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Water, Air, Earth, Plastics, PFAS

From climate change to PFAS remediation, five pioneers explore new frontiers in the quest to protect our planet

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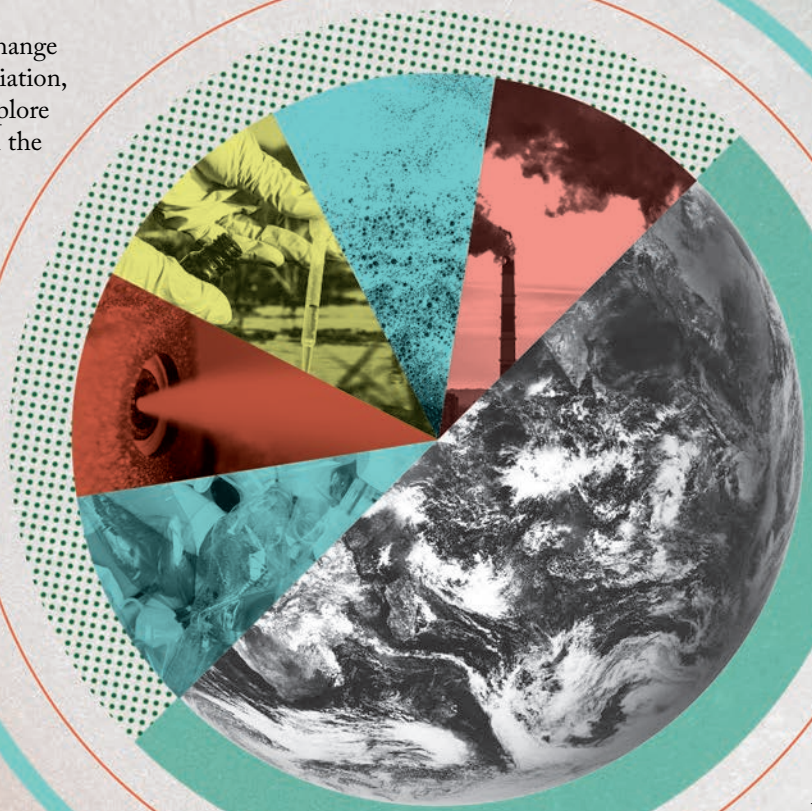

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Do Scientists Really Need Another Twitter?

Are global communications platforms like X a net positive for scientists?

It's a new year and that may mean new diets, exercise routines, and productivity plans. But what about a "Twitter break" – or perhaps an X-odus? Elon Musk's "handling" of the platform has led to considerable soul searching as many, including those in the analytical science community, ponder migrating to microblogging alternative Bluesky – indeed many already have. But I'm beginning to wonder whether scientists really need another Twitter.

Platforms like X are thought to be useful for disseminating research – and several studies have found that widely shared papers on X are more likely to be cited. But what if relevant and impactful papers are simply tweeted about and cited more? As it happens, one study by Branch et al. involving 13 scientists with respectable follower counts randomly selected five papers, and tweeted one while retaining the others as controls; they found that the overall increase in citation counts after three years was not statistically significant.

What about networking and discussion? Although there are important conversations undoubtedly taking place on X, distractions are a feature, not a bug of any cybernetic/algorithmic global communications platform. In other words, when you're restricted in character count and one click away from the latest emotionally charged hot take, it can feel like trying to quietly converse in a crowded bar with music blaring. And with the resurgence of smaller online communities, including e-newsletters, Substack blogs, podcasts, and Discord servers, perhaps scientists would be happier hanging out at the quiet pub over the road (I'll see you there from 8pm).

James Strachan,
Editor

See references online

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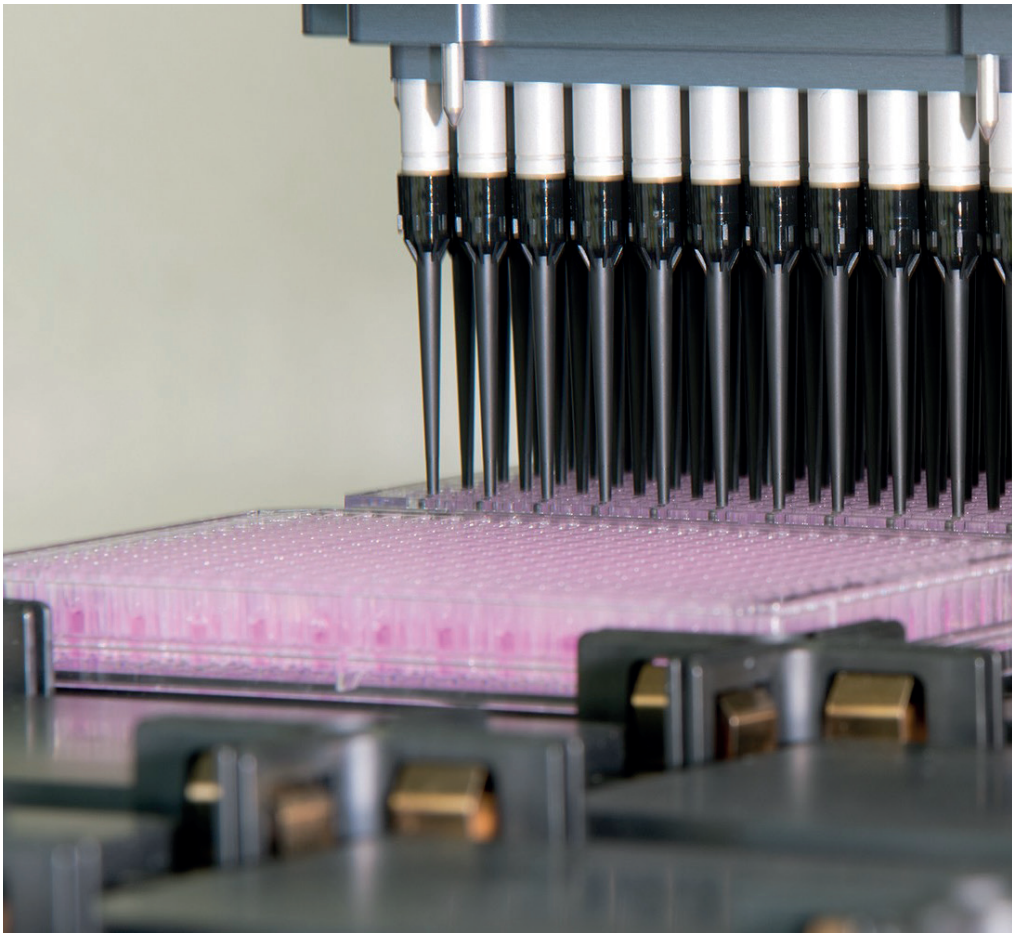
Worse Than the Sum of Their Parts?

Chemical-by-chemical regulation called into question by new research into the cumulative effects of low-concentration mixtures



Automated pipetting platforms for the preparation and measurement of plasma samples and chemical mixtures in high-throughput bioassays at the UFZ. Credit: Bodo Tiedemann

Chemicals typically considered harmless at low concentrations can combine in the human body to form neurotoxic mixtures (1), according to research led by Beate Escher and her team at the Helmholtz Centre for Environmental Research (UFZ).

The team employed high-resolution mass spectrometry (HRMS) and in vitro bioassays to examine the neurotoxic effects of these chemical mixtures. Plasma samples from 624 pregnant women in the Leipzig mother-child cohort (LiNA) were analyzed, testing for 1,000 different environmental chemicals. Of these, approximately 300 were quantified. To evaluate the impact, researchers simulated 80 chemical mixtures in realistic concentration ratios and tested their neurotoxicity on human cell-based assays.

"We've been studying complex mixtures in the environment for years," Escher explains. "This time, we wanted to understand how these mixtures transfer to the human body. By combining target screening methods with suspected neurotoxicants, we could evaluate how chemicals act together."

The research revealed a vast array of chemicals in human blood.

"Ultimately, we were able to view the entire history of chemical production over the course of 100 years; from metabolites and long phased out persistent organic pollutants (POPs) such as dichlorodiphenyltrichloroethane (DDT), to modern chemicals, food contact material chemicals, personal care products, antioxidants, and industrial chemicals," says Escher.

"Despite being present at low concentrations where they wouldn't cause an effect on their own, all of them acted together in mixtures," Escher adds. "In every case the in vitro effects added up."

The study required innovative analytical approaches to overcome challenges.

"Extracting a broad range of chemicals was our first hurdle," Escher notes. "We developed a two-step extraction process using silicone polymer and solid-phase extraction, achieving recovery of 400 chemicals and their mixture effects." The team also used a combination of LC-HRMS and GC-HRMS to broaden the chemical space analyzed, paired with an optimized automatic data evaluation script.

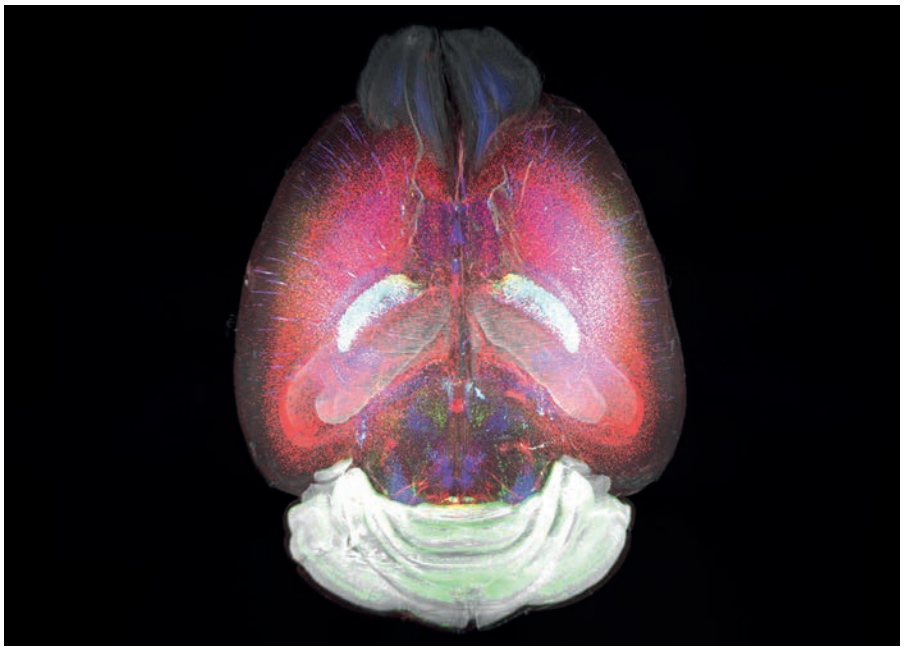
The complexity of the testing was another obstacle. "We used neuroblastoma cells differentiated to mimic basic neural functions," Escher says. "While artificial, this system allowed us to test over 1,000 samples reliably."

This discovery underscores the cumulative neurotoxic risks posed by everyday chemical exposure. One example is perfluorooctanoic acid (PFOA), found in nearly every sample despite its regulatory phase-out in many countries.

Escher emphasizes the broader implications for chemical regulation: "Our findings clearly show that regulating on a chemical-by-chemical basis is insufficient. Risk assessment must address complex mixtures to reflect real-world exposure."

