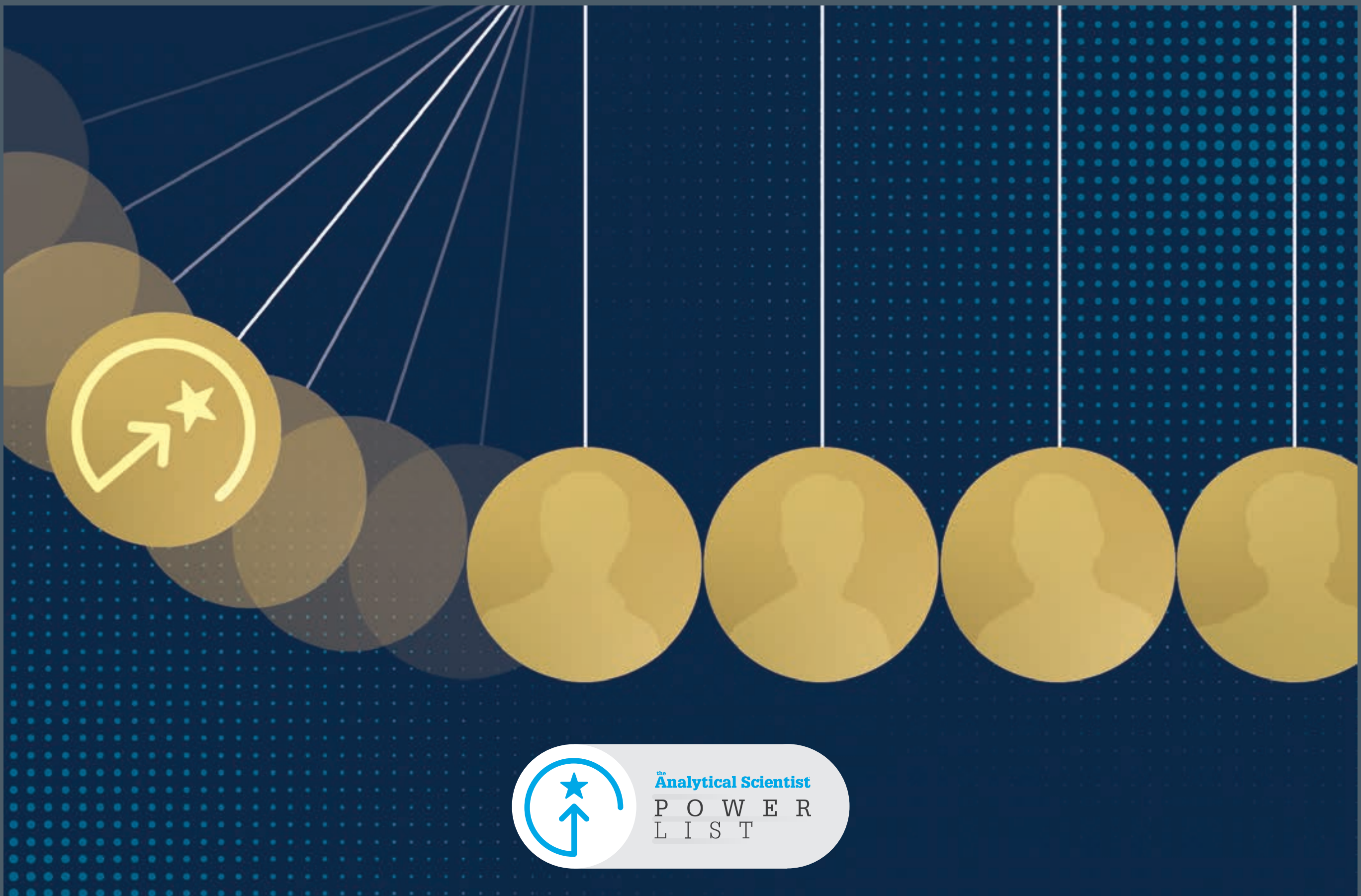
JULY / AUGUST 2023 # 112

the Analytical Scientist®



Ten Years of Impact

We celebrate 100 trailblazers, advocates, interdisciplinarians, and mentors

www.theanalyticalscientist.com

A Future-Focused Power List

Education and attracting talent, data handling and standardization, and raising the profile of the field are the biggest challenges facing analytical science in 2023, according to the Power List

This year's Power List (which begins on page 11) is different for a couple of reasons. First, we're recognizing the individuals whose excellence and impact has stood out over the past decade – a nod to our recent 10-year anniversary. Second, we've split the list into four categories – Inventors and Innovators, Leaders and Advocates, Educators and Mentors, and Connectors and Interdisciplinarians.

