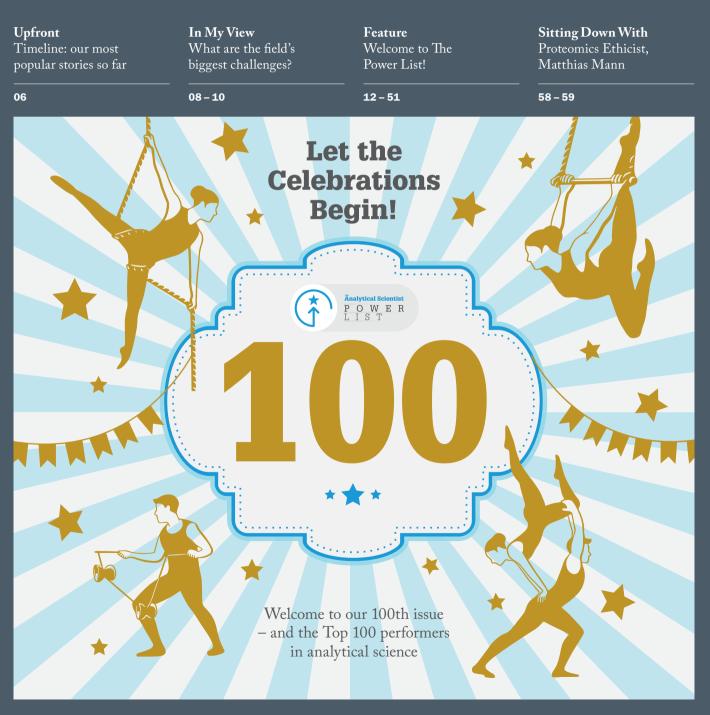
the Analytical Scientist





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Fundamental questions Elemental answers

Celebration and Scrutiny

How can we boost productivity, tackle Big Data, educate the public, and regain our mojo post pandemic? Let's consult The Power List.





t is my great pleasure to welcome you to the 100th issue of The Analytical Scientist – and to the return of The Power List Top 100!

As we said last month, our bold mission is "to record, scrutinize, and celebrate all endeavors in the analytical sciences." Much of this issue is a celebration – welcome to the party! But we also felt it prudent to offer some scrutiny for balance. On page 8, we collated the answers to one crucial question: What is the single biggest issue facing analytical science in 2021 and beyond? Some strong themes emerged.

Ruedi Aebersold highlighted the challenge of extracting meaningful insights from the "increasing quantity and quality of data" being generated today. Jenny Brodbelt, Alejandro Cifuentes, and Erin Baker also agreed. "How can we overcome bottlenecks and integrate huge amounts of data generated by existing analytical techniques from different levels of expression – genomics, transcriptomics, proteomics, metabolomics?" asks Alejandro.

Another important theme was public education – and the "intrusion of politics into science," as Gary Hieftje put it. "I strongly believe that analytical scientists must report the results in a manner that is comprehensible – giving the true meaning of the findings," says Roy Goodacre. "Education is key here."

Finally, several of our Power Listers highlighted the difficulties of "moving on" from the pandemic. "Online conferences have many advantages, but they can't quite replace meeting and discussing in person," says Nicole Pamme.

"We must get our ambition back," says Ian Wilson. "COVID-19 knocked us all off course, and we need grit and determination to catch up."

So, how can the field boost productivity, turn mountains of data into useful information, educate the public (and politicians), and bounce back from the pandemic? Many of the great analytical scientists appearing on The Power List have faced – and overcome – seemingly insurmountable challenges in their careers, so perhaps their combined advice presents the answer...

In their combined words: "Stay curious," "find and follow your passion," and then "remember your purpose." Be "courageous," "patient," and "flexible." "Collaborate." "Think differently," and "never get tired of asking why." "Have a plan B," "hang in there," and "don't be afraid to admit what you don't know." Oh – and "have fun!"

James Strachan Editor

the



Entering the digital age in MS

Introducing the MALDImini-1 digital ion trap mass spectrometer

Shimadzu's first-of-its-kind MALDImini-1 digital ion trap mass spectrometer fits in a space the size of a piece of paper, allowing installation in places where mass spectrometers could not previously fit. It enables ion trapping up to 70,000 Da and the MS/MS and MS³ functionality of the digital ion trap allows researchers to carry out comprehensive structural analyses with ease.

- Fast, simple setup allows for a more convenient workflow
- Software allows switching quickly and easily between MS, MS/MS and MS³ modes for seamless analysis

- Only device capable of MALDI-MSⁿ in this compact size
- Space-saving lightweight design fits anywhere





MALDImini-1

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Features

The 2021 Power List: Top 100 For our 100th issue, we return to our traditional celebration of the Top 100 most influential people

in the world of analytical science

Looking to the future of the

field, we shine a light on early-

career scientists with quickfire research "elevator pitches"

Matthias Mann, Professor of Proteomics and Signal

Transduction, Max Planck

Munich; and Director at the

NNF Protein Research Center,

Institute of Biochemistry,

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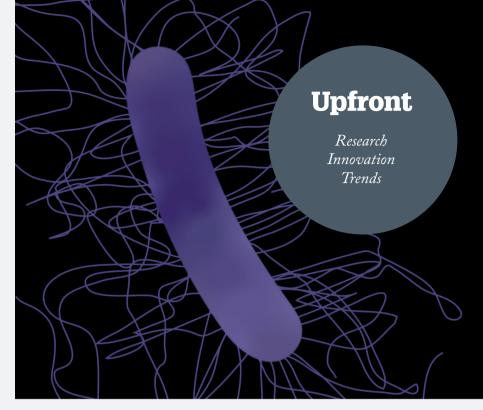
C. difficile, But Not Impossible

Surface-enhanced Raman spectroscopy could be the key to a fast and accurate clinical test for *C. difficile* infection in hospitals

Clositridium difficile is notorious among hospital patients and staff for its ability to infect the bowel and cause (sometimes deadly) diarrhea. Because of its high toxigenicity and increasing antibiotic resistance, early diagnosis of *C. difficile* infection (CDI) is vital to stopping the spread of this disease and ensuring effective treatment. But current testing methods have a number of limitations; they cannot accurately determine infection severity, offer low sensitivity, and do not allow for quantification.

By combining the benefits of a lateral flow assay (LFA) with surface-enhanced Raman scattering (SERS), researchers from the University of Strathclyde and Newcastle University, UK, have overcome these limitations and offered hospital laboratories an ultra-sensitive, fast, cheap, and user-friendly test for CDI.

Their SERS-based LFA platform enables sensitive quantification (down to $0.01 \text{ pg/}\mu\text{L}$) of two key biomarkers, SlpA



and ToxB, in 20 minutes. Importantly, this is the first time a duplex test for both biomarkers has been studied – and it could offer more accurate CDI diagnosis (and pathogenicity determination) without cross-reactivity from similar species. "Also, the use of the handheld Raman spectrometer means this measurement can be done at point-of-care and is highly portable, making it suitable for use in a wide range of situations," says Duncan Graham, Head of the Department of Pure and Applied Chemistry at the University of Strathclyde.

The Newcastle team had previously worked on a *C. difficile* assay with lateral flow, but the method (which relies on a visual assessment with the naked eye) wasn't sensitive enough for use in a clinical setting. "When we started collaborating with Neil Keegan from the Translational and Clinical Research Institute at the University of Newcastle, we recognized that the lateral flow assay could be merged with SERS detection to give the sensitivity required," says Graham.

The team's next step is to move onto clinical samples. "So far we've used simulated clinical samples (synthetic feces), but it's time for the real stuff now," adds Graham.

Reference

1. WA Hassanain et al., Analyst, 146, 4495 (2021). DOI: 10.1039/D1AN00726B.

D TIMELINE

Crème de la Analytical Chem

Showcasing some of our most popular articles over the years

Änalytical Scientist

2013 - FUTURE SEPARATIONS

Emily Hilder and Robert Shellie present a snapshot of separation science (as it was in 2013), and predict how the field will develop in the coming years.



2014 – TOOLS OF THE METABOLOMICS TRADE

Robert Trengove takes us on a tour of the metabolomics field, and how it became what it is today.



2016 - GURUS OF RAMAN SPECTROSCOPY

Volker Deckert and Duncan Graham offer their thoughts on the future of Raman spectroscopy.





A round up of the latest analytical science news – from the world's first net zero MS to multi-capillary CE-SDS

- Bruker has joined the EUfunded PANACEA project, which is working to facilitate the use of solid-state NMR spectroscopy by non-expert users. The aim is to broaden the opportunities for novel chemistry applications by bringing together the necessary instrumentation, research infrastructures and chemical expertise (1).
- Waters Corp recently released its new BioAccord System with ACQUITY Premier – a highresolution LC-MS capable of multi-attribute monitoring of biotherapeutics (2).
- Evotec has entered a collaboration with Biognosys in the hope of accelerating drug discovery and development. The partnership will use Biognosys' data analysis software for data-independent MS-based proteomics as well as its unique workflow for MS facility management (3).
- SCIEX has released the BioPhase 8800 capillary electrophoresis system for biologics analysis – the only



multi-capillary CE-SDS system on the market that processes eight samples simultaneously (4).

 Thermo Fisher Scientific has launched the world's first net zero mass spectrometer, the Delta Q Isotope Ratio MS. As well as improved specifications, the gas IRMS instrument's carbon footprint will be neutralized through "IsoFootprint" – an initiative that permanently removes CO₂ emissions associated with the manufacture and supply chain of all new inorganic IRMS products (5).

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Eau De Boeuf?

Plant-based burgers are on the rise, but how does their aroma compare to the real thing?

As plant-based meat alternatives become increasingly popular, food companies continue to pour time, money, and resources into creating the ultimate no-beef burger. But mimicking the taste, texture, appearance, and smell of the real thing is no mean feat. Now, researchers have used GC-MS to determine the quintessential "meaty" odor of a classic patty.

First, they cooked various patties and simply described the smell – meaty, fatty, buttery, sweet, or roasted. Next, GC-MS (combined with olfactometry) was used to correlate the aromas with specific compounds. Volatiles were injected into the GC-MS and some diverted to a sniffing port where a person described the odor. The rest of the sample was then analyzed by MS to match specific compounds with each descriptor.

So who came out on top? Beyond Meat's burger wins on the odor front, with the compounds 1-octen-3-ol, octanal, and nonanal contributing to its meaty aroma.

Reference

1. ACS (2021). Available at: https://bit.ly/3obn0Pt.

2017 - THE TRUTH ABOUT FRACKING

Doug Carlton Jr discusses the role of analytical chemists in hydraulic fracturing, seeking to add some much-needed objectivity to the debate.



2018 - METABOLOMICS: THE SUPERGLUE OF OMICS

Martin Giera, Mary Spilker and Gary Siuzdak tell us why the metabolome is not simply a "cellular information sink," and share their thoughts on the future of the field.



2019 - THE RAMAN WIZARD

We sit down with Ian Lewis, Director of Marketing, Kaiser Optical Systems, Ann Arbor, Michigan, USA.





2020 -MAKING THE "BREATH BIOPSY" A REALITY

We speak with Jane Hill and Billy Boyle (of Owlstone Medical) about their research into the arena of breath analysis and how it is opening new diagnostic doors.

In *Our* View: The Grand Challenge

Fifteen of this year's Power Listers answer one crucial question: what is the single biggest issue facing analytical science in 2021 – and beyond?

Robert Kennedy: Overall, getting ourselves back to full productivity by overcoming supply chain issues, the pandemic malaise, and lack of interaction with colleagues is a huge challenge for all of us. Another big challenge is creating a more diverse workforce. We'll do better if we develop all the talent and include all the voices working on problems.

Speaking in terms of more scientific issues, I work in a few different areas. For metabolomics, there are many large challenges. We still can only identify a fraction of the compounds that are detected in a given sample. Tracking "features" is much less interesting than tracking known chemicals, so we really need better ways to identify compounds in complex mixtures. It is difficult because the ultimate validation requires having authentic compounds to test. Another issue is analyzing the large data sets generated. For example, in most fields it is straightforward to do a power analysis to determine the sample size needed this simple issue has not yet been worked out for metabolomics.

Graham Cooks: The biggest challenge for any field of research is to have fresh material to explore. We are fortunate in MS to have a wide remit, but this role has a limited lifetime, involving welldefined stages: first it is ignored, then it is embraced enthusiastically, next it is widely used, and finally it becomes routine. We have seen this happen to MS applied to proteins over the past 20 years. The fundamental science of ions – the chemistry and physics of ions – is a more reliable and central concern for MS. This topic includes fabricating new materials and surfaces with ions, synthesizing in a "make-to-measure" fashion small quantities of drug candidates for biological testing, and the fundamental spectroscopy of ions.

Jeremy Nicholson: Understanding human disease complexity at the individual and population level and the global dynamics of disease is and will continue to be of paramount importance. Many of the world's greatest problems are underpinned by analytical sciences – although this is not always obvious – from the Human Genome Project, to understanding global warming, to personalized medicine.

These problems all require measurement and modeling of complex systems to inform us about the changing nature of the world we live in - and how to plan for the future. Humanity currently faces unprecedented environmental changes, upon which we find superimposed new pandemic threats and the emergence of zoonotic pathogens that challenge our healthcare systems and our economies. These changes are with us for good – or as long as human population growth continues to outstrip our resources. And so there are major challenges for analytical science to come up with new metrics and underpinning mechanisms of change that will hopefully enable the creation of mitigation strategies going forward.

Ruedi Aebersold: In our field of MS-based proteomics, the progress achieved over the past two decades or so has been absolutely astounding, and it is the result of the advances realized in analytical chemistry and instrumentation. Today, the pace of progress in generating ever-increasing quantity and quality of data continues unbroken. I think the biggest challenge

In My View

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

Änalytical Scientist

we are facing in our field is the extraction of new biological or clinical knowledge from these data. The computational challenges of the future will focus on questions such as: how do specific proteins operate in the context of the whole proteome? How does the proteome as a whole - in terms of abundance and interactions of proteins - respond to genetic or environmental perturbations? Which observed proteomic changes are causal and which are consequential in terms of changes in their functional state, for example. These and related questions are at the core of the emerging field of personalized/precision medicine.

