

the Analytical Scientist®

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the Analytical Scientist

INNOVATION *Awards*

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in 2023 – and beyond?

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Is Innovation Rational?

Lessons from the Power List: delivering something genuinely innovative requires dogged persistence in the face of rationally justified skepticism, setbacks, and potential failure

Editorial



If you ask the 2023 Power Listers (we did), you'll find that the initial spark of imagination that leads to the birth of the idea, concept, or invention – the seed of an innovation – is helped by several factors. Curiosity, creativity, outside-the-box thinking, an openness to working across disciplines, and the ability to ignore dogma are all important here. But you also need good judgment – “to weed out the interesting but impractical ideas, which will otherwise dilute your productivity,” as James Jorgenson puts it (1).

There is another crucial aspect beyond the ability to see things others can't. As Livia Eberlin says, “The most successful innovators and inventors that I know were also incredibly bold and fearless. They knew people would likely doubt them and criticize them for their creative ideas, and regardless of these challenges they believed in their invention and pushed forward with confidence until others started to realize the potential and novelty of what they had created.”

Should we consider this dogged persistence in the face of expert skepticism “rational” in the empirical-scientific sense – that is to say, lead solely by the evidence? “If yours is a truly innovative or even revolutionary idea, many (most?) experts in the field will tell you that it won't work,” says Rick Yost. Often, the skeptics may well be justified in their disbelief!

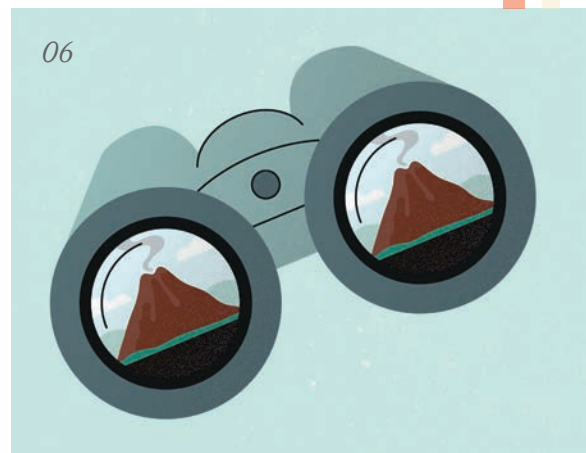
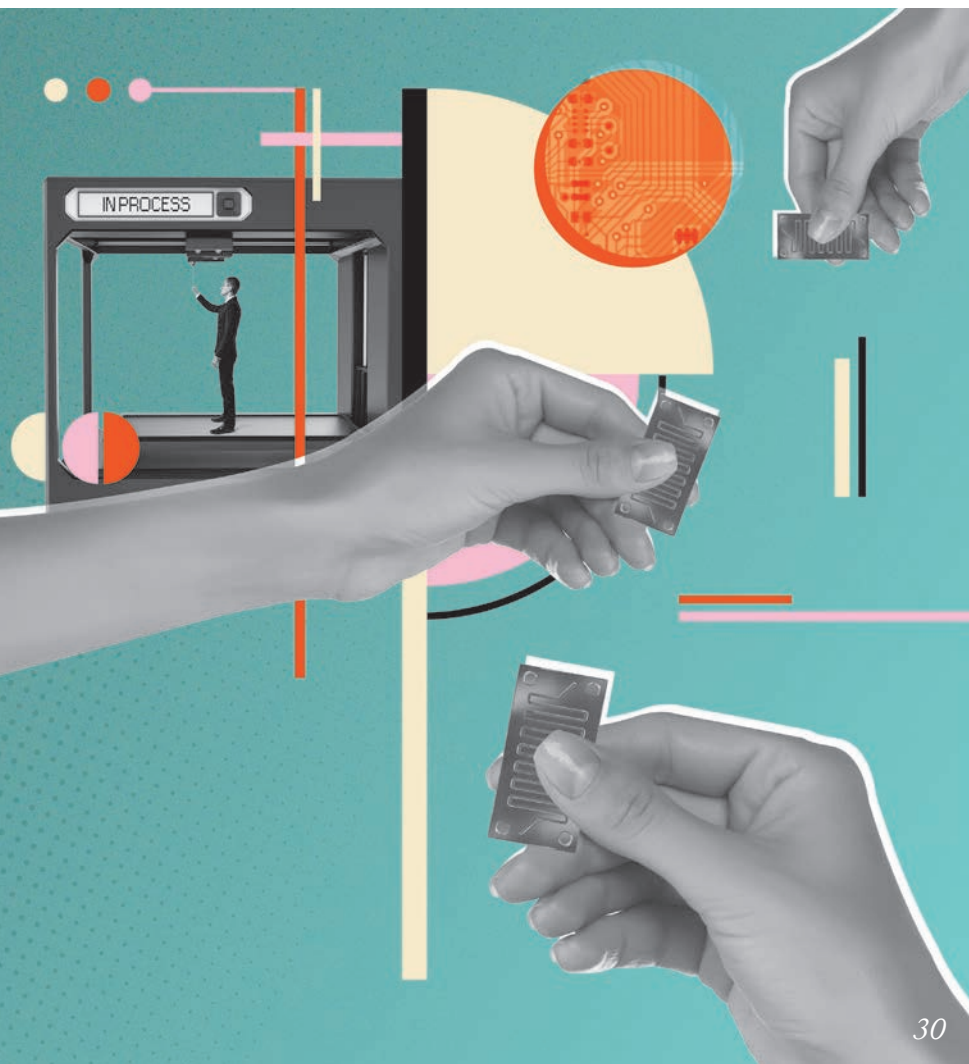
I think the philosopher and psychologist William James can help us make sense of this. He argued that rationality pulls us in two opposing directions: the desire to avoid error and the desire to discover truth, and it's up to us which we prioritize. The truly innovative scientist is, I think, less afraid of error and driven more by the desire to discover truth – even in the face of skepticism, setbacks, and potential failure (“drowning in the ocean of unrealizable ideas,” as Alexander Makarov puts it).

So, in this issue, we celebrate the bold and the fearless. On page 42, we chat with column innovator and recent Uwe Neue Award winner Tom Walter. On page 50, we Sit Down With biosensor legend and National Inventors Hall of Fame inductee, Fran Ligler. And finally, we reveal the overall winner of this year's Innovation Awards (starting on page 16) – with an origin story that stretches back over 20 years, it's an exemplar of persistent innovation.

Reference

1. “What Key Quality Defines an Innovator?” *The Analytical Scientist* (2023). Available at: <https://bit.ly/3QQpC1Q>

James Strachan
Editor



- 03 **Editorial**
Is Innovation Rational?
By James Strachan

On The Cover



*It's the return of our annual
Innovation Awards. See who
made the cut on page 16.*

Upfront

- 06 Reporting on recent breakthroughs, including an answer to the question of what triggers volcanic eruptions, a DNA sequencing-based test for breast cancer, and a new therapeutic target for OCD unveiled by spectroscopy

In My View

- 12 Good interdisciplinary work cannot be forced, you need strong mutual respect and communication to work together seamlessly, argues **Kevin Schug**
- 13 **Steve Martin** discusses how industry and academia can work together more effectively
- 14 How can we give analytical chemistry the sustainable spotlight it desperately needs? Asks **Janusz Pawliszyn**.

Feel free to contact any one of us:
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Change of address: info@theanalyticalscientist.com
Julie Wheeler, The Analytical Scientist, Texere Publishing Limited, Booths Park 1, Chelford Road, Knutsford, Cheshire, WA16 8GS, UK

General enquiries

www.texerepublishing.com | info@theanalyticalscientist.com
+44 (0) 1565 745 200 | sales@texerepublishing.com

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Core Topics

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- 45 **Spectroscopy:** SciX speakers return to discuss key trends and emerging technologies set to most transform spectroscopy

Features

- 16 **Innovation Unlocked**
The Analytical Scientist Innovation Awards are back! Find out which analytical advances are set to open doors in 2023 – and beyond.
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Adam Woolley, Rosanne Guijt, and James Grinias discuss miniaturized separation technology, the rise of 3D-printing capabilities, and recent advances in microfluidics

Sitting Down With

- 50 **Frances S. Ligler**, Eppright Chair and Professor of Biomedical Engineering, Texas A&M University, USA

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Explosive Discovery!

Carbon dioxide exsolution triggers volcanic eruptions from deep Earth

Arguably, the most important question when approaching volcanoes is: “What triggers and sustains volcanic eruptions?”

Esteban Gazel, Professor of Earth and Atmospheric Sciences at Cornell University, USA, and an international team, sought to answer this question – analyzing molten magma, using specialized analytical tools. Here, Gazel reveals the details of the team’s explosive discovery...

What were your key findings – and why are these results important?

We learned that CO₂ exsolution from deep within the Earth, at mantle depths (20–30 km) triggers volcanic eruptions for volcanoes of basaltic compositions – not water in the crust as previously thought. At these pressures, CO₂ is the only dissolved phase; when the pressure is no longer enough to contain the melt, the lithosphere breaks and starts the eruption. By appreciating this process, we can evaluate melt replenishment by focusing on deep earthquakes months and maybe years before magma is too close to the surface. The results from this study

will help us better understand volcanic plumbing and separate magma signatures from the hydrothermal system of a volcano.

What analytical techniques and tools were used in your research?

We used a combination of different micro-beam techniques, with a spatial resolution of 10s of microns. The processes began with quantification of CO₂ in the fluid and melt inclusions by Raman spectroscopy and new techniques we developed at Cornell. To collect all other elements we used secondary-ion mass spectrometry, and applied an electron microprobe analyzer and laser ablation mass spectrometry.

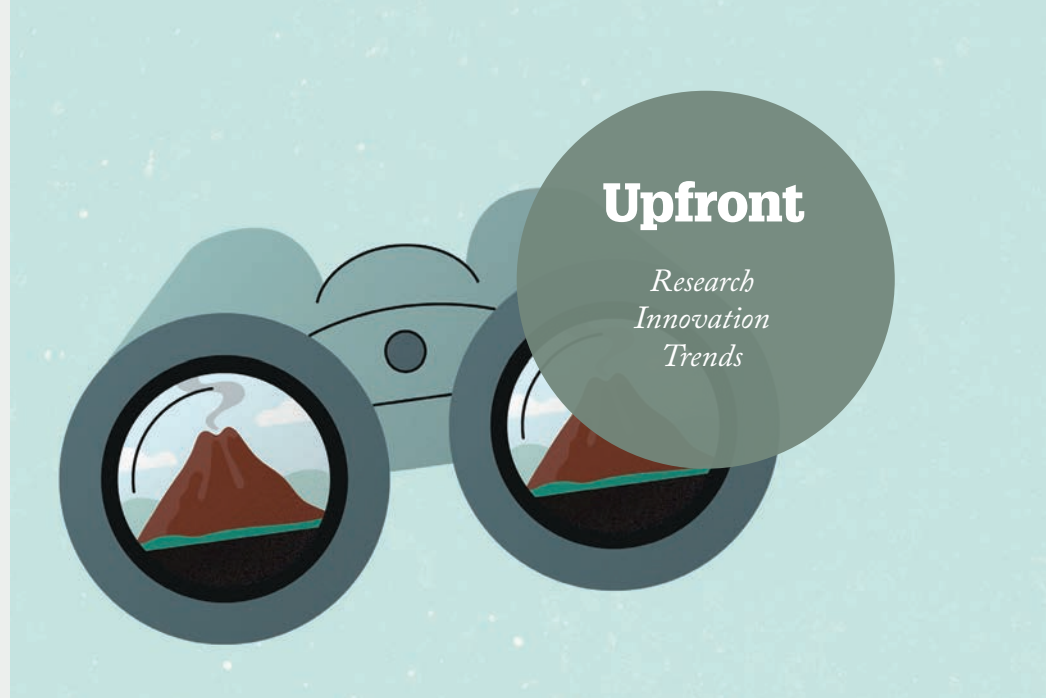
You used a high-precision CO₂ densimeter for Raman spectroscopy in your study – how does this work?

The knowledge of separation between

two CO₂ Raman peaks correlating with the density of CO₂ in a sample has been established for some time. We advanced our densimeter, by incorporating a thermocouple into the optical chamber to maintain precise temperature control and take temperature measurements with our custom-built apparatus. Our protocol also included heating the inclusions to a temperature where all the CO₂ becomes gas. This tool could also be used to explore extra-terrestrial samples, deep crustal rocks, and other scenarios where CO₂ is the dominant volatile phase (<90 percent).

Reference

1. CL DeVitre et al., “Oceanic intraplate explosive eruptions fed directly from the mantle”, *PNAS*, 120, 33 (2023). DOI: 10.1073/pnas.2302093120.



TIMELINE

Celebrating 10 Years of Innovation

To whet your appetite for this year's TASIAs, we explore the number ones of the past

www.theanalyticalscientist.com

2013

M908

908 Devices' handheld high-pressure mass spectrometry system, incorporating a US defense-standard (MilSpec) design for identification of chemical threats



2014

iMScope TRIO

From Shimadzu: a platform enabling high spatial resolution imaging mass spectrometry and an optical microscope for customized analyses of pharmacokinetics and food samples



2015

Full Spectrum Molecular Imaging

From Waters: a combination of MALDI imaging, DESI imaging, and ion mobility for a multi-layered analysis of tissues, small molecules drugs and metabolites



2016

Agilent Intuvo 9000 GC System

A GC system with “click-and-run” connections and no-trim columns – streamlining the GC experience even for inexperienced operators in clinical settings





BUSINESS IN BRIEF

Collaborative research efforts and partnership initiatives to boost cellular therapies, space investigation and clinical research among this month's latest business news

- **Beckman Coulter Life Sciences and 10x Genomics** have formed a partnership to improve automation solutions for single cell assay workflows. As part of the initiative, 10x will develop a suite of automation-compatible consumables and Chromium Single Cell kits for Beckman's Biomek i7 Automated Liquid Handler.
- **908 Devices and Terumo Blood and Cell Technologies** will combine their automation technologies – 908's MAVEN glucose and lactate analyzer and Terumo BCT's Quantum Flex Cell Expansion System – to enable on-line monitoring of critical process parameters in cell culture processing.
- **The Open University, UK**, has purchased the first Syft Tracer – an automated mass spectrometry system developed by **Syft Technologies and Element Lab Solutions** – to facilitate the expansion of its Wolfson Analytical Centre for advanced space studies.
- **LECO Corporation** has joined forces with **Cal State LA** to launch the new LECO Complex Chemical Compositional Analysis Lab – a collaborative educational and research lab for both undergraduate and graduate students.
- **PacBio** has announced the initiation of the HiFi Solves consortium – a partnership involving geneticists from 15 institutions that aims to collect and share the best approaches to study long-read genomic sequencing in clinical research.
- **The Sarawak Infectious Disease Centre (SIDC)** in East Malaysia has joined **Agilent Technologies** to enhance research into neglected tropical diseases (NTDs) – signing a Memorandum of Understanding (MOU). With Agilent's 6475 LC/MS system – based on iFunnel technology – and the development of translational labs, the two bodies are hopeful to accelerate research advancements on NTDs.

Imbalance at the Forefront of OCD Treatment

1H-MRS analysis shows that correcting cortical glutamate and GABA levels could be a therapeutic target for OCD

Around 3 percent of people in the West suffer from obsessive-compulsive disorder (OCD) – but there is little evidence of a neurochemical basis. That's why neuroscientists at the University of Cambridge employed 7-Tesla proton magnetic resonance spectroscopy (1H-MRS) to assess glutamate and GABA levels in the brain.