Reference

1. *G Braun et al., Science, 386, 6719, 301-309. DOI: 10.1126/science.adq0336.*



New Standard for 3D RNA Imaging

A new technique enabling high-resolution three-dimensional RNA imaging across the entire brain, known as Tris buffer-mediated retention of in situ hybridization chain reaction (TRISCO), has been developed in a collaborative effort between researchers from the Karolina Institutet and Karolinska University Hospital, Sweden. The technology addresses inconsistencies with depth and uniformity associated with conventional RNA imaging methods by combining hybridization chain reaction (HCR) technology with Tris-buffered tissue clearing. The result? Enhanced tissue transparency, preserved RNA integrity, and consistent labeling throughout an entire organ (in this case the brain) – all whilst maintaining its structural fidelity.

Reference: S. Kanatani et al., Science, 386, 6724, 907-915 (2024). DOI: 10.1126/science.adn9947.
Credit: Science (2024). DOI: 10.1126/science.adn9947

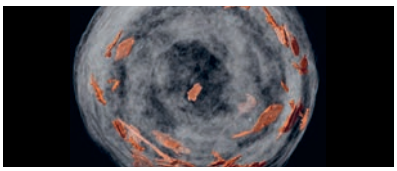
QUOTE *of the month*

"Today with high-end mass spectrometry, we can study thousands of proteins within a single cell in just half an hour. To put that into perspective, 20 years ago, when I worked at a biomarker company, it took us half a day to identify 1,000 proteins from a sample of 1 million cells. So we've gone from 1 million cells to a single cell, and from half a day to half an hour – that's quite an accomplishment."

Koen Sandra (see page 17)

How Dinosaurs Ate Their Way to Dominance

Analyses of fossilized feces, intestinal contents, and vomit reveal how dinosaurs adapted to climate shifts



Fossilized faeces from a large fish with a spiral gut. Credit: Martin Qvarnström

Analyses of hundreds of fossilized digestive remains has revealed details about the dietary habits and ecological strategies that enabled dinosaurs to dominate terrestrial ecosystems (1). By studying more than 500 bromalites – fossilized faeces, intestinal contents, and vomit – scientists uncovered how dinosaurs gradually replaced other tetrapods, leveraging both opportunistic advantages and dietary adaptations during the Late Triassic and Early Jurassic periods.

An international team of researchers, led by Uppsala University in Sweden, employed synchrotron microtomography and GC-MS to analyze bromalites, reconstructing three-dimensional models and identifying microscopic dietary remains, such as beetle exoskeletons, fish scales, and plant cuticles.

The findings indicate that climate-driven shifts in vegetation and the extinction of less adaptable species created opportunities for dinosaurs to expand their niches.

Reference

1. *M. Qvarnström et al., Nature, 636, 397–403 (2024). DOI: 10.1038/s41586-024-08265-4.*

Reexamining Our Driving Force

Sample prep community: it's time to stop, think, and go back to chemistry to explore our methodologies at a deeper level

By Lorena Vidal, Professor, Analytical Chemistry, Nutrition and Food Science Department, University of Alicante, Spain

Analytical scientists often say "the best sample preparation is the one that does not exist." Indeed, the very first of the 12 principles of Green Analytical Chemistry claims that "Direct analytical techniques should be applied to avoid sample treatment" (1). However, those of us who work in sample preparation know that this is a chimera. Developing faster, greener, easier-to-handle, more affordable methods, without compromising analytical parameters, is the main driving force in sample preparation today. But there are some recent trends in the field that lead me to believe that we may be straying from this path…

Taking a step back, the most important advances in sample preparation were made between the 1990s and 2000s, when classical extraction techniques such as liquid-liquid extraction (LLE) and solid-phase extraction (SPE) were miniaturized and different modalities were described, such as the well-known solid-phase microextraction (SPME) in its fiber version developed by Arthur and Pawliszyn (2), and the liquid-phase microextraction techniques (LPME) as single-drop microextraction (SDME) (3), hollow-fiber LPME (HF-LPME) (4), and dispersive liquid-liquid microextraction (DLLME) (5). Since then, the miniaturized techniques have undergone various minor modifications to improve their already outstanding advantages, such as the use of green solvents, magnetic sorbents, the development of portable devices, the use of ultrasound and vortex energy for dispersion, the reduction of waste, the increase of sample throughput, automation, and so on.

As mentioned above, one of the main focuses over the last twenty years has been to reduce the environmental impact of our methods by using green solvents, or at least less hazardous solvents than the traditional chlorinated organic solvents, as extractant phases in LPME techniques. In the early 2000s, ionic liquids (ILs) were introduced to analytical chemistry as extractant phases, mainly due to their "green" nature, but also because of other properties such as low vapor pressure, high thermal stability, high purity and powerful tailoring. Those first and widely used ILs were composed of imidazolium cations with fluorinated anions, such as hexafluorophosphate, due to their viscosity, which is tailored according to the anion and the length of the alkyl chain, and their extraction capacity of organic and inorganic compounds. All those who have developed methods using LPME techniques with ILs as single drop, in hollow fiber or in dispersive mode, claimed that the methods were green. At the time, the use of ILs in analytical chemistry was a hot topic, and the number of scientific publications was growing rapidly. However, years later, when the first toxicity studies appeared, fluorinated anions showed high toxicity – the methods developed were not as green as they should have been, and low-toxicity IL options set the direction of research.

Today, something similar is happening with Deep Eutectic Solvents (DESs) (6) and their nature-origin versions (NADESs) (7). With regard to the latter, there is a misconception that if something comes from nature, it must be green, but hazardous compounds can also be found in nature (8). DESs and NADESs are a hot topic nowadays and publications are springing up like mushrooms, but the toxicity of these solvents is too often not considered. This may be a symptom of a wider problem within the scientific community, which incentivizes quantity rather than quality of scientific publications... In my view, it is time to stop, think, and go back to chemistry to explore our methodologies at a deeper level – to provide genuinely valuable information that can change the course of current research (9). We may even find that many previous studies are invalid – which we ought to welcome!

Another important focus in recent years to reduce the environmental impact of the methods has been to diminish the size of microextraction techniques down to the nanoscale, reducing the amount of sorbents and solvents, and avoiding energy intensive equipment such as stirrers and centrifuges. However, we are still heavily dependent on liquid and gas chromatographs coupled to various detectors, mainly mass spectrometers, which are very energy, gas and solvent intensive. We should therefore put more effort into reducing the environmental impact of these analytical detection systems by making them greener or, where possible, replacing them with others (i.e., smartphones, electroanalytical sensors, etc.).

In conclusion, as a proud member of the sample preparation research community, I believe that we need to look deeper, with the eyes of a chemist, while also taking a broader view of the entire analytical process. We need to think more fundamentally about how we can use more environmentally-friendly detection systems when developing faster, greener, easier-to-use, more sensitive, and more economical analytical methods. This should be our driving force.

References available online:

Empowering Peptide Purification

Peptide drug development has made great progress in recent years – in large part thanks to new purification and separation technologies; however, method development remains an expensive challenge. We spoke with KNAUER's Ulrike Krop to learn more about the company's systematic and cost-saving approach to scale-up.

Why is peptide purification important and what are the main challenges?

Recent approvals of peptide-based drugs highlight their growing importance in therapeutic areas, including metabolic and cardiovascular diseases or oncology. Peptides, often chemically synthesized, require purification to separate desired compounds from synthesis by-products. Reversed-phase high-performance liquid chromatography (RP-HPLC) is the most widely used technique for peptide analysis and purification, with initial separation steps performed on an analytical scale before being scaled up using preparative chromatography.

A significant challenge is the high cost of method development at large scales. To address this, KNAUER develops methods on analytical-scale columns and scales them up later. This minimizes sample loss and reduces eluent usage. Linear scale-up, where column length and particle size remain constant while internal diameter and injection volume increase, ensures safe and efficient scaling.

Can you walk us through KNAUER's approach to peptide purification?

We start with an overview gradient on an analytical system to understand the sample properties and possible impurities. Then, particle size adjustments are made to match those used in purification, overcoming pressure limitations in preparative systems. The gradient is focused around the target peak to enhance resolution and often reduce run time. A high-organic wash step removes late-eluting impurities. Injection volume is then increased to maximize throughput, and a volume overload study determines the maximum sample amount that can be purified without contamination.

One key aspect of the linear scale-up workflow is to increase the inner diameter (ID) of the column, which requires the adjustment of certain method parameters, such as flow rate and injection volume. This can be easily managed with the free KNAUER Method Converter software tool. When the analytical HPLC method parameters are entered, the software tool automatically calculates the appropriate preparative method parameters to scale up the purification process – eliminating the need for manual calculations.

The purified target peak is fractionated, analyzed, and pooled based on desired purity and yield.

What are the key considerations when optimizing a preparative method for peptide purification?

Before optimizing a preparative method for peptide purification, it is important to ensure that your sample is well dissolved. Many peptides are hydrophobic, making solubility a challenge. Proper sample preparation is essential. During linear scale-up, most method development steps should be performed using the same column length and particles; this means that the particle size and modification should remain unchanged.

For further details, we recommend our recent application note, which outlines a workflow for method development and transfer to preparative systems using peptide purification as an example (1).

What trends do you see shaping the future of peptide purification?

Green chemistry and automation are two emerging trends. Efforts to reduce the environmental impact of LC processes include replacing toxic chemicals with greener alternatives; for example, using dimethyl carbonate instead of acetonitrile. These initiatives make LC analysis and purification more sustainable. KNAUER's analytical HPLC systems, certified with the ACT label by MyGreenLab, boast the lowest Environmental Impact Factors (ACT-EIF) in the database as of July 2024.

Automation addresses the growing need for high-throughput purification. Integrating autosamplers, fraction collectors, or liquid handlers increases efficiency and reduces human error. For example, KNAUER's Liquid Handler LH 2.1 combines sample injection and fraction collection into one instrument, enhancing throughput for high-volume labs.

What differentiates KNAUER in the field of peptide purification and method scale-up?

KNAUER is renowned for manufacturing high-end scientific instruments for compound analysis and purification. We provide customizable systems for method development, semi-preparative applications, and high-throughput purification. Our pH-stable columns ensure reliable separation for even the most challenging peptides, while features like eluent heating and column temperature control in our preparative HPLC systems can enhance performance. Our systems are highly customizable and modular – and I think that really sets us apart. Finally – but just as importantly – our fantastic applications team is always on hand to help you develop, optimize, or transfer your method.