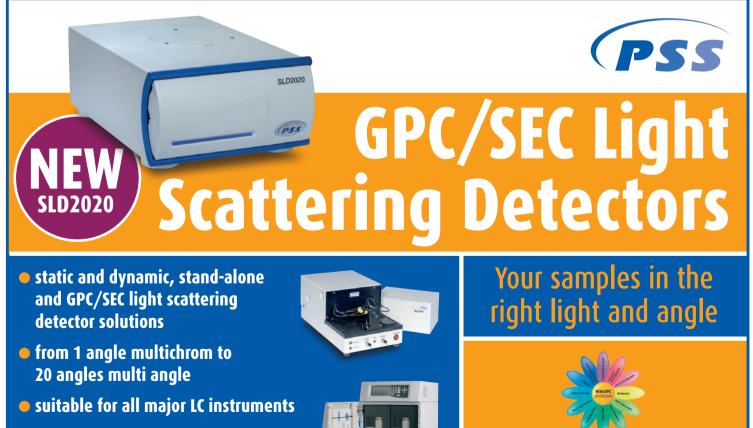
Jenny Brodbelt: Advances in analytical methods have allowed new data to be

collected and new results to be generated in record-breaking time. Integrating all this data and new results into useful information is a daunting challenge, and it requires big team efforts, involving scientists from different disciplines. It can be difficult to maximize the value of all of this new data and end up with significant impact.

Alejandro Cifuentes: In 2021 and beyond, we will still be trying to comprehend the huge complexity of the interaction of food ingredients and our body, and although I believe we will come to a better understanding of the microbiome's role here, we will have to wait a good number of years before we see the expected benefits from this discipline. In terms

of technological advances, we will look for better analytical instruments – faster, more sensitive, with higher resolution – and cheaper. As a main challenge, we will have to solve our current limitations in data treatment. How can we overcome bottlenecks and integrate huge amounts of data generated by existing analytical techniques from different levels of expression – genomics, transcriptomics, proteomics, metabolomics? And more importantly, how will we transform this data into useful biological information?

Erin Baker: I believe the current biggest challenge in analytical chemistry is the rapid evaluation of all the multidimensional or multi-omic data that is collected. Automation and rapid data



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acquisition rates are allowing analytical platforms to collect thousands of datasets each day. However, assessing these datasets quickly is extremely difficult – my students often work in the lab for a week and evaluate data for months to determine molecular significance, as well as the environmental and biological connections.

Claire Eyers: For so long, the field of proteomics has relied on identification of peptides as a proxy for gene expression, which is fine, but limited. Biology is not that simple, with protein function being critically dependent on dynamic regulatory modifications. Our single biggest challenge therefore is moving away from trying to understand biological systems based purely on protein "identification," towards understanding the complement of differentially modified protein isoforms, or proteoforms, that truly regulate function.

Paul Haddad: Despite our collective efforts, chromatographic methods (especially liquid chromatography) are limited by the available peak capacity. Current levels of peak capacity in LC systems are insufficient to enable the resolution of complex samples – especially those of biological origin. The future challenge is to achieve substantially increased peak capacity (for example to 1,000,000) and this is likely to be achieved through the use of 3D systems, which pose immense technological challenges.

Martin Gilar: I think it is the challenge of LC education. Universities are educating very few chromatographers. The pharma, biopharma, and chemical industries are struggling to attract LC experts. Overall, the level of analytical expertise is declining at a frightening speed. This trend, combined with the development of new biotherapies, puts stress on the

"In my opinion, the biggest challenge facing analytical science, indeed science in general, is the intrusion of politics into science, its conduct, and its findings."

industry. Part of the solution is the development of robust and easy-to-use instruments, as well as software-guided approaches to LC method development. Still, somebody will have to pick up the education slack – and this may be an opportunity for the next generation of entrepreneurs.

Gary Hieftje: In my opinion, the biggest challenge facing analytical science, indeed science in general, is the intrusion of politics into science, its conduct, and its findings. Although this problem is not new, it has become more serious and dangerous in the past several years. No doubt, the ongoing COVID-19 pandemic has exacerbated things. Both sides of many political questions claim to have science on their team, when neither has data to support its position. Preliminary findings are asserted to be absolute truth because "science says so," and statistics are frequently misunderstood, applied to inadequate data sets, or intentionally distorted. As always, scientists themselves are likely the only ones who can introduce reason into this fray. They must be

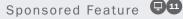
truthful, thorough, and objective, and resist espousing popular positions despite the lure of notoriety and research funding.

Candice Ulmer: The single biggest challenge facing the field in 2021 is establishing diverse, equitable, and inclusive work environments that are supportive of all individuals regardless of race, ethnicity, national origin, gender/gender identity/ sexual orientation, age, religion, culture, and disabilities, to mention but a few. This effort is going to require effective strategies to recruit and retain personnel, data-driven DEI training tools, and enforced corrective actions for issues encountered.

Nicole Pamme: Keeping our scientific communities together across the globe, whilst also managing scientific exchange in a climate friendly way is the biggest challenge. It's been hard to discuss and meet in person in recent months. Online conferences can go some way, and they have many advantages, but they cannot quite replace meeting and discussing in person. How do we best balance this?

Roy Goodacre: I think one of the biggest challenges facing analytical sciences in 2021, and indeed beyond, is to make what we do scientifically understandable to the public. Numerical values mean very little to some people, and few people grasp the concepts of scale, especially when one is talking in orders of magnitude. I strongly believe that analytical scientists must report the results in a manner that is comprehensible – giving the true meaning of the findings. Education is key here.

Ian Wilson: For 2021, I think the biggest challenge is getting the labs working at pace again, rather than just marking time and doing only the MUST DO tasks. We must get our ambition back. COVID-19 knocked us all off course, and we need grit and determination to catch up with all of the things that didn't get done.



Towards an Open Access Future

If we all embrace Open Access, the research community will be better able to tackle pandemics, climate change, resource issues, and more. The most pressing question: How do we get there?

By Sara Bosshart, Head of Open Access Journals, Royal Society of Chemistry

Open access (OA) keeps me up at night. Not the why, or the what, but the how. With the advantages of OA for research so clear now – especially in the midst of a global pandemic – the real question is how we – as researchers, publishers, societies, and institutions – can get

there. How can we co-create the new open research environment we need while preserving integral aspects of the current ecosystem?

As the new Head of Open Access Journals at the Royal Society of Chemistry, these questions form the very core of my role and responsibilities. I'm tasked – in collaboration with my colleagues – with figuring out how we can sustainably transition our successful publishing business that, for decades, has relied on subscriptions to a model that will support OA for the more than 37,000 articles we publish annually.

Luckily, the RSC is no stranger to OA innovation. In 2012, we launched our "Gold for Gold" initiative (1) - a program unlike any other at the time. Put simply, it granted institutions subscribing to the full package of RSC journals credits that they could apply towards OA publication. The program equated to the RSC donating over £1 million worth

of gold OA-article publishing fees to the UK research community and over £5 million worth of vouchers to researchers globally. We were also one of the first publishers to negotiate "read and publish" agreements (a term we coined), which transferred the onus of payment for OA from the author to the institution.

Today we're setting our sights even further – figuring out if, when, and how we want to make all of the important chemistry-related research we publish OA. It's clear that OA is the future; embracing OA is the only way we will accelerate the pace of research to

help us solve the many pressing global issues of today and tomorrow. As a society, our mission is to help chemists to make the world a better place and there's no better way to do this than by making research outputs freely available.

Equally important in our transition to OA is continuing to ensure OA is a viable option for all of our authors worldwide. And means engaging with our communities globally to find OA solutions that work for local research ecosystems — both those with the funds to cover article payment charges and those without. Luckily, although most of the current OA models focus on per-article author payments, there are multiple new models emerging, such as "Subscribe to Open" (2) and PLOS' Community Action Publishing (3) that seek to move away from per-article charges and instead build on existing library budgets to support OA.

Essentially, as we move further towards an OA future, we are going to need to be creative and open to engaging with emerging OA models. We'll need to adapt them to different regional requirements

and emerging trends not only with Open Access but with Open Science and infrastructure developments generally. "We'll need to figure out what we want the future open research landscape to look like – and then work together to get there."

We won't be able to do this alone or in isolation – we'll need the support of our community, authors, members, and partner institutions. We'll need to figure out what we want the future open research landscape to look like – and then work together to get there.

In many ways, as a society, we're uniquely placed to do this – we have an active and invested global community. On the other hand, we also have the extra responsibility to get this right from a financial point of view so that we can continue to support our members and chemists generally – from education, to funding, to resources, and so on.

These are exciting times and, though I may not get much sleep, I'm looking forward to being a part of the OA future we'll be shaping at the RSC; an open future that's better placed to tackle pandemics, climate change, resource issues... you name it.

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For us, the ninth iteration of The Power List feels particularly special because it coincides with our 100th issue – thanks again to everyone who has joined us on the journey! In the spirit of tradition and harmony, we've returned to our original 2013 format of 100 names. As ever, we recognize that no such list can be definitive, but we certainly hope you will find it inspirational.

To celebrate our 100th issue, we wanted to reflect on the future of analytical science by asking our Power Listers about the key challenges facing the field in 2021 and beyond – you may have already read some of their responses on page 8. But we also wanted to celebrate the next generation of researchers, with our "Power List Slam" on page 50.

If you're feeling nostalgic, you may wish to compare this year's List to 2013; some faces are familiar – but there are also plenty of new ones, including analytical scientists from 2014's Top 40 Under 40, 2016's Top 50 Women, and 2020's "Around the World" Power Lists. One question we get asked (and ask ourselves) every year is: How representative is The Power List? Notably, there were no women ranked in the Top 20 back in 2013. So, have things changed? And, if so, have they changed enough? Read on!

Welcome to The Power List!

WANT TO SHARE THIS LIST WITH A COLLEAGUE? IT CAN BE ACCESSED ONLINE FOR FREE AT HTTPS:// THEANALYTICALSCIENTIST. COM/POWER-LIST/2021



ADAM T. WOOLLEY

Dean of Graduate Studies and Professor, Department of Chemistry & Biochemistry, Brigham Young University, USA

Predictions? Significant changes will occur in the model for scientific publishing. I expect that the conflict between the traditional library subscription and open access approaches will result in a restructured publication landscape. Additionally, new and better metrics for evaluating the quality of scientific work (that are less subject to manipulation) will emerge.



ALAIN BERTHOD Emeritus CNRS Research Director DR1; Associate Professor, Institute of Analytical Science, University of Lyon, France

Biggest breakthrough? Miniaturization and increased resolution of mass spectrometers allowed real advances in omics.

Advice? Try to realize what is important and what is less so. (My four grandchildren are so fun. It is tiring but so interesting taking care of them and dealing with their surprising questions – they give me perspective in this matter!)



ALAN G. MARSHALL Robert O. Lawton Professor of Chemistry & Biochemistry, Founding Director and Chief Scientist, Ion Cyclotron Resonance. Program, National High Magnetic Field Laboratory, Florida State University, USA

Heroes? My coworkers: students, postdocs, staff, and faculty colleagues. They have guided me into new techniques and applications, and kept us at the forefront of the field. *Advice?* Don't choose a project because it looks easy. Everything turns out to be hard anyway, so you might as well aim for something important!

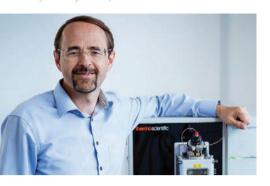
ALEJANDRO CIFUENTES

Professor, Head of Foodomics Lab, CIAL, CSIC, Spain

Controversial opinion? I am not so enthusiastic about the concept of "personalized nutrition." In my opinion, right now this is only a marketing reclaim useful to catch innocent customers (and of course their money). We have a long, long way to walk before we can get enough knowledge about the relation of diet with health and the different answers provided by the different individuals to food, including their specific genetic and environmental conditions.



🐼 Feature



6 A L E X A N D E R M A K A R O V

Director of Research, Life Science MS, Thermo Fisher Scientific; and Professor of High Resolution Mass Spectrometry, Department of Chemistry, University of Utrecht, The Netherlands

Controversial opinion? In MS, I believe that high-resolution accurate mass instruments (HRAM) could exceed limits of quantitation of nominal mass instruments, like triple quadrupoles. And I also believe that HRAM instruments could be produced and sold at much lower price points! *Advice*? Generally, I would advise to learn from others – but not to copy them. Also, for any high-risk research/activity, I would recommend to always have "Plan B" actively developed, in case things go south.





AMANDA HUMMON

Professor, Department of Chemistry and Biochemistry, Comprehensive Cancer Center, The Ohio State University, USA

Advice? Don't be afraid to admit what you don't know. As academics, we want to pretend that we have the answers

and understand everything. The reality is that most of the important problems facing the world today are complicated and nuanced and it is impossible for one person to understand all the salient points. You can still do that important research, just seek out the appropriate collaborators and work as a team.

TOP 20 ANDREW DEMELLO

Professor of Biochemical Engineering, ETH Zürich, Switzerland

Biggest challenge? While the community is extremely good at generating high-quality chemical and biological information on very short time scales, we are still poor at extracting this information at the same rate and with the same richness and contrast. We're definitely making inroads in this direction, but I'd like to see more examples of ultra-sensitive, fast and informationrich detectors able to probe a diversity of molecular species at sub-pM concentrations.

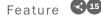


ANTJE BAEUMNER

Professor and Director, Institute of Analytical Chemistry, Chemo- and Biosensors, University of Regensburg, Germany

Controversial opinion? Innovation cannot be limited to making analytical methods

more specific and more sensitive; we also must innovate to lower their cost of fabrication and simplify their use and assay steps. This is not an engineering task, but it is at least as important a task for the analytical chemist as it involves finding new principles, new materials, and new strategies.





BOB PIROK Assistant Professor at the University of Amsterdam, The Netherlands

Biggest challenge? Similar to all other sciences, our field risks being drawn into this pit fight where the focus is not on the quality of our methods but the quantity of meaningless numbers. If I look at multidimensional LC specifically, I am baffled by the increasing number of publications that proudly report complicated systems where the number of dimensions must go ever higher. As a community, we have developed amazingly powerful separation systems combining LC and MS. We ought to learn how to use them more effectively and robustly rather than solving the analytical problem by complicating it further. Perhaps then, after having been here for decades, 2D-LC will find its way into more environments.