“By incorporating the 7-Tesla machine, 1H-MRS allowed us to measure metabolite levels at a more precise level,” says Marjan Biria, Post-Doctoral Research Fellow and lead author.

The researchers discovered a metabolite imbalance; higher levels of glutamate and lower GABA levels in OCD patients compared with healthy participants.

“We could see new treatments for OCD that adjust the balance of glutamate and GABA in the cortex, medication that regulates glutamate, and a non-invasive magnetic stimulation through the scalp.”

References available online

2017

Hyperion Imaging System

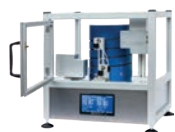
Fluidigm's tissue visualization platform incorporating high-parameter CyTOF technology that simultaneously identifies metal-tagged protein markers



2018

HyperChrom Flow-Field Thermal Gradient GC

Hyperchrom's high-throughput GC measurement system that allows laboratories to achieve much higher sample throughput rates



2019

Solvere Carbon Selective Detector for HPLC

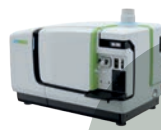
A HPLC advancement from Activated Research employing flame ionization detection (FID) for the universal detection of non-volatile carbon organics



2020

NexION 5000 Multi-Quadrupole ICP-MS

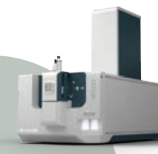
From PerkinElmer: a four-quadrupole ICP-MS system, enabling part-per-trillion concentrations analysis through four stages of mass separation



2021

ZenoTOF 7600 System

SCIEX's QTOF mass spectrometer incorporating a Zeno trap to advance electron activation dissociation for improved structural characterization



2022

iMScope QT

One system from Shimadzu combining two techniques – microscopy and high resolution accurate mass spectrometry – for greener imaging



Milk Monitor

How DNA sequencing of breast milk can replace tissue imaging for early diagnosis of breast cancer in pregnant and lactating women

The lack of sensitive, and non-invasive diagnostic and prognostic tests for early-stage breast cancer in these patients prompted researchers in Barcelona, Spain, to assess the potential of breast milk DNA sequencing (1).

To explore the research, we spoke with Cristina Saura, principal author and Head of the Breast Cancer Unit, Service of Medical Oncology, Vall d'Hebron University Hospital and Vall d'Hebron Institute of Oncology (VHIO).

Why did you focus on breast milk analysis?

A breast cancer patient came to us concerned that she had passed the tumor through her breast milk (BM) to her second daughter during breastfeeding. Despite knowing such thing is not possible, we decided to analyze the sample. To our

surprise, when we examined the patient's BM, we found DNA with the same mutation that was present in her tumor. And thanks to her, we decided to initiate a study to investigate BM-based diagnosis. Due to the proximity of BM to the tumors in the breast, we thought it could be an alternative source for a liquid biopsy.

What were the key findings?

We have shown for the first time that breast milk obtained from breast cancer patients contains sufficient cell-free tumor DNA (ctDNA) to be detected by liquid biopsy. It is even possible to detect ctDNA before the patient can be diagnosed using conventional imaging. We have successfully demonstrated that we would be able to diagnose early breast cancer in women postpartum by our technique – based on DNA sequencing

and droplet digital PCR (ddPCR) analysis of BM.

Some women might develop anxiety about breastfeeding – is this a potential problem?

Breastfeeding is a mother's choice that they must freely take. If women freely choose to breastfeed, participating in the screening should not be a cause for anxiety. In women that may have positive results on breast milk analysis, exhaustive additional exams will be performed to diagnose or rule out a cancer diagnosis. We planned in the prospective trial specific psychological support for those patients to accompany them during this process.

Reference

1. C Saura et al., *Cancer Discov*, 13, 10 (2023). DOI: doi.org/10.1158/2159-8290.CD-22-1340.

Alzheimer's disease (1).

Using nuclear magnetic resonance (NMR) spectroscopy, the team studied the molecular structure, interactions, and dynamics of A β . "This innovative process enabled us to specifically capture and analyze the bound state of A β with GM1 membranes," says lead author Maho Yagi-Utsumi.

The analysis revealed that A β adopts a "U"-shaped structure formed of two A β layers – β 1 (farther from the membrane) and β 2 (closer to the membrane) arranged alternately, which contradicts previous research suggesting a parallel fibril formation.

The team believes this study to be the first of its kind to identify the structural entity responsible for producing amyloid fibrils in brain tissue.

Reference

1. M Yagi-Utsumi et al., *ACS Chem, Neurosci* 14, 15, 2648-2657 (2023). DOI: [10.1021/acscchemneuro.3c00192](https://doi.org/10.1021/acscchemneuro.3c00192).

A Molecular U-Turn

New insights of amyloid β -glycolipid interactions could lead to new treatments for Alzheimer's disease

Alzheimer's disease is characterized by the abnormal aggregation of amyloid beta (A β) into amyloid fibrils in the brain. Recently, Japanese researchers investigated the interaction of A β with GM1 glycolipids – possibly leading to new treatments for





IMAGE OF THE MONTH

*An Ancient Agricultural Time Capsule*

A research team from Denmark isolated and analyzed plant-derived ancient DNA (aDNA) from the core of a clay brick found in modern day Iraq dedicated to Ashurnasirpal II, king of Assyria from 883 to 859 BC. With interdisciplinary efforts, the researchers were able to sequence aDNA and identify plant species from seven different families, including the cabbage ancestor *Brassicaceae*. The team are hopeful that their findings could lead to the eventual establishment of a dataset of ancient biodiversity that explains genetic changes and even agricultural practices of ancient civilizations.

Credits: The National Museum of Denmark

Would you like your photo featured in Image of the Month?
Send it to james.strachan@texerepublishing.com

QUOTE OF THE MONTH

“Democratization of spectroscopy is coming – as more people get smartphones that have more computing power than the NASA computers used to send astronauts to the moon, they can now combine them with innovative accessories that can turn their devices into portable spectrometers ready to measure everything around them on the go.”

Xiaoyun (Shawn) Chen, see on page 46.

Taking the “Lab” to the Plant

Real-time forensic analysis of cannabis samples with miniaturized NIR spectroscopy

Raman and near infrared spectroscopy (NIR) have already been used to identify illicit drugs – setting the foundation for handheld spectrometers, like the Viavi MicroNIR.

The device incorporates a cloud-based data processing service via a mobile app and user interface. This, according to researchers from Switzerland, could allow law enforcement to directly analyze cannabis samples, bypassing the need to send every sample to a lab.

To test their hypothesis, the scientists used the MicroNIR to differentiate between THC-type and CBD-type cannabis samples – an important distinction, especially in countries that have set legal limits for THC concentration, as in Switzerland.

The team successfully analyzed 1,503 cannabis samples with MicroNIR – distinguishing between THC-type and CBD-type cannabis samples and performing comparably to ultra-high-performance liquid chromatography (UHPLC) – a well-established method for cannabis analysis.

Could handheld analytical devices mean the end of specialized forensic laboratories? Not so, according to the authors: “On the contrary, it redefines the contours of forensic laboratories, placing them at the center of the decision-making process, as they can generate tactical advantages and improve efficiency, such as real-time monitoring of illicit markets.”

References available online

Trends and Challenges in PFAS Analysis

We recently asked readers for their thoughts on the challenges involved in per- and polyfluoroalkyl substances (PFAS) analysis. Here, our panel of experts – Marcus Chadha and Day Powell from Agilent, Linx Wacłaski from Metrohm USA, and Ruth Marfil-Vega from Shimadzu – discuss the survey findings, share their perspectives on the latest trends and best practices in PFAS analysis, and present a selection of recent PFAS applications.

What are the main challenges related to PFAS analysis?

Powell: When I first started looking at PFAS, there were only two compounds PFOS and PFOA, but according to the most recent estimations, there could be over 13,000 different PFAS compounds in the environment. Extremely low detection levels and background issues can be a real challenge for labs. Multiple solvents and consumables can contain PFAS, so if you can't get a blank, you'll never get down to the very low detection levels. Regulatory challenges are also very important.

Chadha: Yes, the lack of standards is a key one. For years, we've only had one real provider of standards, Wellington Laboratories. It's crucial that we have a second supplier through the validation process – and we at Agilent are trying to provide an alternative. We also have to make sure that our methods are fast and robust. In addition, we also need to make sure that, as we're detecting more PFAS through our screening methods, we're adding these into our targeted methods.

Marfil-Vega: Without standards, instrument sensitivity or sample preparation are irrelevant, and we're stuck analyzing the same 40-or-so targets.

Wacłaski: Agreed. I'll also add that sample preparation can be quite tedious, with opportunities for human error. And that's why customers are always interested in ways to automate sample preparation. Contamination is another big challenge because it can affect sensitivity; you have to be careful to use high-grade materials for your sample preparation.

Are current analytical methods for PFAS analysis sufficient?

Marfil-Vega: It is true that, in general, we know that for the thousands of chemicals out there, we do not have standardized methods for all sample types. However, I think that in some fields, such as environmental, food, and even clinical, work has been ongoing for decades. We have accumulated a lot of knowledge that can now be transferred to emerging areas where we are just starting to analyze PFAS.

Chadha: A degree of uncertainty is expected because this is an ever-evolving area in terms of regulations, requirements, customer needs, and the needs from different industries. I think we'll always be always catching up.

Wacłaski: I would agree with Ruth and Marcus – and add that there's just so many PFAS compounds out there. We're looking at thousands of potential compounds, which makes it really difficult to quantify. I'm specifically working with a lot of non-targeted methods, which can look at these as a broad class of organofluorine compounds with a little bit of a different approach. But there are limitations with that too because you don't know exactly which compounds you have.

Which areas are currently most important in PFAS analysis?

Chadha: The survey results are broadly what I would have expected and likely reflect where the regulations appeared first. In the coming years, I think monitoring people's exposure at the workplace will increase, as will air monitoring near high risk areas, such as incineration plants. For food, we're going to see more testing of materials that come into contact with packaging.

Marfil-Vega: I would like to add that although drinking water is an important area for PFAS analysis, the PFAS must be coming from somewhere else – either in the products we use daily or industrial waste. So I think we're going to see a greater focus on where the PFAS are created in the first place.

Powell: Agreed. Finding the sources that are leading to drinking water is a big challenge and includes consumable products, wastewater, and more.

Wacłaski: I am seeing an increase in consumer product testing. But the number of sources is growing, and includes food packaging, cosmetics, carpet fibers, clothing – you name it. We see companies trying to make alternate compounds that are certified PFAS free – this is a growing area and there's a lot of testing involved there.

Day Powell is Environmental Application Specialist at Agilent; Marcus Chadha is EMEA Applications Specialist Manager, also at Agilent; Linx Wacłaski is Product Manager for Ion Chromatography at Metrohm USA; and Ruth Marfil-Vega is Senior Market Manager for Environmental at Shimadzu.

Dive deeper with Marcus, Day, Linx, and Ruth as they discuss trends and challenges in PFAS analysis in this on-demand webinar:
<https://bit.ly/3SRILBN>.

How Low Can You Go?

Three approaches to achieve low detection limits

Marcus Chadha and Day Powell: How does Agilent achieve low detection limits for PFAS with its targeted methods? Our strategies include: sample enrichment – an offline SPE step that allows you to preconcentrate your sample and then inject it onto our most sensitive LC-MS instruments. It's more labor intensive, but it does allow us to get down to the parts-per-quadrillion levels. In addition, online SPE LC-MS allows us to do very large injections, followed by an online SPE step. The configuration is more complicated, but, once set up, it's less labor intensive than the offline SPE and the instrument handles the extraction for you. Lastly, we have LC-MS with direct injection. This is the simplest and easiest way to get down to really low levels and optimize blanks.

For these methodologies, we have solutions to help labs get their PFAS methods set up. We have our PFC-Free HPLC Conversion Kit for our instrumentation, which minimizes PFAS from the system. We also have our PFC-Free Columns and Supplies, which includes consumables and helps eliminate PFAS from the actual prep of your samples.

Finally, in addition to Application Services and Support, our PFAS MRM Database contains hundreds of different PFAS compounds optimized across our instrumentation.

Feasibility studies to remove PFAS

Ruth Marfil-Vega: Sensitivity is often cited as one of the biggest challenges in PFAS analysis – often people will say you need a triple quadrupole LC-MS instrument with the highest sensitivity possible. This is driven by regulatory requirements enforcing limits of detection at nanograms-per-liter concentrations. But there are other parameters besides the sensitivity of the instrument that are important to keep in mind. For example, when doing feasibility studies for the removal of PFAS, samples are normally spiked at micrograms-per-liter or even milligrams-per-liter levels. Here, a triple quad is not needed. Instead, a single quad can work well to quantify the individual PFAS present in the sample.

Shimadzu has used a single quadrupole LCMS-2050 to target 28 PFAS. We used the standard DUIS ionization source, simultaneous acquisition in scan, selected ion monitoring, and an injection volume of 1 μ L. We were able to calibrate the instrument between 0.5 and 200 ng/mL, our limits of quantitation were in the ng-per-mL range, with less than 12 percent

relative standard deviation and an accuracy between 80-120 percent. This work demonstrates that you don't always need a triple quad instrument for PFAS analysis.

Combustion ion chromatography for non-targeted PFAS analysis

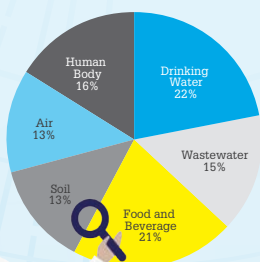
Linx Wacłaski: Non-targeted analysis of PFAS encompasses a broad class of compounds, which include those containing organic fluorine. Non-targeted analysis is thought to be a better risk assessment tool for measuring the true impact of fluorine on the environment. An emerging technique uses a specialized sample preparation, followed by combustion ion chromatography.

There are several approaches for non-targeted analysis of organic fluorine combustion IC. The hottest method today involves measuring absorbable organic fluorine (AOF) by first capturing PFAS compounds from 100 mL of an aqueous sample using granular-activated carbon, then washing off inorganic fluoride with nitrate solution, before combusting the carbon to measure AOF via combustion IC, with an approximate detection limit of 2–5 ppb.

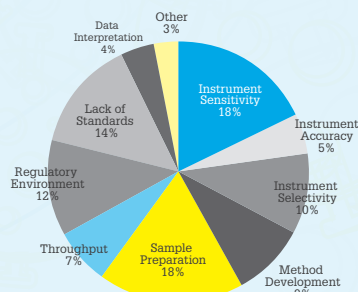
The excitement around this method is reflected in the release of DIN 38409-59 and the development of the Draft EPA Method 1621, both of which incorporate AOF.

A Snapshot of Our 2023 Reader PFAS Survey

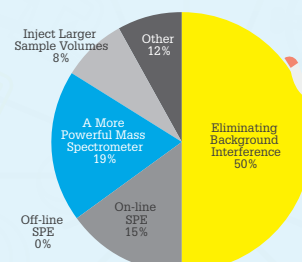
Which areas are currently **most important** in PFAS analysis?



What are the **main challenges** related to PFAS analysis?



Which of the following options are **most desirable for improving sensitivity** for PFAS testing in your lab?