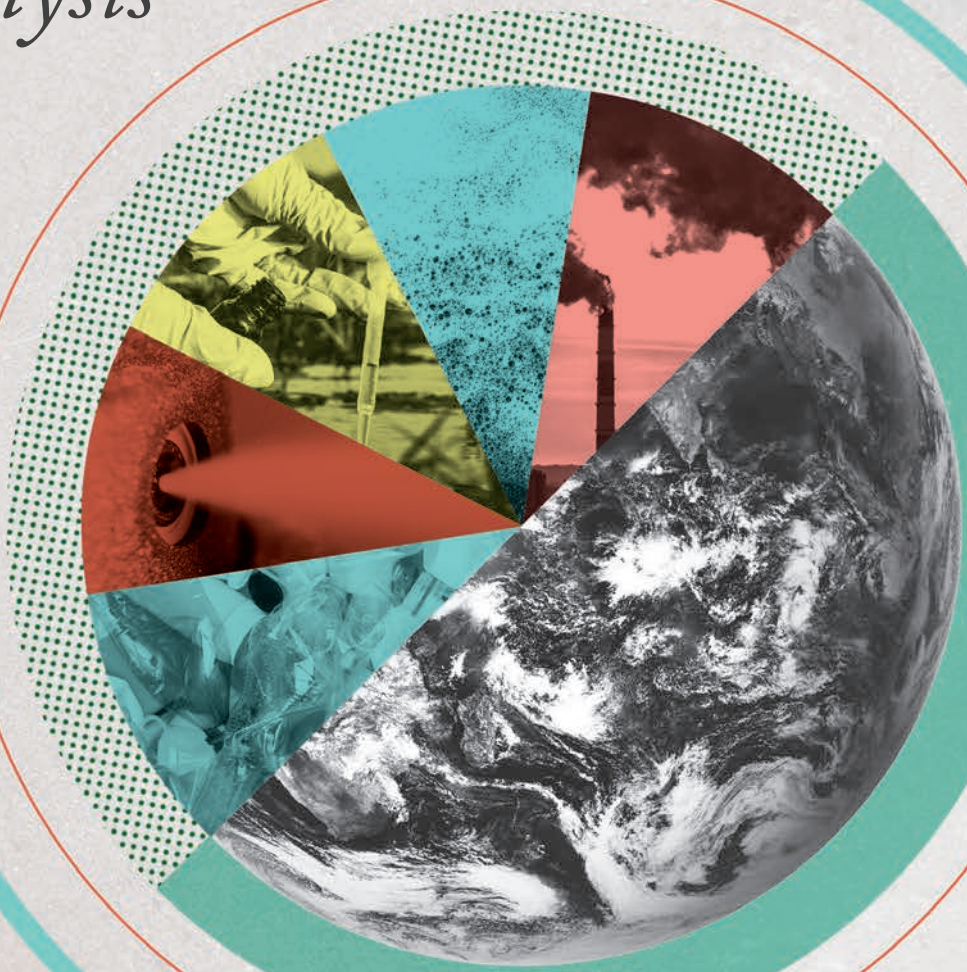
Ulrike Krop is Team Leader Applications & Academy at KNAUER Wissenschaftliche Geräte GmbH, Germany.

Reference

1. *KNAUER, "Systematic and Efficient Method Scale-Up for Peptide Purification" (2024). Available at: https://bit.ly/42ceF1R.*

KNAUER

Five Frontiers in *Environmental Analysis*

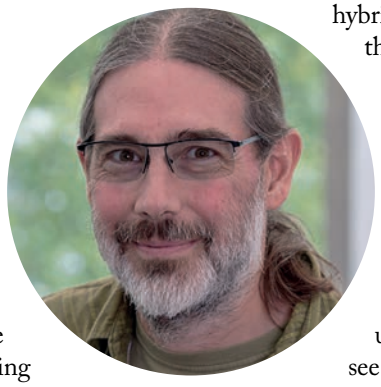


As the world looks to analytical science to guard against the harmful compounds in our environment, the community's imaginative application of increasingly sensitive technologies is helping to paint a more complete contamination picture. It is also driving genuine solutions to the myriad threats we face – from the removal of PFAS from our environment, to delivering a circular plastics economy. Here, five leaders in environmental analysis each highlight a different area where analytical innovation is protecting our planet.

CLIMATE CHANGE

Preventing carbon emissions is the ultimate goal, but analytical science offers key insights into carbon's behavior across systems, guiding breakthrough strategies for climate mitigation and adaptation

With Michael Gonsior, Professor, University of Maryland Center for Environmental Science, USA



What is the most pressing climate change issue right now, and how can analytical science help address it? The simplest solution in theory – and the hardest to achieve in practice – is to prevent carbon dioxide from entering the atmosphere in the first place. While we're making progress, including in alternative energy technologies and developing electric vehicles, the scale of removing CO_2 from the atmosphere is vastly different from preventing it from being emitted in the first place. That's where the real impact lies.

From an analytical science perspective, the biggest challenge is understanding the complexities of the carbon cycle. We're looking at tracking highly complex mixtures and pinpointing specific, indicative tracers. This helps us understand the activity and residence time of carbon in different pools, like the atmosphere and the ocean. Knowing how long a particular carbon molecule stays in a specific part of the carbon cycle helps us predict its feedback effects on CO_2 levels.

To put this in perspective, let's consider the ocean – a massive carbon reservoir. If just 1 percent more of the ocean's dissolved organic carbon were to mineralize annually, it would offset the entire annual anthropogenic CO_2 production. Understanding these large carbon pools and how changes within them contribute to positive or negative feedback loops is essential for predicting climate outcomes and making informed decisions about climate strategies. Analytical science plays a critical role here in uncovering these mechanisms and helping us see where we're heading.

One major area of advancement is in mass spectrometry for analyzing complex mixtures and unknown contaminants. In my lab, we're using an extremely sensitive triple quadrupole mass spectrometer, which is traditionally a targeted tool. But I'm actually using it in an unconventional way by systematically scanning all potential transitions across the entire mass range of organic matter samples. In this case, we're focusing on deep ocean samples, and this approach allows us to pinpoint specific molecular transitions. It's a slow, meticulous process, but it's opening doors to new tracers and even potentially the first structural identifications of deep ocean molecules, especially in refractory organic matter.

In the broader field, the trend has been toward high-resolution instruments, like the Orbitrap and FT-ICR-MS systems. However, a drawback with these high-resolution instruments is that they're typically less sensitive than triple quadrupole systems, which is why I turned to the latter. Sensitivity and speed are still major hurdles for high-resolution instruments.

Looking ahead, I'm excited about the development of hybrid mass spectrometers – systems that combine the strengths of different instrument types. For example, some researchers are pairing triple quadrupole instruments with time-of-flight mass spectrometers to get high resolution and high sensitivity together. These hybrid systems aren't widely commercialized yet, but I think they'll be game-changers, especially for complex environmental samples where precise molecular structures are essential for understanding the system. That's the direction I see making a real impact in Earth System Science.

Thinking about global efforts to address climate change, I could take the pessimistic route – but I'd rather share a different perspective that might seem a bit pessimistic but is actually hopeful in its own way. Often, we speak as though we're separate from the environment – as if we're somehow removed from nature. In reality, that's an illusion. We're probably the only species that sees itself as separate from nature, but that viewpoint doesn't make sense. Nature itself isn't under threat; it's we who are shaping our world, defining how we want it to look and feel. Nature will carry on; the Earth will still be here in a million years, no matter what we do. But what we're really impacting is our place within it, our quality of life, and the balance of ecosystems we depend on.

What gives me hope is that we're slowly – painfully slowly – starting to realize we're part of the environment, not separate from it. We're moving, though gradually, towards understanding our interconnectedness with nature. People are traveling more, and while you could argue that's counterproductive for the environment, it does broaden our perspectives. It lets us experience different environments, ecosystems, and communities firsthand, and that shifts mindsets in powerful ways. The fact that we have access to information more rapidly than ever is helping, too. Despite its challenges, the flow of knowledge allows us to see more of the world and our impact on it.

In the end, I think the biggest shift – and the one we're slowly seeing – is realizing that climate change is about us. We're not really "threatening nature"; we're shaping the conditions for our own survival and the future we want. That's a powerful motivator, and if we can fully internalize that, I believe it'll drive real change.

An expanded version of this article is available online

PFAS REMEDIATION

Analytical scientists are playing a crucial role in the development of technologies to remove PFAS from our environment

By Diana Aga, Professor of Chemistry, University at Buffalo, USA

I first heard about PFAS in 2002, early in my academic career at the University at Buffalo. At that time, a visiting professor from the University of Toronto, Scott Mabury, introduced me to the complexity of analyzing these compounds and highlighted their widespread presence in air, water, and the environment. PFAS are notoriously difficult to detect, and this complexity initially deterred me from working on them. I was an assistant professor, focused on securing tenure, and I didn't want to risk developing a method that might not work. So, for years, I avoided studying PFAS.

Fast forward to about five years ago, PFAS resurfaced in my professional life when collaborators started asking if I had a method for detecting them. They needed it badly, and that pushed me to dive deeper into the field.

Detection remains a central challenge, but it also underpins our response to the PFAS problem, whether it be monitoring or regulation. My PFAS research focuses on potential solutions and detection techniques. In assessing remediation technologies, detection plays a crucial role.

When you're dealing with remediation, you really need to know where the PFAS are going and if they've been fully destroyed. For example, with biosolids or solids remediation techniques like incineration, pyrolysis, or gasification, even at high temperatures, you need to be sure whether you're breaking them down completely or just volatilizing them. The same goes for groundwater treatments using plasma – you blast the PFAS, but where do they go? Are they just broken down into smaller, potentially harmful compounds? You need accurate detection to know.

Though we've made progress in analytical capabilities, there's still a lot of room for improvement, especially when it comes to volatile PFAS and unknown degradation products that emerge from these remediation technologies. I'd say that analytical challenges remain a significant hurdle even today.

CAN WE REMOVE OR DESTROY PFAS?

There are several remediation technologies for PFAS in development; the choice of technology depends on what you're trying to remediate. Right now, biosolids are a big issue. Many wastewater treatment plants used to apply biosolids on agricultural fields, but they're now discovering that these biosolids often contain PFAS, especially if the treatment plant receives wastewater from an industrial source. There are farms in places like Maine that had to close due to high PFAS levels leaching from biosolids, which can contaminate surface water and groundwater, especially when it rains.

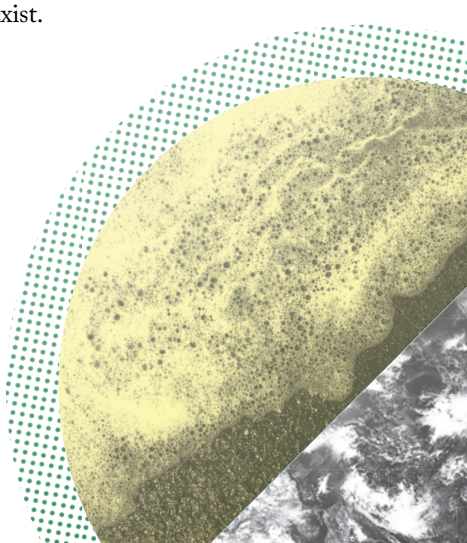
To address this issue, people are exploring pyrolysis or gasification to remove PFAS from biosolids. These processes essentially involve burning the material at very high temperatures, around 900–2,200 °F, to produce biochar or other byproducts (for example, syngas), depending on factors like oxygen levels and temperature. However, the challenge is that we don't always know if PFAS are being fully destroyed or just volatilized during the process.

Several strategies are being explored to remove PFAS from contaminated soil and water environments. For drinking water, activated carbon and anion exchange resin are the most widely used sorbents to capture PFAS. These materials work well, but after PFAS capture, you need to regenerate them or destroy the concentrated PFAS in the spent media. In addition, when using activated carbon filters, a key challenge is knowing when the filter is saturated and thus needs to be replaced. Breakthrough (where PFAS, especially short-chain compounds, start leaching back into the drinking water because the activated carbon has reached its capacity) is not acceptable for water utility companies.