CANDICE ULMER Clinical Research Chemist, Centers for

Disease Control & Prevention, USA

Instrument you couldn't live without? All of my routine and research & development biomedical/clinical work over the past 10 years has incorporated MS. Therefore, it would have been extremely difficult to isolate, identify, and quantify novel markers for various diseases without this type of instrumentation coupled to advanced separation techniques.

Advice? During those challenging moments that at times may seem endless, remember your purpose and be inspired to either ask for help/mentorship or seek the necessary resources.



#3 CAROL ROBINSON

Director, Kavli Institute for Nanoscience Discovery, and Dr. Lee's Professor of Chemistry, University of Oxford, UK

Heroes? I have many heroes but have selected the one who made the most difference to my career: Chris Dobson. He always encouraged me to aim high whether it be with my personal position, grants, or with papers. It is my job now to do this for the next generation.

Advice? Do something – something courageous. Resist the temptation to collect more and more data just because you can, but always have in the back of your mind the question or hypothesis you are trying to explore

CAROLINE WEST

Full Professor, University of Orléans, France

Heroes? Terry Berger is one of the major pioneers in supercritical fluid chromatography, I believe I knew most of his papers by heart when I was a PhD

student. I was also (and am still) greatly inspired by the works and philosophy of

Pat Sandra and Chris Welch. All of these guys have produced fundamental and essential research but also demonstrated applicability in the realworld, which is what I am trying to do. *Controversial opinion*? SFC is not normalphase. And another one: PSI is not an international unit. Sorry to my North American friends but pound is not international, inch is not international, and so PSI is definitely not international! Feature



CATHERINE CLARKE FENSELAU

Distinguished University Professor Emeritus, University of Maryland, USA

Advice? My Dean once bumped into me in the elevator and told me that I should never again come to work at the medical school wearing green shoes.

Eureka moment? My research goal is to exploit MS in the biomedical sciences with ingenuity and dedication; my eureka moment came when our experiments successfully revealed that acyl-linked glucuronides can alkylate proteins.



CATHERINE NGILA Acting Executive Director, The African Academy of Sciences, Kenya

Why analytical science? To apply chemistry to solving environmental problems by qualitative and quantitative measurements. I was always intrigued by the ability of instrumentation to determine chemical structures and the nature of substances. In addition, analytical chemists have the scope to work in different areas, including water analysis, environmental chemistry, nanotechnology, pharmaceuticals, and forensic science – to name just a few.

CHRISTINA JONES

Research Chemist/Advanced Manufacturing Program Officer, National Institute of Standards and Technology, USA

In another life... I would be an attorney and a DJ as a side job or hobby. Law was my first love, but my mother was hospitalized when I was younger and attempting to understand her illness steered me more toward the sciences. Actually, law may have been my second love. My love for music is everything, and I thoroughly enjoy introducing others to new music. I'm usually the person at social functions controlling the music or asked to make a playlist for everyone's enjoyment.



CHRISTOPHER WELCH

Executive Director, Indiana Consortium for Analytical Science & Engineering (ICASE), a joint venture between Purdue University, Indiana University and the University of Notre Dame, USA

Biggest breakthrough? It has been very exciting to observe and to participate in the application of machine learning and artificial intelligence to analytical chemistry, analytical instrumentation, and measurement science. This area is moving by leaps and bounds; progress has been stunning. I'm looking forward to what comes next.

Advice? Follow your passion, ask for advice but make your own decisions. Work hard, but also take time to enjoy family and friends, and to see the world. Have confidence in your vision, speak truth to power, and look for fun in everything you do.

Heroes? I have been very lucky to have some really great mentors, including William Pirkle, Donald Cram, Michael Doyle, Koji Nakanishi, and R Graham Cooks.

Änalytical Scientist



CLAIRE EYERS Professor of Biological Mass Spectrometry, Director Centre for Proteome Research, University of Liverpool, UK

Instrument you couldn't live without? Much of our current proteomics work relies on the Thermo Orbitrap Tribrid series of instruments. We still make good use of the "workhorse" Q Exactive instruments, but the flexibility and the additional

fragmentation capabilities of the Tribrid, particularly electron-mediated dissociation, has been really important for improving the site localization of covalent posttranslational protein modifications, which is so essential for our work.

CORAL BARBAS

Director of the Centre for Metabolomics and Bioanalysis (CEMBIO), San Pablo CEU University, Spain

Biggest breakthrough... Expanding the concept of analytical chemistry from tight quantitative criteria in targeted analysis to semiquantitative untargeted analysis. This has been possible thanks to incredible developments in (mostly) MS technology, but also in chromatography and NMR, and has led to discoveries without needing a-priori hypotheses.

Advice? Put your life and heart into everything you do, even if it's small. That is the only way to enjoy research.



CLAUDIA ALCARAZ ZINI

Full Professor, Instituto de Ouímica, Universidade Federal do Rio Grande do Sul, Brazil

Advice? An academic career includes beautiful, exciting, and enchanting challenges; however, it demands a lot of professional and personal effort. Make your career much more than a profession, make it an opportunity to help students and colleagues grow in their professional and personal lives. But also, make it a mission to help society in terms of human resources development and scientific and technological advancement. Lastly, when I was starting my scientific career, a renowned retired professor gave me a single piece of advice: do scientific work with partners from other countries and build a network with them. Recognition of a researcher's work outside of their own country is much more difficult and such recognition is an important part of career development.

DANIEL W. ARMSTRONG

R. A. Welch Distinguished Professor, University of Texas at Arlington, USA

Instrument you couldn't live without?

Perhaps the simplest, most overlooked answer to this question is the analytical balance. Probably no analytical chemist could do much of anything without it. I would guess that no one has indicated this essential device, but rather put forward much more expensive and grandiose instruments. In that vein, I would say we couldn't have conducted much of our research without HPLC-mass spectrometers.



#10 DAVID E. CLEMMER

Distinguished Professor & Robert and Marjorie Mann Chair of Chemistry, Indiana University, USA

Advice? Keep an eye on the emerging area of accelerated chemistries in droplets. The changes that reagents experience as they interact within and on the surfaces of evaporating droplets appear to resemble aspects of enzymatic activity. The use of rapid and sensitive MS to detect these reactions, combined with learning algorithms, brings new strategies to the field of organic synthesis. It is still too soon to fully appreciate what impact this work will have but some of the early examples are truly breathtaking.





DAVID MCCALLEY Professor of Bioanalytical Science,_ University of the West of England, UK

Advice? If you work in a university environment, try not to end up as a mere research manager; spend at least some time doing things yourself in the laboratory. Analytical science is a practical subject and doing some practical experiments will help you to realize what is possible and what is not possible, as well as how long it takes to do experiments properly! Having said all this, Uwe Neue, a highly successful research scientist, once admitted to me that he had not touched an HPLC for the last 30 years of his life – he could apparently explore all possibilities in his imagination while leaving the practical verification of his ideas to his able co-workers.



DAVY GUILLARME Senior Lecturer and Research Associate, University of Geneva; Associate. Editor, Journal of Chromatography B, Switzerland.

Advice? Today, research is more and more driven by the application rather than by fundamental understanding of the phenomenon. In my opinion, an equal importance should be given to both aspects to make successful research. Communication is also an important aspect of modern research. So, do not hesitate to spread the word on social networks or elsewhere on what you are doing in the lab!

DUNCAN GRAHAM

Distinguished Professor and Head of Department, Pure and Applied Chemistry, University of Strathclyde, Glasgow, UK

Biggest breaktbrough? I think the creation of new probes for sensing conditions/molecules inside cells using Raman and/or stimulated Raman scattering is really game changing. This approach makes use of the vibrational frequency of alkynes being in the cell silent region and then changing in response to different stimuli; for example, pH or glutathione. There's amazing work coming out of Japan and the US in this area.

Änalytical Scientist





DEIRDRE CABOOTER

Professor, Department of Pharmaceutical and Pharmacological Sciences, University of Leuven (KU Leuven), Belgium

In another life... I turned 40 this year, and this seems to be a moment where you ask yourself such questions! Just for the record, I love my job and wouldn't want to be doing anything else. That said, running a wine farm in Stellenbosch (South Africa) sounds like something to do! Closer to home, I might have become a pilot (it runs in the family). Heroes? My mentor/hero/continued source of inspiration is Gert Desmet. It is a privilege and absolute honor to be able to work with someone who is so established, and yet so humble and accessible. Gert always finds the time for scientific discussions, but has also been a great support in so many other aspects of my academic life. I'm forever grateful for this, and look forward to the many adventures still ahead of us.

ELEFTERIA PSILLAKIS

Professor in Water Chemistry, Technical University of Crete, Greece

Controversial opinion? Many priorities and strategies tend to direct research in analytical chemistry to applications and the "known unknowns" – establishing and solving the obvious problems. While delivering known answers to questions is important, solving problems we don't even know exist is far more valuable because that sets our future agenda. To do this, we must defend bottom-up and curiositydriven research, adopt a constructive skepticism in the science we do, and allow "space" in the field for creative scientific debates to happen. Promoting the study of fundamentals will demonstrate that the academic practice of analytical chemistry is dependent upon more than just producing data or copying a method. It will show that research in the field surpasses explicitly knowing things and seeks deeper appreciation of how systems work and especially, how systems fail. The generation and handling of data are of utmost importance in our field; but from a scientific viewpoint, sometimes, we seem to miss the forest for the trees.

ELENA STASHENKO

Director, Research Center for Biomolecules (CIBIMOL), Research Center of Excellence (CENIVAM), Universidad Industrial de Santander Bucaramanga, Colombia *Biggest breakthrough?* Orbitrap technology, because it brought high-resolution to the masses. Although it is still expensive, the alternatives remain beyond the reach of regular research projects.

In another life... I would be either an archaeologist or a geologist.

Advice? I recommend reaching a thorough and deep understanding of scientific concepts, using logic and common sense throughout life, basing judgements on scientific evidence, and never getting tired of asking why.



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EMILY HILDER Chief Maritime Division, Defence Science and Technology Group, Department of Defence, Australia

Instrument you couldn't live without? My scientific passion is chromatography and I can't imagine living without an HPLC. A beautifully simple and powerful technique and the first instrument I would buy in any new lab.

Advice? Stay curious! Don't be afraid to take risks and to fail. Things are generally less risky than your mind tells you they are and every failure is an opportunity to learn that brings you closer to success.



ERIN BAKER

Associate Professor, North Carolina State University, USA

Advice? Patience, persistence, a thickskin and a collaborative spirit are all fundamental in succeeding as a 21st century scientist. These attributes are all necessary to rise above the failures and criticism that are such a huge part of our daily lives, and also address the extremely complex scientific problems affecting us, including the pandemic, environmental pollution, and climate change.



FRANCISCO RADLER DE AQUINO NETO

Head of the Brazilian Doping Control Laboratory, Coordinator of the Laboratory for the Support of Technological Development and Emeritus Professor, Organic Chemistry Department, Institute of Chemistry, Federal University of Rio De Janeiro (UFRJ), Brazil

Nominator comment: Francisco Radler is one of the most influential researchers in analytical chemistry in Brazil. He has a long and solid career exploring useful applications of chromatography and MS, ranging from geochemistry to sports doping control. He is the man responsible for the Brazilian Doping Control Laboratory, which is undoubtedly a great source of pride for the region, having been able to operate for more than 30 years with extremely high standards.

GARY SIUZDAK

Professor and Director, Scripps Center for Metabolomics, The Scripps Research Institute, USA

Controversial opinion? I believe the metabolomics field has not yet recognized the value of neutral loss mass spectral data (NLintensity vs Dm/z), as represented in the new METLIN-Neutral Loss database. Neutral loss spectra's role in identifying unknown metabolites is vastly underappreciated.

Heroes? Think of a world without quadrupole MS. Without the contribution of Nobel Prize winner Wolfgang Paul (a personal hero), quadrupole MS technology probably wouldn't have ever existed.





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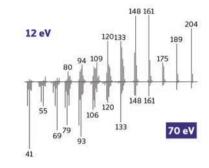
Michael and Tana Powell Associate. Professor, Departments of Chemistry and. Medicine, Siteman Cancer Center, Nutrition Obesity Research Center, Washington. University in St. Louis, USA

In another life... I would love to be a philosopher. I enjoy thinking about big questions and abstract ideas, particularly those related to epistemology. Finding patterns and themes that integrate a collection of seemingly unrelated observations has always fascinated me. I am notorious for raising deontological questions in group meetings and quoting Plato's "The Republic" in lectures.

Heroes? Two of my mentors are Gerty and Carl Cori. They built an empire for studying metabolism at Washington University and ended up training six other Nobel Prize winners. They were among the first to study metabolic pathways between tissues in an organism. Most impressively, they made seminal discoveries with relatively few supplies and without modern technologies, such as MS-based metabolomics.



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GARY HIEFTJE

Distinguished Professor Emeritus, Mann Chair in Chemistry, Department of Chemistry, Indiana University, USA

Heroes? I believe it is important for everyone to have "heroes" – people who serve as role models and who provide a "measuring stick" against which one's own achievements and position can be gauged. The heroes need not be those who are more mature as scientists; indeed, some of my own heroes are former students, colleagues, and contemporaries. Also, the yardstick need not be based on science alone but can be related to such things as character, integrity, consistency, thoroughness, inventiveness, and determination. My science heroes from the past include such luminaries as Richard Feynman and Tomas Hirschfeld but also somewhat lesser-known people such as Jack Frazer, head of the Chemistry Department at Lawrence Livermore

National Lab, J. Harvey Kleinheksel, classroom teacher extraordinaire at Hope College, and Stan Smith, originally of Instrumentation Laboratory.

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GOVERT SOMSEN

Professor of Biomolecular Analysis and Analytical Chemistry, Vrije Unversiteit Amsterdam, The Netherlands

Up-and-comers... I'd like to thank my PhD students for doing the hard work, some marvelous thinking, and for providing me with the material and joy to do my scientific work.



TOP 20 GEORGE WHITESIDES

Woodford L. and Ann A. Flowers. University Professor, Harvard University, USA

Research... Whitesides' research covers a wide range of topics from organic chemistry to materials science, microfluidics, self-assembly and nanotechnology. The goal: to develop diagnostic tools that are of low cost and simple to use.



TOP 20R. GRAHAM COOKS

Henry Bohn Hass Distinguished Professor, Purdue University, USA

Controversial opinion? I think that the stickiest amino acid – serine – played a key role in molecular homochirogenesis – whether this occurred on earth or elsewhere. The basis for this argument is the ease with which the serine octamer, a uniquely stable non-covalent amino acid cluster, undergoes chiral enrichment during sublimation and evaporation.