Connection Breeds Progression

**Understanding the value –
and potential pitfalls – of
interdisciplinary collaboration**

*By Kevin Schug, Professor and
Shimadzu Distinguished Professor of
Analytical Chemistry, University of
Texas at Arlington, USA*

I believe that there are many ways to characterize the term “interdisciplinary.” For me, the interdisciplinary nature of my work stems from the broad utility of analytical measurements, in different research fields, and working with a variety of industrial and academic collaborators. It remains engaging to consider the development of solutions in multiple application areas. At UT Arlington, we have a program that seeds collaboration with specialists across disciplines as varied as computer science, social work, and theater. Working closely with researchers from other fields is rewarding and allows us to learn from each other to improve in our respective disciplines.

One of the biggest problems to tackle through interdisciplinarity is exposomics. Though this is an active area of research, I can't help but think that we are only scratching the surface. By collaborating with trained individuals in fields such as biochemistry, civil engineering, and sociology, we can work to fully capture and understand the effects of nature and nurture on an individual. While we have not worked directly on exposomics in my laboratory, it is interesting to contemplate how the various methods we have developed for measuring chemicals in the body,

organisms, and the environment might be stitched together to obtain a more complete picture of the mobility and fate of different molecules. A hearty dose of data science would also be needed.

On a more modest scale, I've enjoyed working with a variety of engineers, entrepreneurs, and scientists across industry and academia to develop better means for characterization of wastewater from oil and gas extraction activities. Usually, more water is produced than the desired oil or gas. Instead of disposing of wastewater underground, it makes sense to develop treatment and extraction technologies to expand the opportunities for reuse – removing the need for freshwater in activities, such as hydraulic fracturing. These waters have mixed with underground geology and contain valuable metals and minerals that could be repurposed if effective ways can be developed for extracting them. However, treatment technologies must be robust, have good performance, high

throughput, and economic viability to be adapted and implemented. We're currently using various analytical tools to understand the different substances within wastewater, hoping that, by working closely with industry, we can push the boundaries of reuse.

*“Many people
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the exception rather
than the rule.”*

In My View

*Experts from across the
world share a single
strongly held opinion
or key idea.*



Unfortunately, some collaborations don't succeed. Without actively engaged and interested interdisciplinarians, your project is unlikely to progress to completion. The nature of interdisciplinary research is often waiting for one group to finish their part so you can take over, passing your finished work onto the next team, and so on. Projects can stall if groups don't finish their area of work. I've had many collaborations flourish or fail based on this aspect alone. Good interdisciplinary work cannot be forced – you need strong mutual respect and communication to work together seamlessly. With these elements present, the range of problems you can address increases dramatically – as does your success rate.

UT Arlington has been running an internal interdisciplinary grant program for many years – yielding seed funding for some interesting collaborations. Fostering relationships across small businesses and academia often requires funding projects from government agencies, such as the

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs. With this project in particular, a portion of the funding goes to each entity, substantially supporting interdisciplinary work. However, for such projects to work, the teams must meet milestones and undertake separate application processes to develop their initial work.

Much of my research over the years has been supported through industry contracts – but that can only happen when industry partners see value in what your research could contribute to the field. Many people believe that industry-supported research cannot be published – which we've found to be the exception rather than the rule. It is true that some companies enter into contracts that restrict publications. However, peer-reviewed literature in collaboration with a third party can be a great way to prove technology. Publications can be written without revealing important intellectual

property. As a project progresses, discussions of outputs become easier.

Another strong benefit of collaboration with industry professionals is regular interaction. This is especially important for students because it gives them a view of the project through an industry professional's eyes, which helps improve their understanding of important aspects of the work. Oftentimes, these relationships can develop into a job offer for the student once their studies have finished. The most important aspect of successful collaborations is an industry partner who is willing to bring resources to the academic side, and an academic partner that will work towards solving the problems at hand while considering flexibility and importance for their industry partner.

I think that more companies are open to academic collaboration and supporting academic research, but there are many that are still yet to realize the benefits that interdisciplinary work with an academic team can yield.

How Can Industry and Academia Work Together More Effectively?

To get the most out of a collaboration, partners should align on underlying motivations, desired timelines, and long-term vision

By Steve Martin, Vice President of Global Research, Waters Corporation, Milford, MA, USA



COVID-19 instigated new working practices in the life science industries that continue to impact today's work. Now, there is renewed interest in – and, I'd argue, urgency for – global collaboration, workforce agility, patient and customer focus, and digital exchanges.

The past few years have presented new opportunities for research between academia and international organizations in commercial, government, and nonprofit sectors – and these have spurred successful conversations and collaborations. In response to SARS-CoV-2, research and development teams rapidly reprioritized new research, and rallied to produce results. The tremendous output of clinical studies, new diagnostics, therapies, and vaccines have proved that collaborations within and across science communities can drive outcomes in patient health, public policy, and scientific discovery.

As funding for pandemic innovation wanes and as teams adjust to new operations, we must take advantage of

“Bringing cross-functional and cross-industry teams together is imperative for progress; moreover, such relationships can be mutually beneficial.”

the momentum gained from industry working effectively with academic partners. Bringing cross-functional and cross-industry teams together is imperative for progress; moreover, such relationships can be mutually beneficial.

But collaboration is just a word – it requires the right actions and attitude. Below, I outline how both parties can help maximize collaboration.

First, stakeholders across industry and academia must align expectations – there will be decisions regarding

intellectual property (IP) and nondisclosure, technical capabilities, business development, operational structures, and more. And though academia and industry are both committed to solving problems, academia often seeks to push the boundaries of their areas of expertise. They often look to publish the outcomes as high-impact articles in scientific journals – as well as foundation data for raising additional research funding. For successful collaboration, industry partners must recognise academia’s desire for research in areas that can be published and will gain peer recognition.

Once expectations are aligned, the industry partner must develop a problem statement regarding the research and present it to academia before the partnership is formalized. Smaller, more foundational discussions with faculty and staff is also beneficial to agree on objectives, roles and responsibilities, and the scope of the partnership. For example, you might start with a general overview meeting between faculty and industry, then go on to targeted workshops where both sides can delve into strategy, and discuss problems they hope to address. A single point of contact is also useful to ensure that the scope of the program is well articulated,

key experts are connected, and timelines are communicated and managed. In addition, these points of contact help resolve the inevitable challenges that arise in these discussions with respect to IP, project scope, and funding.

Timelines also need to align. Academics work on academic calendars, which could impact the research. Rather than ignoring the problem, all collaborators need to agree on the flow of the research as part of the project plan. Basing these discussions around the Master Service Agreement after the initial conversations is an effective way to ensure alignment and respect for all schedule needs and constraints. Instead of a fully formed project proposal, start the arrangement between the two organizations early in the process to discuss the timeline, and other key research components.

There is a golden thread throughout the challenges we face – it’s about supporting a shared vision rather than a short-term goal. If the aspirations of the individuals and organizations are unknown, it creates an underlying issue that will reveal itself throughout the partnership – ultimately impeding progress. The awareness of the value of teamwork and mutual commitment to addressing the problem is key to any meaningful collaboration.

Painting the Lab Green

Giving analytical chemistry the sustainable spotlight it desperately needs

By Janusz Pawliszyn, Professor of Chemistry, University of Waterloo, Ontario, Canada



Speaking to analytical scientists about sustainability often feels like preaching to the converted – the majority agree that we need to move towards greener, cheaper, and faster processes across the analytical lab. Indeed, there have been many new green and fully functional analytical technologies developed over the past few decades that aren’t all that difficult to implement. But when it comes to actually adopting new technologies, I often encounter legal

and/or mental barriers.

One can argue that analytical chemistry contributes little to the broader environmental picture, but the reality is quite different. There are vast numbers of analytical labs across the world, with almost every chemical synthesis and production controlled by analytical methods. These methods are also typically traditional methods using copious amounts of organic solvents.

We, the analytical community, need to seriously concentrate our efforts to adopt greener alternatives.

Analytical scientists in academia need to ensure courses are up to date and emphasize the importance of new developments in sustainable technologies. Meanwhile, when training young employees, industry scientists should make an effort to build labs in agreement with their economic goals, the company's policy, and a conscious care for the planet.

Unfortunately, there hasn't been much progress outside academic labs to push this green initiative. To be fair, introducing new sustainable technology requires time and direction from supervisors. Many companies are making attempts to reduce use of organic solvents by reducing the size of separation devices and implementing other green ideas. However, the list of validated and reputed solutions is still too short. We're missing regulation-approved methods based on sustainable protocols and technologies.

With the increasingly destructive impact humans are having towards our environment, the aim is to strive for the optimal balance of performance, practicality – and greenness.

To address these challenges, and highlight the efforts of sustainable change in the analytical lab, I would like to draw attention to my latest project: the Green Analytical Chemistry journal (1). There is a

need in our industry for a journal that focuses on the promotion of sustainable analytical methods, protocols, and related technologies. Our objective is to engage readers and join efforts to overcome and reverse the worry of environmental trends we're seeing today.

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The original idea behind the Green Analytical Chemistry journal was prompted by the lack of a title that promoted sustainable analytical chemistry technology and methods, despite the increasing demand in the community. In fact, the existing green chemistry journals dominated by organic chemists don't fully appreciate the advances in analytical chemistry – despite analytical chemists working at micro and nanogram levels for more precise results.

Green Analytical Chemistry was launched in June 2022 and it remains an open access web-publishing journal. All articles published in the journal will support the development

of greener analytical methods – contributing to the reduction of our species' carbon footprint. We seek to promote the development of on-site instrumentation, novel approaches to eliminate or reduce the use of organic solvents and toxic reagents, and complete solutions – particularly validated green analytical protocols.

Additionally, the journal assists in the development of educational programs, providing researchers in academic and industrial sectors with solid support for adopting greener solutions as conveniently as possible.

To accomplish this task, we encourage all members of the analytical chemistry community to submit contributions and propose special issues. We welcome work from scientists across all disciplines, with a special appreciation for methods dealing with characterization of environmental pollution and investigations of human impact on the environment.

Both novel green analytical chemistry approaches and modified traditional schemes fit in line with the journal's themes. The greenness of the method must be transparently assessed considering reagent toxicity, waste production, energy consumption, and user safety. In addition, a comprehensive assessment of the method is required in terms of balancing greenness with functionality. Alongside typical contributions, the Green Analytical Chemistry journal welcomes details of developed sustainable method opportunities from scientists who wish to share their results for convenient adoption across fields.

The details of the Green Analytical Chemistry journals can be obtained through ScienceDirect.

Reference

1. Green Analytical Chemistry (2023). Available at: <http://bitly.ws/RCM3>.



the **Analytical Scientist**
INNOVATION
Awards

Innovation
UNLOCKED

Which analytical advances are set to open doors
in 2023 – and beyond?

15



Brevis GC-2050

A compact, next-generation GC system

Produced by Shimadzu Corporation

The Brevis GC-2050 is a fully scalable system that can connect to auto-samplers, an MS, and other accessories – but is only 35 cm wide. The system also consumes 30 percent less energy than conventional models and minimizes helium usage – saving labs money and contributing to environmental sustainability. The system also boasts intelligent automated functions, such as auto system check, Clean Pilot, automatic start/stop, and remote monitoring. In addition, the new auto injector and flow controller enable continuous analysis with constant linear velocity, flow rate, and carrier gas pressure control to achieve reproducible results.

Potential impact

The Brevis GC-2050 aims to save space, time, and money for labs, while also cutting down on energy use and making analysis less of a burden for users.

What the judges say...

“Not only is this GC compact, it is sustainable and with lower use of precious helium.”

“Simple, compact, and easy-to-use GC.”

INSIGHT-Thermal

A cryogen-free delay loop thermal modulator for GC×GC

Produced by SepSolve Analytical

The INSIGHT-Thermal allows for flexible control of all modulation parameters within ChromSpace software, including the unique ability to apply linear ramps to the cold jet flow rate – crucial for efficient release of high boiling point analytes (C50+). The new “figure of eight” design of the column holder locks the column into the correct position for precise alignment of the delay loop between the jets – improving usability and repeatability. Finally, the INSIGHT-Thermal is compatible with all popular GCs, allowing existing GC(-MS) systems to be upgraded and benefit from the separating power of GC×GC.

Potential impact

The INSIGHT-Thermal overcomes the problem of irreversible trapping and peak tailing caused by excessive flow rates, improving performance. Automated methods can be scheduled in sequences for confident unattended analysis, improving productivity. And the column holder prevents movement of the column, improving reproducibility.

What the judges say...

“This new approach greatly simplifies two-dimensional GC.”

14



CHARON FUSION PTR-TOF

13

Ultra-sensitive real-time analyzer of gas and particle-phase molecules

Produced by Ionicon Analytik

The CHARON FUSION PTR-TOF couples IONICON's next-generation FUSION PTR-TOF analyzer to an improved CHARON particle inlet to reach new limits of detection for organic compounds: <200 ppqv (parts per quadrillion by volume) in the gas phase and low pg m⁻³ in the particle phase. One of its key components is the fast-SRI reagent ion source that increases the primary reagent ion yield while keeping impurities at a minimum. In addition, switching between different primary ions, such as H₃O⁺, NH₄⁺, NO⁺, and O₂⁺, is now possible within ~1 s.



Potential impact

The CHARON FUSION PTR-TOF enables real-time quantification of a wide range of compound classes from non-polar aromatic species, such as polycyclic aromatic hydrocarbons (PAHs) and to highly polar compounds (for example, HOMs), at low concentrations. Researchers in the fields of atmospheric chemistry, environmental research, air quality and industrial process monitoring have new means to identify substances at very low concentrations in real-time.

What the judges say...

"A powerful new tool for the analysis of gasses and particles of interest in environmental and industrial applications."

alphaCART

A mobile, confocal, research-grade Raman microspectroscopy system

12

Produced by Oxford Instruments WITec

alphaCART is a mobile, confocal, research-grade Raman system for all applications that need the lab to go to the sample. Its Raman probe can be flexibly positioned in front of bulky, immovable, or precious objects that can't be transported to a microscope or that don't fit under one. The system's high confocality and signal sensitivity also allow measurements through protective glass and windows, which enables studies of gasses or chemical processes inside reaction chambers and other enclosures.

Potential impact

Investigations in archaeology, the arts and cultural heritage, and geoscience are often conducted in the field or secure storage facilities. And materials science, process and civil engineering, and gas analysis experiments are regularly performed outside of conventional lab environments. WITec and Oxford Instruments developed alphaCART

to equip researchers working in these conditions with real analytical power. The system can characterize paintings under protective glass, be brought into vaults for nondestructive analysis of priceless treasures, and peer through windows into reaction chambers for real-time chemical process monitoring.

What the judges say...

"A very interesting 'field deployable' piece of kit."

"A nice addition to portable Raman measurements – taking a highly respected manufacturer out of the lab and into the field."



11



Alliance iS HPLC

HPLC system for sample analysis in QC pharmaceutical labs

Produced by Waters Corporation

The Alliance iS HPLC is designed to reduce up to 40 percent of common human errors in modern laboratories. The system offers proactive error detection with real-time alerts and pre-run checks, reducing costly re-runs and ensuring product integrity. Its touchscreen interface and guided processes were created to seamlessly integrate with Waters' Empower Software for streamlined data management. The system aims to improve overall efficiency and reliability of pharmaceutical QC processes.

Potential impact

The Alliance iS HPLC System aims to create a ripple effect through the drug development timeline by improving dependability and accelerating the journey to market. The system identifies potential errors early, reducing the number of potential retests and eliminating one of the most common causes for failures in a QC lab that lead to costly investigations, delays and recalls. The Alliance iS HPLC also reduces unplanned instrument downtime and offers a full suite of compliance services.

What the judges say...

"This new QC HPLC instrument from Waters promises to eliminate many of the most common errors observed in QC."