Right now, the typical process is to sample the filtered water on a regular basis for LC-MS analysis at a certified lab. But if there is a backlog, results can take days, or even weeks. To avoid the risk of delayed result reporting, water utilities preemptively replace the carbon filters after a set volume of water has been treated, but this approach can be expensive. Hence, it would be incredibly helpful to have a faster method for detecting low levels of PFAS, ideally something like a PFAS-selective online sensor that could provide real-time data. Unfortunately, sensors for detecting PFAS at such low levels do not yet exist.

SEARCHING FOR A COMPLETE SOLUTION

To truly address the PFAS problem, everyone needs to work together, including regulatory authorities. We are still quite far from a complete solution. The more we regulate PFAS,



the less they will enter the environment. However, the PFAS that are already in the environment will persist – they're called "forever chemicals" for a reason. So, while regulatory measures are essential, we also need to focus on how to remediate what's already there.

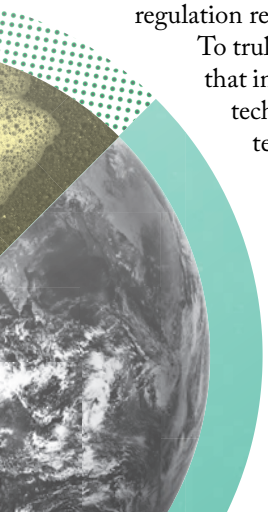
A major hurdle linked to regulation is the lack of toxicity data for many PFAS. We have a good amount of data on PFOA and PFOS, the C8 compounds, but there's limited toxicity information for many of the other PFAS. These compounds often occur in mixtures, so how do you regulate mixtures? It is a significant challenge.

I'd also like to see more progress on sustainable bioremediation technologies. For example, if we could find naturally occurring bacteria that are capable of breaking down PFAS into carbon, hydrogen, and fluorine, it would be the ultimate remediation technology. In this regard, there are some promising lab-scale isolates, but we still have a long way to go to scale-up these solutions to something that can be implemented in real-world environments. Investing more in bioremediation research would be a great step forward.

About 25 years ago, people were concerned about antibiotics and pharmaceuticals in discharges from wastewater treatment plants. Now, many cities have adopted advanced treatment processes following conventional activated sludge systems, such as ozonation and carbon filtration, resulting in very clean water. But we don't have anything like that yet that works well for complete PFAS treatment in highly contaminated water. If we could develop something similar on a municipal scale, it would have a huge impact. If we could inoculate wastewater treatment plants with bacteria that can degrade PFAS, we could prevent these compounds from ending up in surface water, which is often used for drinking water. And if all PFAS are removed during wastewater treatment, the biosolids produced would also be free of PFAS, giving the agriculture industry a valuable and safe fertilizer. Right now, many farmers are hesitant to use biosolids, and they have been banned elsewhere.

As we continue to grapple with the complex issue of PFAS, it is clear that there is no single solution. Remediation technologies are advancing, but challenges in detection, degradation, and regulation remain.

To truly make strides, we need a multifaceted approach that includes stronger regulations, improved analytical techniques, innovative and cost-effective remediation technologies, sustainable substitutes, and greater interdisciplinary collaboration.



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ATMOSPHERIC AEROSOLS

How volatile organic compounds and aerosol particles shape atmospheric processes, influencing cloud behavior, and the interconnected dynamics of ecosystems and climate

With Markku Kulmala, Professor of Aerosol and Environmental Physics, University of Helsinki, Finland

"A central challenge is that many important atmospheric compounds, especially in the gas phase, are present at extremely low levels."

We've established research stations in Finland and expanded to places like China, India, Estonia, South Africa, and beyond. We continuously collect data from these stations, analyze it – using e.g. atmospheric pressure interface mass spectrometry (APi-MS), especially time-of-flight (TOF) instruments. These instruments allow us to measure different compounds and clusters of gas molecules. We can generate a wide range of spectra, capturing the detailed composition of gasses and aerosols in the atmosphere.

We also collect data from the soil, including temperature and humidity profiles. We measure ecosystem functions, such as photosynthesis and gas exchange between tree needles and the atmosphere. We also track tree growth by monitoring diameter and other functional aspects. We measure aerosol concentrations in the air, and we record fluxes – meaning we monitor changes of CO_2 and other greenhouse gasses. We even track various types of radiation, including solar radiation, cosmic radiation, and radon emissions from the soil. As you can see, we cover a broad range of measurements.

What have we found? Let me give you a comparison between a major city like Beijing and our background station in Finland, at Hyytiälä. Hyytiälä isn't the cleanest place on the planet, but it is on the cleaner end of the spectrum, whereas Beijing is much more polluted. Interestingly, some atmospheric processes are quite similar between these locations. For instance, the growth rate of newly formed aerosol particles – about 4–6 nm per hour – is roughly the same in both places. However, the rate at which new particles (around 1.5 nm in size) are produced is about 100 times higher in Beijing than in Hyytiälä.

Moreover, measuring so many different variables with so many different instruments is throwing up a number of surprises. During the COVID-19 lockdown, for example, we observed that in Beijing, nitrogen oxides (NOx) and particle mass concentrations decreased, but ozone levels and particle numbers increased. Surprisingly, the overall particle mass only went slightly down, remaining almost the same before, during, and after the lockdown.

At our station in Hyytiälä, we've observed how increased CO_2 levels lead to more photosynthesis, which in turn emits volatile organic compounds (VOCs) like monoterpenes. These VOCs undergo chemical reactions in the atmosphere, producing low-volatile highly oxidized organic compounds that contribute to new aerosol particle formation. These particles can grow to become cloud condensation nuclei, which influence cloud droplets and, ultimately, precipitation. However, when there are more aerosol particles, clouds live longer, become thicker, and reflect more sunlight. On the other hand, the more aerosol particles we have the more the amount of diffuse solar radiation is enhanced, which penetrates radiation deeper into the ecosystem, further enhancing photosynthesis. It's a fascinating feedback loop with significant implications for both weather and climate.

Longer term, we've observed changes such as a decrease in SO_2 concentrations, both in Beijing and Hyytiälä. We also see how factors like population growth and land-use changes are impacting air quality and climate; in turn, we see how climate changes are influencing processes like photosynthesis. Though our data doesn't span hundreds of years, the data we have – over decades – allows us to clearly see these changes at various time scales.

A central challenge is that many important atmospheric compounds, especially in the gas phase, are present at extremely low levels – often in the parts per quadrillion (PPQ) range, with as few as 1,000 or 10,000 molecules per cubic centimeter, sometimes even less. This makes it incredibly challenging to push the detection limits of techniques, such as API-MS, low enough. Additionally, we need analytical chemistry expertise to help us properly calibrate these measurements. Though we understand some of the basics, the need for better calibration methods and possibly developing standards for these measurements is crucial. And that requires specific expertise in analytical techniques.

That is to say, analytical chemists play a crucial role in efforts to improve atmospheric conditions!

An expanded version of this article is available online

WATER ANALYSIS

PFAS demand attention, but natural and anthropogenic threats create opportunities for innovation in water analysis

With Torsten C. Schmidt, Professor, Instrumental Analytical Chemistry and Centre for Water and Environmental Research (ZWU), University of Duisburg-Essen, Germany

Water research, especially water quality, has been a topic of interest for me since my school days. I started with small projects at school, and I knew early on that I wanted to work on something that would help the environment. For a long time, I considered how best to approach this. I thought about more technically oriented study programs but ultimately settled on chemistry, which led me to analytical chemistry – a field I became passionate about right away.

Today, PFAS are certainly top of the list of emerging water contaminants, but there are several other compounds with the potential to become major environmental issues.

While not a single substance class, compounds that are persistent and mobile (and sometimes also toxic), known as PMTs, are increasingly concerning. Some PFAS compounds fall into this category as well. Over the last decade or so, PMTs have gained attention because they have been largely overlooked in the past but are crucial, especially from a water cycle perspective. These compounds don't degrade easily, and are mobile. They can pass through natural barriers such as soil or bank filtration, and quickly travel through the water cycle. They are very difficult to contain.

Part of the reason they went undetected for so long is because of the limitations in analytical methods, particularly for detecting low concentrations in water. Historically, we relied heavily on gas chromatography (GC) for organic contaminants, which works well for volatile compounds. Later, liquid chromatography-mass spectrometry (LC-MS) became more widespread, but it was primarily based on reverse-phase LC, which doesn't sufficiently retain highly polar organic compounds. However, advances in recent years have introduced new separation methods that better capture these polar compounds. This progress has revealed that many of these compounds are indeed present, sometimes in high concentrations, in aquatic environments – levels we simply couldn't detect before.

The growing awareness has been somewhat of a success story, as these persistence and mobility characteristics are now being considered in the registration of new chemicals under regulations such as REACH. This is a positive shift, helping us avoid the pattern of focusing only on certain properties and then discovering new risks decades later.

We're also starting to recognize that it's not only anthropogenic contaminants we need to be concerned about – naturally occurring compounds can also have serious impacts. For instance, the Oder River disaster on the Polish-German border highlighted this, where higher salt concentrations and warmer temperatures enabled certain algae to grow explosively. The algae then released toxins that killed fish and other organisms. This wasn't directly due to a man-made contaminant but rather a natural toxin exacerbated by anthropogenic influences.

Cases like this emphasize the need for a comprehensive approach that combines chemical data with biological analysis. To address such incidents effectively, we should combine information on chemical composition with data from environmental omics, such as eDNA and RNA-based methods, to see how ecosystems respond to changes in both chemical and biological conditions. This combined approach could advance our understanding of how ecosystem dynamics are influenced by both anthropogenic and natural factors, which is key for developing more effective environmental protections.

While not every individual project or piece of research might have immediate or visible effects, I firmly believe that, as a whole, our work is essential. Environmental analysis provides the data that makes people care, and without it, many of these issues would remain unseen or unaddressed.

An expanded version of this article is available online

THE CIRCULAR PLASTIC ECONOMY

Emerging analytical methods for more precise quantification of hydrocarbon composition and impurity detection may prove essential to realizing a circular plastic economy

By Melissa N. Dunkle, Senior Research Scientist, Dow Benelux, The Netherlands

Plastics are an integral part of our daily lives, found in everything from synthetic fabrics used for clothing to food packaging, building materials, and more. As the global population has grown, so has the production of plastics, which reached 475 million tons in 2022. However, only about 12 percent of this plastic is collected for recycling. So where does the rest go? Approximately 80 percent of the remaining plastic is never recovered; it is either mismanaged, ending up in landfills, or incinerated, following the traditional linear economy model for plastics. A global shift is needed to transition from this linear economy to a circular economy for plastics, requiring action not just from governments and industries but also from consumers.

Governments are beginning to create legislation that mandates minimum recycled content in plastics. For example, the EU's Single-Use Plastics Directive requires that plastic bottles contain at least 25 percent recycled plastic by 2025, increasing to 30 percent by 2030. As we move towards a circular economy for plastics, similar legislation around minimum recycled content for other plastic materials is expected to be implemented by various countries worldwide.