This year's Power List also represents another step in its ongoing evolution. Never before have we received so many words of wisdom from our nominees – far more than we could fit into a single print feature. So a big thank you to everyone who took the time to answer our questions. Today, the Power List is more than just a collection of the 100 most influential people in the world of analytical science, a celebration of past achievements, and a way to unite a sometimes disparate field; it is also a chance for the field's leading figures to paint a picture of the current state of the field – and to consider what the future holds.

What is the biggest challenge facing analytical science today? You'll find a snapshot of the answers we received on page 8. But a (rough) analysis of the full list of responses shows that issues related to education and attracting/retaining talent were most commonly mentioned, alongside data handling and standardization – each making up 21 percent of responses. "We are faced with a veritable tsunami of data that we need to be able to process quickly so that this stage does not become the bottleneck of analytical methods," says Davy Guillarme. Next, at 12 percent, was the reputation of the field. "There is a lack of recognition of measurement science at the molecular level as an intellectual pursuit in its own right," says Scott McLuckey – speaking for many. The final standout challenge at 10 percent was funding for fundamental research, which Gary Hiefje believes will "build the field and break ground for the future."

And what about the future trends on the horizon? Far and away the most popular emerging trend today, according to our Power Listers, is artificial intelligence (AI) – at 36 percent. "AI has the potential to revolutionize the way we tackle global transitional challenges," says Lutgarde Buydens. Then, high-throughput method development (11 percent), and sustainability (8 percent).

I hope that gives you a flavor of the insights gleaned from this year's Power List. But rest assured, nothing will go to waste – there will be plenty more content powered by our 100 Power Listers! As for The Analytical Scientist team? Well, we'll be exploring ways to raise the profile of the field, attract and retain talent, and make use of emerging AI technology to address the data challenge. Watch this space!

James Strachan
Editor

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KEYNOTE SPEAKER

"Fifty years of FACSS and SciX Conferences: The remarkable correspondence with advances in vibrational spectroscopy"

Peter Griffiths
Professor and Chair Emeritus, Department of Chemistry
University of Idaho, USA

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- NESAS and SAS Lester W. Strock Award
  Maria Montes-Bayón
- RSC Joseph Black Award
  Mathew Horrocks
- FACSS Charles Mann Award for Applied Raman Spectroscopy
  Juergen Popp
- The Coblentz Society Clara Craver Award
  Ishan Barman
- SAS and Applied Spectroscopy William F. Meggers Award
  Johannes Pedarnig

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Message in an Ancient Bottle

GC-MS uncovers the mystery contents of Bronze Age ceramic bottles

Gas chromatography-mass spectrometry (GC-MS) analysis of organic residues in ceramic bottles appear to have revealed an ancient trade in scented oils as long ago as the 3rd millennium BCE (1). The ceramic bottles, excavated from an archaeological site in Turkey, were suspected to have contained liquid, but no researchers had analyzed the residues inside them – until now!

A team of researchers at Selçuk University in Turkey analyzed the invisible micro-compounds in the inner walls of the ceramic and extracted the organic residues remaining in the pores of the ceramic structure into a liquid solvent. By putting this liquid through a GC-MS device, they detected organic residue molecules that showed what could have been held within each ceramic container.

Various traces of liquids were discovered, alongside dicarboxylic and oleic acids with large samples of palmitic acids. These substances suggest that a plant-based oil was contained frequently in these bottles. Specifically with diterpenoids presence, the team concluded that other ingredients were contained, such as conifer resin and other plant derived products – indicating that the containers were also used for scented oils.