Thermo Scientific ProPac 3R HPLC Columns

Enabling charge-based protein analysis and viral vector separations

Produced by Thermo Fisher Scientific

Thermo Scientific ProPac 3R HPLC Columns aim to improve protein charge variant analysis and AAV separations in biopharmaceutical research labs by leveraging a novel monodisperse particle platform and strong separation power. The columns are designed with bio-inert materials to reduce secondary interactions, but they also provide improved peak-to-valley resolution of charge variants during late-stage capacity – increasing confidence in the detection and identification of new acidic or basic variants during late-stage development.

Potential impact

Thermo Scientific ProPac 3R HPLC Columns are designed to streamline research processes in biopharmaceutical laboratories performing charge variant analysis of therapeutic proteins, including monoclonal antibodies, and separation of full versus empty AAV capsids used for gene therapy. The new 3 μ m particle size enables ultra-high resolution of charge variants, improved peak resolution, and faster run times.

What the judges say...

"A major step forward in the evolution of high-performance materials specifically designed for the analysis of major classes of biotherapeutics."



10



Syft Tracer

High-throughput real-time trace-gas detection and quantification

Produced by Syft Technologies

Syft Tracer is a real-time, direct injection mass spectrometry (MS) built to solve difficult analytical challenges. Its unique features – in the realm of real-time trace gas detection – include >50 percent greater sensitivity than legacy platforms, high analytical stability, hardware innovations to lengthen system lifetimes, and system optimization for high-throughput environments, where 24/7 operation is the standard.

Potential impact

Syft Tracer enables users to run chemically diverse compounds in one method or between several methods with a single instrument configuration that does not require column changeover or reequilibration steps. A typical CDMO workflow that involves the analysis of residual solvents, nitrosamines, ethylene oxide, formaldehyde, and benzene could, with Syft Tracer, run 70 samples in 9.25 hours, according to the company; in contrast, that same workload would require five GC systems running for over 24 hours.

What the judges say...

"With the potential to streamline gas analyses, this Syft Tracer is one to watch."



MAVERICK

Handheld Raman system for bioprocess monitoring and control

Produced by 908 Devices Inc.

MAVERICK is a Raman-based handheld system built from the ground up for bioprocess analysis. It arrives pre-calibrated using a de novo multivariate model for CHO, HEK, and related cell-lines, and has been validated across more than 30 media types/processes for accurate reporting of glucose, lactate, and biomass – avoiding lengthy empirical calibration approaches. MAVERICK's operating system is entirely embedded, including digital and analog feed controller outputs, so no external computer is required, and the system can be multiplexed to up to six bioreactors. Numerous safety/convenience features are included for process development, such as electronic probe tracking, immersion detection, and remote web access.

Potential impact

Early- and later-stage bioprocess development is dependent on rapid iterative process observation and optimization to improve time-to-market. Experts in cell biology and bioprocess metabolism are rarely also experts in analytical instrumentation and chemometric modeling. And although a Raman spectrometer may cost \$100k-200k to buy, the cost to truly reach productivity can be much higher, with extensive calibration, modeling, and validation phases. MAVERICK aims to make Raman as easy to adopt for the benchtop PD scientists as a pH meter, dO₂ probe, REBEL, or Octet.

What the judges say...

"Looks like a nice economical solution to an economically significant problem."



Autonomous Microscopy

Harnessing the capabilities of autonomous confocal microscopy for AI-based rare event detection

Produced by Leica Microsystems

Autonomous Microscopy enables the automated detection of rare events without the need for human interaction, thus completely automating complex microscopic workflows. Within this autonomous workflow, low-resolution two-dimensional overview images are generated in a first step, which are immediately transferred to the connected AI-based image processing (Aivia) system. This detects the rare events, previously defined by the operator, by means of a pixel classifier and sends the rare event coordinates back to the imaging system, which scans the rare events according to the operator's specifications, such as high-resolution and three-dimensional data stacks. According to Leica, the Aivia-

powered workflow reduces time spent at the microscope by up to 75 percent.

Potential impact

With Autonomous Microscopy powered by Aivia, operator interaction is limited to the initial setup. In addition, objects are detected much faster and more accurately. And the same settings can be applied for other experiments to ensure consistency. Because only objects of interest are identified and captured, data acquisition and final analysis time is significantly reduced. This exclusivity also means significant saving of storage space.

What the judges say...

"AI has been embedded in this confocal 'autonomous' microscope from Leica enabling enhanced object detection and reducing analysis times."

6

EVOQ DART-TQ⁺

Chromatography-free mass spectrometry aimed at the applied market

Produced by Bruker Corporation

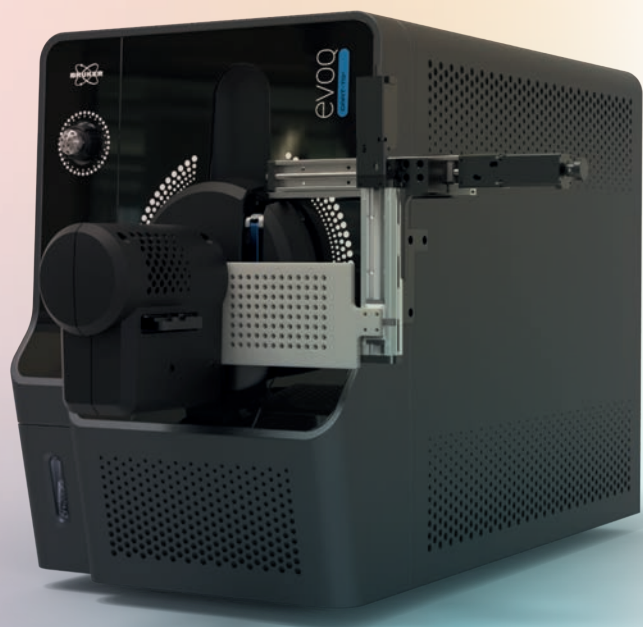
Bruker's triple-quad (TQ) mass spectrometer, EVOQ DART-TQ⁺, features the first and only fully integrated DART (Direct Analysis in Real Time) ionization source. The EVOQ DART-TQ⁺ eliminates complex and time-consuming gas or liquid chromatography for many point-of-need, routine workflows. The system incorporates simplified tuning and method development through data analysis and report generation for improved efficiency and productivity.

Potential impact

Customers in the applied mass spectrometry market require simplified, robust, cost-effective, and environmentally sustainable workflows. With the chromatography-free EVOQ DART-TQ⁺, Bruker aims to “bring MS to the masses” by simplifying workflows with greater ease-of-use, shorter analysis times, lower cost of ownership, and significantly reduced solvent usage.

What the judges say...

“DART in the fast lane allows chromatography free analysis of difficult to access samples.”



Intabio ZT system

Separate, quantify, and identify charge variants in minutes on a single-integrated system

Produced by SCIEX

Analysis with the Intabio ZT cartridge enables separation of charge variants by imaged capillary isoelectric focusing (iCIEF), UV quantitation and electrospray ionization (ESI) directly into a mass spectrometer for further mass analysis and peak identification – all with the use of MS-compatible reagents. To enable electrospray ionization, electrolyte is introduced through the mobilizer channel near the ESI tip to re-ionize the charge variants. The electric field is re-oriented to initiate the mobilization of the peaks toward the integrated electrospray tip. This chemical mobilization process ensures that peak resolution is maintained throughout MS detection.

5

Potential impact

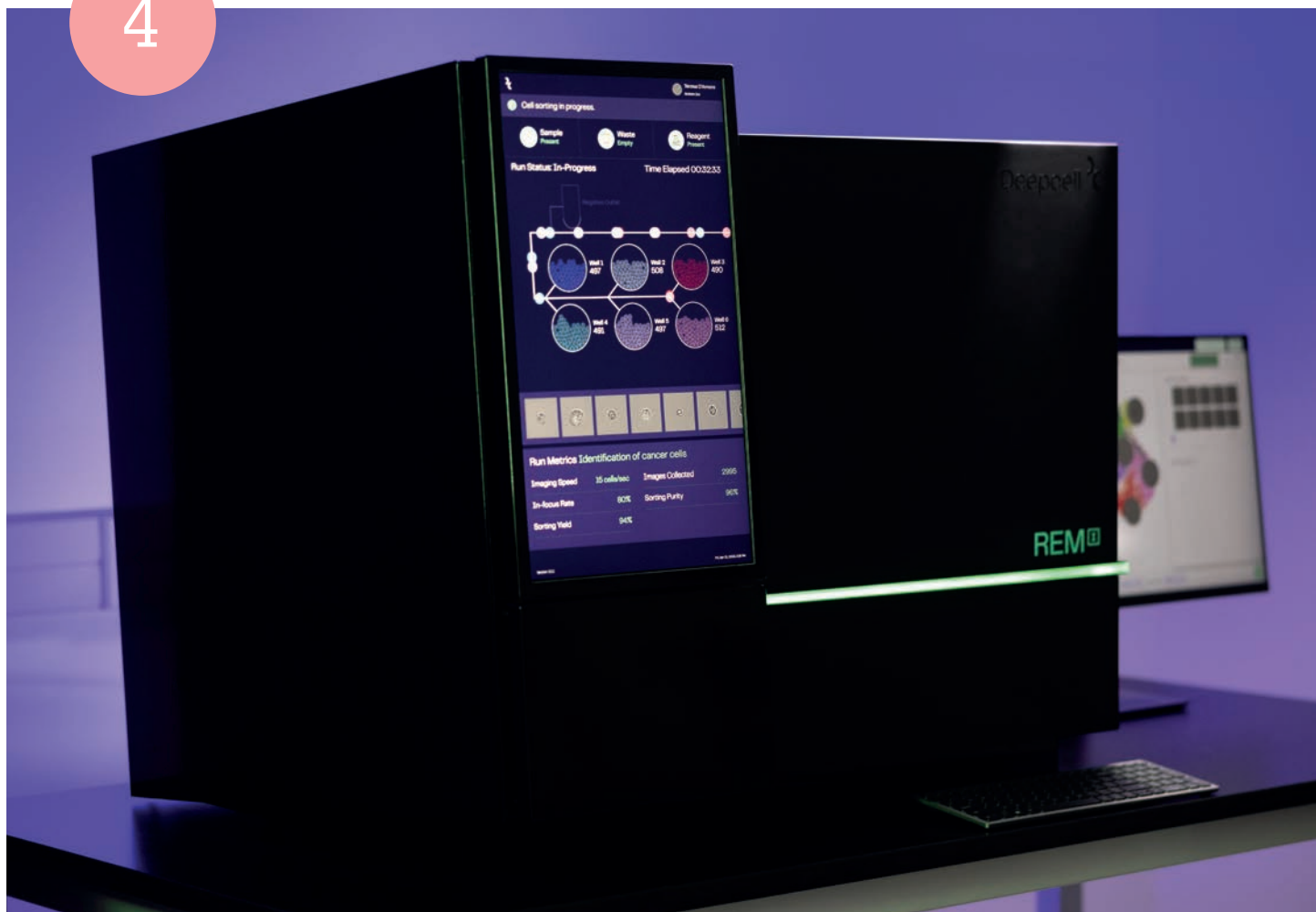
Conventionally, the process of identifying individual charge variant components and interpreting their structural differences takes weeks, and requires the use of multiple instruments with multiple manual steps. Coupling the Intabio ZT system with the ZenoTOF 7600 system enables, in one workflow and on a single platform, rapid monitoring of intact biotherapeutics and identification of charge variants throughout the drug development pipeline.

What the judges say...

“This new instrument platform represents a major advance in the use of isoelectric focusing for characterizing mAb charge variants.”



4



Benchtop REM-I Platform

AI-powered single cell analysis platform to accelerate cell biology discovery and catalyze the field of morpholomics

Produced by Deepcell

Despite recent advancements in microscopy and flow cytometry, existing tools for cellular quantification and characterization have left the field of cell biology hypothesis largely reliant on human interpretation. With the new generation of AI and machine learning models, such as Deepcell's Human Foundation Model, cell morphology can finally join other high-dimensional, single cell analysis methods and enable researchers to realize the full potential of the morpholome.

Potential impact

By bringing together single cell imaging, sorting, and high-dimensional analysis, the REM-I Platform aims to catalyze new methods of discovery in a wide range of fields, including cancer biology, developmental biology, stem cell biology, gene therapy, and functional screening.

What the judges say...

"Cell morphology is an interesting and important parameter within any phenotypic analysis and this AI guided system allows enhanced single cell analysis."

"This new platform provides a substantially improved basis for characterizing single cells."



3

Orbitrap Astral Mass Spectrometer

Faster throughput, deeper coverage, and higher sensitivity with accurate and precise quantitation

Produced by Thermo Fisher Scientific

The Orbitrap Astral Mass Spectrometer combines three mass analyzers: a quadrupole mass analyzer for high selectivity and high ion transmission, an Orbitrap mass analyzer for high dynamic range and high resolution measurements, and the novel Astral analyzer for fast and sensitive measurements. By combining these three mass analyzers and orchestrating the coordination of five separate ion packets within the instrument in parallel, Thermo delivers substantially faster analysis and the highest proteome coverage of any available instrument platform.

Potential impact

The Orbitrap Astral Mass Spectrometer enables a faster

throughput with a run time of 8 minutes per sample, injection-to-injection, allowing users to run 180 samples per day. In addition, each sample injection allows users to identify over 8,000 proteins for a typical cell lysate sample. This faster throughput enables the measurement of tens of thousands of samples in one year with just one instrument, without sacrificing depth or precision. This increases the scale of studies that can be performed in fields such as precision medicine and biomarker discovery, accelerating the discovery of new insights. Thermo believes the Astral will accelerate the pace of omics research, enabling proteomics and metabolomics to reach a scale previously only achievable in genomics.

What the judges say...

"Combining three mass analysers, this Orbitrap Astral solution from Thermo Fisher looks highly attractive for proteomics and metabolomics."

"A breakthrough in high throughput proteomics with increased sequence coverage."

Curio Seeker Spatial Mapping Kits

Whole transcriptome, spatial mapping of tissues at single-cell scale resolution

Produced by Curio Bioscience

Curio Seeker Spatial Mapping Kits are the world's first high-resolution, whole transcriptome spatial mapping solution. They lower the barrier of entry to complex spatial transcriptomic analysis of fresh frozen tissues by plugging directly into existing sequencing workflows; and they require no specialized personnel, instrumentation, or expertise with microscopy. The Curio Seeker Kit generates up to one million continuous whole transcriptomes from any species or tissues at single-cell scale resolution, without modifications to the standard protocol, or optimization of the tissue samples.

2



Potential impact

Curio Seeker Spatial Mapping Kits aim to take discovery beyond what is possible with current single-cell sequencing methods and have applications in both basic and applied research – from developmental biology to viral immunology. The technology enables an understanding of the complex cellular environments of biological systems during development, normal function, disease/injury, and treatment. For example, recognizing the presence of specific immune cell types and their locations relative to tumor tissue has led to understanding the mechanism of immune escape in cancer recurrence and metastasis.

What the judges say...

"This powerful new tool simplifies detailed mapping of tissues at the single cell level."

XCMS-METLIN

The first completely data-driven metabolomics/lipidomics platform with MS/MS data on over 930,000 authentic standards

Produced by Mass Consortium Corporation

The release of the newly created XCMS-METLIN data analysis platform is the culmination of a two-decade-long effort aiming to revolutionize LC/MS/MS data analysis. XCMS has been a pivotal metabolomics and lipidomics technology since the early 2000s when it introduced nonlinear LC/MS retention time alignment combined with statistical analysis. However, its primary limitation has been in structurally characterizing the statistically significant molecules. To rectify this, Mass Consortium has integrated XCMS with METLIN, a comprehensive MS/MS database that is 10 times bigger than the next largest. METLIN has collected data in both positive and negative ionization mode across four collision energies on over 930,000 authentic reference standards.