Änalytical Scientist

TOP 20 GERT DESMET

Professor in chemical engineering, Vrije Universiteit Brussel, Belgium

In another life... After my bachelor degree in engineering, I struggled quite a bit with the choice between starting a masters degree in chemical engineering or construction engineering. Clearly two totally opposite worlds, and I am very happy with my final choice, but what I miss a bit is that the result of what we do is much less visible and tangible compared with building a house or a bridge. No doubt my research interest in the design of chromatographic support structures is subconsciously influenced by the construction engineer that still hides somewhere deep within.





GONGKE LI

Professor, Director of Institute of Analytical Sciences, School of Chemistry, Sun Yat-sen University, China

Biggest challenge? The rapid trace analysis of complex samples. The research of separation, enrichment and detection of complex samples allin-one for on-site analysis should be paid much more attention. In another life... I would be a botanist or zoologist

CHEMISTRY & BIOCHEMISTRY

GUOWANG XU

Administrative Vice-Director, Biotechnology_ Division, and Director, CAS Key_ Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China

Biggest breakthrough? Over the last 10 years the biggest breakthrough in my working field has been in high-resolution MS instruments. Nowadays, people don't need FT-ICR-MS because they can instead achieve the analytical characteristics of high resolution MS with convenient and economical maintenance. On the other hand, UHPLC – which has been commercially available since 2004 – overcomes the limitations of traditional chromatographic analysis and improves the resolution, analysis speed and detection sensitivity to an unprecedented level. UHPLC-MS greatly promotes the development of separation and analysis techniques, and has been applied in different fields including proteomics, metabolomics and other chemical and bio-monitoring.

IAN WILSON

Professor of Drug Metabolism and Molecular Toxicology, Imperial College London, UK

Predictions? Realistically, I hope a lot more will be done to "democratize" analytical science. Things like

microsampling at home by the patient; putting an ion mobility spectrometer on your smartphone to tell you that you have drunk too much (easy) or that you might have cancer (I'm sure there's an app for that!); or making miniature mass and NMR spectrometers that are reliable enough to put on a GP's desk to properly individualize medicine through metabolic phenotyping. I suggest that, if Jim Lovelock could get a mini GC-MS on a Mariner spacecraft to Mars in the 1970's on the "Viking" mission, we should be able to get them into community medical practices in less than a decade (we will of course need the software to remove the analyst from the interpretation of the data but that is what AI is for...).

Advice? Don't follow in my footsteps, I'm happy to get out of the way. LEAD!



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Seature



<mark>#7</mark> ISIAH WARNER

Boyd Professor of the LSU System; Philip W. West Professor of Analytical and Environmental Chemistry; Vice. President for Strategic Initiatives; Howard Hughes Medical Institute. Professor, Louisiana State University, USA

Instrument you couldn't live without? It would have to be a fluorescence spectrometer!

In another life... I would probably be a licensed detective. An analytical chemist is licensed to seek out answers to important chemical questions.

Advice? If you love science, hang in there. Do not let the naysayers turn you off from science.



JAMES W. JORGENSON

Kenan Distinguished Professor of Chemistry, Emeritus, Department of Chemistry, University of North Carolina at Chapel Hill, USA (retired)

Predictions? Relatively inexpensive handheld quantitative chemical sensors of high selectivity and sensitivity would be a most welcome development, especially for at-home use by the general public. This is probably more than 10 years in the future.

Heroes? As a youngster my hero was Jacques Cousteau, and I dreamed of being a marine biologist. As a young scientist, my principal mentors were Milos Novotny and Royce Murray.

JANUSZ PAWLISZYN

Professor, Department of Chemistry, University of Waterloo, Canada

Predictions? Further development of sample preparation and ion mobility/ mass spectrometry instrumentation will have a dramatic impact on the practice of analytical chemistry. The number of new approaches based on rapid chromatography-MS, direct sample preparation-MS and direct sample introduction-MS will grow. Miniaturization of MS and front end devices will result in devices facilitating on-site multicomponent analysis, resulting in rapid diagnostic tools in hospitals, rapid screening methods for food quality determinations, and monitoring approaches for the environment.



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TOP 20

JENNIFER BRODBELT

Professor of Chemistry, University of Texas at Austin, USA

Heroes? Carol Robinson at Oxford continues to be a great role model and hero. She is one of the pioneers of developing native mass spectrometry methods in the realm of structural biology, and she was truly fearless in pursuing the analysis of huge macromolecular protein complexes. The insights gained from her work have opened the eyes of many scientists and established a foundation

JEREMY NICHOLSON

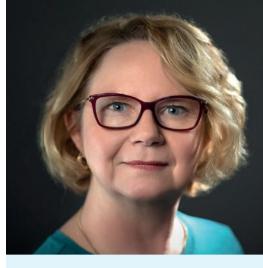
Director, Australian National Phenome Center, Professor of Medicine, Pro-vice Chancellor for Health Sciences, Murdoch University, Australia; Emeritus Professor of Biological Chemistry, Imperial College London, UK

In another life... I am not sure that I am an analytical scientist in the way that most people think about analytical chemistry. My work is almost entirely driven by biomedical problems and spans multiple types of analytical technologies for an entire new field. Another hero is Alexander Makarov of Thermo Scientific Fisher who developed the Orbitrap mass spectrometer. His spirit of innovation led to a transformation in high performance MS.



and modeling/informatic approaches to recovering biological or medical data from complex systems and samples. We do develop new techniques and methods, but they

are always inspired by trying to solve specific types of biological or medical problems (which means that, if successful, they have immediate translational value). So I sit at the interface between medicine and analytical science – I could work at other multidisciplinary interfaces I suppose, but I have ended up doing something I am good at that hopefully also has some beneficial outcomes for society.



JENNIFER VAN EYK

Professor of Cardiology and Pathology, Erika Glazer Endowed Chair in Women's Heart Health, and Director of the Advanced Clinical Biosystems Research Institute at Cedars-Sinai Medical Center, Los Angeles, USA

Up-and-comers? Rebekah Gundry: combines and extends cell surface protein labeling to identify key novel plasma membrane proteins. Combines proteomics in the academic world with industry partnerships to carry out translational work. Lisa Jones: Super cool work to understand protein complexes and their structure in vivo. It is the in vivo part that is mind blowing. Also, she is automating her workflows to allow for higher throughput to address more biological questions and challenges. Peter Nemes: Was carrying out single cell proteomics before it was cool. He directly measures proteins in single cells with the precision and accuracy we all wish for.

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JEROME RANDON

Professor of Separative Methods, Institute of Analytical Sciences, France

Research focus... Jerome's research focuses on monolithic support for sample preparation and chromatographic separations, modification of surface properties of solid materials, and optimization of chromatographic instruments for miniaturized configurations.

JIM LUONG

Fellow, Analytical Science, Core R&D, Dow Chemical, USA

Predictions? Ultra-trace analysis in both targeted and open characterization with ever more complex matrices will be a focus. Matrix complexity will intensify as our society embraces the new norms of circular economies and sustainability, leading to more recycling of the current materials being used by the community.

Advice? Personal growth and change are all about evolution and iteration. The transformation of our lives is about moving into the "adjacent possible."

JOEL HARRIS

Professor of Chemistry, University of Utah, USA

Advice? In my experience, the best research outcomes are driven by curiosity and a motivation to understand and figure things out. Practical or technological applications can derive as a consequence of new understanding. The analytical sciences fit well into this paradigm, where novel and more capable methods of observation of the physical/chemical world can provide new insight that illuminates a path to solving practical problems. Curiosity to gain that insight makes coming to the lab a pleasure, so that working in the analytical sciences doesn't seem like work at all.



#2 JOHN YATES III

Ernest W. Hahn Professor, Departments of Molecular Medicine and Neurobiology, The Scripps Research Institute, USA

Up-and-comers? Rebekah Gundry, University of Nebraska Medical School is doing beautiful research on cell surface mapping. Nikolai Slavov, Northeastern University, re-invigorated the area of single cell proteomics with some breakthrough papers. Jeffrey Savas, Northwestern U Medical School, is doing pioneering research in the area of neurobiology, using studies of long-lived proteins. And Stacy Malaker Yale is taking on the analysis of the very complicated mucins.



#1 JONATHAN SWEEDLER

James R. Eiszner Family Endowed. Chair in Chemistry, Director of. the School of Chemical Sciences. & Professor of Neuroscience and. Molecular & Integrative Physiology at. the Beckmann Institute, University of. Illinois, USA

Heroes? I owe the reason I am an analytical chemist to my first real mentor and the first analytical chemist I worked with – Tomas Hirschfeld. I was fortunate to have worked with him as an undergraduate for three summers at the Lawrence Livermore National Laboratory. He encouraged independence and crazy, novel ideas, while always being available to help ground my ideas with advice and practical experience. After the first summer, he pointed me to a file cabinet full of one-to-two-page measurement science concepts – literally many hundreds of them – and encouraged me to read through the files and pick one or two projects to work on. The limitless ideas, combined with more resources than I ever imagined, not only made these summers exciting and unforgettable, they also influenced my development as a researcher and mentor. Many times I have asked myself, "What would Tomas have done?" when trying to figure out a path forward. I wonder whether my students occasionally ask themselves, "What would Jonathan have done?" when navigating their own scientific careers. I hope so.



JOSEPH LOO

Professor, Department of Chemistry and Biochemistry, University of California-Los Angeles, USA

Advice? Everyone says this: find your passion. I tell all the students I encounter this same message. It might take time to find what drives you, and that's fine. And your passion could change over time, and that's fine too. Some careers go in a straight line, and some zig-zag, with peaks and valleys, and again, that's fine. Trust what your passion is telling you.

KAREN FAULDS

Karen Faulds, Professor, Head of Bionanotechnology and Analytical Chemistry, Department of Pure and Applied Chemistry, University of Strathclyde, UK

Biggest challenge? The COVID-19 pandemic has of course brought major challenges, but it has also brought opportunities for scientists to work

together and quickly share data. On the other hand, it has had a big impact in terms of lost time in the laboratory by researchers, especially PhD students who have limited time to collect the data they need for their thesis. The impact the pandemic has had on the health and wellbeing of researchers is also immense due to increased workloads and the stress of having to carry out lab work in limited periods of time.

KELLY ZHANG

Senior Principal Scientist and Director, Genentech, USA

Instrument you couldn't live without? In the field of pharmaceutical analysis, HPLC is used the most and is indispensable – although some other instruments are critical too.

Predictions? I would expect to see more new analytical methods and technologies for cell and gene therapy, new drug modalities, and drug delivery technologies. There will be more leverage of data science, computation, machine learning, and AI in the field overall.



Feature



KOEN SANDRA CEO and Co-owner at RIC group, Kortrijk, Belgium; Visiting Professor at Ghent. University, Belgium

In another life... In hindsight, I could have chosen another job. I could have decided to pursue my childhood dream and become a pilot. I could have decided to become a professional soccer player like my cousin – if I had been talented enough. I could have decided to stick with my band members and tour the world and play the biggest rock festivals on this planet. No, instead I decided to become a scientist, I decided to step in the footsteps of my scientific father, I decided to marry a scientist, I decided to devote my life to science – life science. And to this day, I've not regretted a single moment.



LANE BAKER Professor, James F. Jackson Chair, Department of Chemistry, Indiana University, USA

Up-and-comers? I think Xin Yan at Texas A&M is doing some really interesting work at the interface of mass spectrometry and electrochemistry; Hang Ren at Texas has some fresh takes on electrochemical imaging; and Ashley Ross at Cincinnati has done some really nice work in expanding bio applications of carbon electrodes and fast scan voltammetry.

Instrument you couldn't live without? Undoubtedly, the scanning ion conductance microscope!



LINGJUN LI Vilas Distinguished Achievement Professor of Chemistry and Pharmaceutical Sciences, Charles Melbourne Johnson Distinguished Chair in Pharmaceutical Sciences, School of Pharmacy and Department of Chemistry, University of Wisconsin, USA

Advice? Analytical science has evolved as the "central science" that enables and impacts multiple areas of discoveries and advancements. Its interdisciplinary nature allows an analytical scientist to work at the interface of chemistry and biology to push the boundaries of each field while solving significant biomedical problems. So have an open mind and seek opportunities to collaborate with researchers from diverse fields and backgrounds.

KEVIN SCHUG

Professor & Shimadzu Distinguished Professor of Analytical Chemistry,-University of Texas, USA

Herocs? It has been a rough past couple of years on this front, because I recently lost my closest heroes and mentors. My father passed away two years ago. He was a retired chemistry professor; I actually took PChem in graduate school from him. He was my foremost role model regarding what a life as a professor could be like. I am not necessarily speaking of chemistry, because his area was hard core quantum mechanics, but rather that you could have a good and happy life as a professor. I saw the flexibility he had and his enjoyment working with and teaching students; he made it seem fulfilling. He retired the same year I completed my PhD. Since then, he was always very interested in the chemistry I was doing. Earlier this year, I also lost one of my best mentors, Harold McNair. There is no amount of praise that would be sufficient to recognize the selflessness of Prof. McNair and his genuine interest in your life and happiness. Alongside that demeanor, he was an amazing teacher. I count myself lucky to be among the many people he touched with his life. I also take it seriously that, what he taught me, I should pass on to benefit others. He taught me to always "pay it forward." I miss these two men in my life.



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S Feature

TOP 20 LISA JONES

Associate Professor of Pharmaceutical Sciences, University of Maryland, USA

Advice? Surround yourself with people who genuinely support you and are not afraid to tell you when you are wrong. Try to ignore the inside voice that says that you don't belong. You worked hard to get here, and you deserve it as much as anybody else. Learn to say no when you can. And have fun!





LJILJANA PAŠA-TOLIC

Laboratory Fellow and Lead Scientist, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, USA

Biggest breakthrough? Over the last decade, the scientific community has embraced the challenge of single-cell and single-particle measurement technologies. The advancements in these technologies are of paramount importance to understand and control biology at the cellular level for human health and the planet's health.

Advice? "You may not control all the events that happen to you, but you can decide not to be reduced by them." This quote by Maya Angelou has helped me navigate through many professional and personal challenges. No matter what happens, you can take the next step, react, and respond in your own way.



