SEPTEMBER / OCTOBER 2022 # 107

the Analytical Scientist®

It's Reconnaissance Time

The Power List: a fantastic excuse to ask leading thinkers and innovators about the current state of the field

We launched the Power List back in 2013 as a celebration. We wanted to highlight great minds and fantastic achievements, while drawing attention to the huge breadth and depth of the field – and the strength of the community despite that fact. Nine years on, much is the same; we are still celebrating all of those things (with a nod to our usual disclaimer about the non-definitive nature of any such list).

Yet some aspects have changed. Back in 2013, we asked our Power Listers for a brief line about their research and a career highlight or two. Now, we ask a wider range of more probing questions. The aim – in addition to eliciting helpful words of wisdom and adding more than a touch of color – is to paint a picture of the current state of the field, according to those at its forefront. And that's why the Power List is one of my favorite issues of the year.

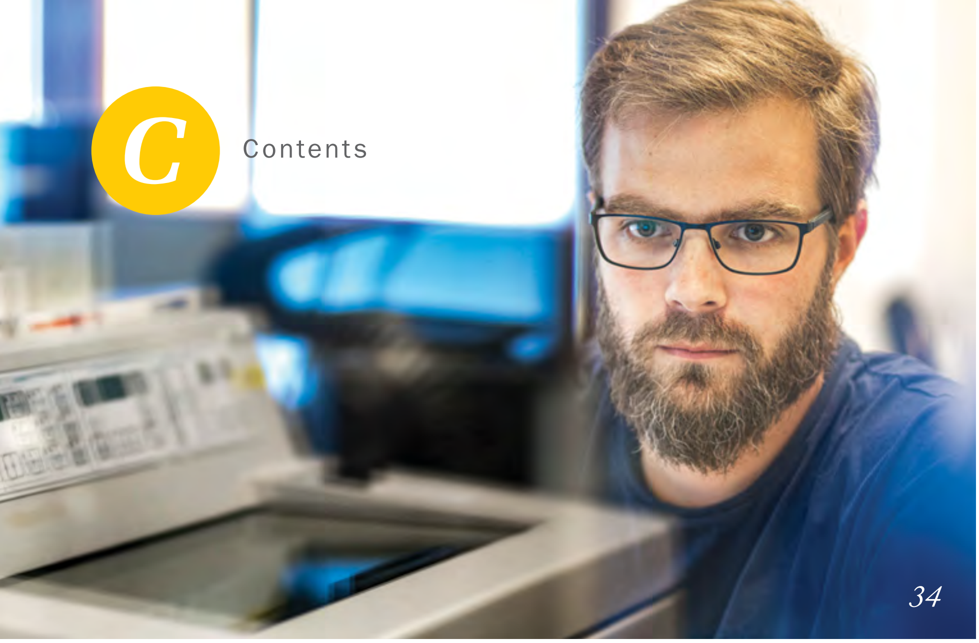
The world has also changed. So it's fascinating to explore what 2022's rising stars think about the problems they are tasked with solving. To give you a teaser, fears include difficulties attracting talent, focusing on tools rather than the questions that need answering, the rise of the "mega lab" (and its impact on funding more widely), a decline in fundamental understanding, diversity (which we explore on page 06), and a lack of standardization in data reporting and processing. And, of course, there are many specific challenges relating to individual specialties. (We're busy compiling responses for another "Musings from the Power List" article series that we'll publish on our website over the coming weeks; keep your eyes peeled!)

But if you're concerned our Top 40 Under 40 Power List is all doom and gloom, I'd suggest dipping into this year's "predictions." The future – according to analytical science's up-and-comers – is miniaturized chromatography, 3D printed columns, portable biosensors, mass spec-enabled clinical decision making, and well-characterized gene therapies. We'll also see all-round faster, easier-to-use, greener, more sensitive, and increasingly automated instruments.

Youthful optimism? Perhaps – but it's worth noting that many of this year's Power Listers are already heading up large groups (despite a relatively young age) – and some even made it onto 2021's Top 100 List. Personally, I think there's cause for genuine excitement when considering what the next 5–10 years may bring.

James Strachan
Editor

Contents



the Analytical Scientist

ISSUE 107 - SEP/OCT 2022

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Distribution: The Analytical Scientist (ISSN 2051-4077), is published bi monthly by Texere Publishing Limited, Booths Park 1, Chelford Road, Knutsford, Cheshire, WA16 8GS, UK. Single copy sales $15 (plus postage, cost available on request info@theanalyticalscientist.com). Non-qualified annual subscription cost is available on request.

In My View

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

In Our View: Diversity in Analytical Science

We asked this year's Power List finalists an important question: what changes would you like to see in analytical science with regard to diversity, equity, and inclusion?

Isabelle Kohler: Everyone should have equal opportunities when it comes to getting their dream job, but unfortunately the reality is different. Climbing the academic ladder as a woman in STEM has made me realize that there is a lot to be done to improve diversity, equity, and inclusion (DEI) in analytical science. Policies exist, but they don't seem to be established by those who would actually benefit from them. When will we start listening to underrepresented communities about what they need to grow and flourish in the field?

I would like to see more attention on people with physical or mental disabilities – be it big, small, visible or invisible, temporary or long-term. Navigating a professional career with a disability can be tough. This adds another layer of stress for those individuals, who often don't dare to share their struggles for fear of being cast aside. Inclusion also means that we should stop glorifying burnout culture and instead actively promote mental and physical wellbeing. I would like to see a work culture in which people with disabilities feel secure and welcome. Many of us struggle to adopt an "all work" mentality for health-related reasons and I don't believe we should be penalized for this.

Candice Ulmer: I am hopeful that DEI will become standard practice in the workplace and a natural component of every institution's culture. In addition, I hope to see a shift – from relying internally on employees to implement and develop DEI initiatives and policies to dedicating a percentage of annual operating budgets to hiring an external DEI consultant, manager, or office.

Michael Marty: The main change I would like to see is greater cooperation between industry and academia to advance DEI. Although most companies want a more diverse workforce, not enough collaborate with academic institutions to achieve this goal. Most academics actively want to support students in achieving their career goals, but resources are limited and academia does not always prepare students with the skill set they need. Greater cooperation could solve a lot of these challenges, but it will require long-term investment at all levels.

Daniel Petras: Though I am very happy about the increased attention and efforts toward improving DEI in science, there is still room for improvement. We need to work as a community to address the socioeconomic barriers that actively exclude a large part of humanity from engaging in science. Especially across borders, some DEI measures might be ineffective or even worsen the situation for economically disadvantaged people by focusing on historically marginalized groups without distinguishing between socioeconomic backgrounds. The introduction of conference fees and increasing article processing charges worries me because they generate a scientific class society that prohibits many researchers from networking and showcasing new science.

More waivers and scholarship programs are needed to enable economically disadvantaged scientists and institutions to participate in the scientific process. Another measure that can have a huge positive impact is free online conferences and the sharing of educational materials over the Internet. Because everyone was stuck at home during the COVID-19 pandemic, having conferences and workshops online made science much more accessible. I believe that having the recordings online increased participation from people all around the globe and effectively removed socioeconomic barriers. I would argue that YouTube is probably one of the most important free educational resources we have.

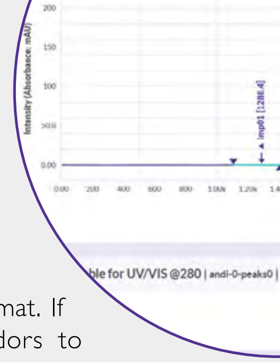
Evelyn Rampler: I am convinced that successful research in a field is dependent on its diversity. There is still a long way to go to reach equality for all underrepresented groups in analytical sciences – and STEM fields in general. For me, it's not only a vision, but a mission to foster diversity, equity, and inclusion in research and teaching. We must promote education about unconscious bias and discrimination against women and underrepresented minorities in science. For that, we need significant changes on institutional and personal levels (1).

We need to move away from the inflexible academic career model that scares away many young and promising scientists. Flexible schedules – and valuing efficiency rather than working hours – would help to balance work and personal demand, dismantling the common belief that working more is directly correlated with higher success rates. Another common belief is that students should move multiple times to succeed in academia, which makes it difficult to start a family. It also makes many scientists struggle with their mental health, because they often lack a functional supporting environment (another major issue during the COVID-19 pandemic). Overall, I strongly believe in the value of a healthy work environment, networks like Females in Mass Spectrometry (FeMS), and role models as major tools to support diversity, equity, and inclusion in our field.

Christina Jones: I want to see the analytical science community become a reflection of the global population. Science and technology innovation impacts our lives and transforms society. If we want to stay at the forefront, we have to innovate. For that to happen in analytical science, we need people with diverse passions and an assortment of perspectives that will challenge us to think differently and introduce new questions to the community that can be investigated.

Reference

1. *E Rampler et al., "Empowering women and addressing underrepresentation in the field of mass spectrometry," Expert Rev Proteomics, 19, 1 (2022). DOI: 10.1080/14789450.2022.2039631.*



Unleash Your Data

Converters and connectors translate locked instrument data into harmonized formats such as AnIML and create bi-directional interfaces with software systems, allowing scientists to visualize, share, reuse and reanalyze data

By Arne Kusserow, Carolin Witte, and Robin B. Shore

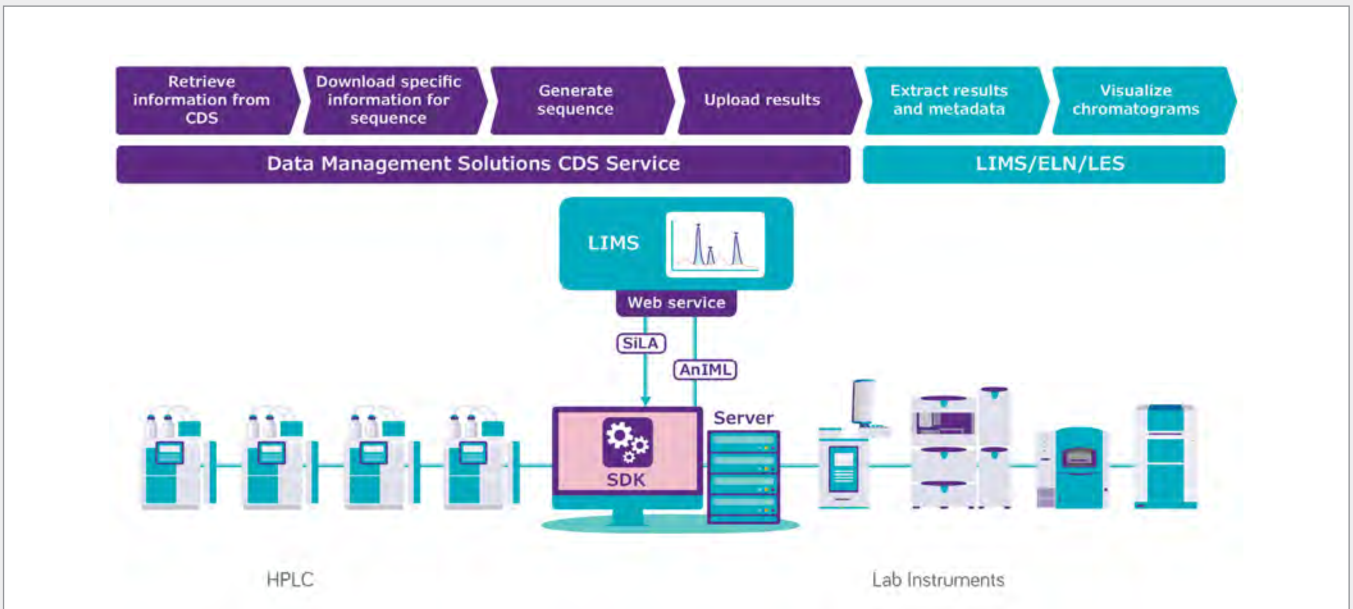
Analytical labs, especially in the pharmaceutical industry, are embracing accessible, community-supported, interoperable data and communications standards such as AnIML and SiLA. AnIML is human readable, clearly structured, flexible, royalty free and available to all. SiLA enables communication between instruments and software systems to let you use your data however you want. Integration of these two standards is creating a new ecosystem – one that allows end-to-end integration of instrument control, data capture, and leading systems such as LIMS, enabling visualization of a sample's entire lifecycle.

But let's take a step back. One barrier to this vision of the lab of the future is that instrument data do not come in AnIML format out of the box (1). Much of the software available today was built years before the current-day appreciation for shared formats or standards, when companies developed their own formats. This has resulted in instrument data often being proprietary, closed and in non-readable file formats – the very antithesis of FAIR (2).

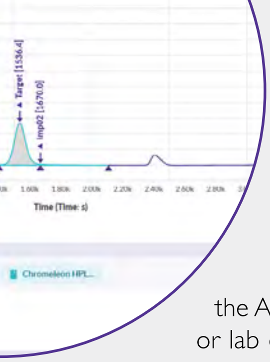
And this is exactly where data converters and connectors come in. First, a Merck data converter reads and decodes the information from the proprietary format. This includes metadata such as instrument name, software version and experiment timestamps; and sample data, which are often just series of characters. How do we decode those data from the proprietary format? If they are human readable, we can fairly easily build a reader to convert them to AnIML's XML format. If not, we work with vendors to solve the problem: they know what's in their data, and they have software we can use to extract those data from their machines.

Next, the converter creates a semantically identical copy of the data in AnIML format and writes this copy to disk. This includes separate AnIML "containers" with sample data, metadata, audit trails and digital signatures. The result is an AnIML file you can use with any XML-compliant software tool.

Connectors are a little more complicated. Once your data have been converted into an AnIML file, you may want to connect that file to a software system such as LIMS or ELN. For this to happen, not only do you need to translate the instrument data to AnIML format, but you also need to teach the third-party software to read the AnIML file. Without disrupting the different software applications already used in the lab, our connectors work bi-directionally, creating interfaces between



Bi-directional interfaces – integrate with LIMS/ELN/LES



the AnIML files and the LIMS, ELN, or lab execution systems you have in place without changing how you use those systems.

The converters and connectors run in the background to automatically track and translate instrument data into AnIML files, which are then saved either locally or to the cloud. At this writing we have converters for more than 300 instruments, including for Thermo Fisher Scientific Chromeleon 7 and Waters Empower 3 (both of which support HPLC, GC, IC, CE and MS) and for Metrohm tiamo and its titration software. On the horizon are connectors for Agilent OpenLAB CDS 2 (anticipated Q4 2022), Metrohm OMNIS (replacing tiamo) and Mettler Toledo LabX.

The lab of the future – today

Merck's "Lab Automation" project illustrates how data converters and connectors can work in practice. Merck's Global Analytical Services group is an association of 21 labs across the globe that offer a wide variety of services in the healthcare and life science industries. The group supports more than 220 analytical methods with a wide spectrum of analytical equipment, such as HPLC, GC-MS and NMR. The aim of Lab Automation was to create interoperable, bi-directional exchange of information between all heterogeneous systems and instruments to support analysts in their workflows (3) – the perfect use case for Merck's data converters and connectors. By translating all proprietary instrument data in Global Analytical Services labs to AnIML and collecting them in a central database, we achieved fully automated data flow, report generation and LIMS upload. In short, all data is captured electronically where it is generated, made available where it is needed and centrally stored using Data Management Solutions Hub software.

After one year, the Lab Automation project had successfully completed the digital transformation of three different Global Analytical Services lab facilities. What did it take? AnIML data converters for more than 20 different scientific instruments, bi-directional software integration with 4 different leading systems and 11 different measurement interfaces, a central data store (Data Management Solutions Hub), and a universal data analysis and visualization tool (Data Management Solutions Workbench).

The project team closely monitored the group's output before and after digital transformation to quantify the project's impact over the first year. Remarkably, Global Analytical Services saved a combined 3,386 working hours across all three labs, an estimated financial savings of approximately €400,000 and a nearly 20 percent increase in samples processed thanks to the automation of key workflows and data processes.

Terms such as "automation" and "digitalization" are buzzwords today, but the important concept underlying them is connecting things in a way that brings value to the customer. Converting locked instrument data to harmonized, standard formats like AnIML is the first step and a valid use case in its own right. But now, using our connectors, we can potentially take all instruments used in a lab, or in a group of labs across the world, and bi-directionally integrate them with a range of software systems to simplify and standardize forms, procedures and data flows in a way that also lets scientists visualize all the data in one system. These data can then be easily shared, reused and reanalyzed by different scientists, labs or companies.

That's what Open Science is all about. The result, as our Lab Automation project shows, is greater efficiency, significant cost savings and more freedom for scientists to do what they do best: conducting experiments and interpreting the results.