Achieving a circular economy for plastics will require different recycling technologies to close the loop. While mechanical recycling for rigid plastic bottles is well-established, not all types of plastics can be easily recycled this way. For this reason, advanced recycling (also known as chemical recycling) is gaining attention as a viable alternative. In mechanical recycling, the polymer structure is maintained, but in advanced recycling, plastics are broken down into their original monomers. Several technology routes can be used for advanced recycling, including solvolysis, pyrolysis, and gasification.

THE NEED FOR ANALYTICAL DATA

Analytical evaluation and data processing are key components in achieving plastics circularity. While this example focuses on advanced recycling through pyrolysis, it's important to note that such evaluations and data are equally crucial when considering mechanical recycling or other advanced recycling technologies.

In advanced recycling via pyrolysis, the importance of analytical data becomes clear. Pyrolysis involves heating waste plastic to temperatures that thermally decompose it into three fractions: gas, oil, and char. For advanced recycling purposes, the oil fraction is considered a potential feedstock for steam cracking. However, depending on the composition of the waste plastic feed, the oil fraction may contain not only hydrocarbons but also undesired impurities. These impurities can include nitrogen species (e.g., from the degradation of polyamide in the plastic feed), oxygenates (e.g., from polyvinyl alcohol, polyethylene terephthalate, or additives), aluminum (e.g., from poly-Al packaging), chlorine (e.g., from polyvinylchloride or additives), and more.

Additionally, the hydrocarbon composition of plastic pyrolysis oils does not align with current steam cracker specifications, where the Platts open naphtha specification is typically used as a guideline. Plastic pyrolysis oils often contain high levels of olefins (e.g., from polyethylene, polypropylene, and other polymers) and aromatics (e.g., from polyethylene terephthalate, polystyrene). Therefore, crude plastic pyrolysis oils cannot be used as a steam cracker feedstock without significant upgrading.

To select an appropriate upgrading strategy, it's essential to conduct a thorough analytical evaluation of the plastic pyrolysis oils to understand both the hydrocarbon composition and the impurity profile. This information is crucial for making informed decisions about which upgrading technologies will effectively remove or eliminate the impurities and improve the hydrocarbon composition, bringing the plastic pyrolysis oil into specification.

While the chemical industry has decades of experience analyzing fossil-based feedstocks, it would be a mistake to assume that these established methods can be directly applied to the analysis of crude plastic pyrolysis oils. Crude plastic pyrolysis oils differ significantly from fossil-based feedstocks in terms of hydrocarbon composition, final boiling point, impurities, and more. As a result, research groups in both industry and academia are actively developing new analytical methods. Significant effort has been dedicated to method development for the accurate quantification of the hydrocarbon composition in crude plastic pyrolysis oils, as well as for the identification and quantification of impurity profiles.

For the analytical evaluation of crude plastic pyrolysis oils, much focus has been placed on gas chromatography (GC). In the works mentioned above, both one-dimensional GC and comprehensive GC (GC×GC) were utilized, and various detector technologies were exploited. One of the newer detectors being evaluated is the vacuum ultraviolet detector (VUV), which is still relatively new to the market. GC-VUV was introduced in 2014, and since then, the technique has shown promise for the characterization of the hydrocarbon composition of various materials, including crude plastic pyrolysis oils. While GC×GC can also provide insight into the hydrocarbon composition of materials, the co-elution of olefins and naphthenes in the same elution band of the 2D plot can complicate data processing when both compound classes are present. However, GC×GC is compatible with various GC detectors, including (but not limited to) mass spectrometry and element specific detectors, making this technique well suited for the characterization of the impurity profile of crude plastic pyrolysis oils.

The evaluation of crude plastic pyrolysis oils is a burgeoning

area of research, with each analysis yielding new and insightful information, making it an exciting time to be an analytical chemist.

MOVING FORWARD

There are many challenges to overcome to make plastics circularity a reality. Change isn't easy, and achieving it on a global scale will require concerted efforts from governments, industry, and consumers.

One perspective not yet discussed in this article is the cost associated with transitioning from a linear plastics economy to a circular one. According to a recent McKinsey report, the plastics industry may need to invest as much as $100 billion to achieve 20–30 percent recycled content in materials. Cost is just one factor that will influence the speed at which plastics circularity is implemented. Other critical considerations include technology readiness and economic feasibility, among many others.

However, before moving forward, it may be necessary to take a step back. As mentioned earlier, only around 12 percent of produced plastic is currently being collected for recycling. Optimizing existing collection and sorting infrastructures and processes is essential to increase this percentage. This challenge presents an interesting opportunity for analytical scientists, as current automated optical sorters have limitations in detecting different types of plastics. Enhancing automated sorting capabilities and possibly integrating artificial intelligence are areas worth watching.

Transitioning from a linear to a circular plastics economy will take time, but the journey has already begun. McKinsey reports that chemical industry players have committed to achieving 7 million metric tons per year of advanced recycling capacity by 2030. It is challenging to predict what the landscape will look like beyond 2030, as this will depend heavily on legislation and the technological advancements that still need to occur.

In conclusion, change is happening, and progress is being made to transition from a linear economy to a circular plastics economy. For those working in this field, this represents a new and exciting area of research, where success means making a positive impact on the environment. Even if you're not directly involved in this field, you can still contribute; we are all consumers, and our choices have an impact.

References available online

Looking Back, Moving Forward

As we enter 2025, Ron Heeren, Deirdre Cabooter and Koen Sandra provide their perspectives on the field's most impressive accomplishments, pertinent challenges, and future directions

What would you say has been analytical science's biggest accomplishment over the past five to ten years?

Ron Heeren: For me, the biggest accomplishment is what I call the "resolution revolution." Over the last five to ten years, all of our instruments – whether it be chromatography systems, mass spectrometers, or spectrometers – have significantly improved in resolution, throughput, and sensitivity. These new instruments have had a profound impact across various disciplines – ranging from battery research, where we can now examine chemical processes in real-time during charging and discharging, to biology, where we're able to analyze a single cell within the context of tissues. Additionally, in agro-food science these advancements let us optimize agricultural processes, such as studying the effects of different spectra of LED lights in greenhouses.

Deirdre Cabooter: One major advancement that has had a huge impact on analytical sciences as well as society as a whole, is the introduction and integration of machine learning and artificial intelligence. They are instrumental in data analysis for instance, as mass spectrometers become more advanced and data more abundant. Machine learning algorithms assist with data interpretation and can even make predictions, such as forecasting compound properties based on their structure. Additionally, AI helps automate tedious tasks like peak identification, integration, and tracking, to assist method development.

Something I also personally appreciate as a daily user is the commercialization of two-dimensional liquid chromatography (2D-LC). In the past, this was primarily a technique used in academic labs with systems built in-house. Commercial availability has made 2D-LC more accessible, and it's now being adopted more and more in industrial settings. This represents a significant step forward in tackling the complexity of modern samples and meeting future analytical challenges.

Koen Sandra: Today with high-end mass spectrometry, we can study thousands of proteins within a single cell in just half an hour. To put that into perspective, 20 years ago, when I worked at a biomarker company, it took us half a day to identify 1,000 proteins from a sample of 1 million cells. So we've gone from 1 million cells to a single cell, and from half a day to half an hour – that's quite an accomplishment.

I've also been particularly impressed by the advancements in speed, sensitivity, robustness, and data-handling capabilities of mass spectrometry. Specifically on data-handling capabilities, I always advise people to look closely at their data. These sophisticated instruments generate brilliant results, but they also produce a lot of irrelevant or "junk" data, and relying solely on software algorithms to make sense of it all isn't ideal. That human touch – critically evaluating the data ourselves – is still essential.

Looking back over the last 12 months, what are the standout accomplishments in the field that you'd like to highlight?

Heeren: Over the past year, I've seen amazing developments in spatial biology and its integration into analytical sciences. If I had to highlight the biggest accomplishment, I'd say it's the fact that we can now routinely perform single-cell transcriptomics, single-cell proteomics, and single-cell lipidomics.

However, these advances also bring significant challenges – primarily, how do we handle and make sense of the vast amounts of highly detailed, high-resolution data we're generating? Analytical scientists are producing so much intricate data that understanding the full complexity of the systems we're trying to study is becoming increasingly difficult.

The topic of AI often comes up when discussing solutions for this, but personally I think we need to be cautious. With funding agencies and organizations heavily investing in AI as a catch-all solution, I think we need to be more critical and specific about the type of AI we are talking about, and the specific problems we would like it to solve.

Cabooter: Something that stood out to me at conferences in 2024 were the numerous talks on oligonucleotides. These therapeutics are drawing a lot of attention due to the challenges they present in analysis, so it makes sense that many groups are focusing on them.

Another trend I've noticed, although not exactly new, has been a renewed interest in green chemistry. It's been around for quite a while, but possibly due to the global emphasis on Sustainable Development Goals, it seems to be regaining momentum. What's particularly interesting is that it's not just about using greener, renewable, or less toxic solvents anymore.

Sandra: There's been a lot of focus on PFAS (forever chemicals) being measured at extreme sensitivities in a wide range of matrices nowadays, including blood, soil, and water. Most methods today are targeted, using LC-MS with triple quadrupoles and sample preparation techniques like solid-phase extraction to concentrate and clean up samples. However, a growing trend is non-targeted screening using high-resolution mass spectrometry and ion mobility. This approach allows us to look beyond the usual suspects, which is important since there are thousands of PFAS chemicals and current methods typically only target a few dozen.

What are the major challenges currently being faced by the field?

Cabooter: One area I often discuss is complex samples. In health and clinical settings, we deal with biological samples and drug development, which are inherently complex. Similarly in environmental sciences, there's a lot of focus on detecting, identifying, and treating contaminants in the environment, with these efforts also involving highly complex samples.

To truly understand what's happening in these areas and drive progress, we need to be able to analyze these samples efficiently and quickly. This requires the development of better methods – high-resolution techniques that can deliver results in shorter time frames. At present, method development is still taking too much time, so we need to find ways to streamline and optimize this process.

Heeren: One key issue is the ethical considerations that arise from our increasing ability to extract detailed molecular information. For instance, antigen profiles are highly personal and reflect what an individual has been exposed to throughout their lifetime. This level of detail could raise privacy concerns, as it essentially reveals someone's molecular phenotype. How do we handle such sensitive information? Who owns this data – patients, researchers, or institutions? Specifically in healthcare, where privacy and ethical issues have always been paramount, these questions are becoming increasingly urgent.

Sandra: For me, one of the most obvious ones is how to inspire and educate the next generation of analytical scientists. I see the field struggling with this – it's becoming increasingly difficult to find skilled scientists with a critical mindset. It's relatively straightforward to find people who can use the equipment, but finding those with in-depth knowledge and a deeper understanding of the technology is much more difficult. And to be honest, I don't blame them entirely. Instrument vendors are developing more and more "black box" systems, meaning users no longer need to think about what's happening behind the scenes.

Thinking about the future, what do you think needs to happen to make progress in the areas discussed? Are we missing anything from the toolbox, or are there other big milestones we need to achieve?