LUIGI MONDELLO Full Professor of Analytical Chemistry, University of Messina, Italy

In another life... From a young age, I have been drawn to chemistry and physics, and I have relished tackling challenges and practical problems. However, my strong passions are linked to motors (motorcycles and super cars), sailing, and diving. I would like to work in one of these fields, as a mechanical engineer or as a marine biologist.

Heroes? Keith Bartle is for sure one of the most important people I met in my life. The period I spent in his lab at the University of Leeds (1992–1993) definitely changed my life. He trusted me and gave me the opportunity to network with many scientists working in my field all around the world. At the same time, he gave me the freedom to start working with natural products and essential oils in his lab, and to focus on really different topics.

LIVIA S. EBERLIN

Associate Professor, Baylor College of Medicine, USA

Biggest breakthrough? Advancements and the availability of high resolution MS instrumentation that allow incredible sensitivity and chemical specificity has really expanded our ability to perform molecular analyses of complex biological samples in a way that is extremely powerful for disease diagnosis, but also to identify molecular changes that were previously undetectable. If I compare the first mass spectra I acquired from human tissue in my PhD to the data we get today from the same samples, it is truly mind blowing to see how many more molecules we can not only detect (over 30 times more!) and chemically characterize today!

Biggest challenge? In the field of MS in particular, I think the pandemic has shown us that MS instrumentation is still behind in terms of robustness, user friendliness, and portability when compared to other molecular-based technologies - like PCR.

So a current challenge is how to make MS instrumentation truly user-friendly and thus broadly expand its use in society.



Stories of Success

The 2021 Power List celebrates the outstanding individuals who have been recognized by their peers as real success stories in the field of analytical science. Here, our industry sponsors explain how they overcame challenges to achieve success in their efforts to support the analytical science community. Stories of Success: Andrew Alliance - A Waters Company Nigel Skinner, Head of Marketing, Andrew Alliance, Geneva, Switzerland, describes how the company's vision has evolved over the years, shares the secrets to success, and highlights lessons learned along the way



What was the original vision of Andrew Alliance?

The company's original vision was based on several observations about life science laboratories made by our co-founders. Firstly, a huge amount of time is taken up by well qualified people doing a lot of manual pipetting – is this really the best use of an analysts' time? Secondly, the more you rely on a human being, the higher the likelihood of errors occurring.

There was a need for something at the right price point that could bring automation to the bench where it's less about throughput and more about freeing up the analyst's time to focus on higher level tasks. And that was the vision behind our first generation of robots.

How has that vision changed over the years?

We've evolved a lot since the original Andrew robot. At the beginning of 2019, we launched a new portfolio of products: the Andrew+ Pipetting robot and the Pipette+ guided pipetting system. These new products were based on five years of working very closely with customers and understanding their needs. Lab research teams have become more dispersed and are collaborating over large distances; to meet this trend, we incorporated cloud file sharing into our products.

Traceability was also an important need for our customers. The Pipette+ system provides the benefit of not having to do the programming yourself, while still allowing a human to carry out the pipetting. This saves as much as 85 percent of the time, and you can essentially run robot or guided pipettes using the same script. This is very powerful, particularly if you're a CRO.

What's the secret to your success?

Without a doubt, amazing agility across all the functions of the business. We work very closely with users and have been able to take their feedback via "INTERCOM" – where customers connect directly to customer support via the software to get real-time solutions to a problem. Not only does this system get customers back up to speed quickly, but it also means we can capture feedback in terms of what customers would like to see. We can then build those improvements and push them out to users via the cloud.

What advice can you offer those navigating a similar journey?

Engage with as many customers as possible. The more you do that, the more you can both understand their challenges and more credibly articulate their viewpoint. And that's especially important when you are the size of Waters; essentially, you must represent the voice of the customer. Also, be prepared to change tack. Rather like a sailing boat, constant course adjustments are normal and not unusual!

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Stories of Success: Tosoh Bioscience

Christian Rohrer, Director of Sales and Marketing, Tosoh Bioscience, shares key successes in the 50 years since Tosoh's initial HPLC column launched, the secrets to these successes, and what the future holds for the company



It's been 50 years since the TSKgel HPLC column launched, kickstarting Tosoh's journey to success in macromolecule analysis. Could you tell me a little about this?

In 1971, Tosoh developed the first TSKgel column for GPC analysis – very shortly after HPLC was first described in a 1966 publication. Later, we developed a full suite of columns for HPLC, but size-exclusion chromatography (SEC) columns are still a core part of our expertise today. Of course, other chromatography media, SEC instrumentation, and MALS detectors have been added in the years since, but it's the TSKgel column brand that really kicked off our chromatography story.

What has been Tosoh's key success over the years?

We are particularly proud of the fact that our columns (and associated SOPs) are used around the world in many different quality control departments. This is a huge achievement for us because it shows that a lot of customers – particularly in the biopharmaceutical arena with SEC – rely on Tosoh's columns for high-quality results. It has been great to see Tosoh continue to be a leader in this space.

What are some of the secrets to that success?

As chromatography experts ourselves, the different teams within Tosoh have always developed methods and products in close collaboration with customers and other experts around the globe to help our clients develop therapies against lifethreatening diseases. I think that has been key to our success; it has allowed us to not only meet customer needs, but also foresee and anticipate future trends.

What are you most excited about for the company's future?

Monoclonal antibodies have been the go-to biomolecule for the last decade. As challenging as the COVID-19 pandemic has been – and still is – it has led to amazing developments in mRNAbased technologies and I'm very excited about the use of such technologies in other disease areas. When you look at biomolecules that are currently approved for therapeutics – such as siRNA or antisense oligonucleotides – I think we'll start to see a lot of new technologies entering this space. Then, there are also the delivery vehicles involved in these therapies, such as virus-like particles and lipid nanoparticles; these are as important as the drug itself.

We're in a very good position at Tosoh. Our background in SEC and our range of current products means that we can help customers across these areas analyze and produce biomoleculebased therapies. I think Tosoh's chromatography solutions will play an important part in the development of these technologies within the medical sector – and that's very exciting.



Stories of Success: PEAK Scientific

Jonathan Golby once wanted to fly planes; instead, he's steering PEAK Scientific's expansion into global markets as its CEO. Now, regardless of where you are in the world, PEAK has an engineer available to support.



Did you always see yourself in business leadership?

The short answer is no, not exactly! I studied business law at university, but my intention was to become an airline pilot ... Sadly, I just wasn't very good at it. After working for the BBC in a number of roles, ten years ago, I joined PEAK, where I was tasked with setting up a global service infrastructure with a particular focus on Asia and Australasia. I spent a lot of time building relationships with instrument manufacturers in Asia to create a service delivery model in addition to the after-market sales model - both significant aspects of our business. I was also involved in setting up many of our overseas entities and offices. After 18 months, I was asked to take on the sales and marketing director role, which I did for about four years before taking over as CEO.

It has been a fascinating journey. I didn't join PEAK with the intention of becoming CEO; I just tried to do the best in the roles I was given. I certainly gave it a lot of consideration before taking the job. But I loved the company and appreciated the fantastic foundation the owners created so, in the end, there was only one answer I could give. It's an exciting job and I've enjoyed every second of it.

What have been the major highlights of your time at PEAK?

The global scaling of the business has been a real highlight. I think we punch above our weight as a small business based in the west of Scotland – we've become a multinational company with a fraction of the resources and headcount you'd expect from such a business. We've set up offices everywhere from São Paulo to Tokyo and most places in between. And the fact that we now have service people all around the world means our clients can feel confident in partnering with us; as a result, we've become the first choice for many instrument manufacturers.

What sets PEAK apart?

We've worked hard to employ likeminded individuals around the world, which is essential to ensuring we remain true to our culture. You get the same familiar feeling every time you walk into a PEAK office, no matter where in the world you are. But we're also obsessed with customer success. We realized early on that the relationship between customer and instrument manufacturer goes beyond making a sale. With that in mind, our aim was to ensure that, regardless of where a customer is located, we'd be able to send a PEAK-trained engineer out to support them. This is something we have achieved that really sets us apart.

We also place a strong focus on R&D and we've heavily invested in our engineering departments, with two bespoke buildings focused solely on R&D. We collaborate closely with instrument manufacturers so that, by the time they release a new product, we've already tested our offering and fitted it to their new system.

Something that can get overlooked is our focus on the supply chain. One of our unique features is that we act like a much bigger multinational "We collaborate closely with instrument manufacturers so that, by the time they release a new product, we've already tested our offering and fitted it to their new system."

company when it comes to bringing supply chains together. We have global distribution centres where we stock finished groups of units so that we can supply more rapidly than any other manufacturer. Have you faced any major challenges as a company?

We're a fast-growing business, which brings challenges. For example, it can be difficult to predict exactly how a new market will react – especially when launching a new product. But we made a conscious decision not to grow for growth's sake; it must be controlled. The most fundamental thing is to ensure that we never forget our existing customers by focusing on new markets. Sometimes, refining and improving existing processes and products is the best way to grow.

What lies ahead for PEAK?

What are you excited about? One area I'd like to highlight is the Internet of Things (IoT). I think that will change the way our model works and the way in which we use our products in terms of remote monitoring and product servicing – helping us toward our goal of zero downtime for customers. I'm also passionate about the work we're doing on the environmental side. We've already put a number of policies in place, such as eliminating gas bottle deliveries with on-site gas generation, and we're looking closely at altering the way we move products around the world and the materials and packaging we use to reduce our environmental impact – ultimately aiming for net zero.

We're also maturing as a company – shifting mindset from that of a small, entrepreneurial company to a more established business. I'm actually really excited about refining our processes, governance, and guidelines – making sure we're growing in the right way to support our customers across the globe. We've come a long way in the decade since I joined, and I can't wait to see where we'll find ourselves in another 10 years.



www.peakscientific.com

Stories of Success: Markes International and SepSolve Analytical Alun Cole, Founding Director of Schauenburg Analytics Ltd, the parent company of both Markes International and SepSolve Analytical, shares how the vision for these companies was realized over the years



What was your vision for Schauenburg Analytics, Markes and SepSolve?

In 1997, my co-partner and I established Markes with the aim of offering supplies, expertise, and product solutions for the measurement of trace level volatile and semi-volatile organics (SVOCs). We later joined the Schauenburg Group and went on to set up Schauenburg Analytics as a parent company to Markes, expanding into other areas of analytical measurement. Our vision was to establish a "family" of small, focused analytical instrument businesses with access to global distribution and a central development capability. Each business retains its specialized knowledge and openness to innovation, while retaining the scale and infrastructure of more conventional global companies.

How has that vision been realized over the years?

The first step was establishing Markes as a market leader in the sampling and enrichment of VOCs and SVOCs using thermal desorption. In line with the desire to offer a broader portfolio, we acquired Time-of-Flight technology (TOF) and subsequently commercialized the BenchTOF GC-MS. When Markes joined Schauenburg International and Schauenburg Analytics was formed, a central development team was created to further refine the BenchTOF platform, develop solutions for comprehensive GC, as well as novel data analytics and software for real-world applications.

In 2016, SepSolve was founded with the mission to provide expertise, application knowledge and support for complete GC and GC-MS workflows incorporating Markes' leading expertise and technology in sample extraction, thermal desorption and the group offerings in BenchTOF, GCxGC and data analytics. SepSolve has since gained widespread reputation, especially in markets such as petrochemicals, flavors and fragrances, and breath biomarkers.

What makes you stand out from your rivals?

We enable our customers to discover more and deliver more outcomes from every sample. How do we do this? We have an intimate understanding of our technology and wide application knowledge across the entire workflow, from sample introduction to data analytics. We've also mastered the unique balancing act between maintaining the strength of independent businesses while harnessing the benefits of a centralized global group.

What are you most excited about for the future of your companies?

There's a tendency today to expect easy access to information – comprehensive information. We've seen increasing demand for our expert knowledge, capabilities and data analytics and I think this trend will continue. Moreover, our business model is expandable, and we have an open invitation to businesses with complementary specialized services or products to join us and benefit from our global infrastructure and centralized technology innovation group.





www.Markes.com and www.SepSolve.com

Stories of Success: Hamamatsu

From working with CERN to developing new medical scanning technology, Marco Mayer, Think Tank leader, Hamamatsu Photonics Europe, explains how Hamamatsu is driven to improve society through optoelectronic innovation



What is Hamamatsu's origin story?

Hamamatsu originated from Tokai Electronics Laboratory in 1948, eventually becoming Hamamatsu Photonics K.K. in 1983. Although particularly known for its pioneering work in photomultiplier technologies, Hamamatsu Photonics has been continually pursuing technologies involving "light" in all its aspects. It was hard to imagine the impact optoelectronics would have in our lives and across such a broad range of industries back then. Over the last 30-something years, we have built upon our original innovation and are now in every corner of the optoelectronic industry.

What makes Hamamatsu different?

Early in the company's development and expansion, we realized our products were very specific – and, therefore, required a specialist team to market them effectively. We are really proud of our people here, who are all specialists in their own right. As a company, we have built a huge wealth of knowledge and experience in this field, which has attracted close – almost symbiotic – relationships with our clients. Our R&D teams, innovators, and sales force keep in close communication, effectively bringing the whole company into direct contact with our customers. We invest heavily in R&D, which is invaluable for our clients. And we pride ourselves on our reliability as we foster long-term relationships.

How do you stay ahead in such a dynamic field?

We are highly focused on our field, which allows us to become more a partner to our clients than a simple sales service – and this relationship is very important to us. Our customers include both small and large companies in a wide selection of industries, including research institutes, analytical service providers and medical equipment specialists. Each and every client has a particular and often unique requirement. Fortunately, we are innovative and flexible, which allows us to meet these specific needs. Just as importantly, we also listen carefully to our customers, which allows us to adapt and ultimately grow with them as they push forward the boundaries of their particular sector. We offer a customized and bespoke service relationship and will support every customer throughout their endeavors – large or small.

What does the future look like for Hamamatsu?

Our overarching spirit here is to help society improve as much as we can. For instance, we are very proud to have been involved with the CERN proton accelerator program since the beginning; we dedicated ourselves to maintaining our role as a sole supplier of a series of components for the project. The same philosophy remains today as we work within the medical field to improve scanning technology – replacing our own older technologies with the new. We can only achieve these things by continually working closer and closer with our clients.