The Regulator's Friend

Data converters can be especially useful for pharmaceutical companies in their interactions with regulatory agencies. Companies often have data associated with the efficacy of their drug product that regulators wish to examine closely – which is impossible if those data exist in an unreadable file format. Manually translating such files, sometimes hundreds of thousands of them, to a human-readable format is a task no one wants to do. Fortunately, we can build a converter that automatically converts these files to AnIML for easy storage and availability to regulators.

Data integrity is another important factor to consider from a regulatory perspective. AnIML has a built-in audit trail that lets you see first-hand whether a data file was opened, by whom and what they did with it, all while ensuring the raw data remain untouched.

Arne Kusserow is Product Manager, Robin B. Shore is Content Development Manager and Carolin Witte is Software Product Owner for Data Management Solutions at Connected Lab of Merck KGaA, Darmstadt, Germany.

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TOP 40 UNDER 40

The Analytical Scientist POWER LIST

Celebrating the rising stars who will save us from the future!

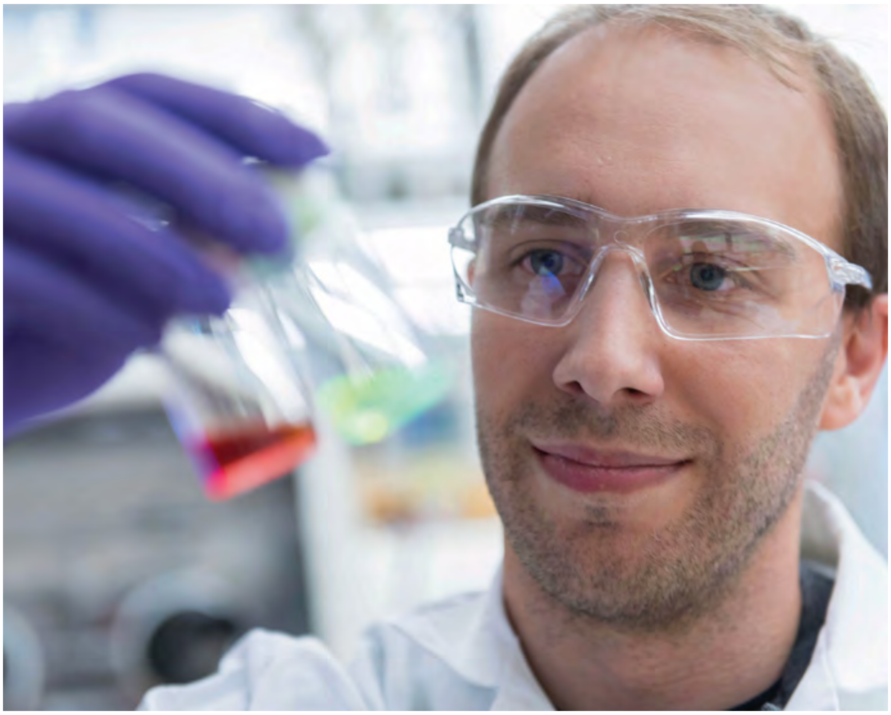
It has been a tumultuous four years since our last Top 40 Under 40 Power List. Just as the world tentatively began to move on from the COVID-19 pandemic, more dark clouds – the events in Ukraine, rising inflation, and the energy crisis – arrived. Also looming large are longer-term issues such as climate change and an aging population.

We've all seen the crucial role scientists played in fighting COVID-19, from developing new diagnostic tests to scaling up and rolling out vaccines. And it's clear we'll need more keen minds to tackle the many crises ahead.

Here, we celebrate analytical science's rising stars, who will, hopefully, provide the answers to the 21st century's biggest questions. The good news is that many of the 40 names below are already working hard on analytical problems in atmospheric science, battery electrochemistry, and cancer diagnosis or developing new instruments and enhancing our understanding of the core techniques. All have the potential to make a profound difference.

Within their analyses of the current state of affairs, their predictions for the future, and their personal mission statements, we hope you find good reason to be optimistic. We're in safe hands, folks!

WANT TO SHARE THIS LIST WITH A COLLEAGUE? IT CAN BE ACCESSED ONLINE FOR FREE AT HTTPS://THEANALYTICALSCIENTIST.COM/POWER-LIST/2022



Russ Algar
Associate Professor, Department of Chemistry, University of British Columbia, Canada

Challenges? I think translation is one of the biggest challenges. Yes, as an academic researcher, I would argue that curiosity-driven research is equally important, but I would also argue that my peers are already quite good at it. The gap between the research lab and societal application has always been one of the largest to bridge.

Advice? Be a flexibly stubborn researcher. Don't be so focused on a particular goal that you miss out on unique opportunities or interesting detours. Hit pause on ideas from time to time, but don't give up on good but challenging ideas that take time to realize. And, even though quantity sometimes looks more impressive, don't compromise on quality. Good scientists still appreciate other good science more than anything else.

Mission? To feel like I know what I'm doing? I've been a principal investigator for 10 years and there is still a lot of flying by the seat of my pants and wondering how I'll keep things going through the next year. Even if I don't figure the job out entirely, the main goals are for my team's research to continue its positive growth and to see some of our work take steps to translate from the lab to society.

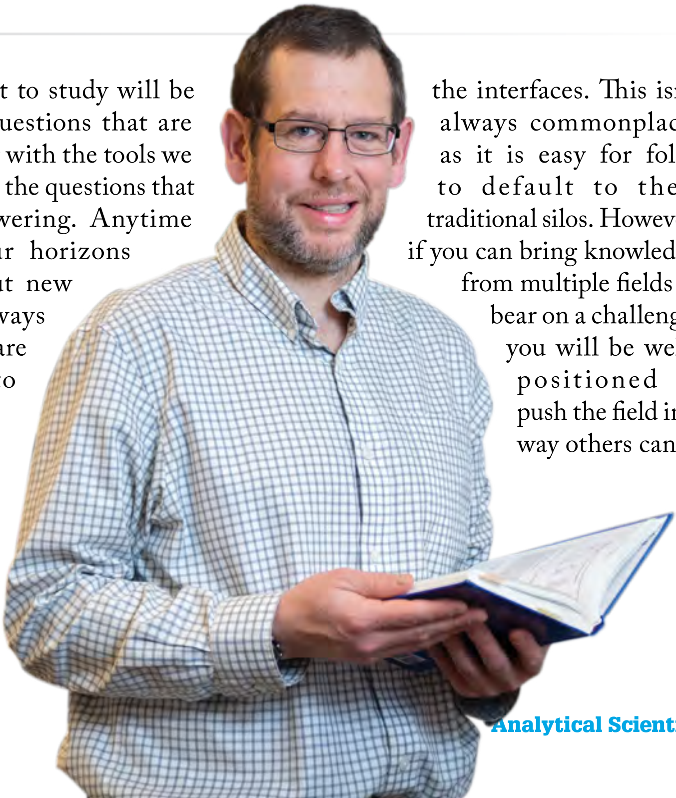
Controversial opinion? HPLC-MS can't do everything!

Andrew Ault
Associate Professor, Chemistry, University of Michigan, USA

Challenges? I think a major challenge for atmospheric chemistry research is that we generate so much interesting data, but that funding primarily focuses on new field campaigns or studies. With typically three-year funding cycles, this means that lots of important data never ends up getting fully processed, analyzed, and written up; as soon as it is collected, funding dictates that we move on to the next campaign.

Fears? My biggest fear is that, with so many amazing tools available, our ideas about what to study will be driven by the questions that are easiest to answer with the tools we have, rather than the questions that most need answering. Anytime we broaden our horizons and think about new tools or new ways to use tools we are taking steps to avoid that.

Advice? Try to keep a foot in multiple fields, as truly cutting edge science is often at the interfaces. This isn't always commonplace, as it is easy for folks to default to their traditional silos. However, if you can bring knowledge from multiple fields to bear on a challenge, you will be well-positioned to push the field in a way others can't.



Zachary S. Breitbach
Principal Research Scientist, Analytical Research and Development, AbbVie Inc., USA

Challenges? One of the biggest challenges in separation sciences is not technical, but rather the decrease in basic research and intense training in the field. Sometimes seen as a mature technique, chromatography groups may be overlooked for the sufficient funding needed to produce high value research programs and the resulting top talent the field needs.

Secret to success? Any success is a direct result of the people I have had the fortune to interact with. I was lucky to have a strong upbringing that taught me the value of hard work and I have an amazing family that understands my drive to go the extra mile in my research. Most importantly, I have always been fortunate to work alongside the best and the brightest.

Advice? Work hard: put in the extra time and be persistent, it will pay off. Work fair: collaborate and recognize colleagues, you can't do it all alone. Have fun: enjoy what you are doing.

Ken Broeckhoven
Associate Professor, Vrije Universiteit Brussel, Belgium

Fears? The difficulty of finding funding for fundamental research for more "common" techniques, such as chromatography; it not only stifles further innovation and development, but also decreases the overall knowledge of the (basic) theory of these techniques.

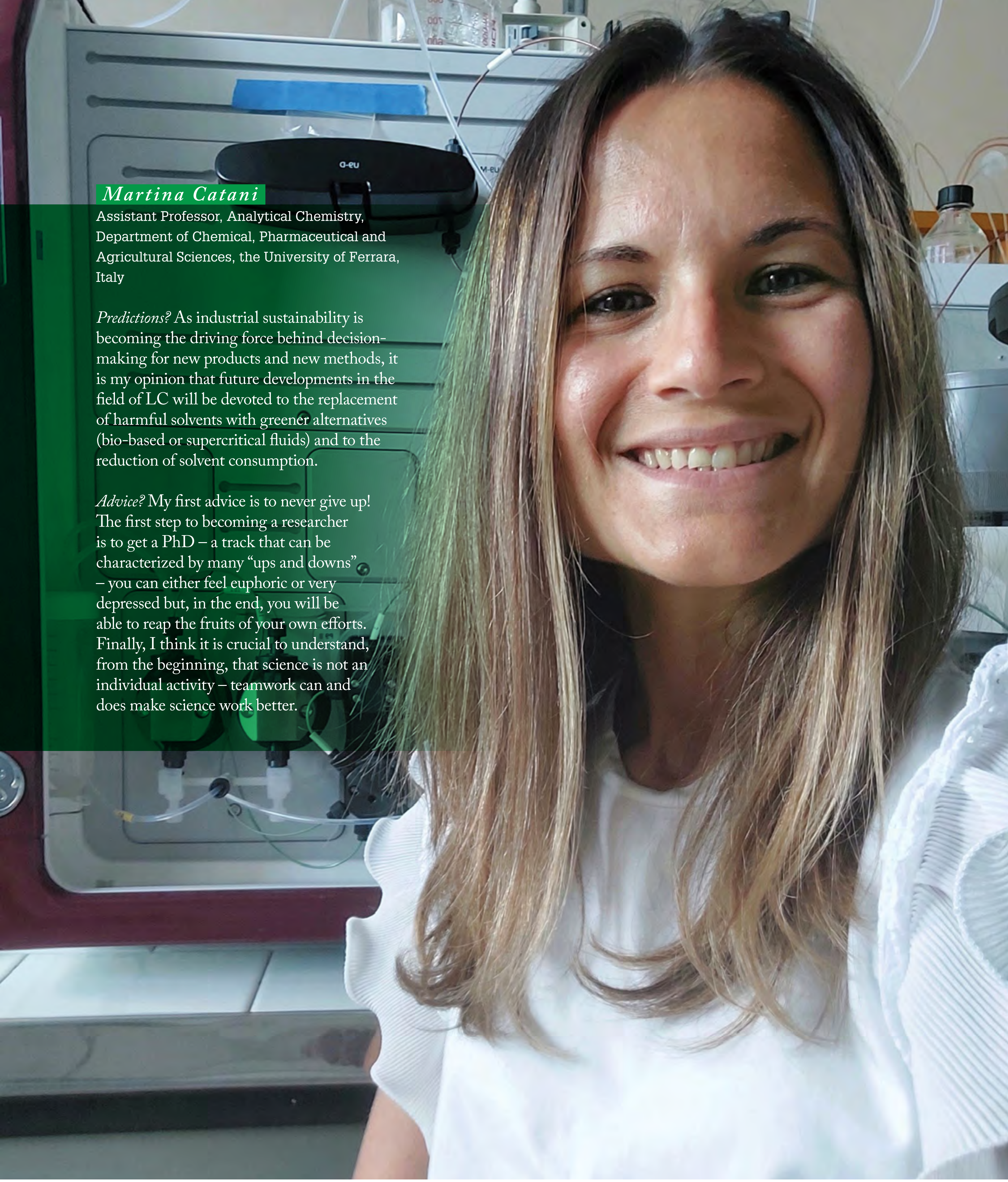
Challenges? Chromatography seems to have reached a limit in separation power without the implementation of drastic technological changes (instrumentation and column technology). 3D printing technology seems promising, but I think it will probably still take at least a decade before it becomes feasible to print high performance columns.

Predictions? I expect to see more work towards user-friendly miniaturization in chromatography. This will resolve certain fundamental issues (such as viscous heating), but will also improve compatibility with emerging technologies, such as 3D printing, which can't print large volume structures with high resolution.

Anna Laura Capriotti
Associate Professor, Department of Chemistry, University of Rome La Sapienza, Italy

Mission? In the next 10 years, my personal aim is to create a solid yet dynamic young research group in the field of separation sciences and omics. Following the footsteps of my mentor Aldo Laganà, who effectively emerged from nowhere thanks to his charisma and willpower, I hope to be a good mentor for the next generation of young scientists – especially following the difficulties faced by the youngest generations following political and economic crises and the COVID-19 pandemic.

Dream dinner party? I would surely invite Mary Wollstonecraft Shelley, the English novelist who, in the 19th century, anonymously published her famous novel Frankenstein, which is considered the first science fiction novel in history. Since science fiction has usually been associated with male novelists, she had to fiercely fight to be acknowledged. Women have always had to fight for seeing their credits recognized – in art as well as in science and research.



Martina Catani

Assistant Professor, Analytical Chemistry, Department of Chemical, Pharmaceutical and Agricultural Sciences, the University of Ferrara, Italy

Predictions? As industrial sustainability is becoming the driving force behind decision-making for new products and new methods, it is my opinion that future developments in the field of LC will be devoted to the replacement of harmful solvents with greener alternatives (bio-based or supercritical fluids) and to the reduction of solvent consumption.

Advice? My first advice is to never give up! The first step to becoming a researcher is to get a PhD – a track that can be characterized by many "ups and downs" – you can either feel euphoric or very depressed but, in the end, you will be able to reap the fruits of your own efforts. Finally, I think it is crucial to understand, from the beginning, that science is not an individual activity – teamwork can and does make science work better.

Livia S. Eberlin
Associate Professor, Department of Surgery,
Baylor College of Medicine, USA

Predictions? I believe mass spectrometry is set to revolutionize medical practice and clinical decision making. I foresee that, in the next 5–10 years, medical professionals including pathologists, oncologists, and surgeons who currently do not have access to the power of mass spectrometry technology for molecular analysis will be using it in a very intuitive way to help define the best treatment options for their patients.

Controversial opinion? For many years, I've been passionate about ambient ionization mass spectrometry and direct mass spectrometry analysis and the value that these technologies have in medicine and clinical practice. Generally, I have perceived that the limitations of these techniques when compared with more traditional chromatography-based mass spectrometry approaches have led many to doubt or disagree with their potential in medical practice, but I think we are now at a stage where there is a more palpable excitement and belief that these technologies can truly make it to the clinic.

Guosheng Chen
Associate Professor, School of Chemistry, Sun Yat-sen University, China

Challenges? My current research focuses on the design of porous organic-framework-confined enzymatic cascades for biosensing. I think the biggest challenge facing this field is controlling the spatial distribution of multi-enzymes within a scaffold. If this challenge is addressed, I believe that it may offer new ways to mimic intracellular biocascades, enabling much higher efficiency and selectivity for next-generation biosensors.

Predictions? I envision that this enzymatic cascading scaffold will be found in devices in the next 5–10 years, serving as a portable biosensor for the point-of-care detection of disease-associated biomarkers. I believe this research direction is highly desirable in personalized medicine and continuous monitoring epidemics.

Secret to success? I think enthusiasm and patience have been the most important elements in the early part of my career: enthusiasm can stimulate a constant thirst for new knowledge and push me to explore the unknown research areas, whereas patience is essential to overcome the continuous barriers in the research journey.

Tao Chen
Principal Scientist, Small Molecule Analytical Chemistry, Small Molecule Pharmaceutical Sciences, Genentech, USA

Predictions? For traditional small molecules, miniaturized instruments with low-cost and high-performance will increase. Novel analytical technologies (standalone or hyphenated) for new therapeutic modalities are expected to boom. There will be an increasing demand for high-throughput analysis as well as the use of data science and machine learning to guide experiment design.