Potential impact

Tandem mass spectrometry (MS/MS)-based metabolomic and lipidomic analyses hold enormous potential for understanding biological systems and play a pivotal role in fundamental biology, drug discovery, personalized medicine, and many related fields.

However, the reliable identification of metabolites remains a major challenge, impeding the field's meaningful contribution. Mass Consortium's integrated XCMS-METLIN platform aims to address this problem with its enormous database. Unlike some other data processing platforms, XCMS-METLIN is a purely data-driven platform, circumventing speculative identifications, thus relying solely on real data for real identifications.

What the judges say...

"This enormous database addresses a major difficulty in the field of metabolomics and lipidomics."

"With MS/MS data on over 930,000 authentic standards this could become the de facto standard library for small molecule analysis."

1





^{the}
Analytical Scientist

The
INNOVATORS

SHOWCASING
THE PRODUCTS
AND COMPANIES
MAKING A
DIFFERENCE
IN 2023



DISCOVER THE VARIUS™ SPECTROMETER

When versatility meets precision

Step into the future of spectroscopy with the Varius™ Spectrometer, an innovation that redefines precision. Its advanced optical design ensures unparalleled sensitivity and resolution across a wide spectral range: from 190 to 1100 nm.

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Enjoy seamless connectivity and data management through intuitive software, simplifying integration into your laboratory setup – empowering researchers, scientists, and educators to push the boundaries of knowledge.

The Varius™ offers superior signal-to-noise ratios, minimal stray light (0.1 – 1 percent), and integration times ranging from 9 μ s to 30 seconds. It connects seamlessly via USB 3.0 and Gigabit Ethernet interfaces, delivering lightning-fast data transfer speeds.

Compact and sleek, weighing just 1,068 grams, it seamlessly fits into your lab setup.

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With almost three decades of experience in fiber-optic spectroscopy instruments and systems, Avantes excels in tailoring spectrometer configurations to meet the diverse needs of our customers. We focus on innovation, with a mission to provide high-quality, customer-oriented optical instruments and solutions.

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Our semi-automated manufacturing process is another differentiator – enhancing precision and efficiency while enabling scalable production and exceptional inter-instrument reproducibility. This approach caters to customers ordering large volumes, ensuring our unwavering commitment to outstanding product performance.

Choose Avantes, and join us in shaping the future of analytical science, where precision and innovation meet to illuminate the unknown. Together, we drive discoveries that make a difference.

BROWSER-BASED, MULTI-TECHNIQUE SOFTWARE

The Spectrus JS portfolio of applications brings you xC/UV/MS and NMR data processing, reporting, access, and databasing from anywhere

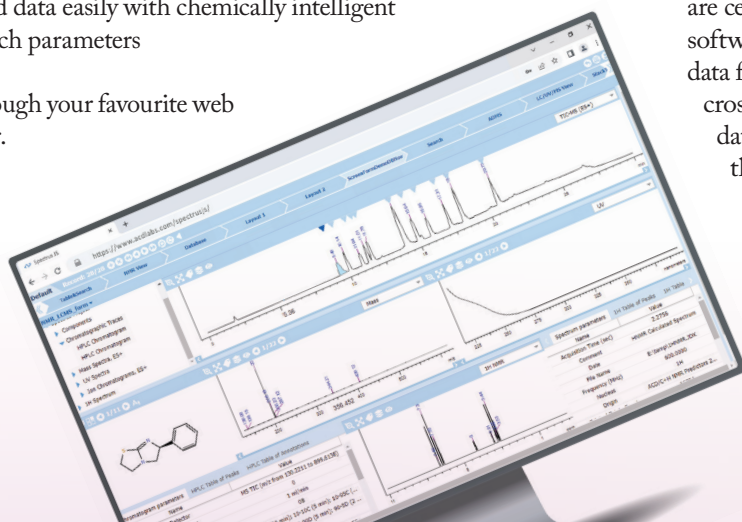
The Spectrus JS family of applications are the first browser-based software for multiple analytical techniques with native support for many instrument data formats. For scientists, this means that the tools they have relied on for decades to extract confident answers from analytical data are now accessible from any device.

Scientists want to access and work with data away from the instrument and without being tied to a location or device; IT teams seek lower maintenance software with ease of deployment, support, and scalability. Browser-based applications meet the needs of both. But such software has been limited to simple, single-technique or vendor applications at best – until now!

Spectrus JS applications enable you to:

- Process and interpret LC/UV/MS, GC/MS, and NMR data in one application
- Import data from varied vendor formats
- Predict NMR spectra and use them to verify structures
- Build dynamic reports
- Store spectra and chromatograms with chemical context (attach structures, meta data, etc.)
- Find data easily with chemically intelligent search parameters

All through your favourite web browser.



ASK THE EXPERT

*Richard Lee, Director
of Core Technology,
ACD/Labs*



What big challenge is driving innovation in the field?

Data accessibility in the pharmaceutical industry poses challenges for both lab scientists and data scientists – with each requiring different points of data access. Chemists in the lab need data on demand, just as it has been acquired or legacy data with a rich interface to view and integrate the data. But accessibility issues arise that include proprietary data formats and isolated data silos. Data scientists, on the other hand, require different access points to use data for deep learning/machine learning purposes. They need tools to abstract required data and engineer that data in a suitable format while also contending with data consistency – which includes non-standardized data and conflicting ontologies.

Practically speaking, how is this challenge impacting users? Scientists in the lab face significant efficiency challenges as they struggle with various informatics systems to access data they require. Historical or legacy data, which can offer insights and critical information, isn't readily accessible. Lab scientists spend a substantial amount of their time querying for data and finding the compatible informatics application to suitably visualize the data. For data scientists, data standardization or unification is the main culprit in data challenges. They spend a considerable amount of effort to ensure the metadata is consistent and normalized before they can use it for further downstream applications.

How can innovation address some of the big challenges facing the field in 2023?

Data standardization and machine learning initiatives are central challenges in chemical informatics. Innovative software such as Spectrus JS can harmonize disparate data formats, making data more accessible and facilitating cross-platform collaborations. Spectrus JS allows for data to be accessible by scientists regardless of location through the browser, but importantly, also enables machines to access data for downstream use. Machine learning algorithms, optimized to work with these standardized datasets, can then provide insights not readily extracted by human review.



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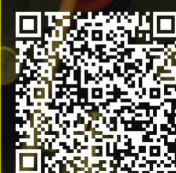


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Image 3: Lab on a chip microfluidics device by luchschenF sourced from shutterstock.com

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Three Gurus of Miniaturized Chemical Analysis

Our trio of experts discuss miniaturized separation technology, the rise of 3D-printing capabilities, and recent advances in microfluidics





What is the current state of miniaturized separation technology?

James Grinias: On the LC side, there are multiple groups working on portable instruments around the world. Many of these systems are also being commercialized, which broadens their accessibility to the wider scientific community. I think one of the biggest milestones in this area has been the emerging adoption of these instruments by major pharmaceutical companies for various analytical needs.

In the broad context of capillary LC, I think there is a major case to be made for the reduced environmental impact of the technique relative to traditional analytical-scale LC. There are several routine methods out there designed for the analysis of relatively simple mixtures that are long (tens of minutes) and run at high flow rates (1-2 mL/min). Capillary LC has advanced to a point where the volume of solvent waste generated from such analyses can easily be reduced by three to four orders of magnitude while delivering comparable results.

However, capillary LC remains a very small part of the broader field because of hesitancy to adopt such methods. Some of this is due to perceived notions of column and instrument robustness at these scales, while part of the motivation is simply a desire to not change methods that are working. As more companies move forward with plans to meet reduced carbon emission and waste generation goals, a shift to capillary LC will be a key tool for chemical analysts to adopt.

Rosanne Guijt: I would also like to highlight the healthcare sector, where there is a financial impetus for miniaturization – with demands for manufacturing (encapsulation of mRNA vaccines), as well as point-of-care diagnostics driving new developments in the field. James is also right about the environmental angle – people are concerned with the sustainability of the materials and reagents they're using, and I anticipate that this driver will gain momentum into the future.

In parallel, with the phasing out of animal models for drug testing, organ-on-a-chip devices have rapidly expanded. With geometries and conditions varying for different cell types (organoids), I anticipate parallel development in 3D printing for cell culture for medical research and drug screening.

Adam Woolley: It has been more than three decades since initial studies on microchip electrophoresis were published, and hype for microfluidics continues to ebb and flow. Initially, microfluidic aspects of an assay were highlighted directly as an end goal, for example, in Caliper's technology in the late 1990s. Now, miniaturized assays use micromachining or microfluidics in their operation as a means to achieve improved chemical analysis, for instance, the micro-chip based chromatography columns from PharmaFluidics (now Thermo Fisher Scientific).

Given the maturity of the miniaturized chemical analysis field, one might assume that innovative work is no longer occurring. On the contrary, novel advances continue in miniaturized analysis, particularly for droplet microfluidics in cell analysis, omics, 3D printing as a tool to create miniaturized systems, and a variety of electrochemical sensing platforms. Many of the drivers of miniaturization remain unchanged from the early days: automation, scalable/low-cost/disposable devices, and reduced chemical consumption. Furthermore, the ability to achieve novel assay designs and outcomes through microfabrication continues to motivate analytical scientists.

But the two key questions remaining to be addressed with miniaturization are: i) how can analytical scientists continue to innovate in a maturing field? and ii) how can multiple "breakthrough applications" be brought to fruition?

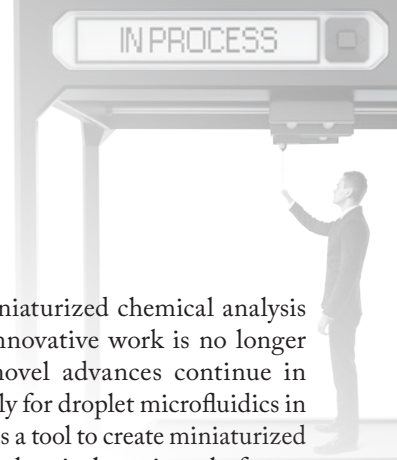
What are some of the most promising developments in 3D printing for analytical applications?

Adam Woolley: One key current direction in 3D printing involves process-specific customization. For example, the creation of custom materials for 3D printing for solid-phase extraction or the development of non-standard 3D printing processes to incorporate new components into devices. These trends illustrate the need for 3D printing practitioners to be able to access the inner workings of the process to achieve novel results.

Another recent focus in 3D printing for chemical analysis miniaturization entails effectively using all three spatial dimensions within devices. Key advantages of this approach include significant miniaturization of devices, dramatically scaling up microdevice fabrication rates, and creating novel architectures and analysis modalities in 3D prints. Importantly, greater utilization of all three dimensions in microfluidic systems also opens the door to using the same 3D printing platform for both prototyping and production.

A final area where important advances are occurring is on the commercialization front. I will avoid specifics because I own shares in a company, but I see promising advances in technology with multiple startups, as well as established 3D printing companies that are now focusing greater attention on the microfluidics and miniaturized chemical analysis market. Broader commercialization will be essential for 3D printing miniaturization to truly make a difference in analytical chemistry.

Rosanne Guijt: With my passion for functional integration, I am pleased to see multi-material options growing across



Meet the Experts



Adam Woolley

“For some time, research in the Woolley laboratory has focused on the interface between biomolecules and miniaturization. Current efforts are directed toward making microfluidic devices that can carry out biomedical assays and using bottom-up self-assembly to nanofabricate electrical structures. Over the past decade, my group has focused increasingly on the development and application of 3D printing in the creation of microfluidic devices. In collaboration with Prof. Gregory Nordin in BYU’s Department of Electrical and Computer Engineering we have developed 3D printers that can readily form truly microfluidic structures, including microchannels, pumps, valves, and mixing chambers – all of which have equivalent functionality to devices made from materials now in use, such as PDMS.

“Two recent publications on our work with 3D printed microfluidics were directed at creating integrated devices for the electrophoretic analysis of biomarkers related to preterm birth risk and the generation and use of concentration gradients in studying chemotaxis. We are currently focusing on increasingly integrated microfluidic systems that carry out sample preparation processes in conjunction with analysis.”

Adam T. Woolley is Professor at Brigham Young University, Utah, USA



Rosanne Guijt

“The focus of my group is the development of new technologies for early detection of threats and disease. So at the core, it is applied/bioanalytical, but the demand for early, point-of-need detection drives the motivation to develop and adopt new technologies. For a long time, my research has been driven by the ambition for functional integration, because I believe that functional integration is the stepping stone towards realizing chemical and biochemical monitoring systems capable of picking up threats early and on-site.

“I was recently fortunate to obtain an ultra-high resolution 3D printer, so I will be deploying that for challenges that cannot be addressed with other printers. At the same time, we will also continue to observe the consumer segment of the 3D printer market, as this provides entry-level access to researchers. Additionally, my passion for functional integration will continue to seek new ways of combining and integrating materials to enable a growing share of the analytical workflow to be integrated on a single device.”

Rosanne Guijt is Professor of Smart Sensors at Deakin University, Victoria, Australia



James Grinias

“Our lab broadly focuses on the development of liquid chromatography (LC) methodology, column technology, and instrumentation. In the area of miniaturization, we have been working with a compact, portable LC instrument in collaboration with Axceed for the analysis of pharmaceutical compounds, clinical samples, and on-line monitoring of chemical reactions. We are also working on a separate platform designed to help scale down 2D-LC methods to capillary-scale flow rates.

“We have demonstrated many applications of small molecule separations using compact capillary LC instrumentation, but recently moved into the area of biopharmaceutical analysis. Results from the analysis of a therapeutic antibody were comparable to that obtained using benchtop instrumentation.

“We hope to expand on the recent biopharmaceutical analysis work by adding additional characterization techniques that rely upon a broader range of LC separation modes. We are also beginning to implement more sample preparation strategies into our workflows that are specifically designed to couple to compact capillary LC methods to enhance the analysis of clinically relevant samples in point-of-need settings.”

James Grinias is Professor in the Department of Chemistry & Biochemistry at Rowan University, New Jersey, USA

different printer types – both in the research and in the commercial space. Because material integration can be done without compromising resolution, 3D printing will become a viable prototyping/small-scale manufacturing approach for lab-on-a-chip devices. It will be really exciting to watch this space over the coming five years. However, because microfluidics is a specialist area within the 3D-printing space, many advances in materials are not yet applicable to printing fine channels. It is important not to extrapolate findings on a mm scale to potential at a μm scale, but experimentally validate suitability.

From a commercial perspective, microfluidics is increasingly used at the heart of pharmaceutical manufacturing and diagnostics – so there's a bandwagon 3D printing can jump onto there. There's also a drive to mitigate climate change – the EU in particular is a driving force – and materials and devices with the potential to aid that mission are anticipated to grow. In particular, there is great potential for the use of advanced nanocomposite materials to replace current energy-intensive chemical processing.

Moreover, with 3D printing also having penetrated high schools, new people entering the field from various disciplines will already bring expertise in 3D printing with them as part

“Because material integration can be done without compromising resolution, 3D printing will become a viable prototyping/small-scale manufacturing approach for lab-on-a-chip devices.”

of their education, which will facilitate adoption.