> HAMAMATSU PHOTON IS OUR BUSINESS





LUTGARDE BUYDENS Full Professor of Analytical Chemistry and Dean of the Faculty of Science, Radboud University, The Netherlands

Biggest challenge? COVID-19 and the climate crises have made it clear that society is demanding a major and accelerated science effort to cope with global challenges. However, without meaningful analytical data there can be no meaningful progress. We will have to collaborate beyond the conventional boundaries of the current technologically-oriented subdomains, such as spectrometry or chromatography. As analytical chemists, we have used and further developed artificial intelligence and data science already for decades. This experience will prove invaluable to accelerate and consolidate the ever-larger volumes of analytical data into sound and meaningful information that can mitigate major global challenges.



MARTIN GILAR Scientific Fellow, Separations R&D group, Waters Corporation, USA

In another life... My teenage aspirations were to spend most of my time on my computer, and grow long hair my parents would not approve of. During the pandemic in 2019-2020, I came dangerously close. That being crossed off my list, I need to come up with a new plan. Write a science-fiction novel? Prospect for gold and minerals? Fly into outer space? I am working on it.

MELISSA HANNAH-BROWN

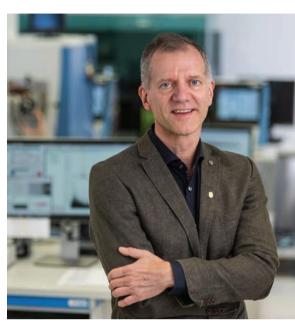
Global Technology Strategy & Partnerships Lead, Worldwide Research,

Development & Medical, Pfizer Medicinal Sciences; Executive Board Chair, Community for Analytical Measurement Science

Biggest challenge? A loss of identity and community which is already impacting the funding, perception

of our field, leadership development opportunities and innovation focus. This is why in the UK and Ireland we have formed the Community for Analytical

Measurement Science (CAMS) which has a core purpose of strategically connecting the community to bring focus and funding a round industry innovation challenges which are being delivered at pace by future leaders in our field.



#4 MATTHIAS MANN

Professor of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Munich, Germany; Director at the NNF Protein Research Center, Denmark

Heroes? By far the largest influence on my scientific life has been the late John Fenn (Nobel Prize in Chemistry 2002). He was the kindest and most modest person you could imagine and treated his lab members more like family than employees. He also always went against the grain and was very successful doing this. Peter Toennies, Director at the Max Planck Institute, where I did my master's degree, was one of the best experimental scientists in Germany and excelled in completely different ways. Finally, Peter Roepstorff in Denmark who really got me to apply MS to biological problems.

Änalytical Scientist



MICHELLE REID

Scientist, Bioanalytical Chemistry, Cristal Therapeutics: Guest Researcher. Maastricht University (M4i). The Netherlands

Biggest breakthrough? Currently, I'm excited about MALDI-2 developments, since we are finally seeing that age-old critique of additional separation of MALDI-MSI data being addressed by timsTOF instrumentation. Biggest challenge? I think we're still navigating how to manage big data, whether it be storage of large datasets or processing big data. Additionally, there are interesting multi-omics approaches and experiments that need optimal data integration tools. *Heroes?* Apart from my academic advisor, Richard Yost, I've long considered Tiffany Porta Seigl, Mike Lee, Alaa Othman, Timothy Garrett, and R Elaine Turner as outstanding mentors. Renã A S Robinson and Emily Ehrenfeld are my (s)heroes.

MICHAEL BREADMORE

Professor of Chemistry, University of Tasmania, Australia

Biggest breakthrough? The advancement in microelectronics and microcomputers and their application in chemical analysis is really starting to change the field of portable analysis.

In another life... I'd probably be a lawyer as I started doing a science/law degree until I saw the light... What I would like to be doing is making bespoke and unique Australian beverages and food products.

Advice? Think differently. Forget the box There is no box

MIKHAIL SAVITSKI

Team Leader and Head of Proteomics Core Facility, European Molecular Biology Laboratory

Instrument you couldn't live without? My research has heavily relied on the Orbitrap mass analyzer invented by Alexander Makarov.

Predictions? I think we will see tremendous further development of functional proteomics which will revolutionize our

understanding of cellular mechanisms. Advice? Strive to find a balance between work and the rest of your life. Identify things that make you happy and energize you. The happier you are, the more things will flow and ideas will appear.



Feature

#5 MICHAEL RAMSEY

Sciences and Minnie N. Goldby

Advice? Analytical Chemistry is tangible in these cases and turning



MILTON LEE

Emeritus Professor of Analytical Chemistry, Brigham Young University; Chief Science Officer, Axcend LLC, USA

Advice? When I started at Brigham Young University some 40 years ago, I was advised to look for opportunities for collaboration. Taking this advice, I've had the pleasure to work with colleagues in environmental biology, developmental biology, microbiology, plant science, chemical, mechanical and electrical engineering, physics, and so on.

NORBERTO PEPORINE LOPES

Professor of Organic Chemistry, Department of Biomolecular Sciences, Faculty of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Brazil

Biggest Breakthrough? At the beginning of the last decade, the development of MALDI-MS/MS allowed us to image substances of low molecular masses. As I work mainly in the area of natural products, this new approach has allowed us to answer important questions about the evolution and physiological function of these substances. With this technology, we were able to prove for the first time the existence of a chemical barrier acting as a photoprotector on the leaf surface of species from Brazilian savannas and the accumulation of substances that prevent ovulation of workers in stingless bees, among others. No doubt this advance will continue to have a major impact on the interface between analytical chemistry and natural products chemistry.



TOP 20 NEIL KELLEHER

Walter and Mary Elizabeth Glass Professor of Chemistry, Molecular Biosciences, and Medicine, Northwestern University, USA

Up-and-comers? Nikolai Slavov, single cell proteomics; Andrea Radtke (NIH), IBEX technology for multiplexed antibody-based imaging. I call them "Generation N.ext" – my informal name for the coming generation of transdisciplinary scholars and entrepreneurs that will take us through 2050.



NICOLE PAMME Professor in Analytical Chemistry, Stockholm University, Department of Materials and Environmental Chemistry, Sweden; Visiting Professor, Department of Chemistry, University of Hull, UK

Instrument you couldn't live without? The humble mobile phone. We have turned to using the cameras embedded in our smartphones as detection devices. We are using these when developing analytical measurement systems for Citizen Science at the river-bank and for farmers in the field. *Predictions?* Diagnostics will play a bigger role. Home diagnostic tests - the COVID crisis has brought their importance to the forefront, and we are likely to see much more activity here in the future.

PAUL W. BOHN

Arthur J. Schmitt Professor of Chemistry and Biomolecular Engineering, Professor of Chemistry and Biochemistry, and Director of the Advanced Diagnostics and Therapeutics initiative, University of Notre Dame, USA

Advice? Don't be afraid to try something new. Science is a conservative social construct, with a strong prejudice that people should "stay in their own lane." Yet, some of the most powerful discoveries come from bringing the insights and experience of addressing one set of problems to a new scientific challenge. In addition to bringing a fresh perspective, scientists moving into a new area are not burdened with already knowing "what won't work." Last, I would note that I think most of us relish our careers in science, at least in part because it continually presents

> us with opportunities to learn new things, and moving into unfamiliar scientific terrain is a great way to do this.

Feature

PAUL HADDAD

Emeritus Distinguished Professor, Australian Centre for Research on Separation Science, University of Tasmania, Australia

Advice? The single, strongest piece of advice I have is to be flexible and to avoid becoming compartmentalized. In my view, there is a tendency for new PhD graduates to feel that they have specialized knowledge in just the field in which they have completed their PhD. This overlooks all the generic skills they have gained along the way – skills in problem-solving, scientific writing, hypothesis testing... If new graduates see themselves as both specialists and generalists, a wide range of career opportunities will emerge.

PETER

SCHOENMAKERS Van't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands

Biggest challenge? The greatest challenge is to identify (health, food, environmental) crises before they arrive. This requires high-resolution non-target analysis and very smart data analysis.

Predictions? Just like we are seeing the progression of selfsteering cars, we will progress more and more towards self-steering instruments. The need may even be greater, because there is a greater shortage of qualified analysts than qualified drivers. Advice? HAVE FUN! Science in general and analytical science in particular is demanding and doesn't pay well. So why be a scientist if you don't enjoy the excitement, the freedom, and the dynamics

of a young

environment.



TOP 20 PERDITA BARRAN

Director of the Michael Barber Centre for Collaborative Mass Spectrometry, The University of Manchester, UK

Up-and-comers? Rebecca Beveridge (University of Strathclyde) for her brilliant work on disordered proteins with MS. Charlotte Uetrecht (HPI and XFEL) investigates structural changes of viral protein complexes with modern MS methods. And finally, Lisa Jones (University of Maryland, Baltimore) uses lasers and MS to locate proteins in cells.

Heroes? So many! But as I get older, it's all the brilliant women who have managed to be academic leaders over the past 50 years – they rock!

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🕑 Feature



PHILIPPE SCHMITT-KOPPLIN

Director of the Research Unit Analytical BioGeoChemistry at Helmholtz Zentreum Muenchen, Germany and Director of the Foodomics Platform at the Institute of Analytical Food Chemistry, Technical University of Munich, Germany

Biggest breakthrough? After a decade in microseparation sciences with capillary electrophoresis coupled to MS in the 1990s, I discovered Fourier transform ion cyclotron resonance MS in the early 2000s – versatile high throughput applications to profile simultaneously and rapidly tens of thousands of small molecules in food chemistry, environmental sciences, space chemistry and health metabolomics, describing the chemical diversity of biomes and abiomes. Real breakthroughs have been made over the past 10 years to boost resolution and sensitivity in magnetic resonance-MS systems.



PURNENDU DASGUPTA

Hamish Small Chair, University of Texas at Arlington, USA

Instrument you couldn't live without? A high-resolution digital microscope. In another life... I'd be writing poetry! Advice? Read the newest – but don't forget the classics.



PHILIPPE WILSON Professor of One Health, Nottingham Trent University and Chief Scientific Officer, NHS Willows Health, UK

Advice? Dare to innovate. Some of the best projects I've become involved in have been at the fringes of my (then) expertise but have made me learn, grow, and succeed - all in that order. If something fascinates you, go for it and see where it leads. Don't listen to the Imposter Syndrome on your shoulder; we all get it. My trick has been to acknowledge it is there, and plough on ahead regardless. Also, it's important to understand how you work best. Personally, I know that I work well when a large team is working with me on my projects, and with a huge variety in these programs of work. However, that is not for everyone, and others prefer to really concentrate on very specific areas. Understanding how you work best from an early stage can go a long way to charting out a successful career trajectory.

RACHEL POPELKA-FILCOFF

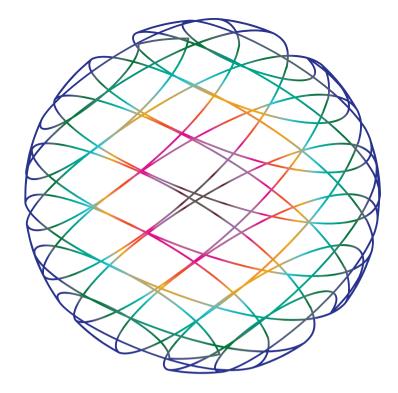
Rock Art Australia Minderoo Chair in Archaeological Science, School of Geography, Earth and Atmospheric Sciences, Faculty of Science, The University of Melbourne, Australia

Heroes? I'd like to acknowledge all my mentors and supervisors throughout my career, but particularly women analytical chemists and mentors who are 5–10 years ahead of me in their careers. These

women not only demonstrate excellence in science, but are also role models in leadership that supports everyone. They are: Claire Lenehan (Flinders University), Amanda Ellis (University of Melbourne) Liz Mackey (NIST).

Advice? Explore and stay true to your passions. As archaeological science and analytical science crosses disciplines, you may feel encouraged to be limited to a particular direction. The intersection of natural and social science and their perspectives is where the excitement happens.





OPPORTUNITY PITTCON TOGETHER

Pittcon is a catalyst of scientific advancement for you, your research, your career, your company, and together, our world. Our aim is to provide you with unparalleled access to the latest advances in laboratory science, to the instrumentation enhancing your work, and to an international assembly of scientists experimenting, discovering, and innovating within areas of focus that include:

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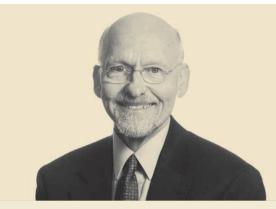






RENÃ ROBINSON

Associate Professor of Chemistry, Dorothy J. Wingfield Phillips Chancellor's. Faculty Fellow, Department of Chemistry and Department of Neurology; Leader of Outreach, Recruitment, and Engagement, Vanderbilt Memory and Alzheimer's. Center; Training Faculty, Vanderbilt. Brain Institute, Vanderbilt Institute of Chemical Biology, Vanderbilt University, USA; NOBCChE President-Elect *Biggest challenge*? Accessibility. The amazing technologies that exist currently across the field of analytical chemistry are helping to solve a number of biological, environmental, medical, and multidisciplinary applications. However, to realize their full potential these technologies have to be accessible to individuals outside of our field. This will require innovations in instrument design that include easy user interfaces, portability, affordability, and simple readouts.



TOP 20RICHARD SMITH

Chief Scientist and a Battelle Fellow in the Biological Sciences Division, Pacific Northwest National Laboratory, USA

Controversial opinion? With the power and flexibility of IMS approaches, and other ion manipulations, such as those possible with SLIM (particularly extended ion storage and reactions), I believe the use of relatively slow liquid phase chromatography separations will be increasingly displaced. In some cases LC may be used for off-line fractionation, but in many others it will become unnecessary.

In another life... I'd be working with a new technology of some sort. I am a hopeless technophile, and love problem solving – I'm endlessly fascinated by the challenges involved in everything from robotics to constructing a quantum computer.

RICHARD VAN BREEMEN

Professor of Pharmaceutical Sciences, Linus Pauling Institute and College of Pharmacy, Oregon State University, USA

In another life... Instead of pursuing a career as an analytical scientist, I would probably have focused on the development of fuel cells or batteries. Growing up during the Apollo space program in the 1960s, I was fascinated by the fuel cell used to generate electricity from hydrogen and oxygen on board the Apollo spacecraft.