Secret to success? I found chemistry fascinating back in high school; I was inspired by my first chemistry teacher. Over the course of college and graduate school, I was fortunate to work with my advisors who are leaders in the field of analytical chemistry; they cultivated my interest in this field. Here at Genentech, I am grateful to have managers who promote scientific research and innovation, and encourage me to push my boundaries.

Advice? I benefited a lot from the working principles of my PhD group: "work hard, work smart, work together, and be happy." In addition, be flexible and open-minded – face up to fear and embrace new opportunities that could lead to exciting adventures and pleasant surprises.

Daniel DeBord
Vice President of Research & Development, MOBILion Systems, USA

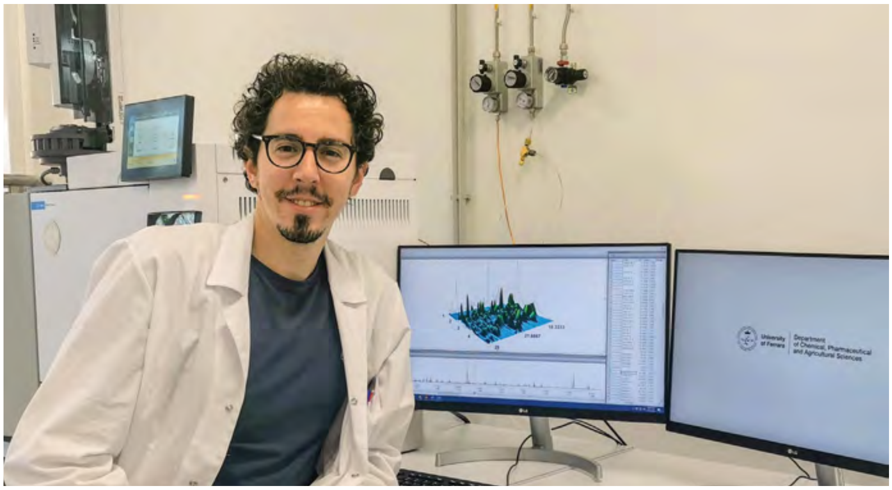
Controversial opinion? Anyone familiar with the field of mass spectrometry likely knows the story of the Orbitrap mass spectrometer. It is a beautifully elegant mass analyzer that was invented roughly 20 years ago and has grown to become the most ubiquitous type of mass spectrometer for discovery applications. It has been adapted, optimized, and demonstrated for an incredibly diverse range of applications, with most common users recognizing it as the de facto standard. However, I'm of the opinion that there is no "end all, be all" mass spectrometry solution for all applications. The patchwork quilt of analytical problems in the real world means that the various other types of mass analyzers – time of flights, quadrupoles, magnetic sectors, and so on – each have redeeming qualities and complementary capabilities that allow them each to surpass the almighty Orbitrap in certain areas. The diversity of technologies is one of my favorite aspects of the mass spectrometry field and is something I advocate for to ensure that we maintain a healthy ecosystem – one where we reserve a place for each of these unique branches of the mass spec family tree.

Shane Ellis

Australian Research Council Future Fellow, Molecular Horizons, School of Chemistry and Molecular Bioscience, Australia

Fears? We get a bad rap as a "boring" field – just titrations and routine analysis. But it's so much more – and truly multidisciplinary, bringing together engineering, chemistry, physics, biology and informatics. For example, look at all the cool instrument development that has occurred in the MSI field. People are developing highly complex instruments all the way from ion optics simulations, electronics, design and construction to their eventual testing and deployment. I would classify this as analytical chemistry too. To attract more younger scientists, we need to communicate how fascinating and broad analytical chemistry can be, as well as the many career opportunities it can open up.

Mission? I recently set up a new MSI laboratory at the University of Wollongong. A primary goal is to grow this into a world-class MSI laboratory with a broad and complementary set of capabilities. I also want to develop MSI techniques to the point where we know exactly what molecules and what biochemical processes we are visualizing. And after losing a very dear friend and colleague to cancer, I am also passionate about contributing to improving the capabilities for MSI so it can be deployed to help guide tissue diagnosis and treatment decisions and eventually improve the lives of patients.



Flavio A. Franchina

Assistant Professor (tenure-track), University of Ferrara, Italy

Challenges? In my opinion, an important current and future challenge is the exploitability of the immense volume of data in our hands. Nowadays, we have available (thank goodness!) powerful, accurate, and high-resolution modern analytical instrumentation, which allows us to acquire and store a huge amount of data. This, in combination with the elevated number of samples required for statistical relevance in research studies, makes the extrapolation, fusion, and conversion of the data into knowledge very challenging. Although exciting and motivating, we are trying to address increasingly complex questions, encompassing several disciplines – thus the skills and knowledge required for a scientist are increasingly demanding. More than ever, sharing and collaboration can help us progress this quest faster.

Advice? First, identify and master the fundamentals of your discipline. Then, don't be afraid of the novelties and challenges – these squeeze the best out of you. Go experience 360° integration (scientific, cultural, organizational, and so on) abroad and be open to new fields. Throw out the worst and melt the best of these experiences to shape your scientific and personal profile. It is not (at all!) an easy trail, but passion and persistence are qualities to develop, embody, and shape to reach your objectives.

Justin Godinho

Investigator, Drug Substance and Product Analysis, GlaxoSmithKline

Predictions? I believe there will be increased demand for simultaneous characterization of large proteins and their supporting sample constituents. Currently, a series of separation techniques is required for complete analytical characterization. We have seen some research directions shift towards innovative methods to elucidate multiple critical quality attributes simultaneously. I also expect greater adoption and drive towards multidimensional separation technologies and MS based instrumentation in QC settings to safely deliver well-characterized molecules to patients with fewer more comprehensive analytical tests.

Advice? Find opportunities to collaborate. More specifically, seek out colleagues that have different skill sets. Your work will benefit if you are challenged to think differently.

Andrea Gargano
Assistant Professor (tenure-track),
van't Hoff Institute for Molecular Science,
University of Amsterdam,
The Netherlands

Fears? I fear that the opportunities we have to expose our research are insufficient to disseminate our results and interact with other scientific communities. I fear that we are not doing enough to bridge the analytical community with other applied and fundamental sciences. Analytical science research groups should not be an ensemble of research islands focused on developing complex methods. Ideally, we should be organic/integrated parts of institutes, universities, and international research efforts. However, for young academics like me, it is not common to be part of international research efforts, to be involved in research that crosses disciplines, or even to teach in a different context than the one in which they work. I think analytical science needs to grow even more into a more multidisciplinary and broader community rather than following a spiral of hyper-specialization.

Alexandre Goyon
Senior Scientist, Small Molecule
Pharmaceutical Sciences (SMPS),
Genentech

Predictions? The development and application of multi-dimensional liquid chromatography mass spectrometry (mD-LC-MS) methods to solve unmet characterization needs for complex drug modalities and sample matrices.

Controversial opinion? The pharmaceutical field is quickly evolving and a variety of drug modalities and delivery systems are now being investigated. However, the application of analytical chemistry to solve diverse real world challenges may not be valued as much as fundamental studies. Industrial partners are often underrepresented in journal editorial boards and conference scientific committees, which may create a disconnect between fundamental and applied research. For example, liquid chromatography plays an essential role to support quality control in the industry while exploratory techniques such as mass spectrometry are given more importance in academia.

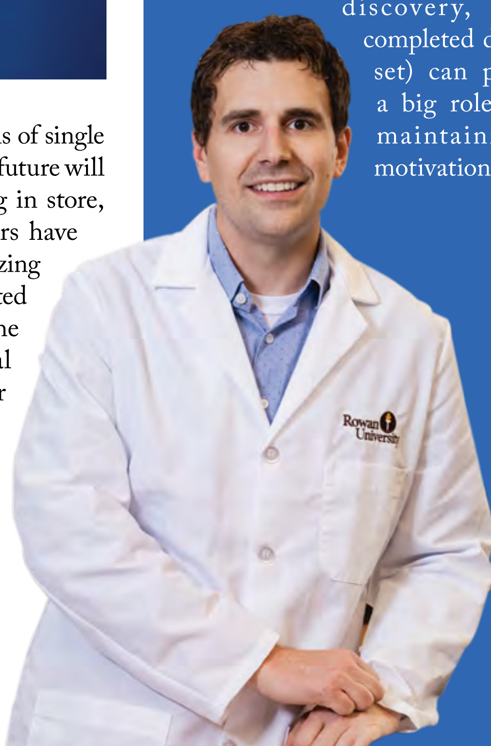
Advice? Stay focused, keep being curious, and consider challenges as an opportunity to learn and make a difference.

Bram Heijs
Group leader MS Imaging, Center for Proteomics & Metabolomics, Leiden University Medical Center, The Netherlands

Predictions? Given the rate at which mass spectrometry imaging (MSI) is currently developing, there's no doubt that incredible new developments will be unveiled. About 10 years ago, routine measurements were performed at 100 μm spatial resolution. The current state-of-the-art is performing measurements at subcellular spatial resolution to enable the analysis of single cells. It is a no-brainer that the future will have single organelle imaging in store, as modern mass spectrometers have already proven capable of analyzing the molecular content of isolated single organelles. Besides the ever ongoing push for spatial resolution, spatial molecular identification and annotation tools will likely become more commonplace, which should be the end of "putative identifications" commonly seen in MSI-based work.

James Grinias
Associate Professor, Department of Chemistry & Biochemistry, Rowan University, USA

Advice? The American Chemical Society's ChemIDP is a great tool that helps young scientists identify careers that align with their interests. I highly recommend it to any student that asks me for advice on how to find a job. Part of the program focuses on setting goals, which I also think is a critical aspect to advancing as a scientist – try to figure out where you want to be in 1, 5, or even 10 years, and then set manageable and achievable benchmarks that will help you guide you there. Finally, don't forget about the fun parts of science. Persistence is key in research because failure is unfortunately a frequent part of the scientific process. However, making sure you celebrate the "wins" along the way (a new discovery, a completed data set) can play a big role in maintaining motivation.



Liam Heaney

Senior Lecturer, Bioanalytical Science, School of Sport, Exercise & Health Sciences, Loughborough University, UK

Fears? My biggest fears relate to the funding landscape. I have noticed an interest in moving the funding approach for mass spectrometry away from the individual lab setting and towards an approach where there are "mega labs" and national/regional facilities. Though these approaches might make sense to a funding agency (you can fill a lab with the best equipment and best scientists), the reality is that these setups will massively detract from the next generation of scientists' capacity to learn.

Mission? My personal goal is to continue in my attempts to expose analytical science to a wider audience. I am aware of how little content for laboratory analysis is included across sports science courses, especially when considering the total reliance on analytical science for anti-doping monitoring. This is a major part of sport, and I really believe our sports science students should be learning about this to complement their other studies. From a research perspective, I am excited to continue building a reputation within the anti-doping sector both for myself and for our School/University.

Benjamin-Florian Hempel

Head of Proteomics Laboratory, Department of Veterinary Medicine, Veterinary Center for Resistance Research, Freie Universität Berlin, Germany

Challenges? The exponentially increasing data sets of high-dimensional complexity that analytical instruments generate in short time scales. Current analysis tools are still lagging behind to take full advantage and extract the highly complex information enclosed in the dataset.

Predictions? This question can be answered in three simple words: speed, handling, and miniaturization. Current instruments already enabled analyses of large sample cohorts on very short time scales, which will be further developed in future. The simplified handling is another upcoming trend, which allows many more end users an ease of use in clinical routine, for example. Last but not least a step into the future is miniaturization of instruments. The already existing benchtop instruments will become even more compact so they can be directly used in field studies.

Secret to success? Freedom to implement my own ideas – within reason! – and learn from resulting successes and mistakes.

Jared O. Kafader

Research Assistant Professor and Director of Instrumentation, Proteomics Center of Excellence, Northwestern University, USA

Predictions? Over the next 5–10 years we will see significantly more automated studies taking place. Automation unlocks high-throughput studies for the clinical arena, which reveal important trends that are not captured in more fundamental investigations. The pandemic has jump started this push with advanced testing and diagnostic studies.

Advice? Continually teach yourself something new every day and surround yourself with other driven scientists. As you become familiar in a subsection of your field, regularly turn your attention to additional experimental, computational, or informatics based tools. Collaborations both internally within your research institution and beyond is the only way to stay at the forefront of your field and grow as an investigator.

Christina Jones

Partnerships and Outreach Strategist and Research Chemist, Advanced Manufacturing National Program Office, National Institute of Standards and Technology, USA

Secret to success? ISIAH WARNER. Even putting his name in all caps isn't enough to emphasize the great, positive impact our mentor-mentee relationship had on both my professional career and personal life. He took me under his wing as a scared undergrad with no knowledge of the impact that science and technology research has on the quality of our lives. He gave me a space as an undergraduate chemistry major to grow comfortable and confident in my abilities as a scientist, analytical thinker and problem solver, and, more importantly, he showed me that analytical science is a place where I too belong and empowered me to be ambitious and reach for the stars in my career.

Advice? Don't compare yourself to others because that's a losing battle. Get in tune with your own abilities and evaluate yourself based on what you know you are capable of – thinking of your progression, not perfection. Also, establish a Board of Directors for yourself. Surround yourself with mentors, sponsors, and peers who have your best interest at heart, understand your goals, and can provide encouragement and resources to help you accomplish them.

Joaquin Rodriguez Lopez

J. Andrew and Susan S. Langan Professorial Scholar, and Associate Professor of Chemistry, University of Illinois Urbana-Champaign, USA

Challenges? Figuring out ways to electrify as many technologies as make sense to turn the tide on anthropogenic greenhouse gas emissions. My group's grain of sand to this major challenge is to introduce new ways to observe, understand, and re-invent electrochemical interfaces using tools of analytical and materials chemistry.

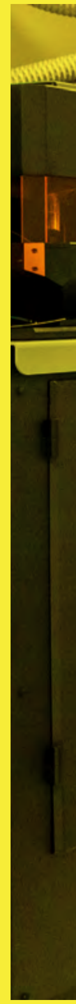
Advice? Actively seek a network of people and mentors that can help you propel your career. Regardless of what scientific problems you pursue or your sources of funding, make sure you have room to pursue topics that interest you personally, beyond the influence of current trends or what is "hot." Diversity also means introducing new ideas that are generated in the long, integrative process of becoming a scientist. I've found some of my greatest satisfactions – and the things that motivate me to work at my best – come from problems I have been slowly stewing on for decade(s!).

Isabelle Kohler

Assistant Professor, Amsterdam Institute of Molecular and Life Sciences, Vrije Universiteit Amsterdam, The Netherlands

Mission? My personal mission for the next 10 years (and, actually, the rest of my life) is that every day I wake up in the morning, I feel content, fulfilled, connected to my core, and ready to learn something new during the day. For me, this can only happen when my mind and my body are aligned – in other words: that my work-life balance is under control and healthy. This remains a challenge in the academic world, where overwork is the rule rather than the exception.

Dream dinner party? I would organize a Power List-themed dinner and gather all my past and current colleagues, mentors and supervisors who have been featured in the Power List since 2013. From the beginning of my career during my PhD in Geneva until my current position as Assistant Professor in Amsterdam, I have been fortunate enough to be surrounded by such talented people who are recognized as the most influential analytical scientists by the community. Luckily, with international borders opening again after the COVID-19 pandemic, there's a chance that this dinner actually happens in the foreseeable future! I'm sure I don't need to list here who will receive an invitation card to this dream dinner – they know who they are!



Benjamin T. Manard

Research Associate, Analytical Chemist; Chemical Sciences Division; Oak Ridge National Laboratory, USA

Secret to success? Mentors – hard working and assiduous mentors who are dedicated to analytical science. My mentors have really shaped my career, each instilling unique aspects of how to be a good analytical scientist. Some pushed thinking outside the box and problem solving, while others pushed the value of high-quality data.

Advice? Initiate collaborative efforts across disciplines. Analytical science is a critical necessity across all fields. Your career doesn't have to be a solo endeavor. Reach out to others not only in analytical chemistry, but in multiple areas of science for collaborations. That is one of the nice things about analytical science, it can be applied to everything.

Lawrence Madikizela
Associate Professor, Analytical and Environmental Research, University of South Africa, South Africa

Fears? Research productivity is assessed by one's ability to publish and attain research funding. With the latter becoming more difficult, some researchers are attempting to publish poor quality research. As an editor and reviewer in various journals, I have seen a high number of research articles being declined based largely on a lack of novelty, poor experimental design, and poor quality of the research manuscript itself. Sadly, some reviewers and editors overlook these shortfalls, which result in the publication of mediocre work. I'm most worried about the impact this will have on younger researchers, who benchmark themselves against what has already been published. In some cases, they might even be reading research published by a predatory journal and using that to conceptualize future research ideas. In the long run, this will have severe consequences.

