MS in silico is possible. Genome-guided MALDI-TOF MS had not previously been thought possible using commercially available applications for bacterial identification. Now, however, it was.

When science benefits consumers, laboratories and companies

Combining genome-based references for identifying toxin producers with rapid and cost-effective MALDI-TOF MS analysis – in contrast to expensive genome sequencing – has now resulted in a new and advantageous ability to routinely differentiate all *Bacillus cereus* group species and their potential virulence in food. For the first time, all species can be identified under routine conditions using MALDI-TOF MS and assigned a toxin profile using a genome-based database. Depending on the findings and the matrix/product, critical food products can thus be proactively removed from circulation.

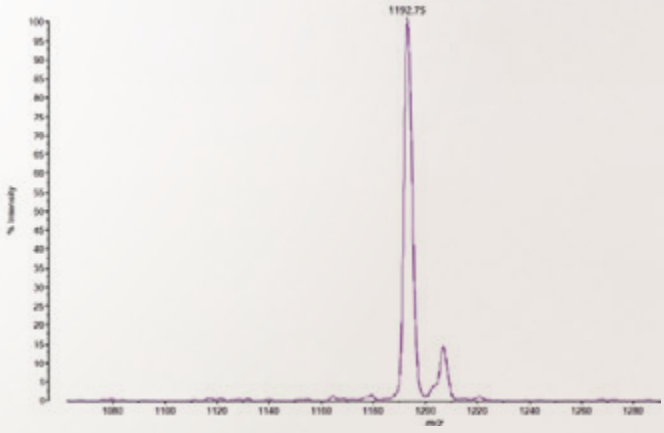


Figure 2: Detection of cereluide *m/z* 1,191 (potassium adduct) directly from cultured strain MB8. The spectra were acquired without matrix in LDI in the mass range 700–5,000 Da on a MALDI-8020 EasyCare.

This new method can be used in the food, pharmaceutical and cosmetics industries along the entire production chain, from raw materials through production/processing to the final product. It allows quality managers to better interpret the frequently detected *Bacillus cereus* group, improve food safety and better protect consumers. The method is already routinely used in the Mabritec laboratory where more than 1,600 *Bacillus cereus* group isolates originating from food and industrial samples have been identified.

Good tools help good people make things better

Genome-guided MALDI-TOF MS enables reliable species-level resolution within the *Bacillus cereus* group and links isolates to characteristic toxin and virulence profiles that remain invisible to conventional CFU-based and routine identification approaches. The work of the scientists at Mabritec demonstrates that rapid MALDI/LDI-based detection of cereulide from cultures and suitable food matrices is technically feasible, sufficiently sensitive and compatible with routine workflows, thereby strengthening risk assessment and surveillance for emetic *Bacillus cereus* group strains. Using Shimadzu equipment, a clever Swiss company came up with a new way to better protect the health of consumers, which also saves companies from costly and embarrassing product recalls.

Note
For more information and references, please refer to the digital version of this edition.

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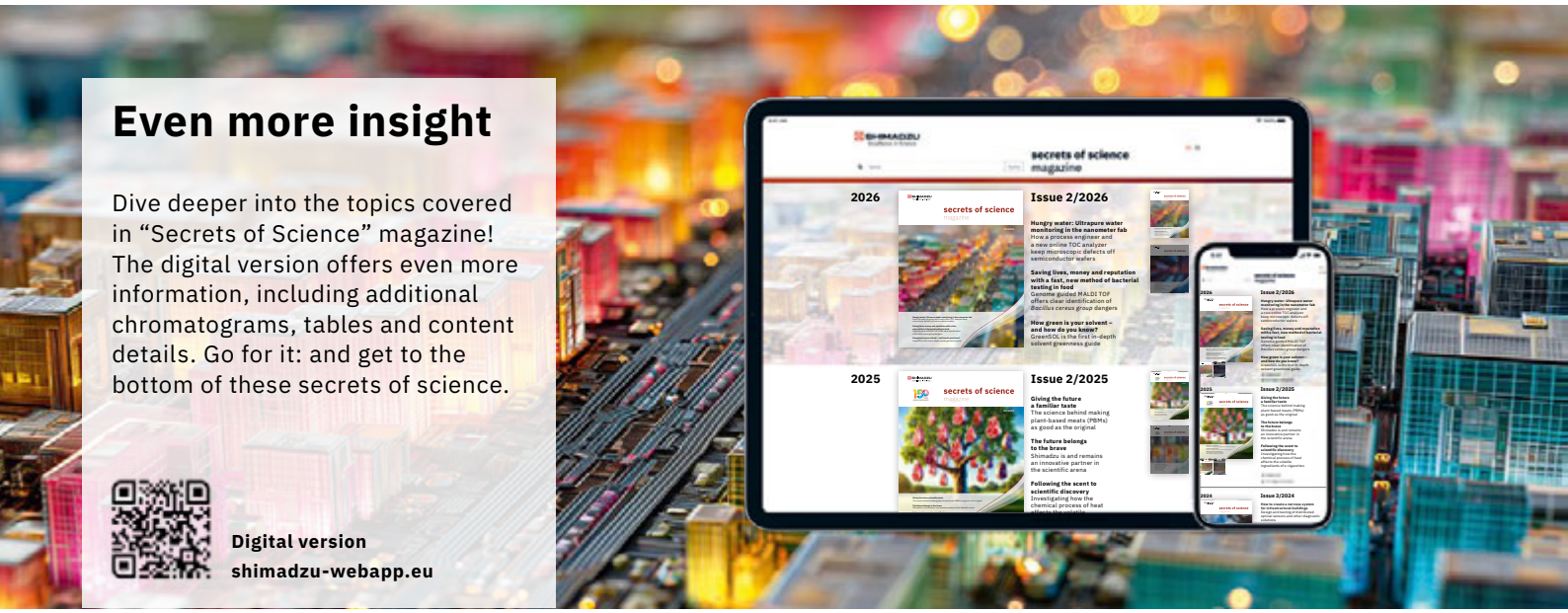

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