Sandra: The toolbox will never be truly complete, which is part of what keeps our field exciting and full of opportunities. For example, in the biopharmaceutical field, there's a clear need for technologies that can provide deeper insights into large molecular assemblies like lipid nanoparticles and viral vectors.

One specific need is for a mass spectrometer capable of measuring in the mega-Dalton range – having such a tool could reveal whether mRNA is encapsulated within lipid nanoparticles or if a transgene is present in a viral vector. In an ideal scenario, this same mass spectrometer would also work in the kilo-Dalton and Dalton ranges, enabling it to handle antibody measurements and lipidomics. That might be asking for a lot, but it would be a game-changer – especially if the instrument could be made affordable.

Sticking with the biopharma domain, we often use dozens of different methods to gather complementary information about these molecules. Combining these methods into a single technology capable of assessing multiple structural and functional attributes would be a major step forward. There's already work being done in this area, and the concept has even been given a name: MAM, or Multiple Attribute Method.

Cabooter: As Koen mentioned earlier, I think another area we need to focus on is education. It's not exactly about "adding new tools to the toolbox," but rather ensuring we train people properly in analytical sciences. Sometimes I feel that students are content with simply pressing the "start" button on an instrument and generating data, without fully understanding how the system works.

In our group, we emphasize the importance of understanding the instruments – how they work, how to troubleshoot when they break, and the fundamentals behind their operation. This focus needs to start early, even at the bachelor's level. We need to ensure that students grasp the instrumentation, the core concepts and the working mechanisms, as this foundational knowledge equips them to excel in their future careers and adapt to the evolving challenges in the field.

How would you sum up your current perspective on the potential future of analytical science as a whole?

Heeren: I'm positive by nature, so I'm very optimistic about the future of analytical sciences. That said, there is one significant caveat: data. The challenge is that we need to do something counterintuitive for analytical science – to reduce the data so we can make it comprehensible. This goes against our instinct, as we're trained not to throw away data or oversimplify, but rather to embrace complexity.

There are already promising developments in the field, however, that aim to tackle data management and interpretation. Overall, I think analytical sciences are in a strong position, as long as we continue investing in the talent that drives our field forward.

Cabooter: Ask me again in five or ten years, but for now, I'm very positive about the future. I still wake up inspired by the challenges and opportunities ahead – whether it's improving hardware, advancing software, or tackling exciting new applications. Every day brings new possibilities, whether in clinical analysis, food safety, or environmental monitoring.

I'm particularly excited about interdisciplinary projects, where we collaborate with people from other fields to brainstorm, solve problems, and develop new techniques and solutions for societal challenges. These opportunities keep the work fresh and meaningful.

Sandra: I'm also quite positive. It's truly amazing what we've achieved over the past decades, building on the incredible work of the early pioneers in the field. Looking ahead, I see a bright future for analytical science. There's so much exciting potential in the advancements coming our way. I'm optimistic about the contributions we can make – to health, the environment, and beyond.

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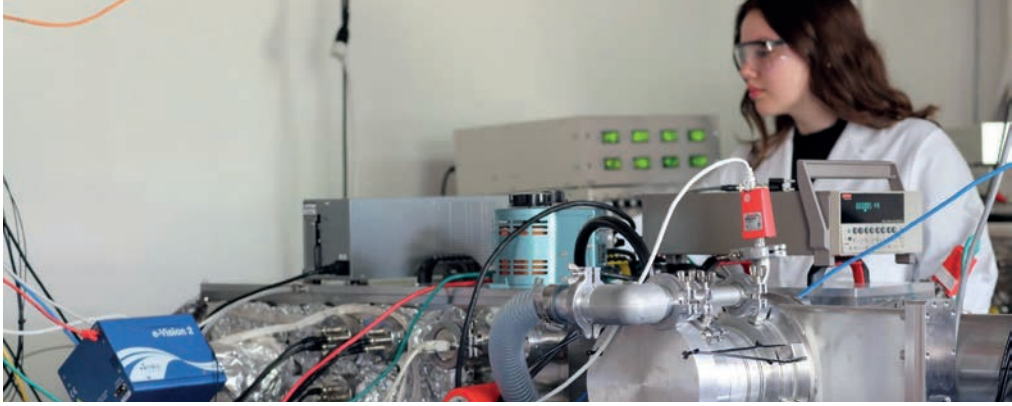

MASS SPEC

CD-MS: To Megadalton and Beyond

Charge-detection mass spectrometry (CD-MS) has extended the range of MS to gigadalton-sized viruses and polymers; and with a commercial instrument in development and exciting new applications in complex protein mixtures, maturity beckons

By Martin Jarrold, Distinguished Professor and Robert & Marjorie Mann Chair, Indiana University Bloomington, USA

The origins of CD-MS date back to the 1960s. During the Sputnik era, as satellites were being launched into space, there was concern about the impact of dust on these satellites. Researchers aimed to accelerate particles to high velocities and then impact them onto surfaces to observe the effects. As a result, the concept of measuring the m/z and charge of a particle by passing it through a conducting cylinder was introduced. Then, in the mid-1990s, Henry Benner and colleagues adapted this idea by adding an electrospray source to study electrosprayed ions. Their approach involved single-pass measurements, which limited the size of the particles they could analyze to very highly charged particles in the megadalton range.

But my CD-MS story starts in 2006 – basically because I was looking around for something different to do. I had colleagues here in the chemistry and biochemistry departments at IU who were looking at viruses and I thought I could try to use mass spectrometry to measure their masses.

Of course, with conventional mass spectrometry, there's a mass limit to what you can measure – usually around a megadalton, if you're lucky, and if you have a fairly homogenous sample. But many samples are either heterogeneous or have high molecular weights, such as vaccines or viruses.

As is often the case when you start something new, we had many failures to start with. Then I came across several publications by Benner, who was then at the Lawrence Livermore Lab, on charge detection, which seemed perfectly suited to the task at hand.

To understand how charge detection works, we have to go back to the limitations of conventional MS, where you're measuring the m/z spectrum. If you have large, multiple-charged ions, you also have to figure out what the charge is. You can do that if you have well resolved peaks in the m/z spectrum, thanks to the ions being in different charge states. But if you have a heterogeneous sample, each mass in the sample gives you a distribution of charge states, which overlap – and you end up with a featureless blob. You can't figure out what the masses are because you can't figure out what the charges are. With CD-MS, you perform a single-particle measurement, which gives you the m/z and charge for each individual ion. The m/z multiplied by charge gives you mass, so you have the mass of each individual ion. Once you do that for thousands of ions, you can take the masses and bin them into a histogram – that's your mass distribution.

In other words, by individually measuring each ion's charge and m/z ratio, you avoid the confusion caused by overlapping signals, allowing for the measurement of large particles and heterogeneous samples. The problems with CD-MS at that time was that it was limited to highly charged ions, and it had very poor resolution – in a nutshell, it wasn't practical. I thought we should try it because it seemed to be such a cool technology, and I was sure we could find a way to make it better. So, we started doing CD-MS with a simple, single detector setup – with the ions just flying through. As soon as we had a working instrument a retired colleague, George Ewing, heard about what we were doing and got us interested in looking at the charge on water droplets. It was a good match because the CD-MS detectors we had in those days were really poor and highly charged water droplets were one of the few things we could measure. George led us astray and kept us distracted with water droplets for several years.

"You really need to start a company"

It took us close to a decade to really build upon Benner's work and engineer the CD-MS technology into a practical measurement tool – it wasn't until 2013 that we got our first ion trap CD-MS to work. The key improvement was the ability to measure the charge accurately, which had hindered Benner's measurements. An important development here was using Fourier transforms to analyze the data. Initially, we used Gaussian signal processing, but incorporating Fourier transforms significantly expanded what we could analyze. Suddenly, we could examine much more lowly charged particles, and the frequency measurements obtained were a much more reliable and accurate way to determine the m/z. From that point on, our focus shifted to increasing the precision of charge measurement and ensuring the accuracy of frequency measurement – an engineering challenge that involved extensive simulations to optimize the process. We became proficient at conducting computer simulations, diligently working to achieve a level of accuracy and reliability sufficient for commercial use.

"A WHOLE NEW BALLPARK FOR MASS SPECTROMETRY"

CD-MS technologies have the potential to address challenges in viral particle analysis, synthetic nanoparticle characterization, and single-cell analysis – areas where traditional methods fall short

With Evan Williams, Professor of Chemistry, UC Berkeley, USA

I first became interested in this area well over 20 years ago when I attended an electrostatic ion trap workshop and saw some of the cone traps from Daniel Zajfman's group at the Weizmann Institute of Science, Israel. They were being used for ion storage in rings, performing isolation and storage tasks. Unfortunately, it took us about eight years to secure funding to build our first instrument, which set us back considerably because it was essentially a ground-up build. Despite the challenges, we stuck with the cone traps, which is a bit different from Martin Jarrold's approach.

In an FTMS-type instrument – whether it's an Orbitrap, an ICR, or these electrostatic ion traps – the frequency is always directly related to the mass-to-charge ratio (m/z). The idea is that by measuring a frequency, you can determine m/z. Most people prefer the frequency to remain stable so they can measure it over a long period, which allows for very precise mass measurements. Orbitraps and ICRs, for example, are known for their high accuracy in this regard.

However, in electrostatic ion trap devices, ion frequency is energy-dependent. Martin's strategy has been to try to minimize this energy dependence by designing harmonic traps. While you can never achieve a perfectly harmonic trap – there will always be some energy dependence – you can minimize it over a narrow range of energies.

In contrast, our approach involves trapping ions with energies ranging over 60-70 eV per charge, which is a significant range. The advantage of this with single-ion techniques is that if you have multiple ions with the same m/z, you can spread their energies out, so they each have different frequencies. We continuously track the m/z, charge, and ion energy throughout the entire time that an ion is trapped. This results in fewer interferences and allows for a much higher degree of multiplexing. We can introduce more ions into the device without their frequencies interfering or stacking up, which is a limitation in techniques like the Orbitrap. In the Orbitrap, if you fill it with ions of the exact same m/z, all their signals co-add, and you lose information about the number of ions or their charges. Our approach helps avoid this issue.

This field is wide open right now because accurate mass measurement of very large particles, such as synthetic nanoparticles, has been challenging. We now have collaborations with several groups where CD-MS is proving to be the best, and sometimes the only, method for characterizing these particles. Traditionally, microscopy has been the primary tool, but it has its limitations. For example, techniques like TEM (transmission electron microscopy) require drying out the sample on a grid, which can introduce artifacts. Additionally, microscopy isn't well-suited for obtaining kinetic information, as it typically involves pulling samples out at different times.

The advantage of CD-MS for large particles is similar to the advantage of conventional mass spectrometry for smaller molecules (below a MDa): it provides very accurate mass measurements, quickly, with high sensitivity and specificity. This is valuable for characterizing anything involving large particles, whether it's viral particles, synthetic lipid nanoparticles, or other examples we've been working on. For instance, we can determine how much RNA is in lipid nanoparticles, what the average size of the particles is, and how they are affected by processes like freezing.

We'd like to be doing single-cell analysis right now, and there are many good reasons to pursue cellular analysis based solely on mass. However, once you get into the micron size range, other techniques might be more suitable. The challenge of heterogeneity becomes more significant at that scale, and high mass accuracy becomes less critical.