Having said that, training is still a big challenge! 3D printing is a combination of understanding the technology, the materials, the fluidics and the application; as a result, it relies on a cross-disciplinary skill set. This reliance is associated with a risk that if the depth in one or two of these aspects is lacking,

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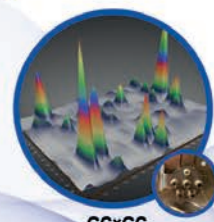
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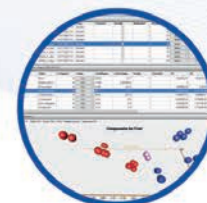
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CAD models of a porous tube developed for growing lung epithelial cells, which were 3D printed. Credit: Neelabh Gupta and Yi-Chin Tob, Queensland University of Technology

elements may be overlooked. And that may lead to a loss of time reinventing the wheel or in the delivery of an inferior product. So communication and collaborative skills to work in a diverse team are at least as important as the technical aspects.

James Grinias: I continue to be excited about the prospects of 3D printing in separation science, especially in the area of sample preparation. People are combining novel geometric designs with advances in material science to come up with more effective analyte extraction devices that can be manufactured by anyone with a low-cost printer. This area is sure to continue emerging in coming years.

We are still in the early stages of a “fully printed” LC column. A number of advances have been made for preparative-scale separations, and I think there is a wide-open area to explore as we move into more traditional analytical separations. Many experts in the field have demonstrated that printer resolution is a current limitation, with the platforms that can effectively “print” stationary phases with sufficient resolution still being far too slow for routine use. The growing adoption of pillar array columns has shown that there is an appetite for perfectly ordered columns for specific applications, and 3D printing will only expand what can be achieved in this area over the coming decades.

What does the future of miniaturized analysis look like?

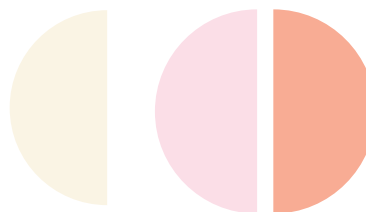
Rosanne Guijt: I am convinced of the need for technology able to translate the full analytical workflow to a system that

can be operated at a point-of-need setting – and preferably autonomously to provide the time-resolved data required for understanding where the disease or environmental hazard/chemical process sits relative to its life cycle.

Focusing on the devices made by 3D printing, I feel it currently fills a void demonstrating performance using a scalable manufacturing route, addressing a significant obstacle in the prototype-to-market translation. For product manufacturing, it may only be possible to deliver on projects where the 3D-channel geometry is quintessential and cannot be made for a similar cost using traditional approaches. On the horizon, sustainability of materials and resins may come into play, as well as a desire to decrease transport kilometers in the supply chain – 3D printing would be compatible with decentralized, demand-driven manufacturing. With the cost and throughput of 3D printing, however, in the near future applications will remain mainly in prototyping and small scale production, with the exception of boutique applications that cannot be realized using any other manufacturing approach.

I would welcome a move away from 2.5D to 3D thinking in the design phase and understand how and where the 3D geometry and design provides the opportunities. As a community, we have remained too traditional and not truly embraced the 3D build space. We must embrace what 3D printing has to offer in design – the lab-on-a-chip community has yet to do this, which is impeding progress.

James Grinias: I am hopeful that compact separations-based platforms



will eventually play a role in routine clinical diagnostics. Most LC-based clinical assays rely upon third-party testing services conducted in off-site laboratories. As the performance of miniaturized LC systems continues to improve, I think that these tools can eventually be used to help deliver real-time results in clinical settings. The MasSpec Pen is already demonstrating what MS can do in surgery rooms and I think LC could play a comparable role for applications like routine drug testing.

Scaling up commercialization and broader adoption can be a “chicken-and-egg”-type problem. I am hopeful that members of the academic community can continue partnering with emerging companies to demonstrate the power of new, miniaturized technologies in various industries, which can eventually lead to wider use and overall commercial growth. Specifically for compact capillary LC systems, I think that a wider array of columns in the 0.1–0.3 mm diameter range could broaden the application space, as most column manufacturers typically stick with 2.1–4.6 mm diameter columns.

Adam Woolley: I am excited and optimistic for the future of miniaturization in chemical analysis. In conjunction with the longstanding emphasis on bioanalytics, I anticipate a strong push toward implementation of miniaturization technologies in omics, particularly in studying single cells.

Environmental analysis is a field where miniaturization has untapped potential, particularly where “drone” technology and 3D printing customization can provide previously impossible remote access with customized analytical capabilities. Miniaturized chemical analysis tools are ripe for advancing food security, from pest sensing/abatement to water and fertilizer sensing and optimization.

Nonetheless, there are challenges to overcome for miniaturization to reach its full potential. The funding environment, particularly for academic research in the US and Europe, remains stubbornly tight, hindering the exploration and development of innovative miniaturization technologies. Furthermore, effectively bridging the divide from academic concept to commercial assay continues to be an issue in need of

better solutions. Another key need is to decrease device costs, particularly for more complicated assay systems; this may require novel or improved materials and fabrication processes.

Finally, I conclude with opportunities for introspection for those in the field. Are there changes that can be made in the funding ecosystem to enhance innovation? How can the publishing world disincentivize the proliferation of “me too” microdevice assay publications? How can miniaturized chemical analysis practitioners shift focus from device operation innovation to application and problem-solving innovation? Is there more that can be done to foster the transition to commercialization? What are novel approaches to incentivize investment in the most promising technologies? How can we facilitate key conversations between academic, healthcare, government, and industrial stakeholders to advance solutions that analytical scientists can direct at the greatest problems our world faces today?

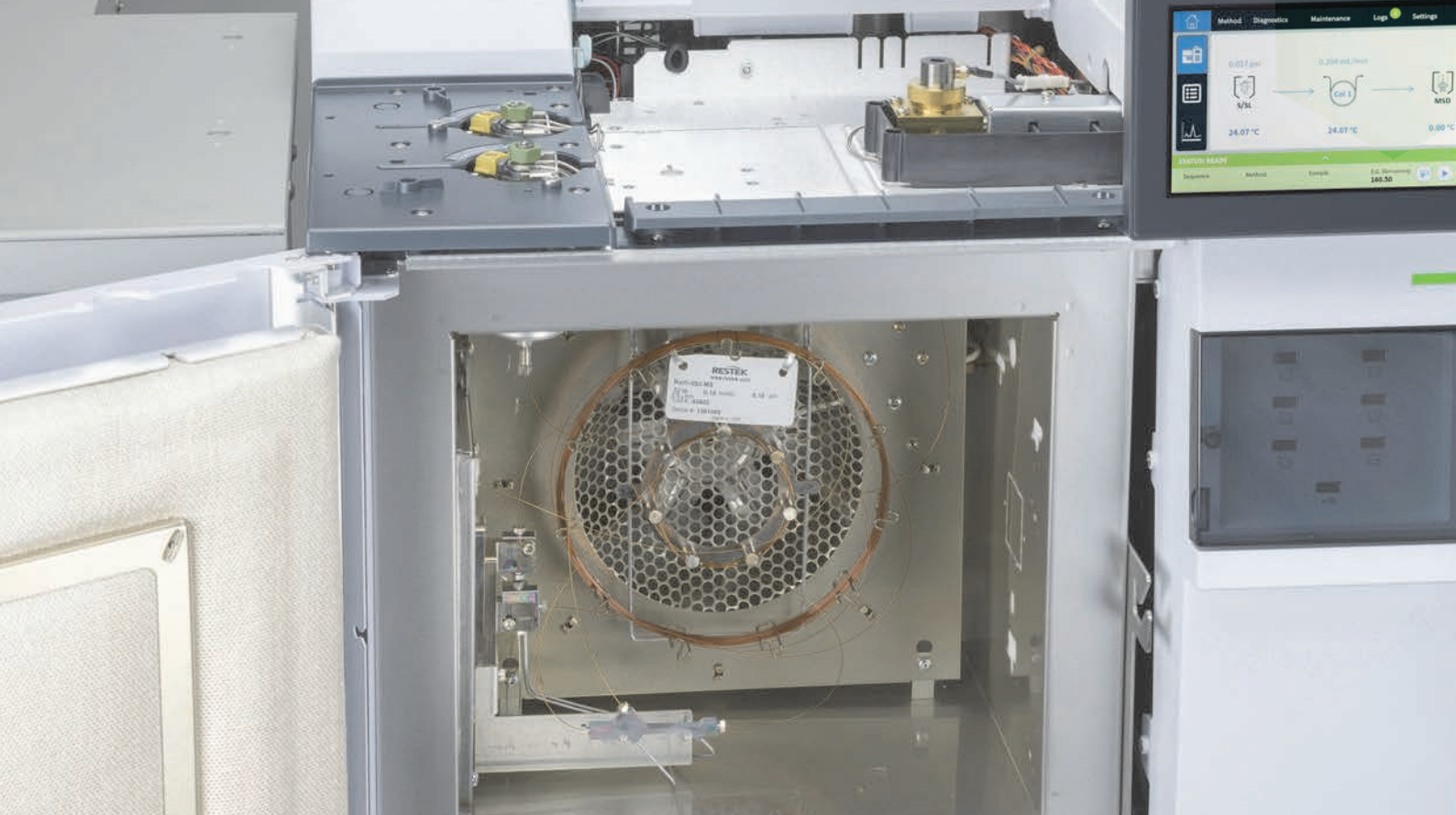
Working together to answer these questions will help miniaturized chemical analysis practitioners remain relevant for decades to come.

References available online



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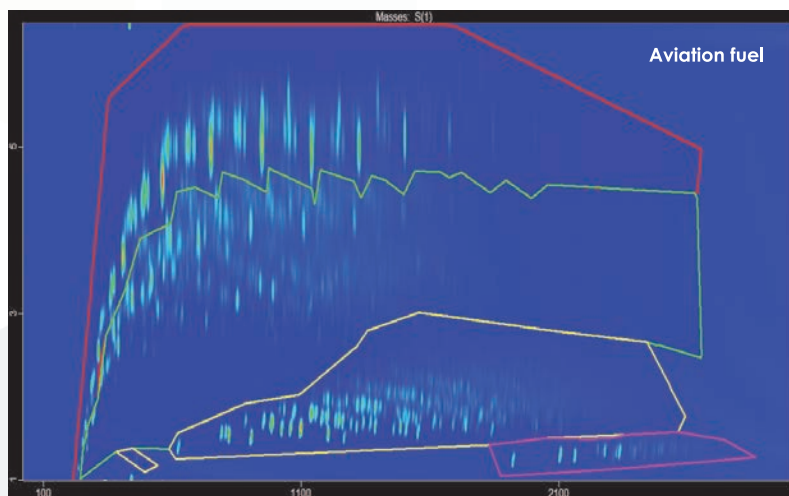
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Core Topic Mass Spec

Natural defense. To protect themselves against predators, velvet worms (*Onychophora*) expel a protein based slime – forming stiff and stable fibers after dehydration. An international research team recently examined the molecular structure of the worm’s defense slime – in hopes of characterizing the chemical modifications occurring to create those threads. The scientists employed high-resolution nuclear magnetic resonance (NMR), natural abundance dynamic nuclear polarization (DNP), and mass spectrometry to reveal phosphonate as the key compound responsible for this fiber-turning modification. “These fibers can dissolve back into their precursor proteins in water, after which they can be drawn into new fibers, providing biological inspiration to design recyclable materials,” said the authors.

Revealing Ryugu. Following the Hayabusa2 space mission, researchers have performed preliminary chemical analysis of samples from the Ryugu asteroid that orbits the sun between Earth and Mars. The samples were digested in acids and subjected to inductively coupled plasma mass spectrometry (ICP-MS) and thermal ionization mass spectrometry (TIMS). The researchers found variance in isotopes of chromium depending on where the sample was collected on the asteroid, which indicates that water was moving around on the parent body of Ryugu, shaping the distribution of elements.

Structural surfaceomics. Despite cellular therapies becoming increasingly popular, there are still significant challenges to overcome – such as the lack of cancer related surface biomarkers. Researchers from Canada, Germany, and the USA have collaborated and introduced a new strategy to target and characterize cancer-specific protein conformations on the surface of tumor cells. “Structural surfaceomics” combines cross-linking mass spectrometry with cell surface capture (CSC) to define protein-protein interactions, specifically of surface N-linked glycoproteins. The team successfully applied surfaceomics to an acute myeloid leukemia (AML) model – identifying the activated form of integrin beta 2 ($\beta 2$) as a potential immunotherapeutic target.

Towards a differential diagnosis of BD and MDD. Bipolar disorder (BD) can be distinguished from major depressive disorder (MDD) during episodes of low mood by profiling biomarkers in patient dried blood spots (DBSs), according to a study from the University of Cambridge, UK. The researchers used a targeted mass spectrometry-based metabolomic platform to analyze DBS metabolites and a questionnaire to assess current depressive symptoms.

References available online

IN OTHER NEWS

Researchers from Canada, Germany, and the USA introduce a new strategy combining cross-linking mass spectrometry with cell surface capture to target and characterize cancer-specific protein conformations on the surface of tumor cells.

Scientists suggest stricter health policies for beauty salons and barber shops, as BTEX compounds – carcinogenic chemicals found in beauty products – were found in high concentrations following analysis with gas chromatography-mass spectrometry.

Xin Ma and Facundo M. Fernández report, for the first time, triboelectric nanogenerators (TENG) hyphenated to coated blade spray-mass spectrometry (CBS-MS) for the analysis of small drug molecules.

Researchers implement surface-induced dissociation in an electrostatic linear ion trap and describe initial results for protein complexes generated under native conditions.

Operation Moonshot: Lessons from the Landing

Lessons learned from Operation Moonshot, which developed a LC-MS/MS-based COVID-19 test – from research to routine clinical use – in just five months

In the summer of 2020, Operation Moonshot was set up by the UK's Department of Health and Social Care (DHSC) to fund various diagnostic approaches for the detection of SARS-CoV-2 – involving scientists from across academia, industry, and the NHS.

One of the project's primary aims was to develop a state-of-the-art targeted protein assay utilizing liquid chromatography tandem mass spectrometry (LC-MS/MS) to capture and detect low levels of tryptic peptides derived from SARS-CoV-2 virus. The result? The successful development, translation, and validation of a SARS-CoV-2 test using nasopharyngeal swabs – in just five months (1).

Rachel Carling, Director of Newborn Screening and Clinical Lead for Biomedical Sciences at Synnovis, worked as the lab lead for both St Thomas' and the "P2" labs in this initiative. We spoke with her to find out what lessons she learned during Operation Moonshot.

How important was collaboration during Operation Moonshot?

The interdisciplinary expertise between academia, industry, and the NHS was key to the success of this project. First, academia used their expertise



to rapidly create a specialized mass spec method and continually improve it. Next, industry provided advanced technology and valuable support for method development – bringing equipment and materials not typically available within the NHS. Finally, once the mass spec method was established, the NHS optimized and validated it to meet the high standards needed for UKAS accreditation.

Why did you opt for a mass-spec-based approach?

We predicted that mass spec methods had poorer sensitivity than PCR methods because they lack the amplification step of PCR. However, we considered mass spec worthy of investigation due to its ability to separate and detect signature peptides derived from the SARS-CoV-2 virus while maintaining a high output. The nature of mass spec also suggested it would be able to handle variants with only minor modifications required.

“We should reconfigure existing mass spec services, giving us a smaller number of centralized mass spec hubs with direct connections to academic labs – streamlining the translation of new tests into the NHS.”