Michael Marty

Associate Professor, Department of Chemistry and Biochemistry, University of Arizona, USA

Fears? My biggest fear is that we are not attracting enough talented students into analytical graduate programs. Traditional analytical chemistry or quantitative analysis courses tend to start with topics that most students find boring like error propagation or statistics. These are undoubtedly important, but they don't draw students in. When I started teaching our undergraduate analytical chemistry course, I flipped the curriculum so that we start with the analytical methods to solve key problems and then cover the statistics once they have some context for why they are important.

Secret to success? Excellent mentors. At every stage, I have been surrounded by people who believe in me more than I believe in myself. They encouraged me to take leaps that I did not think I was ready for. Also, I think I have been extremely lucky to be in the right place at the right time.

Advice? Learn to code. Start with a brief tutorial to learn the syntax. I recommend Python, but other languages are good too. Then, pick a problem that you want to try to solve with it. Start with something simple like integrating a peak. Then, just keep building on that foundation, focusing on things most useful for you rather than arbitrary exercises. Ask for help from colleagues, social media, and web searching.

Vladimir Michaelis

Associate Professor and Canada Research Chair in Magnetic Resonance of Advanced Materials, Department of Chemistry, University of Alberta, Canada

Challenges? Sourcing and securing a safe supply of liquid helium is the biggest challenge ahead of us. Liquid helium is critical for superconducting magnets and associated research including magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) within the physical and applied sciences. These disruptions lead to decommissioning of magnets and facilities worldwide.

Predictions? Major technological advances in analytical hardware will continue for the foreseeable future in solid-state and dynamic nuclear polarization (DNP) NMR spectroscopy. Higher magnetic fields, faster magic-angle spinning, 2D and 3D multidimensional approaches and polarization boosting methods will enable exploration of exotic quadrupolar nuclei, which make up the majority of the NMR active nuclei in the periodic table. The evolution of data mining, repositories and artificial intelligence will allow the field of NMR spectroscopy to be used more broadly.

Advice? Each journey is unique. Be open to listening to other experiences (good and bad) and map out your own path. There will be many failures along the way but celebrate every success no matter how small – the rest is noise.

Daniel Petras

Junior Research Group Leader, CMFI Cluster of Excellence, University of Tuebingen, Germany

Predictions? I assume mass spectrometry and metabolomics will be further standardized and will be mainly performed as a service measurement in core facilities – similar to sequencing today. Non-targeted analysis will thereby largely replace targeted assays. I assume we will reach annotation rates akin to proteomics/genomics experiments once in silico prediction of MS/MS spectra and retention/drift times are solved. I am waiting for the "AlphaFold moment" here.

Fears? My biggest fears for the analytical sciences is the continued division of different sub fields in their silos and the blocking of technological and conceptual progress by sticking to established dogmas. In a sense I'm not too worried because, if this happens, analytical science will be simply swallowed or replaced by other fields that embrace the culture of change and adapt to roadblocks and new opportunities.

Dream dinner party? Albert Einstein, Rosalinde Franklin, Kary Mullis, and Timothy Leary.

Katelynn Perrault

Associate Professor, Forensic Sciences and Chemistry, Laboratory of Forensic and Bioanalytical Chemistry, Chaminade University of Honolulu, USA

Predictions? One of the big shifts I think we will see over the next 5–10 years is a reduction in our reliance on helium in the world of gas chromatography. I've been having a lot of trouble sourcing helium and when it is available, the costs are increasing exponentially each year. I would love to see a shift to more sustainable approaches to gas chromatography, involving the use of different carrier gases that can be generated in the laboratory. Luckily, gas generators have come a long way and can provide reliable, clean, and high flow rates required to use them in chromatography. I personally don't think I'll ever purchase another GC instrument without the capability for hydrogen carrier gas use and a hydrogen generator!

Controversial opinion? Optimization is a really important tool in chemical analysis. But – one has to know when "good enough" is sufficient. Sometimes we have to sacrifice the use of fully optimal settings to make our lives easier and be more productive. That might sound like bad science, but it is really important in a lot of the work I do because we typically need to deal with batch analysis and high throughput data processing. Sometimes we have to accept that "good enough" is actually synonymous with "fit for purpose," a term that I tend to much prefer! I don't think everyone will agree with me on this, and I know it can be a point of contention with reviewers of manuscripts when they are viewing a single study in isolation from the bigger picture of a large research platform.

Secret to success? I had a few amazing mentors who taught me several really important lessons. First, they taught me to work with a sense of urgency. This has served me well in my role since I feel that, as faculty, we are often pulled in so many directions at once. Learning to focus on which direction merits urgency has been extremely helpful in my career. Second, they taught me to always treat important things as if they are important. This has really helped me to manage team projects and interpersonal relationships in my career. Lastly, they taught me to always keep an open mind when it comes to connections.

Bob Pirok

Assistant Professor at the University of Amsterdam, The Netherlands

Fears? That we forget the past. I am someone who always looks ahead, but when it comes to science, I think we – including myself – must be more careful that we do not lose touch with everything the scientists before us have published in the literature.

Advice? Follow your own path. Take note of what others say, but also reflect and verify your own personal view.

Missions? To continue developing tools that allow everyone to use the full potential of state-of-the-art separation technology. It amazes me how we are all developing the next best technology whereas almost no one can use what we have right now. Modern separation technology, especially multi-dimensional, has the capabilities to crack many analytical problems in public and private labs. It is unacceptable that you rarely see this stuff applied in routine environments. We must do better.

Georg Ramer
University Assistant, Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria

Secret to success? I wasn't that good at chemistry during my undergrad – I lit my hair on fire in my first analytical chemistry lab course!

In the Austrian university system, switching from chemistry to another undergrad curriculum would have meant losing most of my already accrued credits, therefore I had decided to finish as quickly as possible and move on to something else.

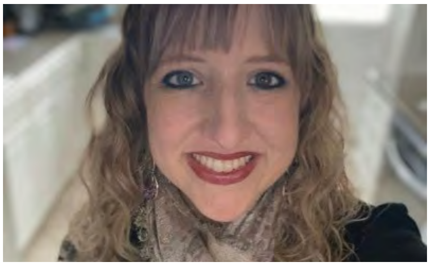
When I started looking for a thesis project I found a group in the chemistry department who were using all the things that were hobbies to me for their actual research.

The group lead, Bernhard Lendl, offered me a project based on my enthusiasm alone. In his group, I was able to take on projects I found interesting, to spend long evenings coding or tinkering with valves and pumps and turning data into pretty plots. Instead of switching to a different field or dropping out of academia I ended up going for a PhD in analytical chemistry.

Evelyn Rampler
Group leader, Department of Analytical Chemistry, Faculty of Chemistry, University of Vienna, Austria

Challenges? The future of analytical chemistry lies in innovation and cooperation! As we continuously face new challenges to separate, identify, and quantify matter, improved instruments and workflows are the foundation for novel discoveries to answer questions in all fields of science. Science is becoming increasingly complex, so the days of the single genius scientist solving mysteries all by herself/himself are over. I am convinced that we need to cooperate but also compare and combine diverse approaches to lay the bases for innovation and research breakthroughs in all scientific fields.

Advice? I can recommend my 3P strategy developed on the basis of discussions with our University of Vienna Women in Chemistry (WoChem) network. Passion: go for an inspirational and supporting research environment. Persistence: don't give up – every challenge is a chance for change, and if some obstacles are too big to handle alone, get help and stay motivated (return to your supportive environment). Perspective: have your goals and role models – don't forget to go for a healthy work-life balance (saying no is an option and often essential) and stay open to adapt your goals on the way.



Ashley Ross

Research Assistant Professor and Director of Instrumentation, Proteomics Center of Excellence, Northwestern University, USA

Biggest challenge? As we learn more and more about the brain and other biological systems, we realize that we have a huge issue when it comes to specificity with electrochemistry. We are really good at looking at a few analytes at a time in very controlled experiments; however, measuring in tissue is not a nicely controlled in vitro experiment. There are likely many other neurochemicals that are signaling that haven't even been discovered yet and that presents a real challenge for us electrochemists who are developing methods to measure biological signaling.

Advice? I love to tell those who aspire to do research: "Do not be afraid to take risks." It is so tempting as a young faculty member to play it safe and do the science that you are comfortable with, especially because of all the pressures we are under to get tenure, be successful, and so on. Of course, it's smart to be strategic in your early career, but it's also important to push the boundaries a bit with your research. Some of the best projects going on in my lab at the moment are projects that I would have never dreamed we would be doing a few years ago. Sometimes it's necessary to get out of your comfort zone and go for it. I have found that that creates amazing opportunities for collaboration across disciplines and raises the overall impact of your work.

Laura Sanchez

Associate Professor, Department of Chemistry & Biochemistry, University of California, USA

Predictions? I hope our ability to annotate known unknowns in imaging mass spectrometry datasets increases with expanded instrument capabilities. It will also be exciting to see the development of subcellular imaging techniques for measuring protonated molecules.

Secret to success? Both my advisors valued collaborative science during my training and, with that in mind, I am most excited to continue exploring the boundaries of bioanalytical chemistry. Interdisciplinary collaborative research has been central to my lab's ability to take risks. I would also like to credit the brave students who joined a new professor's lab – without their hard work and dedication, I would not be where I am today. Thank you, Alanna Condren, Jess Little, Katherine Zink, and Melissa Galey.

Advice? Don't be afraid to fail and take risks.

Mission? To help ensure that science continues to be a more inclusive field.

Ali Salehi-Reyhani

Lecturer, Faculty of Medicine, Department of Surgery & Cancer, Imperial College London, UK

Challenges? Ultimately, I think the biggest challenge we face is the public perception of science, which should lead, one would hope, to the public support of science. Despite having come through a global pandemic on the back of biomedical science, the public perception of science seems more strained than ever. We might feel a little removed from the public but, as the field develops and as we translate instrumentation and techniques out of our labs into the clinic or the home, we will inevitably be faced squarely with public attitudes and perceptions.

Pierre-Hugues Stefanuto
Lead Scientist and Lecturer, Molecular System Organic Biological Analytical Chemistry Group, University of Liège, Belgium

Mission? On the research side, I want to demonstrate how exhaled breath analysis could change the lives of patients and help us to evolve towards personalized medicine. I aim to tackle this question by developing multi-omics approaches focusing on identifying the origin of small molecules. On the education side, I want to continue to promote analytical science and to make the knowledge available to everyone. With the Multidimensional Chromatography Workshop team, we demonstrate every year that access to scientific events should not be about money but about the passion to share the knowledge.

Predictions? The rise of data! I am really curious about how far we will go with the modeling tools for method development, prediction, and data processing. All analytical scientists must be prepared to master the data side of the field. I believe that we have to prepare ourselves and the next generation to be comfortable discussing processing, statistical tools, coding, and more.

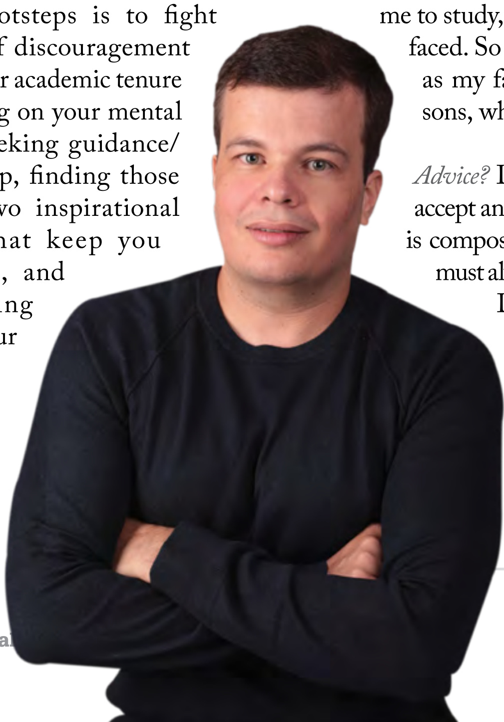
Controversial opinion? A lot of people believe that separation science will disappear with the rise of always more powerful mass spectrometry. In my opinion, chromatography will always have a seat at the table.

Dream dinner party? I am a huge science enthusiast, but I'd have to leave work behind and invite Philippe Gilbert and Wout van Aert, my two cycling heroes.

Candice Z. Ulmer
Chemistry Branch Chief, Eastern Laboratory, US Department of Agriculture, Food Safety and Inspection Service, USA

Secret to success? I credit most of my success in the early part of my career to my involvement in high school STEM outreach programs, participation in mass spectrometry-related undergraduate research, and long-lasting mentorship opportunities through organizations like the South Carolina Alliance for Minority Participation (SCAMP), the McNair Scholars Program, and the McKnight Doctoral Fellowship Program.

Advice? My advice for someone following in my footsteps is to fight feelings of discouragement during your academic tenure by focusing on your mental health, seeking guidance/mentorship, finding those one or two inspirational quotes that keep you motivated, and never losing sight of your end-goal.



Boniek Gontijo Vaz
Professor, Chemistry Institute, Federal University of Goiás, Brazil

Secret to success? I came from a small city in Brazil's countryside and grew up on a small farm with my family, where I always helped my dad with farmers' duties, as well as studying. At that time, we didn't have electricity on the farm, so I didn't have access to a TV or a computer. I think "without the distractions," I turned my attention to the nature surrounding me. I am very curious about natural things. My parents sometimes helped me with some intriguing questions, but sometimes they could not. So, through books, I used "travel" to different worlds and find answers. My parents always encouraged me to study, despite the challenges we faced. So I credit my parents as well as my family – my wife and my sons, who have been my anchor.

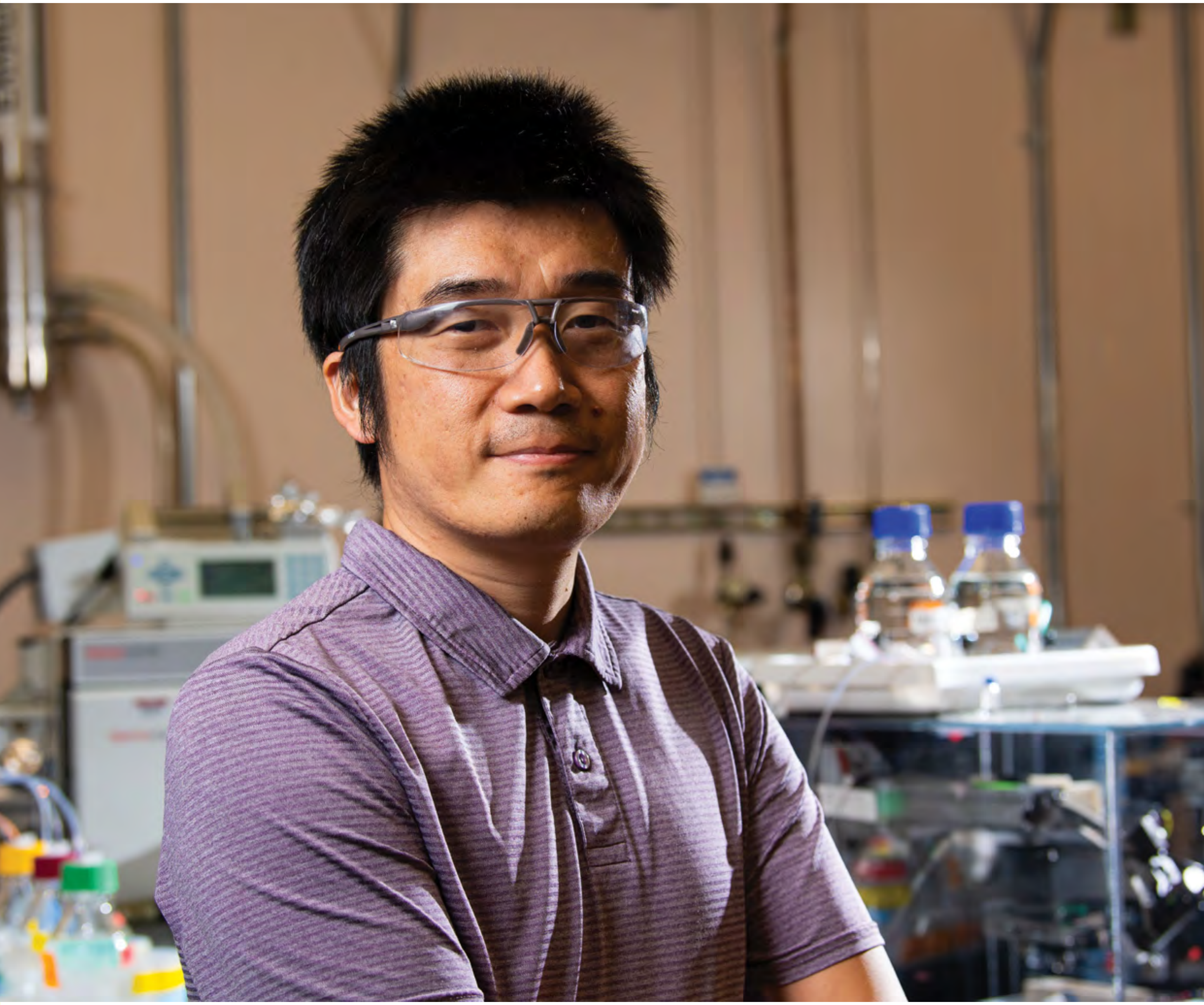
Advice? Don't fear failure; instead, accept and grow from them. Science is composed mostly of failures. We must always keep going and trying. Dedication and consistency are the way. Dream and maintain a deep desire for your goal to find persistence and give you the energy and focus to keep trying to reach your goals. Never give up.