In terms of the current limitations, we're starting to learn a lot more about the technique, particularly with electrospray ionization, which is how most ions are introduced into the instrument. Getting large particles through electrospray, at least the way we currently do it, is likely to be a significant challenge. While we haven't hit the limits yet, we believe this area will require further development.

Another significant issue is the speed of the devices. A lot of the data being published involves long accumulation times – sometimes an hour or two just to get a decent ion count. That's acceptable when you're developing a new technique, but in practical applications, it's not something most users are willing to endure. Our goal is to reduce this time to be more in line with an LC time scale.

Nevertheless, I'm actually surprised that more companies aren't interested in commercializing the devices we're currently developing. This technology really does open up a whole new ballpark for mass spectrometry.

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As we were working on this, David Clemmer – who I've known for many years and who now works with us at Megadalton – was always telling me that we really need to start a company and commercialize our CD-MS technology. I would always reply: "Yeah, right! I'm a chemistry professor, not a businessman!" But around 2018, we began getting interest from people in the pharma industry using AAV vectors for gene therapy.

When researchers are encapsulating DNA inside a viral vector, one of the first analytical questions is the ratio of empty to full particles and how much partial packaging is going on. Given the size of the particles, answering this question is quite challenging. You might have a selection of capsids ranging in mass from 3.5 to 5 megadaltons (for example), depending on how fully packaged they are. With CD-MS, you can accurately determine the ratio of full-to-empty capsids in some detail. In fact, you can glean quite detailed insights into the protein composition of the AAV capsid, as well as the DNA inside the capsid, too. But more on that later.

Initially, we were fulfilling requests to measure samples for free – just as something on the side. But I realized this wasn't the best use of student's time, so we started charging people for it and paying students on the side to do the measurements. The requests kept coming and we just couldn't keep up. David's comments about commercialization started to make a great deal more sense!

We started the company, Megadalton, in 2018. Ben Draper, a graduate student of mine, was the first employee. In fact, he was all set to work for Intel, until we offered him less money to stay… Thankfully, he accepted! He'd been working on the technology and was excited to get involved in trying to commercialize it, and he has done a fantastic job developing the analytical capabilities of CD-MS.

Waters supported us from the get go – initially giving modest funds to keep us afloat, before we were measuring enough samples to survive on our own. They continued to invest and eventually visited to check out our instrument, had their own scientists run it, and so on. In the end, they acquired the IP from Indiana University and Megadalton in 2021, and we've continued to work closely with them.

They've been building prototype instruments – what they call "technology demonstrators." And they're currently working on a version of the instrument that is close to the one they'll end up selling. The projected date for the instrument to hit the market is, I believe, sometime in 2025. So watch this space!

Maturity beckons

CD-MS has come a long way, but it is by no means a mature technology. I think we're going to see the resolution of the m/z measurement get much better – this is what we're focused on. And when you've got a technique where you can measure m/z very accurately, and you can assign a charge state to that m/z, you can look at very complex protein mixtures. This wasn't one of the original ideas behind CD-MS – it was really to look at big things. But I think it's going to look at medium-sized things as well – and have a profound impact there. For example, I think it will soon become possible to take a sample of serum and, with very little cleanup, electrospray it, and then look at it with CD-MS to get a readout of what proteins are there.

Going back to the original intention, CD-MS has extended the range of mass spectrometry from around a megadalton, depending on the sample, to around a gigadalton. Now we can look at very large particles, such as polymers and very large viruses.

I mentioned the demand for a technique like CD-MS in AAV analysis, but AAVs are actually relatively small compared with other viral vectors, and they are also limited in terms of the size of the genome that they can encapsulate. So, there's interest in using larger viruses to act as gene therapy vectors, such as adenoviruses and lentiviruses. CD-MS can analyze these much larger viruses; we've published an analysis of a 150 megadalton virus, for example.

We've also done some CD-MS work on the COVID-19 spike protein, which is another example of its utility. The spike protein is very heterogeneous due to the 22 glycosylation sites on each of the three trimers, resulting in a total of 66 sites. This creates a heterogeneous mixture of masses that conventional MS cannot analyze. However, CD-MS can measure the mass distribution, even though it's broad and cannot yet resolve individual components with very high resolution.

We have also started investigating lipid nanoparticles, spurred by the success of COVID-19 vaccines, which led to increased interest in their other applications. Using CD-MS, we have also measured the masses of DNA, particularly looking for genome truncations in AAVs. By extracting DNA from gene therapy vectors and measuring its mass, we can determine if it matches the expected mass. If the DNA is shorter, it indicates truncation, which is another significant issue in AAV gene therapies.

It's an exciting time for CD-MS. We've recently significantly reduced the time it takes to measure the charge accurately. We're now at a threshold where we can truly improve the m/z resolution, which will, in turn, enhance the mass resolution. For a long time, we were stuck at a resolving power of around 700. However, we've recently improved the resolving power to 14,000. I believe we can push this up by another order of magnitude, making CD-MS competitive with very high-resolution MS technologies. I'm very excited about the next couple of years. I think these advances are achievable within this timeframe.

Is there an upper limit to the size of particles we might be able to analyze using CD-MS? At some point, as particles become larger, gravity will start to play a role. We're not at that stage yet, and it's not clear if measuring into the gigadalton range, such as measuring cells, is necessary. Personally, I'm not yet convinced that exploring tens or hundreds of gigadaltons is essential. Having said that, a few decades ago, people likely had similar doubts about the scales we currently work with, so perspectives could well change in the future.

CHROMATOGRAPHY

Chromatography Free: It's Closer Than You Think

In an era of increasingly sophisticated ion mobility–mass spectrometers, isn't it time we jettisoned chromatography altogether? Well, it isn't quite that simple – yet.

By Oliver J. Schmitz, Full Professor, Applied Analytical Chemistry, Faculty of Chemistry, University of Duisburg- Essen, Germany

In the age of ultra-high-resolution mass spectrometry, why are we still tethered to chromatography? Chromatography not only demands significant resources and time but also poses environmental concerns, all while offering a limited separation power when compared to the capabilities of today's mass spectrometry (MS) technology. Yet, here we are, with chromatography still embedded in our workflows. Why?

For quality control and simpler analyses, traditional methods such as HPLC-UV or GC-FID might suffice, but these are targeted applications. In the realm of non-targeted analysis, especially for complex samples, MS is typically coupled with chromatographic pre-separation to achieve the required precision. The pairing of triple quadrupole MS with gas or liquid chromatography has long set the standard for targeted analysis, yet as MS technology advances, we need to question if this approach is still necessary.

Non-target analysis is governed by an established framework, such as the identification levels defined by researchers like Emma Schymanski. Their five levels of identification culminate at levels 1 and 2, which demand rigorous structural confirmation and increasingly complex MS data. But while MS can deliver remarkable information, it often falls short when striving to reach these higher identification levels in complex samples – unless, of course, chromatography steps in to bridge the gap.

Therefore, despite its many limitations, chromatography has proven indispensable in complex non-target analysis, allowing separation and identification of compounds that MS alone struggles to differentiate. But challenges persist. Even with high-resolution MS, signal intensity for MS/MS often isn't adequate across all signals in complex samples. Chromatography is required to distinguish isobaric compounds effectively, but even when coupled with advanced MS instruments like Orbitraps or FT-ICR-MS, technical difficulties emerge. These systems, while high-resolution, are simply too slow to keep up with rapid chromatographic separations, making the combination less than ideal.

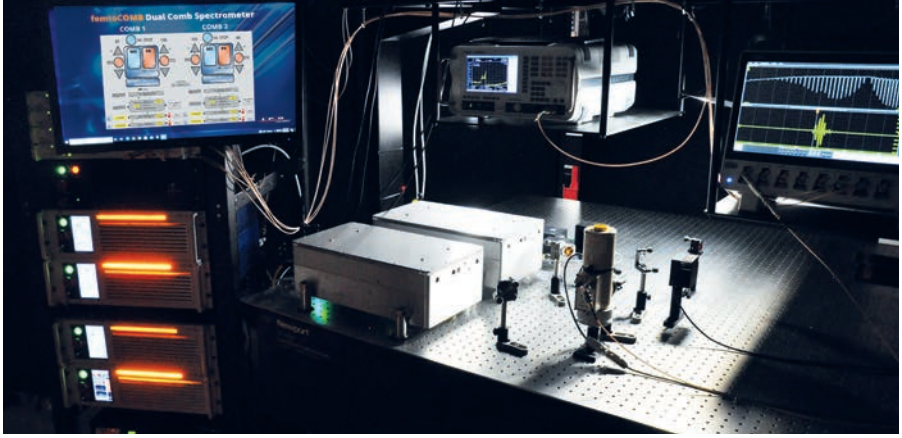
However, promising alternatives are on the horizon. Innovations such as the 21 Tesla FT-ICR-MS, equipped with dynamically harmonized FT-ICR cells, offer extraordinary resolutions and data precision. Systems like these have demonstrated mass resolutions as high as 80,000,000 with long transient lengths. Alan Marshall's group has shown the potential of this setup, yet practical limitations remain – namely, the narrow width of typical chromatographic peaks, which restricts the number of data points that can be collected, posing a major challenge for broad adoption.

Another intriguing alternative is the qTOF-MS coupled with ion mobility spectrometry (IMS). Though the qTOF has lower resolution than FT-ICR-MS, its pairing with IMS provides an extra dimension of separation through collision cross section (CCS) calculations. This two-dimensional separation effectively compensates for the qTOF's lower mass resolution and significantly enhances identification accuracy.

"Coupling mass spectrometry with liquid or gas chromatography has long set the standard for non-targeted analysis, but given the advances in MS technology, we must ask ourselves whether this approach is still necessary."

The growing CCS database, recently expanded by Erin Baker's team to nearly 28,000 entries, heralds a transformative future for non-target analysis. Paired with advanced ion mobility spectrometers, this growing resource promises to simplify and expedite the identification of complex compounds.

With advancements like these, we're moving toward a workflow where chromatography might no longer be required, achieving both depth and specificity in chemical analysis without the downsides of traditional chromatographic techniques.



SPECTROSCOPY

A New Era for Infrared

"The spectroscopic equivalent to trading in a pair of binoculars for the James Webb Telescope" – can dual frequency combs catapult infrared spectroscopy into application spaces long dominated by mass spectrometry?

By Mikhail Mirov, General Manager; and Sergey Vasilyev, Laser Scientist; both at IPG Photonics Corporation

Mass spectrometry and infrared (IR) spectroscopy are the preferred analytical techniques to identify and quantify unknown compounds. IR optical measurements are often easier and faster, yet mass spectrometry remains the gold standard for chemical analysis, especially for identifying low concentrations of unknown chemicals.

However, since the 2005 Physics Nobel Prize recognized John Hall and Theodor Hänsch's development of laser-based precision spectroscopy based on optical frequency combs (OFC), the extension of the concept to dual OFCs (1) and the first experimental demonstration (2), efforts gathered steam to realize fast, sensitive, and broadband IR spectrometers. We believe that OFC-based instruments are now poised to realize this potential – complementing and, in some applications, replacing mass spectrometry as the tool of choice.