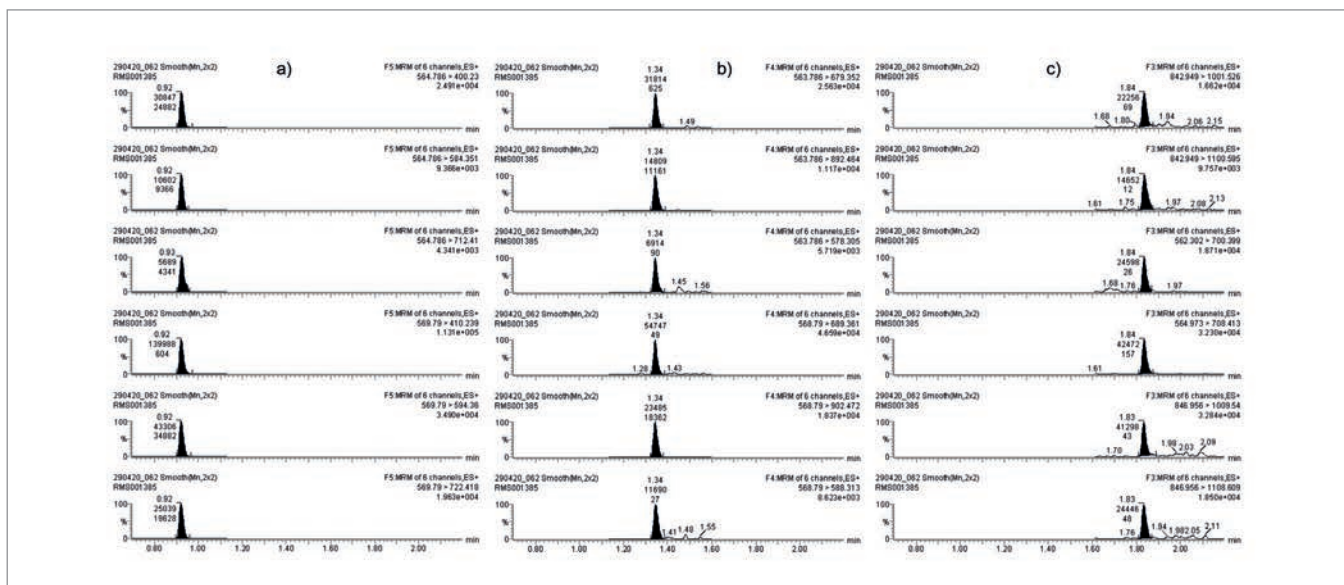


Figure 1: Extracted ion current chromatograms for the three target peptides a) AYN b) ADE and c) DGI for a SARS-CoV-2 positive sample with a RT-qPCR cycle threshold value of 23.

What challenges did you face and overcome?

The main hurdle for academics was balancing sensitivity and speed during analysis. Solid phase extraction (SPE) was proving inadequate, but once the “game changing” immunocapture reagent stable isotope standards and capture by anti-peptide antibodies (SISCAPA) became available, we had a breakthrough.

Our clinical biochemistry labs were challenged with optimizing and accrediting the method with UKAS. And that meant a lot of my time was spent simplifying sample preparation steps and working out how to interpret the data. We hit a turning point when Waters provided us with the Andrew+ pipetting robot – cutting our sample preparation time in half.

What lessons did you learn throughout Moonshot?

Operation Moonshot perfectly demonstrated what can be achieved when academia, industry, and the NHS work together. It highlighted the importance of a collaborative mindset,

advanced technology access, automation, and dedicated time for development in order to succeed. Post-pandemic, we aim to continue with this “triplex” approach.

We also confirmed the benefits of investing in mass spec and pre-analysis within the NHS. Providing a critical mass of equipment and staff enables better training and increases the capacity for development of new tests. With a drive towards automated mass spec and CE marked/IVDR compatible tests, questions are being raised for the future impact of clinical analysis and the translational pipeline going into the NHS.

I think we should reconfigure existing mass spec services, giving us a smaller number of centralized mass spec hubs with direct connections to academic labs – streamlining the translation of new tests into the NHS. This reconfiguration would improve efficiency, expertise, and investment in analytics – enhancing NHS services.

Are we now better prepared for another pandemic?

We’re undoubtedly more prepared for a pandemic than before 2020. From a mass

spec perspective, we are aware of the limitations of the COVID-19 method while understanding external factors – such as the time it takes to create specific antibodies, the requirement for standard specimen collection tubes, and accessing specialized facilities.

At the end of the Moonshot project, I worked on a “lessons learned” exercise so we could collate feedback and highlight areas for improvement moving forward – especially in managing rapidly changing plans and effectively communicating them.

What does the future hold?

Moonshot has opened doors for a range of new tests in our routine clinical lab. Typically in these areas, mass spec is used for small molecules, but Moonshot shows us that we can apply it to peptides and further expand on our testing capabilities. The legacy of Moonshot could see a plethora of clinical testing and advancements.

Reference

1. J Hällqvist et al., *Clin Chem Lab Med*, 61(2), 302–310 (2022). DOI: 10.1515/ckm-2022-1000.

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Core Topic Chromatography

Nuclear water. Despite undergoing treatments to reduce radioactivity of the Fukushima nuclear plant wastewater before its controversial release in the Pacific Ocean, isotopes can still be found at trace concentrations – though it demands a highly complex and time consuming separation process. To simplify seawater analysis, researchers from Japan and China developed an anion-exchange chromatography-based method, which they used to successfully extract neptunium from seawater surrounding the Fukushima nuclear plant.

Toy story. In addition to inhalation and injuries, plastic toys now pose another health risk to children: exposure to hazardous compounds – particularly when made with recycled plastic. Wu and colleagues from the Toys & Juvenile Products Testing Institute and the Sun Yat-sen University, China, set out to establish an advanced screening strategy for children's plastic toys. In a three stage testing process, the team employed static headspace gas chromatography-mass spectrometry (GC-MS) to successfully identify unknown volatile compounds from 11 virgin and 12 recycled plastic toys – specifically acrylonitrile-butadiene-styrene (ABS). The researchers also designed various chemometric models to discriminate between the materials in ABS toys for a complete safety assessment.

Au de Naturelle. Amid the perfumery industry's shift towards natural raw ingredients, a French research group set out to develop new fragrant compounds from “forgotten” perfume plants. Using headspace solid-phase microextraction coupled with GC-MS, they analyzed and characterized the volatile compounds within *Crataegus monogyna* – a plant, commonly known as hawthorn, with a rich history in perfumery. They then successfully developed a new and non-toxic natural ingredient, which will undergo further screening for use in commercial perfume products.

Intense focus. As the popularity of nootropic supplements has increased – especially among students keen to enhance their academic performance – so have adulteration cases, with unapproved compounds circulating in the market, posing a health hazard for consumers. With this in mind, Korean scientists optimized liquid chromatography-tandem mass spectrometry (LC-MS/MS) according to the international guidelines – improving specificity, accuracy, and the limit of detection – to enable simultaneous fragmentation of nootropic substances. The research group tested their updated method on 54 different samples – identifying 11 nootropic compounds, including vinpocetine and omberacetam.

References available online

IN OTHER NEWS

GC-TOF-MS-based metabolomic analysis of Yujiangsuan – a traditional Chinese fermented fish–chili paste – sheds light on the fermentation process, paving the way for safer production and consumption.

Liquid chromatography combined with elemental and molecular mass spectrometry could improve nuclear medicine tracer manufacturing – enabling rapid and sensitive impurity control in commercial radiopharmaceuticals.

Researchers detect PFAS in Chinese cosmetic samples, including products marketed for pregnant women; perfluorobutanoic acid, with high placental transfer efficiency, was the major PFAS found in cosmetics for pregnant women.

Scientists develop an immuno-affinity LC-MS/MS assay for early detection of HIV and tuberculosis – successfully determining disease-associated peptides; p24 and CFP10.

Tom Walter: HPLC Column Innovator

After receiving the Uwe Neue Award, Tom Walter discusses his career in chromatography at Waters

Please tell us about your career – how did you get into column specialization and what is your current focus?

I joined Waters as an NMR spectroscopist after completing my chemistry PhD back in 1987. I was mainly responsible for carrying out NMR analyses – focusing on stationary phases for HPLC columns and sample preparation devices.

As the years progressed, I moved up in the company and worked on a new family of HPLC columns based on high purity silica particles – these became the Symmetry Column brand. Here, I oversaw the development of the bonding processes, chromatographic evaluations, and analytical characterization. I was also responsible for setting the product specifications, which remain the most stringent in the industry. I'm currently a Corporate Fellow working in the Consumables and Lab Automation Division – writing technical articles, presenting at conferences, and consulting with colleagues in R&D and Marketing.

What was it like working with Uwe Neue – and how do you feel about receiving the Award bearing his name? I learned much of what I know about HPLC from Uwe, who was mentored by pioneers István Halász and Heinz Engelhardt. We were colleagues for 23 years – from when I first started at Waters until his untimely death in 2010.



During his 34 years at the company, Uwe developed stationary phases, chromatographic tests, and column packing technology and applications. His efforts contributed to our understanding of gradient separations, column selectivity, method development, and temperature and pressure effects in UHPLC. Uwe became an established expert in HPLC and received the Halász Medal in 2005, which commemorated his late mentor. Of all the awards Uwe received, this was the most meaningful to him. I feel the same way receiving the Uwe Neue Award.

Could you share your career milestones and describe their impact on analytical labs?

One important milestone was being involved in the development of hybrid organic/inorganic particles for HPLC. In the late 1990s, our research team sought to create columns with improved stability with alkaline mobile phases, which was requested by chromatographers in the pharmaceutical industry. We hired a materials chemist for this project, and the prototype hybrid silica/methylsiloxane material he made became the foundation for the

first commercial hybrid particle HPLC columns, called XTerra Columns. I wrote some of the first articles and gave the initial presentations as these columns were launched in 1999.

Following the success of the XTerra Columns launch, I took the role of Director in the Chemistry R&D group, overseeing the development of the next generation of general-purpose HPLC columns. I took inspiration from an article on bridged polysilsesquioxanes, which are hybrid materials with an organic group connected to two silicon atoms. I believed that this chemistry could lead to a material similar to XTerra particles but with improved mechanical strength.

The timing of this discovery was serendipitous; our research in ethylene-bridged hybrid (BEH) materials coincided with the need for high-strength particles to create the first UltraPerformance LC (UPLC) columns. Combining our most versatile particles with the new speed and efficiency capabilities of UPLC was a huge success. We introduced these columns as ACQUITY UPLC BEH Columns in 2004, and they remain our most popular columns today.

ACQUITY UPLC BEH Columns have been used for a wide range of applications, including separating small and large molecule pharmaceuticals, conducting biomedical research including proteomics and metabolomics, characterizing traditional Chinese medicine, and food and environmental testing. As one example, these columns play an important role in the analysis of nucleic acid therapeutics, including mRNA-based COVID-19 vaccines, verifying their identity and purity.

Analytical science is sometimes viewed as a “service” – with analytical scientists “simply delivering results.” What is your view on this?

I believe that the work of analytical scientists is of equal importance to the work of other scientists. Though one subset of analytical science involves applying well-established methods to similar samples

(for example, quality control of chemicals), there are also many innovations in this field – from new applications of existing technologies to the development of new analytical instrumentation.

Analytical science has played a leading role in many areas; for example, in genomics, proteomics, and metabolomics.

What are your thoughts on bringing industry and academia together?

The general role of academic scientists is to generate new knowledge and educate students. Industry usually has a shorter term focus, aiming to deploy innovative science to develop new products and grow their company. Many ideas generated by academic scientists were further developed by industrial researchers to create new products. The hybrid organic/inorganic particles and UPLC work I mentioned earlier occurred in this way. Waters has also benefited from collaborations with academic separation scientists, such as James Jorgenson, Georges Guiochon, David McCalley, Peter Schoenmakers, and Davy Guillarme. Conferences like the International Symposium on High Performance Liquid Phase Separations and Related Techniques (aka HPLC) play a key role in fostering these collaborations.

What are your predictions for the future of separation science?

There have been many developments in the HPLC column industry over the course of my career that weren't predicted by experts. Some examples include the creation of hybrid particles for HPLC columns and the high impact of UHPLC. Though there are current trends that will almost certainly continue, I expect that

“There are many innovations in this field – from new applications of existing technologies to the development of new analytical instrumentation. Analytical science has played a leading role in many areas; for example, in genomics, proteomics, and metabolomics.”

there will be innovations emerging that are not currently on the radar of today's industry watchers. These could be new technologies being developed in secret or innovations that occur through serendipity and chance collaborations across different fields. Either way, it should be exciting!

Tom Walter is Senior Director of Consumables Separations at Waters Corporation



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Toxic palette. Leonardo da Vinci is known for his unusual painting practices, one of which has recently been unveiled by a French research group. The scientists employed X-ray diffraction and infrared spectroscopy to analyze microsamples from two of his most famous creations – the Mona Lisa and the Last Supper – to shed light on the pigments and techniques he employed. Plumbonacrite – a toxic and rare lead compound that results from a reaction occurring between the oil and lead oxide – and shannonite were found in both art pieces. Despite the polymath not discussing the use of lead oxide in his manuscripts extensively, the study suggests the compound was indeed part of his palette – possibly being the first one to use it, as plumbonacrite and shannonite have yet to be found in other historical paintings.

Imaging wars. Visualizing enzyme activity in cancerous cells could be critically useful for diagnosis and prognosis, but the lack of highly specific imaging tools has been a roadblock. Now, researchers from the US and China developed NanoSABER – an enzyme-responsive intracellular Raman imaging nanoprobe. The team successfully obtained an optical output of the tumor-

specific enzyme, legumain, using their design – paving the way for Raman-based multiplexed molecular imaging.

Ancient seawater. In the hope of answering how life started on Earth, scientists from the University of Oxford, UK, and the University of Cape Town, South Africa, recreated Archean seawater – studying the minerals and metals that favored early evolution. The team employed X-ray absorption spectroscopy to directly study seawater chemistry – confirming the speculations of biologists that greenalite was necessary for early life forms.

Decoding smiles. What really makes a smile healthy? Scientists from Finland, Sweden, and Austria have collaborated to investigate and identify, for the first time, the metabolic signatures of oral diseases. The team characterized 157 metabolites – employing nuclear magnetic resonance spectroscopy – linking them back to periodontal inflammation, gum bleeding, and other symptoms of oral conditions. The authors conclude these mouth diseases and caries could be associated with cardiometabolic diseases, such as heart attacks and diabetes.

References available online

IN OTHER NEWS

Penn State scientists spectroscopically confirm – with NASA's James Webb Telescope's Near-Infrared Camera (NIRCam) – the existence of two of the most distant galaxies.

Proton magnetic resonance spectroscopy images show how heart defects disrupt metabolomic processes in the developing brain – opening pathways to improve medication and care for newborns with congenital heart disease.

Research informed by Raman spectroscopy finds that a lithium ceramic could act as a solid electrolyte in more powerful and cost-efficient generation of rechargeable lithium-ion batteries.

Researchers identify the oldest pieces of Baltic amber found on the Iberian Peninsula using infrared spectroscopy – imports began over 5,000 years ago.

What's Trending in Spectroscopy?

Which key trend, emerging technology, or killer application is set to most transform spectroscopy over the next 5–10 years? We present answers from six SciX speakers.