Elena Dominguez Vega
Assistant Professor, Center for Proteomics and Metabolomics, Leiden University Medical Center, The Netherlands

Predictions? The biopharmaceutical industry is betting on gene therapy products. Analytics for their characterization are still in their infancy and many questions are still open in regards to their structure and composition. I can foresee many analytical groups making great contributions in technology development in this area.

Secret to success? Working on a hot topic like biopharmaceuticals gave me a lot of visibility and also opportunities for collaboration. But most importantly, the support of many people that I have worked with over the years, from my early times during my PhD to the people in my own group. They all helped me grow into the analytical scientist I am today, while still keeping a smile on my face.

Advice? Don't be afraid. Enjoy your work and the people that you work with. If things do not turn out as you expected there will always be alternatives. Working with anxiety, fear, and stress is not going to provide you with a better outcome.



Ying Zhu
Senior Research Scientist, Pacific Northwest National Laboratory, USA

Fears? I worry people put too much emphasis on data science or artificial intelligence that attempts to rescue unreliable or noisy data. Though data science has proved to be critical, as analytical chemists, we should always focus on delivering the most accurate, precise, and reliable measurement data.

Secret to success? In the early part of my career, I have been extremely fortunate to work in five different academic laboratories. These experiences allowed me to gain combined expertise, including microfluidic engineering, robotic automation, chemical biology, proteomics, and liquid chromatography-mass spectrometry.

Advice? Everyone has his/her own path to success. My suggestion is to follow your passion and be brave in the face of change. Even if you feel very comfortable staying in one lab or location, you should try to join a different lab in a different country; the diverse academic and cultural background will benefit your whole life.

APPLICATION SPOTLIGHT:

Sync into your Chardonnay

What, exactly, is the difference between a buttery Chardonnay and a traditional one? Finding the analytes responsible for the change in flavor can help producers monitor the quality of production, catching concerns before they become issues. What used to be tedious busy-work of comparing data set to data set can be sped up by using a statistical analysis tool such as the new ChromaTOF® Sync.

Spend more time looking at your data, not through it.

READ MORE AT

info.leco.com/blog/sync-into-your-chardonnay-with-the-pegasus-bt

Core Topic
Mass Spec

Sniffing out a test for Parkinson's. A few years ago we reported on Joy Milne's unusual gift: her ability to smell Parkinson's disease. Perdita Barran set out to isolate the molecules that make up the distinctive odor. She's done that and more! Barran and her University of Manchester, UK, colleagues found that there are lipids of high molecular weight that are substantially more active in people with Parkinson's, and then developed a paper-spray-ionization-ion-mobility-MS-based diagnostic test, which can be performed in as little as three minutes. "We are tremendously excited by these results which take us closer to making a diagnostic test for PD that could be used in the clinic," said Barran.

Introducing the Omnitrap. When it comes to mass spec innovation, we often hear about sensitivity gains and miniaturization – but what about consolidation? The Omnitrap is the first attempt to integrate the entire fragmentation toolbox into a single unit, while also alleviating limitations for processing ions in the gas phase. Dimitris Papanastasiou, Roman Zubarev, and the rest of the team at Fasmatech – plus collaborators at Thermo Fisher Scientific, including Orbitrap inventor Alexander Makarov – have published their latest developments.

The authors hope the Omnitrap will open doors in biomolecule characterization by top-down MS. And based on some of the #TeamMassSpec chatter, it seems a number of groups are looking forward to testing out the new instrument later in the year.

Our oxidation aura. Many of us spend most of our time indoors, in enclosed spaces, where we are exposed to all sorts of chemicals. Outside, hydroxyl (OH) radicals, formed when UV light from the sun interacts with ozone and water vapor, are largely responsible for "cleaning" the air. But what about indoors? Should we be worried? It turns out that we humans generate our own oxidation field and change the indoor air chemistry around ourselves – according to a study involving proton-transfer-reaction-MS and fast GC-MS systems.

But we can't rest on our auras: "We need to rethink indoor chemistry in occupied spaces because the oxidation field we create will transform many of the chemicals in our immediate vicinity," said project leader Jonathan Williams. The press release points out that oxidation processes can lead to the generation of respiratory irritants and small particles in the immediate vicinity of the respiratory tract, which can have adverse effects especially in children and the infirm.

IN OTHER NEWS

Researchers from Uppsala University, Sweden, develop "direct infusion probe" for rapid metabolomics of low-volume samples.

How soft is secondary electrospray ionization (SESI)? Softer than electrospray ionization, say Renato Zenobi and colleagues; but proper soft tuning of instrument is essential to fully benefit from SESI.

Max Planck Institute researchers present a cryogenic MS protocol with ability to detect peptides in attomole dilution range from ice films.

Karen Butler and Erin Baker describe high-throughput drift-tube ion-mobility spectrometry coupled with MS screening method for opioid profiling.

Microfluidic chip combines microdialysis and MS for in vivo monitoring of nanomedicine pharmacokinetics in real time.

PTR3: The Innovator Behind the Innovation

Catching up with PTR3 inventor Martin Breitenlechner

In 2020, Ionicon's PTR3-ToF 10K, a high-performance PTR-TOF for detecting highly oxygenated organic molecules, was featured in The Analytical Scientist's Innovation Awards. The fundamental invention behind PTR3 is the decoupling of ion-molecule reaction chemistry from the axial transport of reagent and analyte ions, increasing reaction time and boosting instrument sensitivity.

PTR3 was the brainchild of Martin Breitenlechner, who was working as a postdoctoral researcher at University of Innsbruck when inspiration struck. He patented the underlying technology behind PTR3 – a multiphase-multipole device to heat ions homogeneously. Ionicon was soon spun out of the University of Innsbruck and, as the leading PTR-MS manufacturer at the time, the company exclusively licensed and commercialized the technology.

We caught up with Breitenlechner, now a researcher at the USA's National Oceanic and Atmospheric Administration, to find out what it takes to come with a new analytical instrument.

Did you always want to be an "inventor?"

I always wanted to know how and why things work, so science became my passion – I wanted to be a scientist more than an inventor. But, because observation is the foundation of scientific discovery, I became an inventor incidentally by developing new scientific instruments and trying to contribute to the advancement of atmospheric science.

Do you think your physics background gives you a unique perspective?

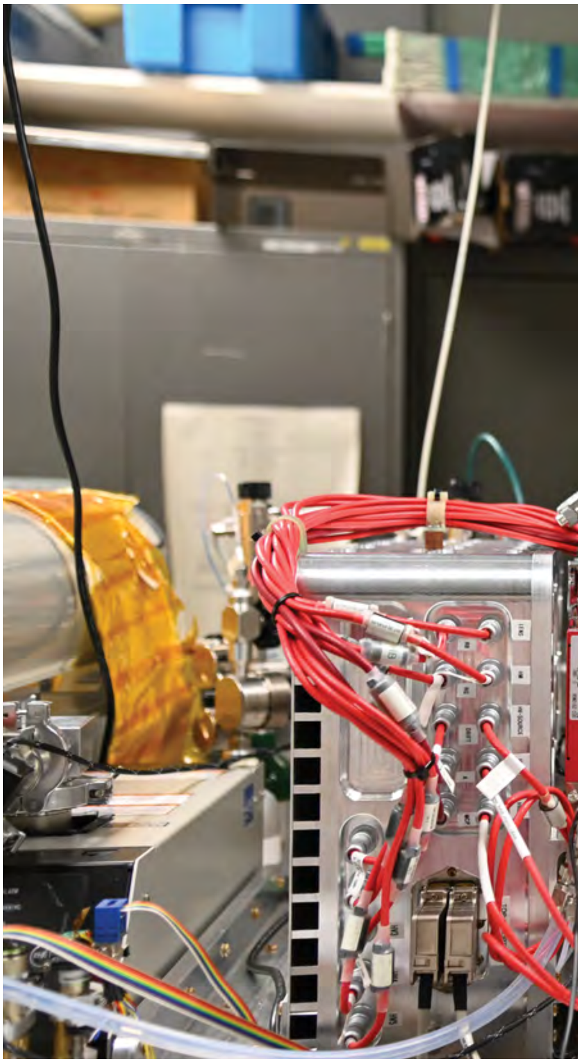
It's not unique in the sense that most people working in our field of atmospheric science are either physicists with some knowledge of chemistry or chemists with an understanding of physics. Mass spectrometry is an interesting hybrid of disciplines – the workings of a mass spectrometer are a physics problem, its application is chemistry, and the ion chemistry in the ionization process is in between the two. It's a really interesting field.

How did you get involved in the development of PTR3?

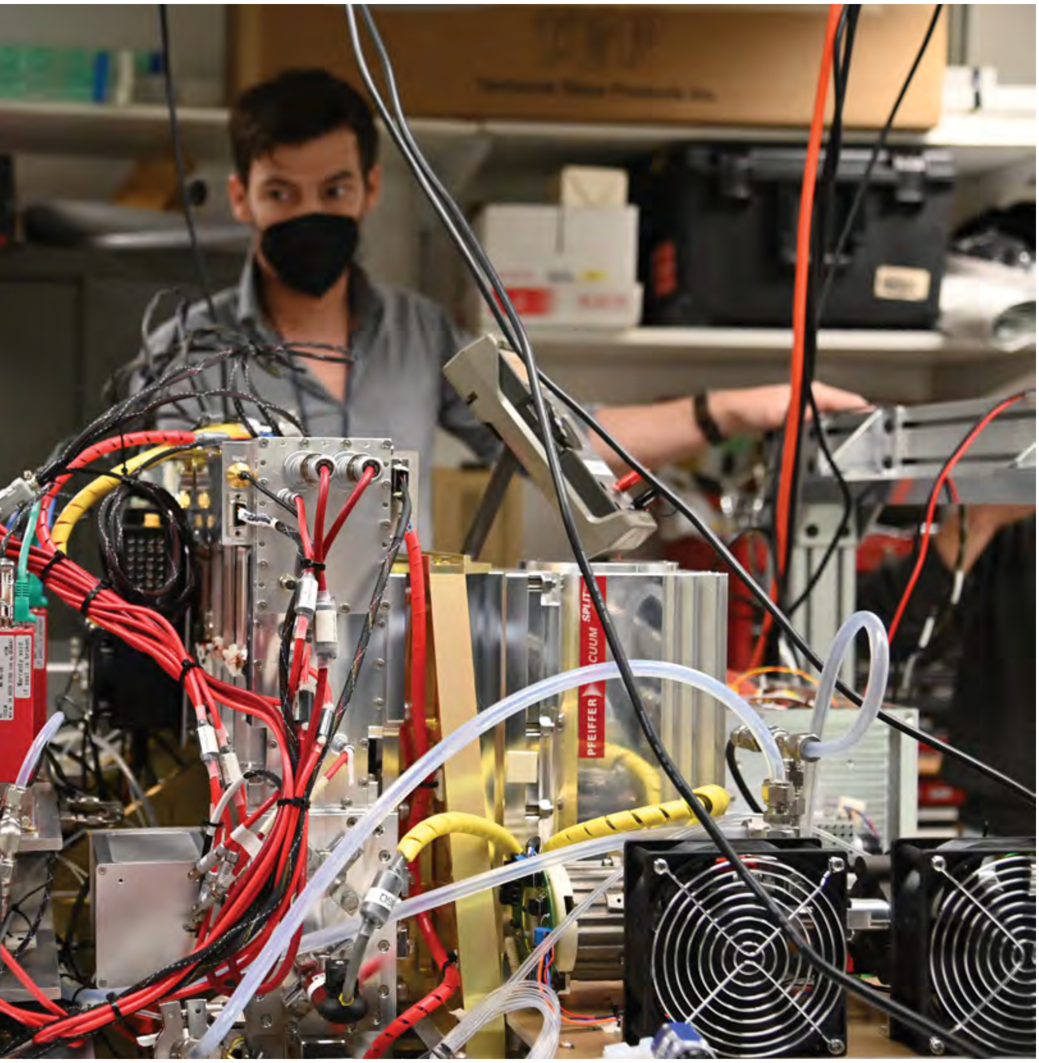
PTR-MS (proton transfer reaction mass spectrometry) is a well-established technology for observing gas-phase organic molecules in complex samples such as ambient air. It was developed in the mid-1990s by scientists at the University of Innsbruck, Austria, in whose research group I happened to do my PhD. But these instruments were not sensitive enough to apply PTR-MS to atmospheric science – they could not detect many organic compounds in the atmosphere – so I became interested in improving existing methods. One day, I pitched a new ion source design to my PhD advisor, hoping we could increase the sensitivity by an order of magnitude – but we only achieved a factor of two, not really a big enough step forward to justify the increased complexity. I came to the realization that a radically new design of the reaction chamber between the ion source and the mass spectrometer was necessary to make a significant step forward.

Did you have a "eureka" moment?

Absolutely. I was simulating various geometries and concepts of reaction



chambers. In PTR-MS, it's vital that ions experience a homogeneous electric field during their journey through the reaction chamber. That is usually achieved by applying a voltage gradient over a stacked ring electrode configuration, with the caveat that ions move through the chamber very quickly, limiting the reaction time and therefore the sensitivity. One of the first ideas was to generate a cylindrical geometry surrounded by a double-helix ion RF ion guide. It almost worked; ions moved through the chamber 100 times slower,



"I always wanted to know how and why things work, so science became my passion – I wanted to be a scientist more than an inventor."

thereby increasing sensitivity. However, though the electric field was spatially homogeneous, it was not temporally so; it oscillated between zero and a maximum value, as in any two-phase ion guide. The eureka moment was the realization that a three-phase tripole had the desired properties – it generates an electric field vector in its center that is constant in magnitude. That was the key to the development of the PTR3 and also the origin of its name.

What gets you out of bed in the morning?

I work at the Chemical Sciences Laboratory in the National Oceanic and Atmospheric Administration (NOAA) in Boulder, Colorado. NOAA is leading a multi-year research project to advance our understanding of processes in the stratosphere that impact the climate system. Chemical processes in the stratosphere are inherently difficult to study, because the concentrations of trace gases involved are minute. However, the sensitivities of chemical ionization mass spectrometers have greatly improved over the last decade to the point where we can now increase our understanding of stratospheric chemistry by deploying a chemical ionization mass spectrometer on board a high-altitude research aircraft. At NOAA, we modified an off-the-shelf instrument for that mission so that it could be operated completely autonomously onboard NASA's WB-57 aircraft. After successful technical test flights earlier this year, we are currently preparing the instrument for its first science mission, scheduled for February 2023. We are very excited; it is without a doubt the most exciting project I've been involved in during my career.

What is the biggest challenge in your field today?

Today, the most sensitive instruments already have detection limits in the parts per quadrillion range, which is close to being low enough to detect anything that can – from a kinetic point of view – be relevant to the climate system. So I think, in atmospheric science, we will see a shift in focus away from new developments that further improve sensitivity and toward improvements in instruments' analytical capabilities.

Faster HPLC – Without the Downtime

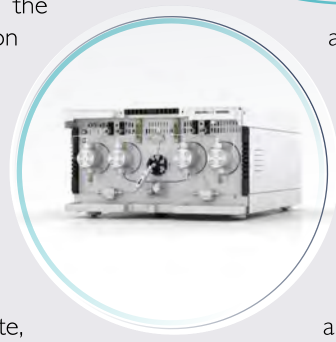
How KNAUER's new pump and liquid handler for the AZURA system help bridge the gap between classic HPLC systems and the demand for fast, reproducible high-resolution methods – especially in the biopharma industry.

By Christian Schmidt, Product Manager, KNAUER

Over the past decade, there has been a steady trend towards faster and higher resolution HPLC methods – but that also means higher operating pressures. Here, improved stationary phase materials combined with smaller particle sizes and column diameters have helped. In addition, to achieve the separation efficiency required with significantly smaller peak volumes, we've seen optimization of the tubing and other system components in the liquid path. However, optimizing liquid paths in this specialized way isn't possible with most conventional HPLC systems. The major challenge is getting the system to operate reliably and reproducibly at ultra-high pressures – without frequent maintenance downtime.