As an undergraduate chemistry major, I had planned a summer internship during 1979 at the Lewis Research Center near Cleveland, Ohio, (now the NASA Glenn Research Center) where the Apollo fuel cell was developed. When this internship was canceled due to budget cuts, I was fortunate to obtain an amazing summer position in the pharmacology laboratory of the late Larry Fischer at the University of Iowa, where I operated a quadrupole MS for the first time. During that internship, I used GC-MS for the quantitative analysis of human metabolites of the anti-seizure drug diphenylhydantoin. In 1981, I joined the biomedical MS laboratory of Catherine Fenselau at the Johns Hopkins School of Medicine for my dissertation research on phase II drug metabolism and have continued to carry out related research ever since!





ROBERT KENNEDY

Hobart H. Willard Distinguished Professor of Chemistry, Chair, Department of Chemistry, University of Michigan, USA

Instrument you couldn't live without? It is not an instrument exactly, but we have cleanroom for fabricated microfluidic devices. Life was exceedingly difficult before that. Now we can make designs rapidly in glass or PDMS based on designs developed the day before. The cleanroom yields high success rates. It makes me much happier.

Heroes? In the past, when I answer this question, I have emphasized Ralph Adams, a pioneering bioanalytical chemist, and my mentors Mark Wightman and Jim Jorgenson. I'd like to add Isiah Warner to my hero list. Isiah Feature C45

overcame much to become one of the most accomplished analytical chemists ever. Further, he used his stature to assist other African-American students to succeed as scientists. He is an inspiration in many ways.

ROHAN THAKUR

Managing Director, Bruker Daltonics, Germany

Nominator comment: Rohan led the team that introduced the timsTOF Pro as a commercial instrument, which researchers have used to advance the field of proteomics. Rohan has since helped launch an instrument for single cell proteomics. His mind is always on the science and how to progress the field.









ROHIT BHARGAVA Founder Professor and Director, Cancer Center at Illinois, University of Illinois at Urbana-Champaign, USA

Biggest breakthrough? The biggest breakthrough in our field has been the ready availability of tunable lasers across the mid-IR spectral region. With the availability of quantum cascade lasers, a widely tunable, high intensity source became available. This technology has changed our field. It has spurred the development of new instrumentation, fast imaging, and novel capabilities, and it promises to be the basis of many more advances.

In another life... I would probably be a material scientist, focusing on specialty polymeric materials. Having joined graduate school to learn more about polymer processing and making composite materials, I instead got interested in characterizing them and the tools that we used.



ROY GOODACRE Professor of Biological Chemistry, University of Liverpool, UK

Advice? Find a research area, perhaps a little bit niche, that you are passionate about and committed to. Think about translating science - and I don't mean from analytics to the clinic, I mean look at other disciplines and see how those principles can be translated into the research arena that you are passionate about. And remember to walk before you run! It takes years to establish something that you can feel proud of, so patience and perseverance are essential. It's not a race and I believe it's better to be right than first.

SHAOPING LI

Distinguished Professor and Deputy Director, State Key Laboratory of Quality Research in Chinese Medicine, University of Macau, China

Biggest challenge? In terms of Chinese medicine, the single biggest challenge facing quality control is the discovery of effect related components that may greatly contribute to the efficacy of herbs by affecting the solubility, stability, bioavailability, and interaction of active compounds.

Änalytical Scientist

Advice? Be happy to work, diligent to learning and insistent on success.





#9 RON HEEREN

Imaging, Maastricht University; Director of M4i. The Maastricht MultiModal Molecular Imaging

I would coach students to take full

#8 RUEDI AEBERSOLD

Professor of Molecular Systems Biology and Chair, Department of Biology, ETH Zurich and Faculty of Science, University of Zurich, Switzerland

Instrument you couldn't live without? An ESI tandem mass spectrometer. Essentially all our work depended on these types of instruments. Without these, proteomics as we know it would not be possible. The progress in the performance of the instruments over the last couple of decades has been incredible. Today, even the protein contents of single cells can be analyzed – to some extent. Some speculate that other powerful approaches will displace MS as the key technology in proteomics, but I can't see that happening anytime soon. For sure, some aspects of proteomics will be taken over by faster, simpler or cheaper techniques, which are now emerging. But the incredible flexibility of MS to not only identify protein species, but to also determine their functional state, their interactions with other proteins or nuclei acids, or to identify the site and type of PTM's will remain key tasks for MS.

Feature



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SUSAN RICHARDSON

Arthur Sease Williams Professor of Chemistry, Department of Chemistry & Biochemistry, University of South Carolina, USA; President of ASMS

Feature

In another life... I would be hunting dinosaur fossils in Wyoming!

Heroes? I have many heroes and mentors through the years. In addition to Fred Menger, my PhD advisor who taught me physical organic chemistry, Mary Jane Mattina and Al Thruston taught me most of what I know about mass spectrometry. And I would like to give a special shout-out to Sam Karickhoff, who was a great mentor to me at the US EPA. He was the one who created the log KOW concept and the SPARC chemical prediction model. He taught me how to put my mind in the mind of a chemical.



SHELLEY MINTEER

Dale and Susan Poulter Endowed Chair in Biological Chemistry, University of Utah, USA

Advice? The life of a scientist is an exciting ride, but only if you aren't afraid of trying new techniques and going in new areas. Enjoy the ride, but remember that sometimes the pot holes in the road are more educational than the scenery.



SUSAN OLESIK Professor, Ohio State University, USA

Predictions... I predict the field will develop smaller and more sensitive analytical measurement devices. *In another life...* If I wasn't an analytical scientist, I'd probably be a farmer!



VALÉRIE PICHON

Professor, Sorbonne Université in Paris; Director of the Department of Analytical Chemistry (LSABM) and Co-director of the Institute of Chemistry, Biology and Innovation (CBI), ESPCI Paris, PSL University, France

Biggest challenge? We must think more and more about developing green methods and thinking about the impact that our methods, as a whole, can have on the environment.

In another life... If I were not an analytical scientist, I would be bored! This field can, depending on our specialties, lead us to work with all socio-economic sectors, which makes our work so exciting and rewarding.

TOP 20 VICKI HOPPER WYSOCKI

Professor of Chemistry and Biochemistry, Ohio State University, USA

Heroes? John Fenn was a great colleague and mentor when I was at Virginia Commonwealth University. He was a talented scientist who went on to win the Nobel Prize, but he was also one of the most humble scientists I have ever met. He attended our joint analytical chemistry group meetings at VCU and he would say, "I'm just another student." Because both of us had grown up in Kentucky, he would also sometimes say to me, "I'm just a simple Kentucky boy." He was a great role model for our graduate students, always asking questions when he didn't understand something – he never worried that he might not look "smart," if he asked a basic question.





VICTORIA SAMANIDOU

Professor of Analytical Chemistry, School of Chemistry, Aristotle University of Thessaloniki, Greece

Controversial opinion? LC-MS/MS is not always the most efficient equipment. Humble, simple HPLC systems can make miracles when used appropriately. Thus we have to put emphasis on improving chromatographic separation despite the benefits offered by hyphenated techniques. your own that follows your vision, your dreams, and your passion for analytical science.

Advice? Don't follow any path, create

YI CHEN

Principal Investigator, Institute of Chemistry, Chinese Academy of Sciences; Professor, University of Chinese Academy of Sciences; Professor, Huaiyin Institute of Technology, China Feature 🚭

Biggest Challenge? How to effectively perform in vivo analysis of biologically significant compositions, with spatiotemporal resolution.

Predictions? It would be great if the ratio of AI-related analytical strategies and methods could be increased gradually. *Heroes?* My hero is James Clerk Maxwell.

YING GE

Professor of Cell and Regenerative Biology, and Chemistry, Director of Human Proteomics Program, University of Wisconsin-Madison, USA

Advice? Be perseverant and follow your passion. You can do anything you set your mind to; you will accomplish something amazing during your lifetime.

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THE POWER LIST SLAM

As part of our 100th issue celebrations, we invited a handful of early career researchers to tell us what they're working on, why they're passionate about analytical science, and whether they have a "grand plan" for their careers. Join us – as we celebrate the potential Power Listers of the future.



ADAM M.A. SIMPSON PhD Candidate.

Mitch Lab, Civil & Environmental Engineering, Stanford University, USA

The elevator pitch... Food disinfection is necessary to help prevent food-borne pathogenic outbreaks. However, many chemicals used during food disinfection, such as chlorine, can react with internal biomolecules and biopolymers in the foods (for example, proteins, lipids, carbohydrates, vitamins, and pigments). These transformation products are covalently bonded inside of foods and are only liberated in consumers during digestion. Research on F-DBPs is very young – but, based on my findings, the transformation products are toxic.

The "grand plan"... I hope to continue my research as a tenure-track assistant professor at an R1 institution. I'm mostly excited to develop young researchers and see them thrive in any career direction they want to pursue. I also have a strong interest in Science Communication: I have a YouTube channel (titled: "Adam MA Simpson") where I aim to humanize academia with a focus on STEM higher education. As a Jamaican-American Dual Citizen of mostly African descent, I also often feature underrepresented minorities in Academia, where they talk about their road to academia, how their research impacts society, and common misconceptions they'd like to dispel. The aim is to show the public that there is a space in STEM for everyone. In the long run, I'd like to produce a talk show where I can help scientists answer questions from everyday people and pop-culture icons.



ALBA ALVAREZ-MARTIN Postdoctoral

researcher, AXIS Research Group, NANOlab Center of Excellence, Department. of Physics, University of

Antwerp, Belgium

The elevator pitch... My father is a sculptor, so I grew up surrounded by all kinds of materials (wood, metal, paints, varnishes, and so on). From a very young age, I learned to appreciate the immense work that goes into both the creation and preservation of a piece of art. While seeing my dad deal with problems associated with the yellowing of coatings, the loss of consistency or cracking, an obsession started to grow in my head: how can I contribute to maintaining the beauty of art? I did not inherit any artistic skills, but I have focused my

scientific career on understanding the chemical interactions associated with the degradation of museum artifacts. Today, I study the degradation of historical organic pigments that have been used by painters such as Van Gogh, Gauguin, or Rembrandt. These complex pigments are metal-dye clusters that change their conformation over time. With ESI-Orbitrap, we can detect those small changes over the lifetime of a painting. In addition, these clusters can interact with other components in oil paint, leading to the gradual loss in vibrancy of the original color. These chemical changes can be monitored by using a combination of spectroscopic and high resolution-MS techniques. The ground-breaking aspect of the project is the unique approach of using micro-destructive techniques to drastically improve our understanding of the molecular fragmentation pathways of organic pigments and to expose their triggers.



BREN MARK B. FELISILDA

Postdoctoral Fellow, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

The elevator pitch... Society's increasing need to transition into a sustainable

entries will be

future requires an energy sector dominated by renewables - especially for energy conversion and storage. At the heart of these developments are breakthroughs in materials design and synthesis. Conducting polymers are a known material for such applications, but the use of additives, such as surfactants, in manufacturing changes their properties, leading to decreased performance. My research aims to explore the use of the electrochemistry at soft polarized interfaces as a disruptive platform technology to enable controlled interfacial electrosynthesis without the need for additives. Exploring the use of "greener" alternatives, like Fenton's reagent, as polymer oxidant will also combine the advantages of "green" chemistry and interfacial electropolymerization.

The "grand plan"... As a first-generation scientist and coming from a minority background, I know first-hand the struggles of having limited resources and not having someone to look up to in my chosen field. However, all of these did not stop me from trying to achieve my dreams and, hopefully, I can be that "someone" for any aspiring scientists from the "barrios."



GEORGIA MAY SINCLAIR

PhD Candidate at RMIT University. Victoria, Australia

The elevator pitch...

There are over 4700 manmade compounds in the environment right now, including poly- and perfluoroalkyl substances (PFAS). We know the dose makes the poison, but we don't know what impact PFAS are having on ecosystems at the concentrations they are being detected – little is known about the effects of PFAS, especially the longterm biochemical effects on organisms. I want to determine the effect of PFAS on aquatic organisms, using metabolomics. I want to contribute to the development of molecular markers for PFAS exposure to aid in the development of environmental PFAS regulations that are effective in fully protecting the environment.

The "grand plan"... I aim to continue in environmental toxicology research and to contribute to understanding the overall effects of contamination in our wetlands and our terrestrial systems using analytical science. I want to contribute to policy and guideline regulations to protect the environment from anthropogenic

causes.

SRISHTI JOSHI

Postdoctoral Research Fellow. Centre of Excellence. **Biopharmaceutical**

Technology, Indian Institute of Technology, Delhi, India

The elevator pitch... My research domain is the "analytical characterization of biopharmaceuticals," with a focus on characterization of critical quality attributes. The in-built quality of these products is a result of precisely controlled processes that result in structurally homogeneous products. Analytical characterization is essential for process control, as well as for evaluating the eventual outcome of the bioprocess (i.e. the drug product). The unambiguous evidence gathered for structural integrity or similarity from these exercises forms the bedrock for regulatory approval of these products. Therefore, a well-designed analytical characterization

platform is critical to manufacturing safe and efficacious biodrugs. My research involves using multiple chromatographic and spectroscopic techniques towards development of precise, accurate, robust, and affordable analysis for biotherapeutics.



Postgraduate Research Student, Low Carbon Energy and Technologies (LCERT), The University of Nottingham, UK

The "why"... I enjoy the multidisciplinary nature of analytical science. There are so many research teams that will, at some point, need an analytical scientist to help answer their really important questions. My days are incredibly varied as I get to collaborate on projects across a vast array of fields - one day I am looking at petroleum fractions and the next single cells or skin tissue. This means I am always learning about new areas and being exposed to cutting edge science.

The elevator pitch... We are investigating ways to prevent the formation of insoluble fuel deposits in internal combustion engines. Deposits are prolific and lead to significantly higher levels of vehicle emissions, especially particulates. They are also tricky to analyze, so we are using state-of-the art MS techniques (mainly using 3D OrbiSIMS) to tell us what's in our samples and where the key chemical species are located. We collaborate with Innospec, a specialty chemical company with manufacturing and research centers across the world. They use our crucial data to develop new chemical additives to clean engines by removing deposits - and that means our work has a real-world impact and will help to reduce vehicle emissions and improve global air quality levels.