Alexis Weber: For me, it's the downsizing of spectrometers. When applying for grant or fellowship funding, I have noted that most solicitations have a large focus on the need for developing methods and technologies that are applicable in the field. This is not restrictive to a specific agency, but all scientific solicitations I have reviewed within the last couple of years. This trend will have a large impact on the spectroscopy field as a whole as more novel applications are able to be developed due to the smaller size but increased capabilities of spectrometers.

John Wasylyk: Advances in machine learning should greatly enhance the way we evaluate and apply spectroscopy-based analyses. We currently have an array of commercially available tools that search spectral files and help predict spectra of new compounds. Applying machine learning to kinetic studies, including kinetics of side reactions, will provide a new level of prediction and control, ultimately reducing excess testing and advancing process knowledge in early development cycles.

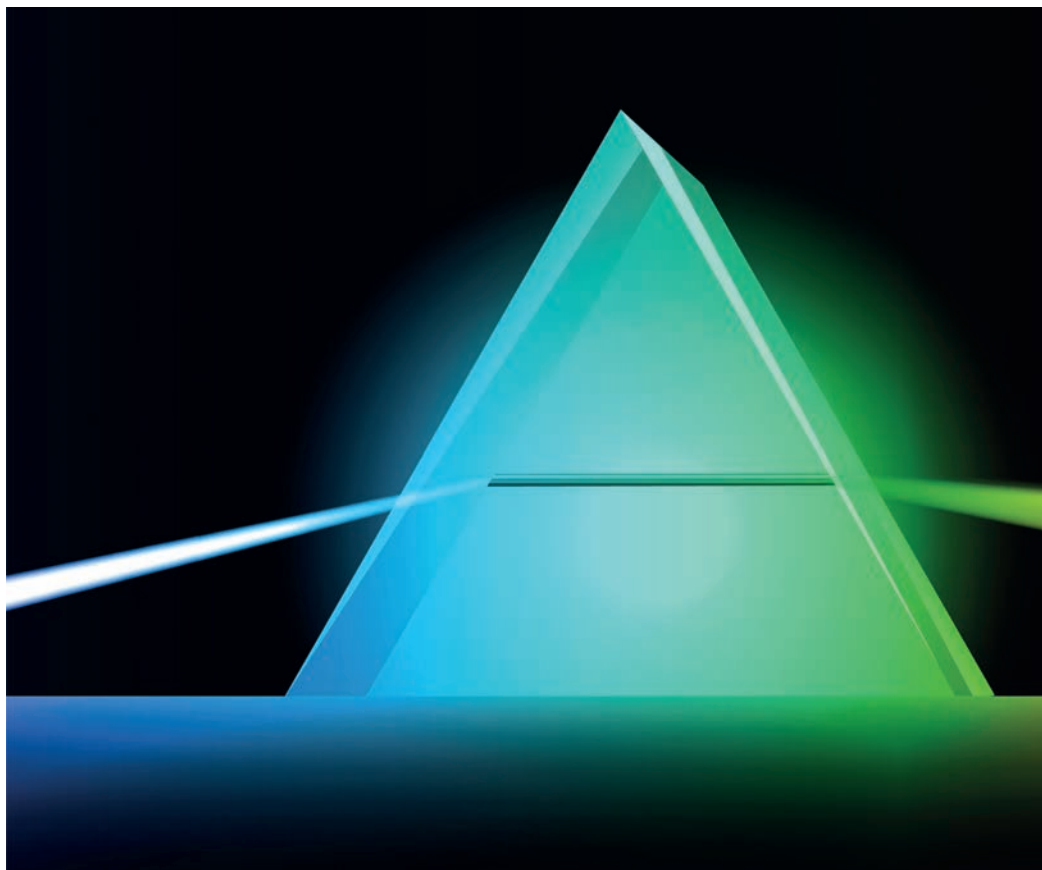
Sian Sloan-Dennison: I believe the next killer application is the SERS analysis of lateral flow devices with portable spectrometers, which would create a point-of-care platform that will provide

rapid, sensitive, and quantitative data on a plethora of clinically relevant biomarkers. In the next 5–10 years, we should expect to see portable automated systems that read lateral flow devices, relate SERS intensities to biomarker concentrations, and translate this into an easy-to-interpret result for the end user in emergency departments – leading to improved patient stratification. If SERS analysis can prove itself as a gold-standard analytical technique, it can finally move out of the lab and into real world scenarios.

Xiaoyun (Shawn) Chen: Democratization of spectroscopy is coming – as more people get smartphones that have more computing power than the NASA computers used to send astronauts to the moon, they can now combine them

with innovative accessories that can turn their devices into portable spectrometers ready to measure everything around them on the go. This allows users to use spectroscopy to authenticate their purchases, judge the quality of produce at their local market, and even combine the spectral measurements with BlockChain technology. The sky's the limit and the spectroscopy community should be prepared to welcome more citizen scientists and help them maximize the utilization of their handheld spectrometers.

Roy Goodacre: I agree with Shawn. Science is funded by the people and thus for the people, and I think democratization of science – or spectroscopy – is important and will be the future.





If we cast our minds back a few years (!) during the pandemic, people were regularly testing themselves. In other words, there was no need for them to visit some experts to have a test done. And I think this will continue. With the rise of wearable technologies people are used to having themselves continually monitored for personal activities, heart rate, and so on. It's therefore compelling that spectroscopy can be used for personalized medicine or personalized healthcare – this is certainly a future killer application (and, I believe, not that far away).

As Shawn said, we all carry mobile phones, and therefore a potential spectrometer. It might be relatively straightforward to design something that hijacks this technology to allow for measurements to be done. In addition, we all have toilets in our home and

there's been a great deal of discussion of the intelligent toilet; when you urinate or defecate into it, the toilet makes measurements and reports them to you and/or a physician. I think spectroscopy could play a role here as well.

Is this too far-fetched? I don't think so! If we look in other areas, the killer application for chemical sensing has been automatic diabetes checks with under the skin sensors that are linked to your mobile phone. I'm not suggesting that spectroscopy will replace a glucose monitor, but spectroscopy could be used to assess a plethora of other biomarkers so that we can monitor our health and

Chemistry at the University of Strathclyde, UK. She specializes in SERS and point-of-care. She is a SciX session chair for Raman spectroscopy.

Xiaoyun (Shawn) Chen is a senior research scientist at Dow Chemical Company, where he focuses on vibrational spectroscopy – especially for in-situ reaction monitoring. He is a SciX session chair for process analytical technology.

Roy Goodacre is a Professor of Biological Chemistry at University of Liverpool, UK. Roy's research interests include mass spectrometry-based metabolomics and developing Raman spectroscopy approaches for bioanalysis.

C. Derrick Quarles Jr. is a Sr. Scientist working for Elemental Scientific in the areas of automation for ICP and ICP-MS, elemental speciation (LC-ICP-MS and LC-ICP), and laser ablation (LA-ICP-MS). He is a SciX session chair for Atomic spectroscopy.

spot disease earlier than we otherwise would have. The earlier the better!

C. Derrick Quarles Jr. Over the last 10 years, there has been an increase in single particle- or single cell-ICP-MS based applications. I would expect that this trend continues and we see instruments continue to reduce in size and become faster and more sensitive, leading to the ability to detect smaller and smaller particles (for example, <5 μm).

SciX took place on October 8–13 in Sparks, Nevada, USA. For more information about the conference, visit: scixconference.org/scix2023

Charge Heterogeneity Characterisation of an IgG4-Based mAb Using AEX Coupled to MS

This application demonstrates that the charge heterogeneity of an IgG4-based mAb with a pI of 6.6 (proprietary mAb) can be successfully evaluated using a strong anion exchange column, BioPro IEX QF, coupled to MS detection (1).

Three basic and two acidic charge variants can be separated from the main species (Figure 1). This method is highly sensitive to the Fc N-glycosylation

A1: deamidation, glycation
A2: deamidation
B1: PG species
B2: NG species
B3: 1 x C-term Lys

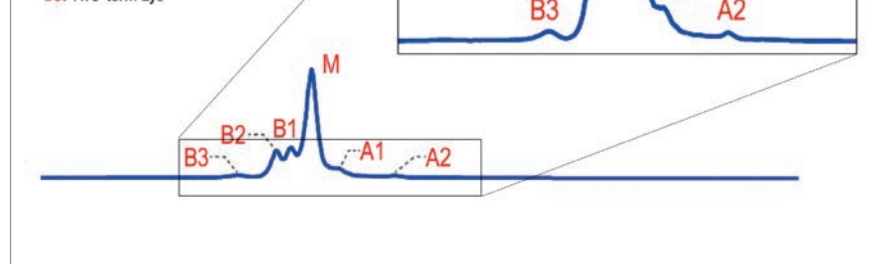


Figure 1: Native AEX-MS charge variant analysis, shown basic (B) and acidic (A) variant peaks as well as the main species (M) (1).

macroheterogeneity because the fully glycosylated main species is separated from the partially glycosylated (PG) and the non-glycosylated (NG) species, which elute earlier. The surface charge rather than the intrinsic charge seems to be decisive for the AEX separation.

The resolution of the glycosylated variants can be further improved by PNGase F-mediated deglycosylation.

The method is suitable for monitoring critical Fc quality attributes of IgG4-based mAbs.

Reference

1. A. Liu, Y. Yan, S. Wang, N. Li, *Anal Chem*, 94, 6355–6362 (2022).

Full method details can be accessed here:
<https://ymc.eu/d/brDpu>

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SEC-MALS Characterization of Copolymers Used for Drug Delivery

Biodegradable polymers are an important class of macromolecules that can be employed as drug-delivery agents to solubilize hydrophobic therapeutic molecules in water. The pharmacokinetics of the polymer within the body is greatly dependent on their molecular weight and size.

Size exclusion chromatography (SEC) has been widely used to study the molecular characteristics of polymer-drug systems. A series of PEO homopolymers and a PEG-PGA copolymer were analyzed and

compared using SEC with conventional calibration and multi angle light scattering. The use of conventional calibration provides accurate molecular weight if the structure and the chemistry of the calibration standards and the samples are identical. The PGA block in the copolymer modifies the conformation of the PEO chain, resulting

in an overestimated molecular weight when using a PEO calibration. The use of a light scattering detector is required to determine the true molecular weight of polymers, regardless of their chemistry and structure.

Find out more at:
<http://bit.ly/Copolymer-characterization>

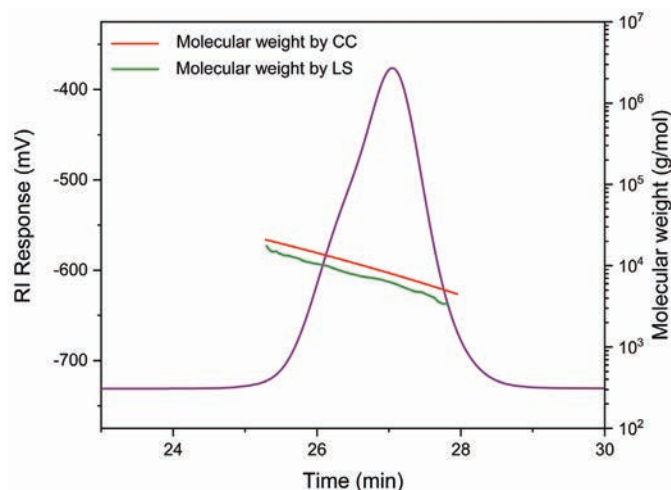


Figure 1. RI chromatogram and molecular weight traces obtained for PEG-PGA by light scattering (LS) and conventional calibration (CC)



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A portrait of Frances S. Ligler, a woman with short, wavy, light brown hair and blue eyes. She is smiling and wearing a dark blue, ruffled-neckline top. She has blue beaded earrings and a necklace with several colorful gemstones. The background is a plain, light gray.

Scientist, Engineer, Inventor

Sitting Down With... Frances S. Ligler,
Eppright Chair and Professor of Biomedical
Engineering, Texas A&M University, USA

Did you always want to be a scientist? I grew up in Kentucky spending a lot of time in the woods and on horseback, so I aspired to be a forest ranger or a cowgirl. However, in college I became interested in biologically oriented research, which led to graduate school at Oxford University, UK, where I fell more in love with lab work and research. From there, I completed my first postdoc in biochemistry and a second in immunology – becoming more involved in clinical research.

I really am still fascinated with discoveries in nature – which is the essence of science for me – and new ways of creation, fueled by engineering know-how. I don't know if you'd call the realization of an invention a "eureka moment," but invention certainly generates moments of excitement that prevent me from ever getting bored.

You take a very practical approach to your research – why did you shift your focus?

When I was midway through my career, I decided I wanted to make things to put in the hands of others to solve their problems. So I became half scientist, half engineer. Even when I started out as a scientist, I focused on practical tasks such as developing diagnostics for cancer based on blood samples. Using the tools of engineering has been very liberating, because instead of trying to develop or prove theories, I could actually solve problems and generate theories to fit the facts! This approach worked perfectly in terms of how my brain works and the results validated the process. I basically figured out what I wanted to do and learned whatever I needed to learn to accomplish the goal.

I also have a policy where every five years I try to figure out what's the most exciting thing going on in science or engineering and put a foot in that door. This is how I worked in regenerative

medicine and pharmacoengineering while collaborating with others that want to broaden their perspectives and opportunities outside of their own lab or institution.

What achievement has made you most proud?

I'm certainly best known for my work with biosensors. My group invented four different types of optical biosensors – creating some of the first practical methods for incorporating biological molecules into optical devices while keeping the biological recognition molecules functional for long periods of time. This led to 11 commercially produced biosensors – I believe five or six of these are still on the market today.

In 2017, I was flabbergasted to receive the National Inventors Hall of Fame (NIHF) Award – I hadn't realized how impactful my work had been because much of the results of use were classified at the time. I've now become quite involved with NIHF and have been attending the summer camps that they sponsor – teaching elementary school children to appreciate their creativity, learn how to solve problems, and be inventors. Some of these children have opened my eyes and spontaneously thrown out solutions to technical hurdles we've never been able to solve in the lab. It's been a very rewarding experience to work with such a wonderful organization.

But I think what I'm most proud of is my postdocs. I've had over 60 postdocs – 50 of which were during my time at the Naval Research Lab that went on to work within industry, academia, nonprofits, governmental labs, and so on. In my lab, they learned to work with people across disciplines and generate the intellectual property critical for translating research into products. Seeing where they're at now makes me feel so proud that I played a part in their

career development. I've learned just as much from my students as they've learnt from me.

What drives your curiosity and keeps you motivated?

Much of my motivation stems from the realization that I have a chance to make a difference – whether it's saving lives or worrying about what happens if I don't. That's certainly what kept me focused to work 60–80 hours week after week. I've certainly got a reputation for my "get it done" mindset. But ultimately, it's a fascination with what could be or explaining why something is the way it is.

What advice do you have for others following in your footsteps?

Follow your passions so you have the energy to pursue your goals. But it's also key to work on hard problems – somebody's sure to solve the easy ones so you need to take the mantle. Take that leap into the unknown, and see if you can swim. If you can't, just look for another door. You must take advantage of opportunities and get out of your comfort zone, but also be sensible.

I highly recommend working in teams – finding people on a similar or higher playing field than you (don't be afraid to ask for help!) – this can help you build a key infrastructure and broaden your knowledge.

Another thing I often tell young people is not to plan more than five years in advance. Your priorities are sure to change, and your interests will evolve. This doesn't mean your career will change every five years, but it's important to be open to new opportunities – this is how I combined science with engineering.

Ultimately, appreciate the professional and personal people in your life – these folks are the influencers that will shape you into the person you aspire to be.



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