To meet the challenge, KNAUER has launched a range of (U)HPLC pumps and a new liquid handler for high-throughput applications – the LH 8.1. These innovations overcome the challenges of pumping LC solvents at ultra-high pressure and analytical flow rates, bridging an important gap between classic HPLC systems and the demand for faster, high-resolution methods.

Our aim in developing the P 8.1L pump was to deliver high-end performance alongside robustness and reliability. We also wanted to improve the user experience through greater automation. For example, the pump determines the compressibility of the solvent in real time, which means the operator does not need to enter the value manually. With the liquid handler, even complex chromatography tasks can be automated – and I should also highlight the loss-free sample feed and high injection precision. Together with the automatic purging function of the pump, seamless switching between different methods is possible without user intervention.



The overall result? Outstanding retention time reproducibility – regardless of the flow rate, back pressure, and eluent type used. This feat is achieved thanks to adaptive pulsation compensation, the aforementioned eluent compressibility monitoring, and variable piston stroke. The pump also features a highly efficient microfluidic mixer, which increases system sensitivity by reducing detector noise caused by compositional fluctuations – especially when using trifluoroacetic acid as an ion-pairing agent for peptide and protein separations. Finally, the outstanding flow-pressure-footprint of the pump gives research laboratories the freedom to choose from any type of modern stationary phase technology – opening up new possibilities for method development.

Tackling biopharma complexity

The fastest growth area for HPLC and LC-MS is in the biopharmaceutical industry, which is itself blossoming. The increasing complexity of biopharmaceutical modalities – from oligonucleotides to intact proteins, and more – means developers and manufacturers are increasingly turning to LC-MS/MS as a characterization tool. This need coincides with another trend: increasing demand to reduce instrument operational complexity and simplifying sample preparation through intelligent automation – two key features KNAUER is targeting with new products.

Importantly, our products are suitable for use across many stages of pharmaceutical development and production; once methods incorporating the new pumps and liquid handlers have been finalized and validated in the development stage, they can be transferred and used for quality control in the manufacturing laboratory. In particular, we see benefits for the identification and quantification of active pharmaceutical ingredients, their impurities and degradation products, as well as characterization of the dissolution properties of solid dosage forms and pharmaceutical formulations.

In short, the AZURA system – the new pump and liquid handler are available now – checks three essential boxes for the evolving biopharma industry: reduced user intervention, increased reproducibility, and improved laboratory efficiency.

A new truffle in town? Truffles: a scarce delicacy with an unusual taste and even more distinctive smell. So, what properties give the truffle its unique odor? Researchers from Laval University, Canada, investigated *Tuber canaliculatum* – also known as the North American Appalachian truffle – using headspace solid-phase microextraction paired with gas chromatography-mass spectrometry to identify the chemical fingerprint culpable for its aroma. Results showed 30 different compounds, including 2,4-dithiapentane, the main offender of the classic truffle oil scent. However, six compounds were unique to *Tuber canaliculatum*. The authors highlighted that this study may prompt further research into the species, in the hope that this North American gem will be commercialized and eventually share the same celebratory status as its fellow European cousins.

Deep breath. Exhaled breath analysis – less intrusive than blood or urine sampling – shows significant promise for disease diagnosis. But it has one problem: a distinct lack of standardized sampling and analysis procedures. A recent study examined the performance of two different comprehensive two-dimensional gas chromatography coupled to mass spectrometry platforms in different laboratories. Following the "Peppermint Initiative" – aiming to establish standards for breath analysis – guidelines, the participants were given a peppermint capsule, while the researchers followed a standardized workflow to collect exhaled breath samples at certain time points, monitoring selected peppermint metabolites. Both platforms enabled the longitudinal tracking of the peppermint oil metabolites in exhaled breath, and the increased sensitivity of comprehensive two-dimensional gas chromatography enabled the monitoring of 10 target compounds over a 6.5 hour period.

A piece of the neuron puzzle? The evolutionary history of neurons has long puzzled scientists because their genetic and psychological properties remain largely ambiguous. Wanting to explore neuron evolution, scientists in Japan used LC-MS/MS to analyze short peptides belonging to different basal metazoans. Twenty-eight of these short peptides were extracted from sponges, comb jellyfish and cnidarians and their amino acid sequence translated. Results revealed some shared short neuropeptides but most significantly, both neurons showed similar proteins crucial for neuronal function. "We already know that cnidarian peptide-expressing neurons are homologous to those seen in more complex animals," said Hiroshi Watanabe, one of the authors of the study in the press release. "Now, comb jelly neurons have also been found to have a similar 'genetic signature'." This suggests that these neurons share the same evolutionary origin – as such, it's likely that neurons only evolved once.

IN OTHER NEWS

Thin-layer chromatography method developed to improve size- and shape-selective separation of semiconductor nanoparticles known as quantum dots.

University of Texas at Arlington electrical engineering researcher, Yuze "Alice" Sun, receives $550,000 National Science Foundation (NSF) grant to develop portable, wearable chromatography device for rapid gas analysis that could detect illness immediately.

Gas chromatography-mass spectrometry reveals chiral monoterpene emission in plants fluctuates differently depending on stressful conditions – particularly drought.

Research using gas chromatography-mass spectrometry reveals that blending propanol with biodiesel can reduce polycyclic aromatic hydrocarbons (PAH) emissions, as well as improve engine performance and lower toxicity.

How You Can Help Your Ukrainian Colleagues

ScienceForUkraine provides information, job opportunities, and equipment to Ukrainian scientists. Here's how to get involved

Many watching Russia's invasion of Ukraine unfold have wondered how they can help. Millions of Ukrainians have been forced to flee their homes. European countries – and others too – have taken refugees in, offering the basic provisions of life, such as shelter, safety and security. But as the conflict continues, many Ukrainians are concerned about their futures. Will they be able to continue their current profession? How will they support themselves and their families? For scientists, whose livelihood relies on funding, the future is especially uncertain. But there are ways the wider scientific community can support their Ukrainian colleagues.

Modest Gertsiuk, a researcher at the Institute of Environmental Geochemistry, National Academy of Sciences of Ukraine, Kyiv, and President of the Chromatographic Society of Ukraine; Matiss Reinfelds, Association of Latvian Young Scientists; and Maciej Maryl, Institute of Literary Research of the Polish Academy of Sciences; are involved in an initiative – ScienceForUkraine – that provides information, job and collaborative opportunities, and equipment to Ukrainian scientists. Here, Gertsiuk, Reinfelds and Maryl explain how the war is likely to impact scientists in Ukraine over the long term, and how you can make a difference.

What was your first reaction to news of the invasion?

Gertsiuk: It was shocking news. Although the possibility had been discussed in the media since the war began in 2014, it was hard to believe that a direct invasion on such a scale would take place. But it happened. Sirens sounded in Kyiv and other cities warning of an air attack. People hid in bomb shelters – it was impossible to predict where the missile would hit. We heard loud cannonade and explosions in Kyiv as Russian troops were stationed in the suburban towns of Irpin, Bucha, and others in the immediate vicinity of Kyiv. A significant number of people working in Kyiv and, in particular, in scientific institutes of the National Academy of Sciences and and higher educational institutions lived in these suburbs.

How has the Russian invasion affected analytical scientists in Ukraine?

Gertsiuk: Many people from Kyiv and other towns and villages attacked by Russian troops have been forced to move to safer cities in Ukraine or migrate abroad. Territories near to the war zone are constantly being fired on, which makes it impossible to carry out experimental work. And the activities of scientific institutions and scientists in occupied territories has stopped entirely.

Personally, I went to the west of Ukraine, and then to Germany, then to Slovenia for the 26th International Symposium on Separation Sciences, and back to Ukraine. Analytical scientists, like other scientists, are mostly working remotely. This has inevitably led to a sharp decrease in the number of experimental studies being published. With the liberation of the territories, work in scientific institutions will continue and experimental research will once again become possible. But as we speak, in all Ukrainian territories, the threat of rocket attacks – with sirens often sounding – remains.

What lasting impact will the war have for scientists in Ukraine?

Gertsiuk: In addition to the immediate problems associated with displacement, there has been a significant reduction in the financing of scientific institutions, leading to a decrease in salaries and potential job losses for scientists. In particular, experimental research is practically not being funded right now.

And that's why I believe ScienceForUkraine is very important. It is an initiative of volunteers providing information about temporary job opportunities for scholars fleeing Ukraine with a wide international reach. Over 2000 scientific groups all over the world have already joined our movement – and we hope that you will be able to open your door to Ukrainian scholars as well.

How did ScienceForUkraine begin?

Maryl: ScienceForUkraine was launched on February 26, 2022, as a rapid-response central database for collecting offers of support for the Ukrainian academic community. By introducing the #ScienceForUkraine hashtag and creating a Twitter account, @ScienceForUkraine, the aim was to disseminate the support available to the Ukrainian academic community.

How can researchers help?

Maryl: We strongly encourage funders, academic institutions, and companies to provide remote collaboration opportunities for Ukrainian scholars. Two years of the COVID-19 pandemic have taught us that research can be performed remotely, and we should think about funding such opportunities for Ukrainian colleagues. For instance, COST Action Virtual Mobility grants could be used for the purpose of data collection (see NEP4DISSENT for an example). But it's not only about financial support, it is also about providing colleagues with contacts and career development opportunities despite the raging conflict. Other examples include unlocking online

courses for Ukrainian scholars or setting up mentoring schemes. These are relatively low cost, yet very meaningful for those remaining near war zones in Ukraine (see the example of Project Fleck).

Reinfelds: Chemistry is a very instrument-based science. Laboratories could offer to run analyses free-of-charge for various samples or allow scientists from Ukraine to use their equipment during short-term visits. In an ideal scenario, we'd love to see more long-term collaboration and joint research papers or project proposals.

Often, there will be a piece of equipment that stands in the far corner of a lab practically unused – either the projects for which the device was purchased have ceased or new generations of PhD students have shifted to other devices. The equipment may be kept under the assumption that it may return to active use some day, but often this does not happen. (I can easily imagine all the dual wavelength detectors, which were replaced with DAD some years ago, sitting under HPLC tables "just in case.") Unused equipment could be extremely useful for a Ukrainian colleague!

We invite everyone who thinks they could contribute in some way to register their offer on our webpage.

Can you share any success stories?

Reinfelds: We have a lengthy Twitter thread containing a list of success stories. But these are just a relatively small selection. Many offering help don't want to sound the trumpet – and we don't push people to go public. However, we have published a detailed report on the first three months of the initiative and are working on an anonymous survey, collecting information from Ukrainian scholars who had to leave Ukraine after the invasion (1). This effort should also give us a clearer picture about the stories of displaced scholars in the future.

Reference

1. *ME Rose et al., SSRN Electronic Journal (2022). DOI:10.2139/ssrn.4139263.*

A CHANGING SOCIETY

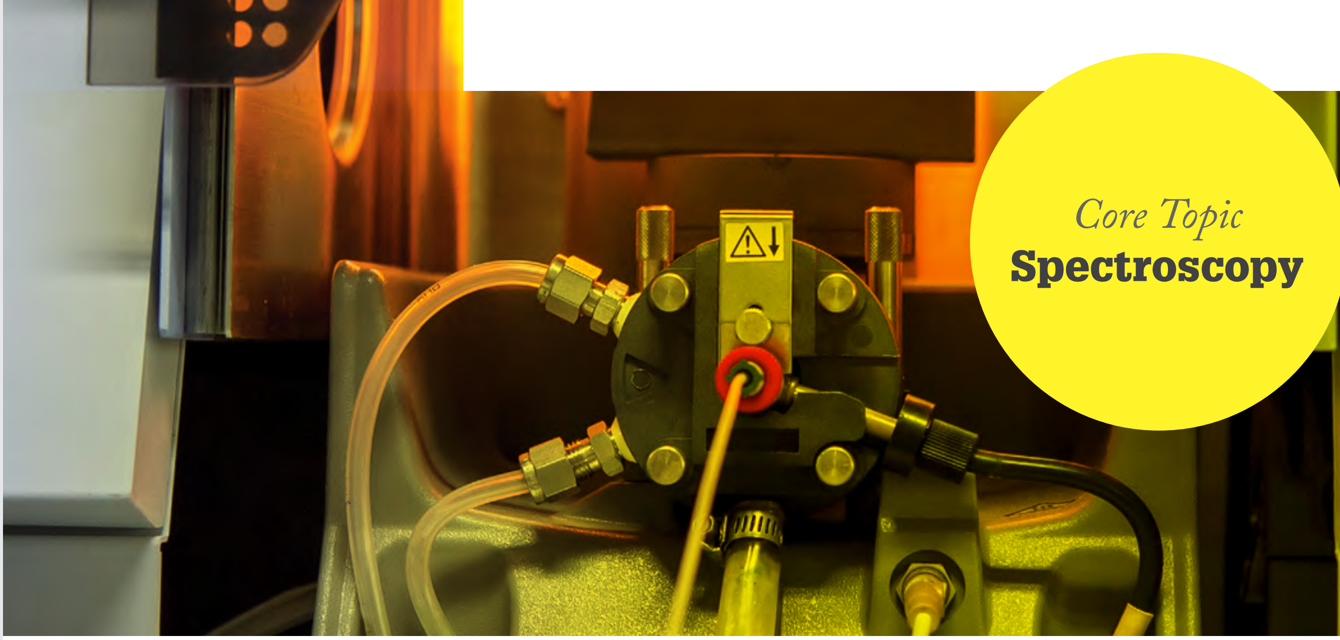
With Modest Gertsiuk

Tell us about your work with the Chromatographic Society of Ukraine...

The Chromatographic Society of Ukraine brings together both scientists and specialists who perform chromatographic research. The society goes back to the All-Union Association of Chromatographers in the former Soviet Union. After Ukraine became independent, I was tasked with uniting chromatographers in Ukraine, which is how the Chromatographic Society of Ukraine was born. We launched a scientific publication in 2001, the Journal of the Chromatographic Society, which publishes articles on basic and applied research in the field of chromatography – with a focus on the activities of scientists and research centers working in Ukraine.

Did the Russia-Ukraine war in 2014 affect the society?

Yes, we held international conferences – "Methods of Chemical Analysis" – annually in Ukrainian cities, such as Lviv, Truskavets, Sevastopol, with local branches of the Chromatographic Society taking part in the organization of these conferences. However, with the war in 2014 and the occupation of Crimea and part of Donbass, the conference venues had to change. And due to the urgency of security issues, conference topics have also changed. Conferences with names like "Chemical and Radiation Safety: Problems and Solutions" began to be held, with foreign scientists also taking part.



Core Topic
Spectroscopy

"Pimp my spec" – an upgrade for NMR spectroscopy. NMR spectroscopy is a vital method for describing the atomic structure of biomacromolecules in their native solution state – but this method suffers from low sensitivity. So, how did researchers from the University of Vienna, Austria, go about solving this problem? They used hyperpolarized water in a method dubbed "Dissolution Dynamic Nuclear Polarization" to achieve a 1,000-fold signal amplification in NMR measurements, measuring biomolecules at concentrations as low as 1 micromole/liter. In the press release, one of the co-authors, Dennis Kurzbach, compared NMR spectroscopy to an electric guitar. "If the amplifier is too weak, you will hear very little if you do not hit the strings strongly," he said. "Meaning that you need a lot of material to see an NMR signal. With the new hyperpolarization amplifier, you can now see something even at low concentration".

Drink up. Green coffee beans currently go through rigorous quality control measures with experienced analysts to determine whether the coffee is considered "special" or "traditional." However, there have recently been suggestions that testing should have limited human input for maximal consistency. As such, researchers have developed a method combining multispectral imaging with machine learning models to distinguish specialty coffee from traditional coffee. One of the four algorithms tested, dubbed "SVM," showed exceptional performance, with an accuracy of 0.96. The authors concluded that the use of multispectral imaging combined with machine learning is an effective method for screening special and traditional green coffee beans, with rapid results that do not require pretreatment or destruction of samples.

A promising breast cancer diagnosis method? Current methods of breast cancer diagnosis are time-consuming, costly and often dependent on physician experience. In search of a more reliable diagnosis method, a group of researchers combined serum Raman spectroscopy and different classification algorithms. Analyzing the serum Raman spectra of 171 invasive ductal carcinoma patients and 100 healthy volunteers, the researchers built four classification models: support vector machine (SVM), decision tree (DT), linear discriminant analysis (LDA), and Neural Network Language Model (NNLM). The LDA, SVM, and NNLM algorithms achieved 100 percent accuracy, thus demonstrating high reliability and validity in breast cancer diagnosis.