Extraction of Pesticides and Flame Retardants by the Empore[™] SDB-XC Disks



EPA Method 527 is a targeted list of 26 semi-volatile organic compounds in drinking water designed to detect and quantify various pesticides and chemical additives in flame retardants. For example, numerous pesticides in EPA 527 are classified as pyrethroids, which are a chemical class of pesticides that are highly effective insecticides. While pyrethroids generally have low mammalian toxicity, they are known to be toxic to aquatic organisms, including fish. Examples of herbicides and organophosphate pesticides can also be found within the list of target compounds. Other major chemical classes of interest in EPA 527 are polybrominated biphenyls (PBB's) and polybrominated diphenyl ethers (PDBE's). Chemical species belonging to these classes are often used as additives in flame retardants and are also known carcinogens to humans.

In this application note, multiple extractions are performed simultaneously by the Empore[™] EZ-Trace (catalog #8000) to extract semi-volatile organic compounds from reagent grade water samples using the 47 mm Empore[™] SDB-XC SPE disk (catalog #2240). Extractions are performed on the EZ-Trace under the negative pressure of a vacuum pump.

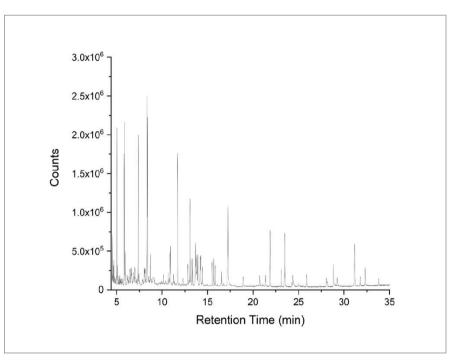


Figure 1: Chromatogram of 26 analytes, three surrogates, and three internal standards. Analytes have a concentration of 2 μ g/L in the water sample.

| Water | Reagent | Grade Water |
|-----------------|--------------|--------------|
| μg/L | 1.0 | 2.0 |
| 70-130% | 24 | 26 |
| avg Rec. (%RSD) | 102.7 (15.8) | 102.6 (12.7) |

Table 1: Summary of results for three different concentrations of PDS (primary dilution standard) in reagent grade water and one sample of tap water.

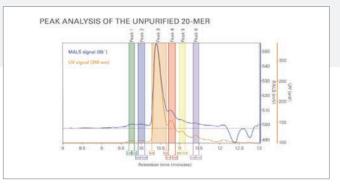
The extract is evaporated, diluted, and then analyzed via GC-MS. The extract analysis was performed on a Shimadzu GC-2010 Gas Chromatograph with a splitless injection port interfaced to a Shimadzu GC-MS QP2010 (Kyoto, Japan) and a $30m \ge 0.25 \mu m$ MilliporeSigma GC column. The accuracy and precision for the recoveries of 26 analytical standards are determined from the four-point calibration curve of each standard (Figure 1).

As allowed by EPA Method 527.1, the permissible recovery range is between 70% and 130% with \leq 20%. For the both samples of the reagent grade water, the average recovery was 103% with 16% and 13% RSD for 1 and 2 µg/L respectively (Table 1). Recoveries were within the acceptable limits for 92% of analytes while 96% of analytes were within the acceptable RSD limit. For the five compounds known to produce high recoveries, their accuracy and precision were all within the limits set by the EPA method. These results demonstrate that the CDS Empore[™] EZ-Trace, combined with the Empore[™] SDB-XC SPE disk, provide a clean and efficient screening method while still producing high analyte recoveries for the compounds listed by EPA Method 527.1.

A Perfect Match for Oligonucleotide Analysis: Size Exclusion UHPLC and MALS Detection

Oligonucleotide-based therapeutics such as antisense oligonucleotides and siRNAs are already being used as therapies for previously untreatable diseases and further molecules are being developed. The characterization of the product and its impurities is a challenge as both are structurally similar, while their effectiveness differs. Detection and characterization of oligonucleotides and impurities is simplified by combining the high resolution TSKgel® UP-SW2000 size exclusion column with the highly sensitive LenS3 multi-angle light scattering detector (MALS).

An unpurified oligonucleotide with a length of 20 bases was injected onto a UHPLC-SEC column (TSKgel UP-SW2000) resulting in a profile containing the product, shortmers as well as components larger than the product. Subsequent MALS



| Peak | Retention time | % RSD | MW (Da) | % RSD |
|------|-------------------|-------|---------|-------|
| 1 | 9.774 | 0.1% | 13,599 | 2.1% |
| 2 | 10.012 | 0.0% | 11,550 | 1.9% |
| 3 | 10.398 | 0.1% | 6,398 | 0.7% |
| 4 | 10.776 | 0.1% | 5,751 | 1.5% |
| 5 | 11.053 | 0.1% | 5,177 | 2.3% |
| 6 | 11.422 | 0.2% | 4,446 | 5.5% |

detection with LenS3 determined the molecular weight of product and impurities for precise sample characterization.

Read the full application note here: http://bit.ly/Oligo-Analysis



PERFECT MATCH FOR OLIGONUCLEOTIDE ANALYSIS

- HIGH RESOLUTION UHPLC COLUMN FOR SIZE EXCLUSION: TSKgel® UP-SW2000
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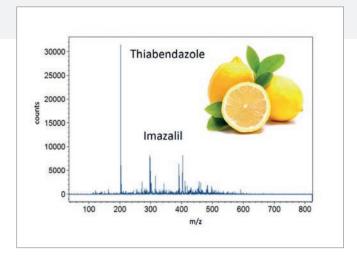
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TOSOH BIOSCIENCE

Detection of Residual Pesticides on Fruits and Vegetables Using Portability[™] Miniature Mass Spectrometer

Mass spectrometry can now be deployed for on-site pesticide screening in real time

A case study for residual pesticide screening on fruits and vegetables is reported. All produce was purchased from a local market in San Jose, California and immediately analyzed by TD-ESI coupled to the PortabilityTM mass spectrometer without any sample preparation. The portable analyzer was able to detect ppm levels of pesticides such as thiabendazole, imazalil, flutolanil, and permethrin. Featuring light weight and compact size, BaySpec's novel mass analyzers based on linear iontrap technology are the most sensitive portable devices



available on the market with parts-per-trillion detection sensitivity. These extremely compact instruments are simple to operate and maintain, and they are ideal for a variety of bulk or trace on-site detection in real time. Learn how you can bring the lab to the sample with portable analytical tools from BaySpec by reading our educational application note for pesticide screening of produce.

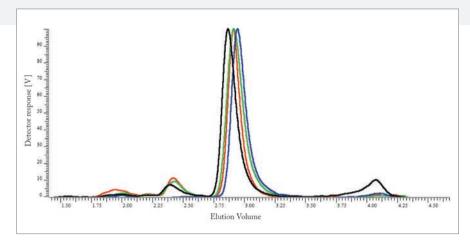
Read the full app note at http://tas.txp.to/1018/ANBaySpec



Solutions 🗐 55

Analysis of Bevacizumab by SEC-MALLS using a YMC-SEC MAB column

Size exclusion chromatography (SEC) is a standard technique for analyzing monoclonal antibodies (mAbs). It is also a standard separation mode used in quality control to obtain information about aggregation and/or fragmentation of the mAb. Detection by light scattering, e.g. multi-angle laser light scattering (MALLS), can provide additional information, as the signal intensity is also influenced by the molar mass in contrast to usual concentration



detectors such as UV or RI.

In this application note, YMC's dedicated SEC column for antibodies, YMC-SEC MAB, has been used to develop a method for Bevacizumab (Avastin®) using MALLS detection. Different buffers, flow rates and injection volumes were tested to achieve a robust method with good resolution. Compared to UV detection, the MALLS signal shows two higher molar mass species, aggregates of Bevacizumab. A phosphate buffer with 0.3 M NaCl and a flow rate of 0.33 mL/min appeared to be the most suitable conditions.

Download the application note with the full method details here https://ymc.de/files/Bevacizumab.pdf



Spotlight on... **Technology**

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The PAL Dynamic Headspace module is a plug-and-play option for CDS 7000C concentrator. This module adds dynamic headspace capability to PAL RTC/RSI rail in a closed system that is compliant with USP 467, EPA 5035A and 8260C soil methods, with max temperature of 300 °C. *https://www.cdsanalytical.com/ purge-trap-7000c*



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UCT's all-new Micro-Prep[™] is a 96well micro-elution plate that features SPE disk technology designed for streamlined sample clean-up and analyte enrichment. It is ideally suited for automated, high-throughput sample prep workflows for biological sample types such as urine, serum and plasma. https://www.unitedchem.com/producttag/micro-prep/



MET ONE 3400+ Series Portable Airborne Particle Counter

An air particle counter from Beckman Coulter Life Sciences that helps GMP cleanroom users simplify their routine environmental monitoring and improve data integrity. This counter features Microsoft Active Directory for User Name and Password control for logon and electronic signatures to support 21 CFR Part 11 compliance.

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cryoRaman – Cryogenic Raman Imaging Microscope from WITec and attocube

Designed for existing and emerging challenges, cryoRaman offers VIS to NIR excitation lasers, 1.8K to 300K operating temperatures, high magnetic fields to 12T, unique cryogenically compatible Ramanspecific objectives, an exceptionally precise piezoelectric scan stage, TCSPC modes, low-wavenumber Raman peak detection, and full polarization control. *https://www.witec.de/cryoraman/*



New PTR-TOF 10k Trace VOC Analyzer

The new IONICON PTR-TOF 10k offers real-time VOC analysis with the unprecedented insights of a mass resolving power of up to 15,000 m/ Δ m. The novel combination of high-resolution time-of-flight with reliable and robust PTR-MS technology is an asset for challenging samples and complex gas matrix that can be monitored in real-time with this analyzer. *https://www.ionicon.com/products/ details/ptr-tof-10k*



Next-Generation Time-of-Flight Mass Spectrometers for GC and GCxGC

The new BenchTOF2TM series of instruments deliver increased sensitivity and enhanced spectral quality and selectivity to maximise the amount of information extracted from every sample. An extended dynamic range, hydrogen carrier capability and the option to carry out both hard and soft EI help you discover more and deliver more in your laboratory.

https://chem.sepsolve.com/Spotlight/BTOF2

The Proteomics Ethicist

0

Sitting Down With... Matthias Mann, Professor of Proteomics and Signal Transduction, Max Planck Institute of Biochemistry, Munich; and Director at the NNF Protein Research Center, Copenhagen

What drives you forwards?

I'm immersed in developing proteomic technologies – and understanding how these precision tools can impact the study of cancer and other diseases. However, we are also very concerned with the ethics around the applied use of proteomics. Technology is advancing at pace, and it is imperative that we stop to consider the ethical implications of our efforts, and how, importantly, this is put into practice.

Throughout my career I have mostly been driven by technology. For instance, as a PhD student I was intrigued by how MS works and how this could be applied to studying biology, which was not as commonplace then as it is today. Some 30 years on, the technology has advanced considerably, and we are able to interrogate more and more complex systems. This forward motion shows no sign of abating, and it still captures my attention just as much now as it did when I was a PhD student.

How did you get to where you are today? I had a chance encounter with a visiting professor – John B. Fenn – from Yale whilst studying for my master's degree at the Max Planck Institute in Goettingen. He encouraged me to move with him to undertake a PhD. He is the inventor of the electrospray ionization technique for the analysis of biological macromolecules, and was awarded the Nobel Prize in Chemistry in 2002 – making this choice in my career a particularly fortuitous one!

I realized that, though physics and chemistry were well served by this kind of technology, John had demonstrated applications that stretched into biology – a very underserved discipline.

Molecular biologists at the time were starting to unravel complex biological processes, which required understanding and characterizing specific proteins. They would painstakingly purify the proteins using gels only to struggle with analysis because they only had access to techniques that required a lot of source material. And unfortunately, gels were not compatible with MS. We figured out how to make these proteins available for MS, devised the nanoelectrospray technique to increase sensitivity and created peptide sequence tags to allow protein identification. With the human genome sequencing project underway, we were able to identify various proteins for the first time, including telomerase and key proteins in the immune system.

How has modern computing impacted upon your work?

Computing power has ramped up significantly over the years. I'm somewhat unusual in that I come from a physics and mathematical background, which has stood me in good stead when it comes to harnessing such advances. I could write new algorithms and programs to handle complex MS data. I would say my perspective – very much shaped by my multi-disciplinary background – has helped me see biological problems in a different way and given me the ability to drive the technology forward.

Tell me about your interaction maps?

We work with and derive interaction maps that highlight the connections between various biological systems. It's basically network analysis – akin to the social network mapping used by Google and the likes. One such map is the protein interaction map, where protein—protein interactions can be mapped to help elucidate their function.

We became involved in a project to map a whole organism – the "holy grail" of interaction mapping! A network describing a cell is already in place and we have since been involved with repeating this work for a significantly more complex yeast cell. This work illustrates the progress the field has made in the last 20 years. Modern advances have allowed us to analyze these interactions using a fraction of the material required previously – and at much greater speeds and resolution. The impact of this progress is seen in human biology, where a newly identified protein can be dropped into a map to shed light on its possible function and utility. The next step is to explore these maps in a dynamic process, during some cellular activity or response over a specific timeline.

What are the implications for COVID-19 research?

The multiple waves of COVID certainly spurred us to see what our technology could add to the research landscape. In a fruitful collaboration, we used COVID-infected cell cultures to look at what was happening in the infected cell, including posttranslational modifications. We discovered that the virus uses cellular proteins to modify its own, which was not known at the time. We also looked at the interaction map to determine which proteins were interacting with which. These findings led to the postulation that some drugs could be repurposed for fighting COVID-19. We are also investigating patient body fluids and post-mortem tissues to aid disease prognosis and tissue-specific mechanisms.

What is the future for proteomics?

Proteomics has developed greatly over the last 20 years or so, with many good research groups in the field - and that's been coupled with the emergence of enhanced computer power and commercial collaborations. However, we still have a long way to go! That said, we now have higher sensitivity, we can mine a wider range of data and, critically, we need less sample. Modern techniques have real clinical utility as a small blood sample can be analyzed as a diagnostic for diseases. Such an approach can also be prognostic; for instance, where a breast or prostate cancer has not yet manifested but the patient is predisposed to such changes. These techniques may be used in determining the potential severity of the disease and inform better treatment stratagems. But such a direction calls into focus the ethical positioning of such tests as we do not want to over-diagnose. Specificity and sensitivity are critical to make it ethical to use such tests, especially when screening a large number of people.



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