Today, mass spectrometry delivers best-in-class sensitivity. That technique splits samples into ionized fragments, then separates the fragments based on their mass-to-charge ratio to produce signatures that are interpreted to identify molecular weights and structures, as well as that of the original compound. But mass spectrometry has tradeoffs in terms of cost, complexity, and throughput.

Fourier transform infrared (FTIR) spectroscopy, on the other hand, is more reasonable cost-wise, and with a broad spectral range. In FTIR, broadband infrared light interrogates a sample by interacting with the vibrational and rotational modes of the constituent molecules. Because FTIR is non-destructive, it avoids the ambiguity associated with interpreting mass spectrometry data. Until recently, the lack of bright infrared sources and the associated need for mechanical scanning limited the speed, resolution, and sensitivity of common FTIR instruments. Quantum cascade lasers (QCL) solve the brightness issue, offering high speed measurements with excellent resolution. But a QCL can only be tuned over a narrow (a few microns) wavelength range. Enter OFC, which combines broad wavelength coverage across the full molecular fingerprint region with the high brightness of a laser.

Last year, Professor Vodopyanov's team at the University of Central Florida demonstrated, using a commercially available mid-IR dual OFC laser source, molecular spectroscopy with unprecedented resolution and dynamic range (3). Their study reveals for the first time in full detail the Doppler-limited spectroscopic signatures of a mid-sized molecule at low pressure. Traditional FTIR lacks the resolution and dynamic range to capture such detail. In contrast, the intense, broadband illumination, high resolution, and high dynamic range detection of the dual OFC spectrometer is capable of revealing the new spectral information. Compared to traditional FTIR, the UCF results are the spectroscopic equivalent to trading in a pair of binoculars for the James Webb Telescope.

In addition to unprecedented sensitivity, dual OFC spectrometers capture data in real-time. When methanol gas enters the cell, the oscilloscope immediately displays the captured spectrum, including fine structures that a less sensitive technique is unable to resolve.

Equally promising, the hybrid fiber/solid-state laser source incorporates mature, robust technologies, with the addition of proprietary crystals to provide its unique mix of watt-level broadband mid-IR light with ultra-low noise. A commercially available mid-IR dual OFC laser source (see above) already fits on a tabletop. As with other fiber-based laser technologies, ongoing optimization and cost-reduction will enable the platform to shrink further in both size and cost, allowing fast, ultra-sensitive broadband dual OFC laser spectrometers to proliferate.

Dual OFC's newfound ability to make fast, broadband, high resolution, high dynamic range optical measurements is an exciting development for the analytical science community – promising to extend the application space of IR spectroscopy into areas dominated by mass spectrometry. Affordable, compact dual OFC spectrometers may even enable new applications, such as real-time point-of-care breath analysis for disease diagnosis and monitoring, real-time fence-line emissions monitoring, and standoff detection and analysis of trace chemicals.

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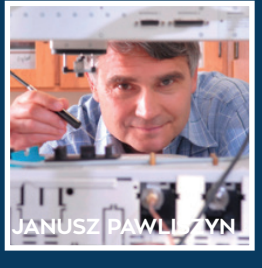

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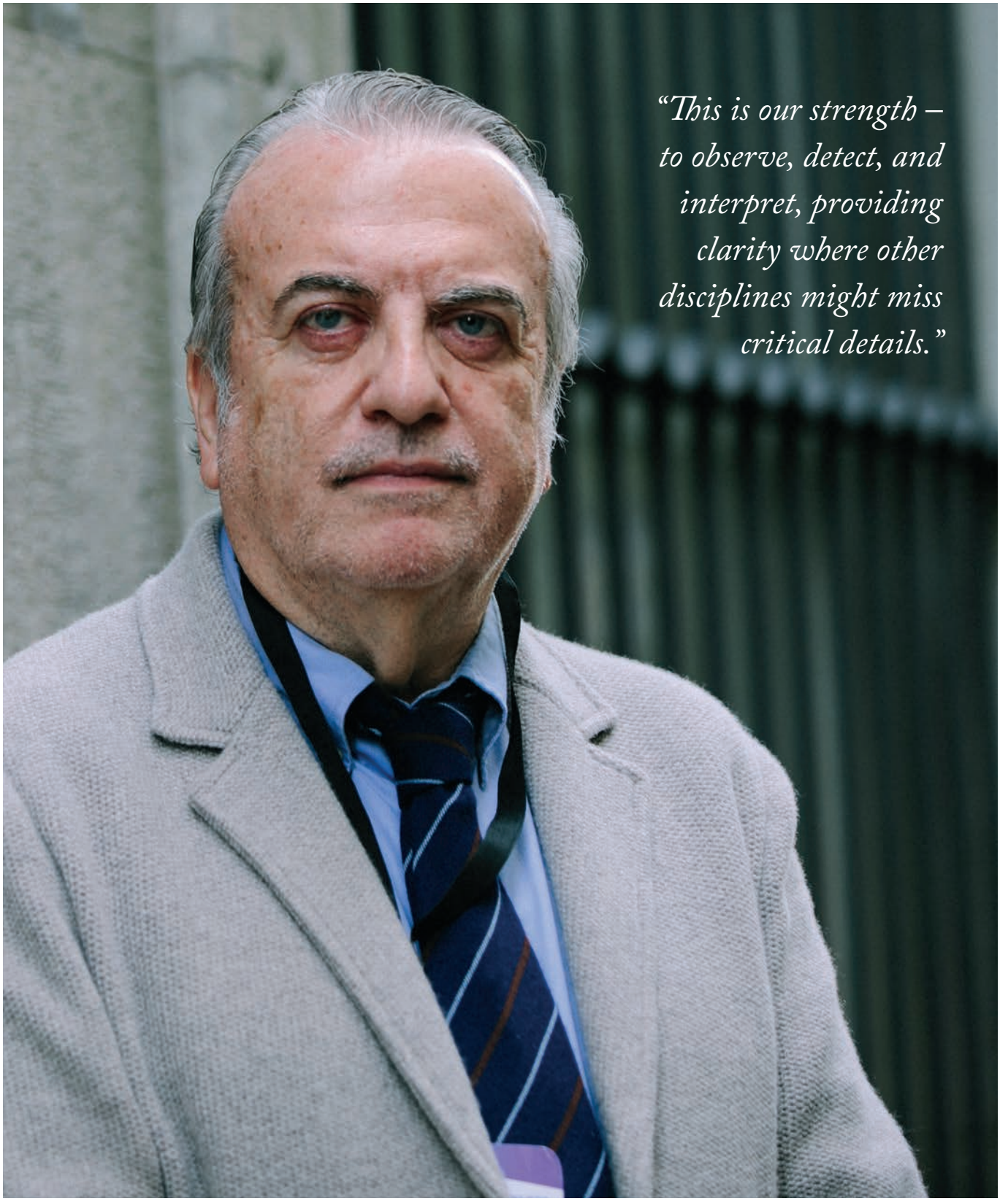
"This is our strength – to observe, detect, and interpret, providing clarity where other disciplines might miss critical details."

The Planet Protector

Sitting Down With…
Damià Barceló Cullerès,
Honorary Adjunct Professor,
Chemistry and Physics
Department, University
of Almeria, Spain

The main environmental issue that you're working on is microplastics. Could you explain why you're interested in this area?
Microplastics are a very interesting area because, in many ways, they're similar to nanomaterials. In water, they act as vectors for contaminants, somewhat like carbon-based nanomaterials. Microplastics absorb a range of harmful substances – metals, organic pollutants, and even pathogens – so they create a harmful system beyond the plastic particles themselves. This system has a destructive effect because it's not just the microplastic that's hazardous, but what it carries with it. That's one aspect.

The other side is that "microplastic" encompasses many different types of polymers, such as polyethylene, polypropylene, PET and others. Each has its own properties, sizes, and ages, making the chemistry involved quite complex and, to me, very intriguing. For example, the age and degradation level of a microplastic influence its chemical interactions. A degraded microplastic, detectable by its spectral profile, might have different functional groups that interact in new ways with pollutants.

What is your personal driving force behind your research?
Well, I think it's the sheer number of challenges still present in the field, especially as an analytical chemist. Take microplastics, for example – there are so many open questions. There aren't standardized analytical methods for their analysis, and it's incredibly complex. If you look at the literature, you'll find significant variation in how measurements are conducted and reported. Some report particles per liter or particles per kilogram, but what kind of particles? What sizes? There are so many unresolved issues, and this makes the field incredibly challenging and exciting.

I recently gave a lecture to encourage young researchers. I told them there are ample opportunities for PhD theses in this area because almost everything is still uncharted – even basic things like inter-laboratory standards. Recent studies comparing standardized polymers, like polyethylene, across expert labs showed discrepancies in identification, indicating how far we are from consistent methodologies. Labs rely on different techniques, such as pyrolysis GC-MS, micro-FTIR, and micro-Raman spectroscopy, and no single lab has all of these techniques to cross-validate results. We still need international collaboration to standardize these methods and measure the impact on fish and biota accurately. If we can't measure precisely, it's tough to determine the environmental effects.

I don't know how many years I have left to work on this – I'm 70 now – but I intend to do my best to make meaningful contributions in this area.

Analytical scientists are often viewed simply as data providers – the people who deliver results. What's wrong with that?
Well, if analytical chemists only deliver results, they risk being limited in their role and impact. I believe that analytical chemists should work more interdisciplinarily, with fields like medicine, toxicology, and engineering. We should be involved not only in producing data but also in interpreting it – explaining what a nanogram or microgram level actually means in practical terms. We need to take that extra step beyond data delivery. If we remain data providers only, we'll continue to be viewed as mere analysts.

However, if we collaborate with others and apply our skills to broader contexts, we can attract more interest and demonstrate the unique contributions analytical chemistry can make. Many in our field already work across disciplines – food safety, environmental health – but there's always more we can do to learn from others and expand our impact.

Finally, could you summarize where analytical scientists should go from here – or what direction should they choose?
We need to prioritize precise measurements and collaboration across various fields. Take ecotoxicology, for instance; they often model but still rely on us to measure actual pollutant levels in organisms like fish or crustaceans. This is where analytical chemistry becomes essential – our measurements provide the baseline data they need. The same applies to engineers, who might want to know how much of a contaminant is removed during wastewater treatment. But as I always have to explain – their methods can create new metabolites that might be harmful. Analytical chemists are crucial because we can identify these metabolites and look beyond the primary compound to see what else is produced in these processes.

There are strong points we bring to our colleagues in fields like toxicology and engineering; we can help explain what's actually happening in a plant, a fish, or a wastewater system. If, for example, a medication like carbamazepine breaks down, it can result in numerous secondary chemicals, each with its own potential impacts. Our work reveals this complexity, while other fields may focus only on the disappearance of the parent compound, assuming the issue is resolved.

This depth of insight is what makes analytical chemistry an indispensable discipline. Yes, it's expensive work, with advanced instruments sometimes costing millions, but it allows us to give highly accurate data and explain what's occurring in different environmental contexts. And this is our strength – to observe, detect, and interpret, providing clarity where other disciplines might miss critical details. From my experience, these strengths help foster respect and collaboration with engineers, ecotoxicologists, and soil scientists, and it reinforces the essential role of analytical chemistry in solving complex problems.

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