IN OTHER NEWS

Novel machine-learning tool may facilitate interpretation of X-ray photoelectron spectroscopy spectra by accurately predicting the spectrum of disordered material made of carbon, hydrogen and oxygen.

Promising liquid-liquid interface assembly method vastly improves SERS sensitivity – reducing the detection limit by 2-3 orders of magnitude compared to traditional dry-state SERS methods.

Optical spectroscopy guru Curt Marcott, Light Light Solutions, will be presenting two webinar sessions on IR and Raman database searching on 13 and 14 September.

Raman spectroscopy demonstrates high diagnostic potential for oral squamous cell carcinoma – showing high specificity and sensitivity.

Exciting Times For… Spectroscopy: with Geoff Winkett

Geoff Winkett, General Manager and Vice President of Molecular Spectroscopy at Agilent, discusses developments in molecular spectroscopy and the growth of the biopharma market

Tell me a little about your background in spectroscopy…

My background and experience are somewhat atypical for an Agilent Vice President (VP) and General Manager (GM). I have a commercial – as opposed to scientific – background; my time with Hewlett-Packard/Agilent over the past 29 years has been in various business finance functions.

I have worked all over the world – including Australia, the UK, and the US – and, after spending five years in California, I returned to Australia in 2011 to take on the role of Chief Financial Officer of Agilent's recently acquired Spectroscopy (Atomic & Molecular) and Vacuum businesses. After taking a lead role in driving the growth of the business' top and bottom lines, I was appointed GM and VP of Agilent's Molecular Spectroscopy business in November 2020.

What is the most exciting development in molecular spectroscopy today?

There are many exciting developments underway in molecular spectroscopy right now, but one area of particular interest is growth in the biopharma market. Given the amount of investment going into biologic drugs, there is a strong belief that large-molecule pharma will outweigh traditional small-molecule pharma in the years to come. This creates a significant opportunity (and challenge!) for molecular spectroscopy products to support customers in this area with their testing needs.

Molecular spectroscopy solutions based on techniques such as Fourier-transform infrared (FTIR), fluorescence, ultraviolet-visible, and Raman spectroscopy can complement other techniques such as high-performance liquid chromatography (HPLC) in multiple areas of the biopharma value chain, from early discovery all the way through to quality assurance (QA), quality control (QC), and production. Such techniques are powerful tools for application areas such as protein quantification, protein stability, oligo QA/QC, raw materials identification, and more – uses that can help customers in the molecular spectroscopy field improve time to market, reduce the cost of ownership, and ensure compliance with regulatory bodies.

Another key area of development is the role molecular spectroscopy plays in detecting and monitoring key environmental challenges, such as the consumer-led concern around microplastics. The infiltration of plastics in our environment and their impact on human health has been a hugely important topic in recent years. As a result, we've seen increased demand from customers who need to be able to identify these particles in water supplies.

We've discussed exciting developments, but what major challenges is the field facing today?

Significant challenges laboratories and analytical scientists face are data integrity, security, and compliance with regulatory authorities' requirements. These are complex, quickly evolving areas and customers need to have peace of mind when using testing equipment. As a result, we have made key investments to help our customers navigate these challenges. In fact, we recently released an updated version of the software behind our Cary 3500 UV-Vis spectrophotometer, which builds controls around signatures, access administration tools, electronic signature workflows, and audit trails into the software – a reflection of the industry's increasing data security concerns.

Any advice for an early-career spectroscopist?

Regardless of the discipline, my advice for anyone early in their career is not to restrict yourself to one area – instead, get as much experience in as many fields and disciplines as possible. I am a firm believer in backing yourself and trying something different.

In fact, I think people early in their careers should look for opportunities to gain international and cross-cultural experience. One of the best career decisions I ever made was to spend time working in different countries. Though it was extremely challenging at times, I learned so much from these experiences that I am convinced I would not be in my position today were it not for those bold moves. After all, we are operating in a global environment – these experiences are invaluable!

On a related note, focus on building your network of contacts both internally and externally. Seek out opportunities to meet and connect with other people, particularly in leadership positions. These networks will be vital not only to help equip you in your current role, but also to facilitate the advancement of your career in the future.

MORE EXCITING TIMES

Refresh your memory – what were our previous spectroscopists excited about?

Juergen Popp, Scientific Director at the Leibniz Institute of Photonic Technology, Germany

In my opinion, the latest developments in IR spectroscopy (the sister method to Raman spectroscopy) are particularly exciting. For many years, a major problem in IR spectroscopy was the lack of suitable IR excitation sources with a high photon density. This problem has since been solved with the introduction of quantum cascade lasers as highly brilliant light sources; indeed, using these lasers as an excitation source for IR spectroscopy or imaging in the spectral range from 950 to 1800 cm-1 can be seen as a significant milestone.

Jean-Francois Masson, Full Professor at the University of Montreal, Canada

I view two major fields as being exciting. The first one involves the use of spectroscopic sensors as point-of-need devices – and eventually wearable devices. Though it has been a promise of the field for the past 20 years, all the tools are now available for analytical scientists to design sensors that will fulfill this promise and help humanity.

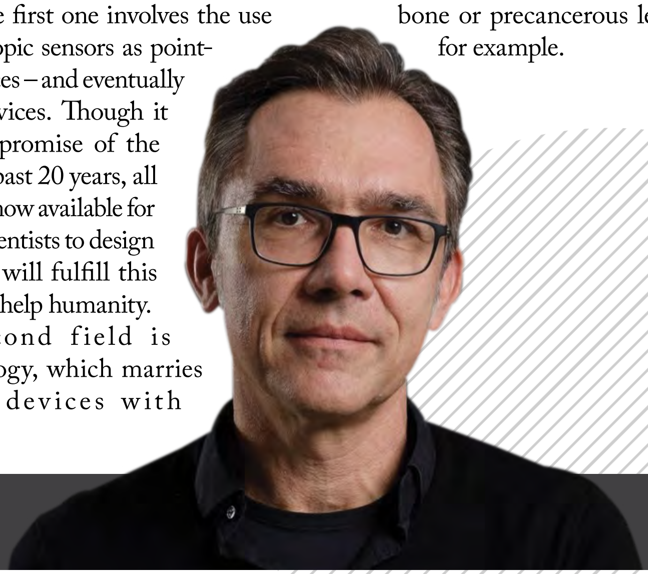
The second field is optophysiology, which marries photonic devices with the measurement of physiological parameters. I dream of the opportunity to reveal minute metabolite changes at the cellular level that will help to better understand disease progression and treatment efficacy. Designing nanosensors able to do this is what drives my current research.

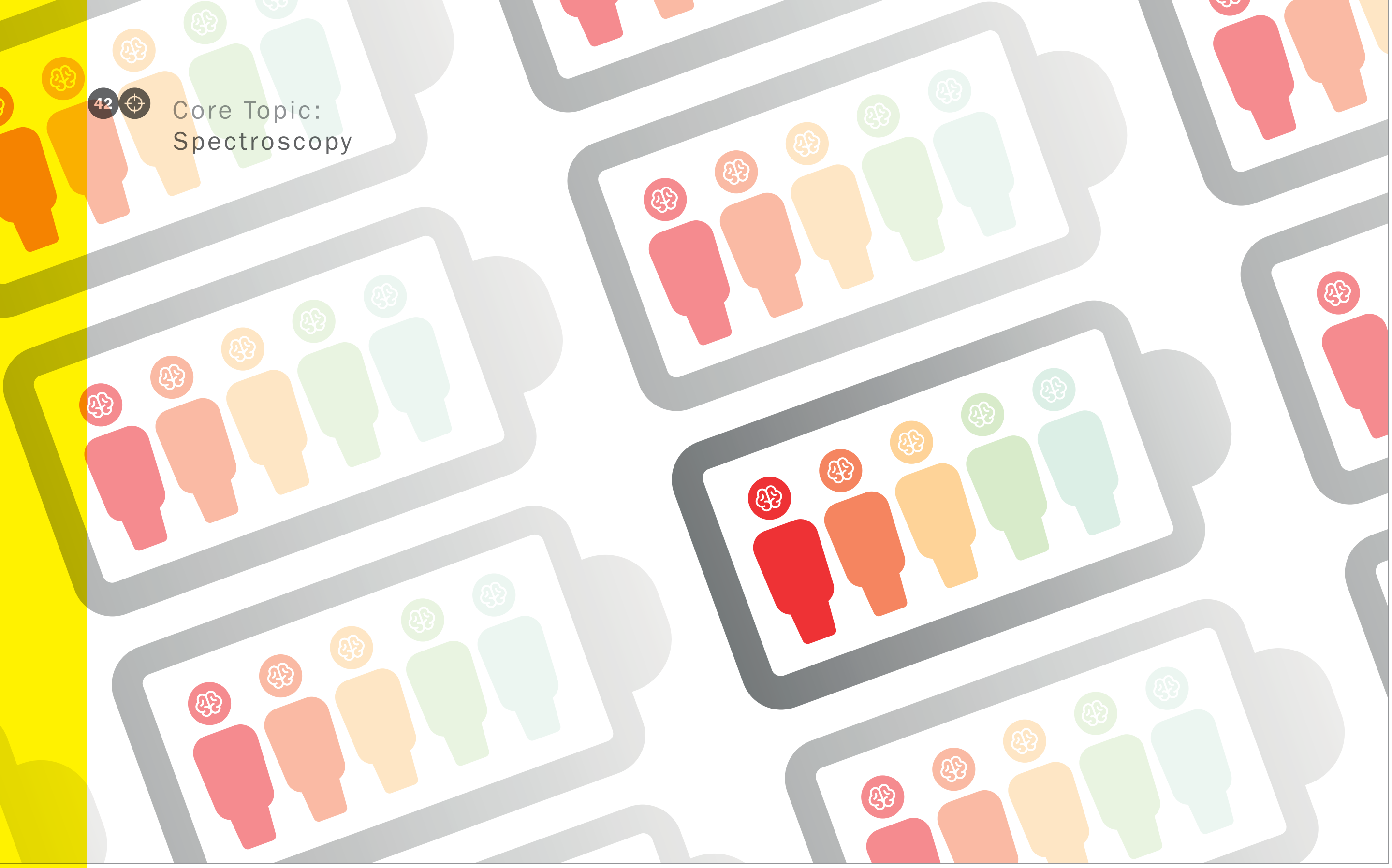
Rob Lascola, Senior Fellow Scientist at the Savannah River National Laboratory, USA

There are many choices, but I'm really impressed with spatially offset Raman spectroscopy. It's exciting because we're able to see light and make measurements in environments where you wouldn't expect to.

Karen Esmonde-White, Product Manager at the Endress+Hauser Group, USA

I would agree with Rob on this. The realization that we can do Raman spectroscopy in turbid media and in layered samples and collect spectra from buried layers has been revolutionary for Raman spectroscopy. It's especially important in the biomedical field where now you can get measurements through the skin to analyze subsurface bone or precancerous lesions, for example.





Losing (Cognitive) Control

High-demand cognitive work causes a build up of glutamate in the brain – according to real-time magnetic resonance spectroscopy analysis – which, in turn, may alter economic decision making

By Georgia Hulme

Mental fatigue has long puzzled scientists. Why do we feel it? What generates it? These questions nagged researchers from Pitié-Salpêtrière University in Paris, France, as they contemplated why machines can do cognitive tasks continuously without fatigue but the brain cannot. They hypothesized that fatigue arises from an increase in the cost of exerting cognitive control – which stems from glutamate accumulation in the brain (1).

To test this theory, two groups of participants executed either high- or low-demand cognitive tasks, interlaced with economic decisions, while researchers measured the levels of metabolites in their brains. The researchers found that, when intense cognitive work is prolonged for several hours, some potentially toxic byproducts of neural activity, such as glutamate, accumulate in the prefrontal cortex. "This alters the control over decisions, which are shifted towards low-cost actions (no effort, no wait) as cognitive fatigue emerges," explains Antonius Wiehler, co-author of the paper. Other signs of fatigue in the group performing mentally challenging tasks included pupil dilation and increased levels of glutamate in the synapses of the inferior prefrontal cortex.

In previous studies, the researchers used fMRI – but this technique could not explain why the cost of cognitive control increases over time. Instead, the team used magnetic resonance spectroscopy (MRS), which meant that they could measure brain metabolites while human subjects carried out the tasks.

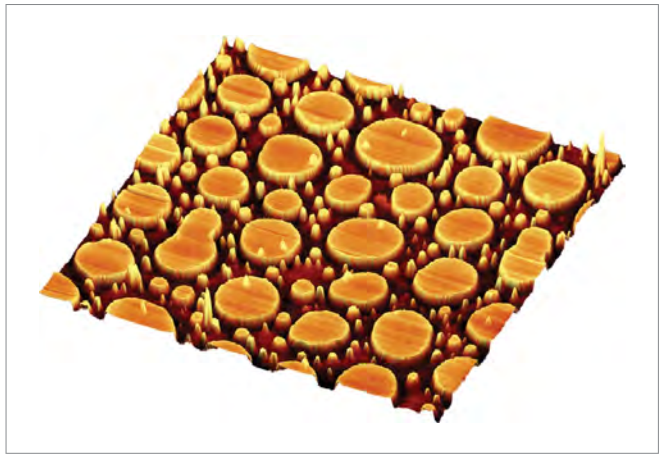
Although the study had minor limitations – such as the low spatial and temporal resolution of MRS – and the results were only correlational, they do offer an explanation as to why cognitive control is harder to mobilize after a strenuous workday. Wiehler hopes that, in the future, "prefrontal metabolites could be monitored using MRS to detect cases of severe fatigue/burnout in many different situations, such as employees after work, athletes during heavy training programs, or students during revisions before their exams."

In further studies, the researchers hope to learn why the prefrontal cortex is more susceptible to fatigue and glutamate accumulation than other brain regions. Wiehler seeks to understand how metabolite buildup could be prevented or removed from the synapses. He adds, "Going forward, we may also be exploring whether markers of fatigue are predictive of clinical outcome across diseases such as cancer or depression."

Reference

1. *A Wiehler et al., Current Biology, 32, 1 (2022). DOI: 10.1016/j.cub.2022.07.010.*

Correlative Raman Imaging of Polymeric Materials



Polymers have widely varying chemical, mechanical and optical properties. Knowledge of their morphology and composition is crucial to advancing their development and monitoring their production.

In this application note: a thin-film mixture of PMMA-SBR is investigated and its components are differentiated with Raman-AFM, a Raman-AFM-SNOM measurement of a PS-SBR-EHA mix is presented, depth-profiles of a polymer coating and an adhesive layer are shown, and the topography and chemical composition of bioinspired nanofibers are characterized with Raman-AFM.

The instrument used for all measurements was a WITec alpha300 RAS correlative Raman-AFM-SNOM microscope. This system fully integrates all three techniques in a modular architecture with a common software environment. The speed, sensitivity and resolution of the alpha300 series, along with its intuitive user interface and configurability, enables researchers to carry out challenging experiments quickly and routinely.

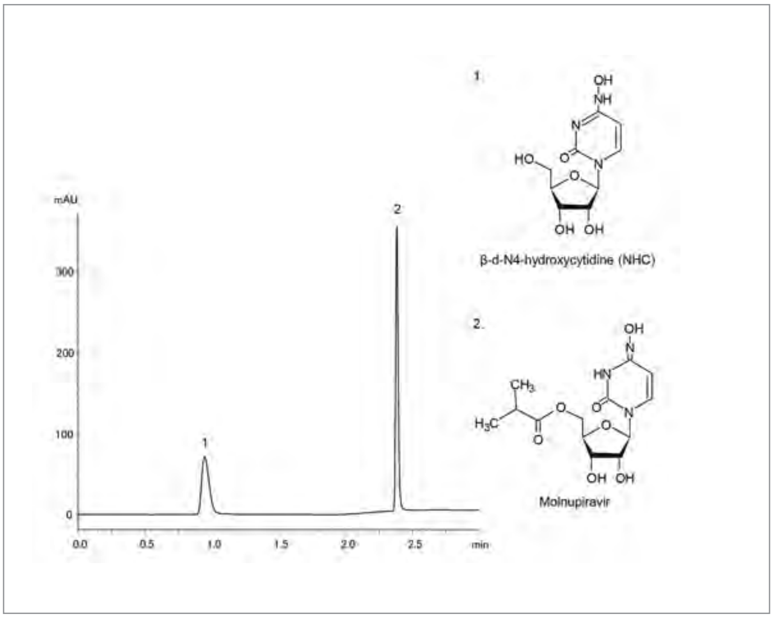
See the App Note here (PDF):
https://bit.ly/WITec_AppNote_Polymers

UHPLC Analysis of COVID-19 Agent Molnupiravir

Molnupiravir (Lagevrio®) is an antiviral medication to treat mild to medium COVID-19 infection. In fact, Molnupiravir is a prodrug of the active substrate *N*⁴-hydroxycytidine (NHC), a synthetic ribonucleoside analogue. The treatment leads to the introduction of copying errors during viral RNA replication and thus inhibits the viral reproduction.

Molnupiravir and its active agent β-d-*N*⁴-hydroxycytidine can be separated in only three minutes by using a YMC-Triart C18 UHPLC column and a MS compatible mobile phase at pH 4.3 and relatively mild temperatures of 40°C.

Full method details can be accessed here: https://ymc.eu/d/brDob



Quick separation of the prodrug molnupiravir from its more polar active agent NHC using a YMC-Triart C18 UHPLC column.

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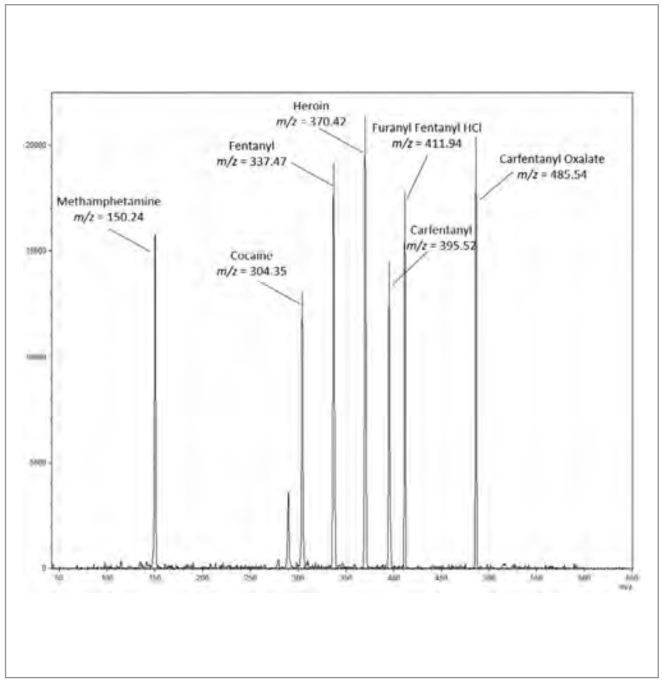
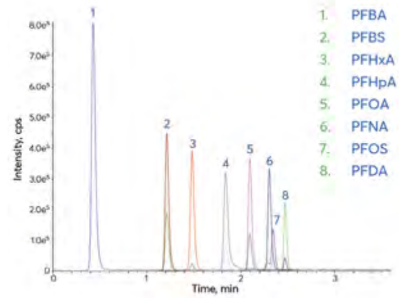


Sub-3 minutes LC-MS/MS analysis of PFAS with Avantor® ACE® HTP-MS Columns



Column: Avantor® ACE® HTP-MS
Particle Size: 2 µm
Dimensions: 10 x 2.1 mm
Mobile Phase: A: 20 mM ammonium acetate in H_2O
B: 20 mM ammonium acetate in $MeOH/H_2O$ (90:10)
Gradient:

Time (mins)	% B
0	0
0.1	25
2.1	75
2.2	100

Flow Rate: 0.5 mL/min
Injection: 0.5 µL
Temperature: 22 °C
Detection: Sciex QTRAP® 6500+ LC-MS/MS system.
Ionisation mode: ESI, negative mode
Source temperature: 450 °C
Curtain gas: 38 psig
Ionspray™ source voltage: -3500 V
Ion source gas 1: 40 psig
Ion source gas 2: 70 psig
Sample: 12 ng/mL for each analyte

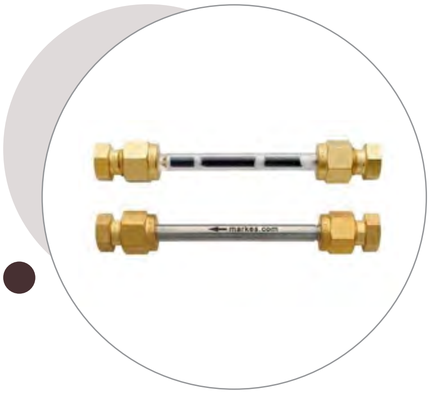
Figure 1 demonstrates the use of an Avantor® ACE® HTP-MS column for the separation of PFAS analytes. The high-efficiency particles, coupled with the low-dead volume design means that full resolution of seven of the eight analytes is readily achieved in less than 2.5 minutes on the 10 x 2.1 mm column.

Many laboratories across multiple sectors are facing increasingly high sample volumes. The specificity offered by LC-MS (LC-MS/MS or LC-HRMS) provides opportunities to simplify analysis, reduce chromatographic run time and increase throughput; however, there are challenges. Ion suppression and isobaric interferences must be addressed, so it is important to perform chromatography prior to MS detection. One option is to use very short column lengths (e.g. 10 mm), which provide sufficient chromatography for matrix removal and analyte retention, whilst achieving substantial increases in sample throughput compared to standard format LC-MS columns.

Read the full article on the product page at vwr.com

Spotlight on...

Applications



PFAS Sampling Tubes

Newly launched: a range of thermal desorption sorbent tubes for sampling up to 500 L of ambient air for analysis and detection of PFAS. With such high volumes of air available for analysis, a wider range of PFAS compounds can be identified, and low pg/m3 detection limits can be reached for analysis.
https://bit.ly/3dwvnlN

Quick Comparisons: ChromaTOF® Sync

Learn how ChromaTOF Sync can effortlessly align your data sets, making data comparison faster and more efficient. Statistical analysis tools can effortlessly highlight analytes of interest, calling out even subtle differences that have significant meaning. Read more with our Baijiu Aroma Profile app note.
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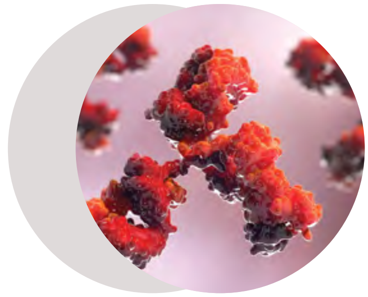
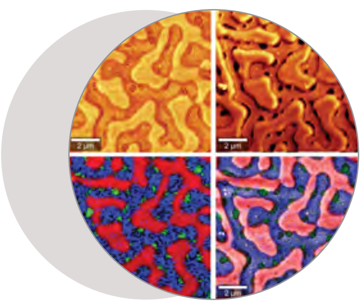


Selecting the Optimal Column for Native SEC-MS of Monoclonal Antibodies

Three different size exclusion columns were compared for their compatibility with mass spectrometry. The TSKgel UP-SW3000-LS column was superior to other columns due to its low shedding and long-lasting high ionization efficiency.
https://www.separations.eu.tosohbioscience.com/OpenPDF.aspx?path=~/File%20Library/TBG/Products%20Download/Application%20Note/an0081a-l.pdf

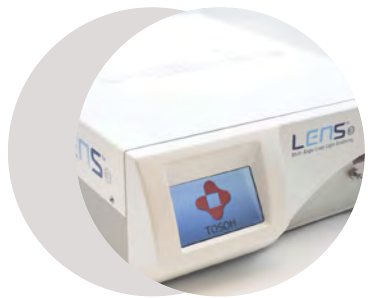


Correlative Raman Imaging of Polymeric Materials

In this app note a thin-film mixture of PMMA-SBR is investigated and its components are differentiated with Raman-AFM, a Raman-AFM-SNOM measurement of a PS-SBR-EHA mix is presented, depth-profiles of a polymer coating and an adhesive layer are shown, and the topography and chemical composition of bioinspired nanofibers are characterized with Raman-AFM.
https://bit.ly/WITec_AppNote_Polymers

Spectral Phenotyping Helps Preserve Our Food Security

This article examines how NIR spectroscopy can be used to create data models to analyze the stress of drought on maize leaves. Predictive spectral models were created that can be used to estimate the impacts of varying drought conditions on food security.
https://www.spectravista.com/?utm_medium=print&utm_source=tas&utm_campaign=oct2022



Monitoring Structural Changes in Polysaccharides

Pullulan and dextran samples were analyzed by SEC-MALS to assess their structural differences. In order to detect structural changes also in the low MW and low Rg region, the highly sensitive LenS3 MALS detector was used. The analysis revealed that both polysaccharides are linear polymers at low MW, while dextrans exhibit branching at higher MW.
https://bit.ly/3ClJlz9

Spotlight on...

Applications

Multiresidue Pesticide Analysis with the 6475 Triple Quadrupole LC/MS System

Here, we describe the development and evaluation of a comprehensive LC-MS-MS method for over 500 pesticide analyses in three food matrices (wheat, olive oil, and black tea). The work was completed using the Agilent 6475 triple quadrupole LC/MS (LC/TQ) system coupled with the Agilent 1290 Infinity II Bio LC system and MassHunter Workstation 12.0.
https://bit.ly/3T7RnT8

LC/Q-TOF Analysis and Profiling of Meats and Plant-Based Alternatives

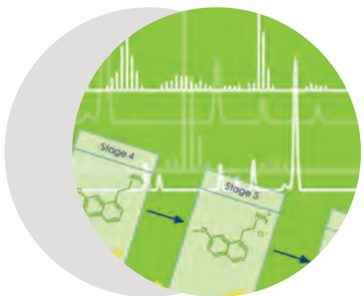
This application note describes a nontargeted profiling method to characterize chemical components of animal and plant-based foods , using a high-resolution accurate mass 6546 LC-Q/TOF. Also, various statistical tools are presented that translate accurate mass 6546 LC/Q-TOF data into more easily understandable information.
https://bit.ly/3EvVZ1k

Micromilling of uniform nanoparticles for NASA space applications.

A NASA lab's ability to develop optimized ceramic nanoparticulate materials for demanding research applications in energy storage, power generation, and other advanced application areas has been enhanced by FRITSCH micromills.
www.fritsch-us.com

Overcoming Barriers to NMR Data Processing with Browser-Based Software

Moving NMR data processing to the web browser provides unique benefits over traditional desktop software. A natural products researcher shares his experience of switching to browser-based NMR data processing with Spectrus JS and how it streamlined his workflow while also improving lab-wide practices and allowing him to report more accurate results.
https://bit.ly/3CTbFJF



Streamlining Forced Degradation Data in Development

Forced degradation studies are an essential task in pharmaceutical development. This work requires consolidating large amounts of analytical and chemical data, which is often spread across multiple teams. This application note describes how decision support software can support forced degradation research.
https://bit.ly/3ejI7wl

Using Infrared Laser Imaging (QCL) for High-Throughput Screening of Surface Contaminations

FTIR microscopy is a proven method to locate and identify unknown substances and contaminants based on their molecular vibration. This kind of analysis provides reliable, unambiguous indications of where a contamination is coming from and how to troubleshoot processes.
https://bit.ly/3enmAD6

Spotlight on... Technology

IONICON FUSION PTR: VOC Analysis Now with 4x Higher Sensitivity

The FUSION PTR revolution continues: experience a 4x higher sensitivity with our 2022 FUSION performance update! The best-in-class Next-Gen IONICON PTR-TOF technology solves your real-time VOC analysis challenge. Detection limits in the ppqV-range give new insights in atmospheric chemistry research, air quality monitoring, and climate studies.
https://www.ionicon.com/fusion

Accelerate Drug Development with the ZenoTOF 7600 System

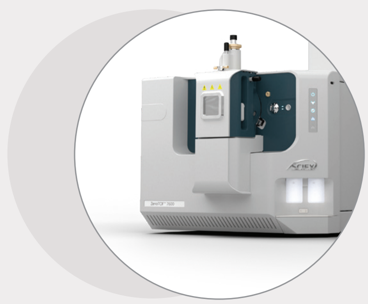
Driven by the power of electron-activated dissociation (EAD) coupled with the Zeno trap, the ZenoTOF 7600 system unlocks sensitivity gains, allowing you to uncover new information about your complex biotherapeutics with certainty in your results to make better-informed decisions, faster.
https://sciex.li/3tzaqz

Real-Time VOC Analysis for Pharmaceutical and CDMO Applications

SIFT-MS delivers high-throughput solutions that eliminate bottlenecks in development, production, and QA/QC. Learn how to increase your capacity and operational efficiency in residual solvents analysis, detergent and sterilization monitoring, and nitrosamine characterization.
https://www.events.syft.com/pharma

The SCIEX 7500 System

Enter a new era of sensitivity and LC-MS/MS innovation with the SCIEX 7500 system. GO BEYOND current limits of sensitivity, productivity targets, ruggedness and robustness challenges with the new D Jet ion guide, OptiFlow Pro ion source and integrated E Lens probe. Pioneer new discoveries with this innovation.
https://sciex.li/04yeq0



Enhance biomarker research with the ZenoTOF 7600 system

The SCIEX Z enoTOF 7 600 h igh-resolution accurate mass system unlocks sensitivity gains that reveal new, rare, or even previously undetected information on an everyday basis. Detect up to 20 times more ions in every experiment and access a spectrum of tunable fragmentation techniques to uncover new perspectives for every molecule in every experiment.
https://sciex.li/3tzaqz

On a Collision Course

Sitting Down With…
Vicki Wysocki, Professor, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio, USA

Tell us about your main line of research, surface-induced dissociation…

When I joined Graham Cooks' research group at Purdue, the group was trying to intentionally collide ions into surfaces as an additional activation method for tandem mass spectrometry. They successfully implemented the surface-induced dissociation (SID) method, but instruments of the time could only ionize and transmit small molecules (up to about 10,000 Da if ionized via fast atom bombardment). As it became possible to ionize and transmit much larger ions into mass spectrometers, my lab incorporated the surface collisions of these species into a variety of instrument types. Surface collisions, by virtue of increasing the energy in a large step, fragment large non-covalent protein complexes into structurally meaningful subcomplexes.

Though collision-induced dissociation (CID) can provide structural information, its low energy, multistep activation can also significantly restructure protein complexes. If researchers are careful and know what they are doing, they can use CID in a structurally meaningful way for non-covalent complexes, but they may also inadvertently produce misleading data. Currently, we use native mass spectrometry and SID as complementary techniques with other structural biology tools such as cryo-electron microscopy.

Why do you so frequently collaborate with experts outside your group and across different cultures?

One of the wonderful things about science is that the main things that you need to bring to the table are your willingness and ability to think and your tenacity. Bringing together people of different backgrounds leads to the greatest progress. Group members learn by working with others from different personal and scientific backgrounds. A recruiter from industry once told me, when I asked, that what they look for in new hires is people who can work well as part of a team. By working with a diverse group internally and collaborating with others outside the group, including making regular presentations to collaborators, group members become mature scientists who work well in their future environments.

What gets you out of bed in the morning?

The main thing that drives me is scientific curiosity – the need to discover something – but also the drive to share findings with others and to make it possible for them to use our discoveries for their own purposes. I also love watching students learn and mature as they carry out their research. It is very rewarding to see them branch out into their own careers in which they innovate and improve daily life for others. Each person may think, at times, that their contribution is not enough, but all of us are needed to improve the world.

Looking back at your career, what has been your biggest reward?

I would say that my biggest reward has been seeing my PhD students move on to careers in universities, government labs, chemical companies, clinical labs, biopharma, and instrument companies. Most of them have stayed in the mass spectrometry field and make innovations regularly. They are enthusiastic about what they do, and I enjoy seeing their progress. I've also enjoyed taking a particular scientific path (collisions of ions with surfaces to provide structurally informative fragments) and building it over what has become decades.

Which characteristics have helped you most?

Persistence is a characteristic in which I think I excel. When I find a problem interesting, I like to continue tackling it until we solve it or at least make good progress. Insight grows from persistence; the more time you spend on a problem, looking at it from different angles, the more likely you are to gain insight into it. Often, and especially if you think you are not making progress, it's good to take a break from the problem and come back to it with fresh thoughts.

Maybe I should also comment on originality. I don't always think of myself as original or creative, but I do enjoy taking a body of data and trying to generate new meaning from it. In that sense, I think I can be original by finding the hidden stories in datasets or planning experiments that have not been done previously.

How have you found serving as ASMS President?

ASMS is a wonderful society. The members are a loyal group and we always have large numbers of volunteers for any job. During, before, and after my term, the society has worked on increasing diversity, equity, and inclusion (e.g., in selecting session chairs and speakers, in committee selections, in publishing, and so on) – making sure multiple voices are heard throughout the society's functions. There is still a long way to go though so I hope all members continue to work hard to make the society more inclusive.

The presidential term is not just the time spent as President. It's a six-year term in which you first serve as the Vice-President for Programs, putting the annual conference program together for two years; next, you serve as President for two years; and, finally, as Past-President for two years. It is an honor to serve in the position and to witness the large number of volunteers who give their time to make the society successful, working with a fantastic Scientific Association Management team.

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