Not only does this study highlight the importance of GC-MS in archaeological investigations, but it also provides the oldest evidence for trade in such commodities in the region dating back to the late 3rd millennium BCE.

"The different organic residues indicate that a range of different recipes were used and contained within the containers for an undisclosed period of time," says Ismail Tarhan, Associate Professor of Biochemistry at Selçuk University, Turkey, and lead author of this study.

"There are many studies that we'd like to conduct as an extension of this research," says Tarhan. "We're planning to consolidate the results of GC-MS analysis with the results of stable isotope analysis alongside colleagues in Europe and have received offers to conduct similar research with different excavations."

"We hope that exploring these avenues allows for more comprehensive analysis into our ancestors' livelihoods."

Reference

1. *I Tarhan et al., Archaeometry, 65, 4, 833–849 (2023). DOI: 10.1111/arcm.12852.*

ASD: Precision Medicine Powered by Metabolomics

Could a more detailed understanding of the metabolome lead to personalized treatments for autism spectrum disorder?

Given autism spectrum disorder's (ASD) complex interplay of genetic and environmental risk factors, a team of researchers from Brigham and Women's Hospital and Harvard Medical School in Boston, USA, wondered if the metabolome would reflect changes in pathways, providing a better understanding of ASD.

To test their hypothesis, they classified individuals with ASD into groups based on relevant clinical and diagnostic characteristics, before using UPLC-MS/MS to explore the differences between phenotypically-derived subgroups in terms of their plasma metabolomic profile (1).

They found distinct metabolic patterns between phenotypic subgroups – providing new information about the underlying biology that gives rise to diverse ASD traits. Co-author of the study, Rachel Kelly, says: "These identified pathways may represent important targets for more personalized medicine approaches to alleviate the burden of symptoms."

Reference

1. *N Prince et al., Brain Behav Immun, 111, 21–29 (2023). DOI: 10.1016/j.bbi.2023.03.026.*

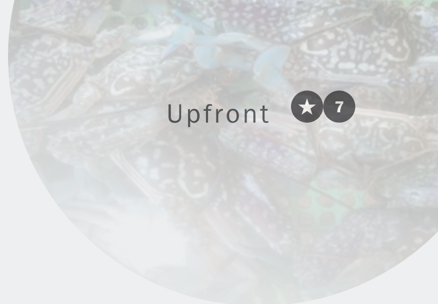
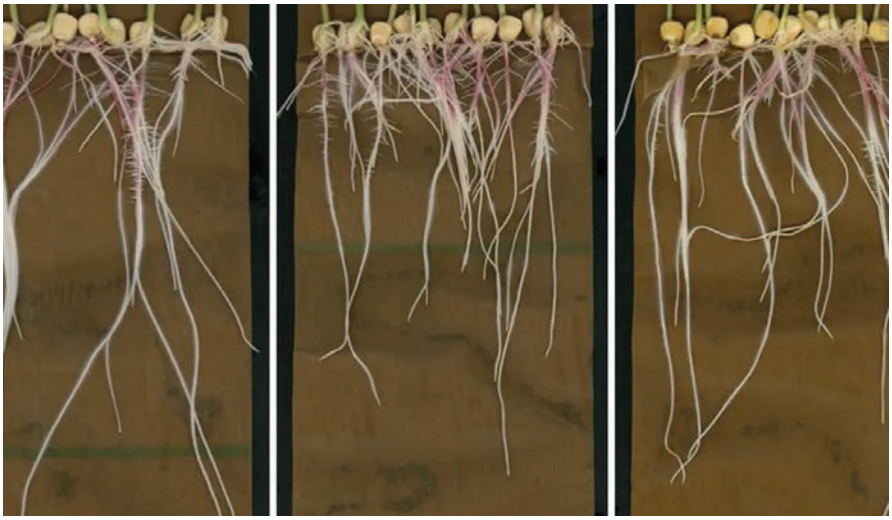


IMAGE OF THE MONTH



Below the Surface

Desorption electrospray ionization mass spectrometry imaging (DESI-MSI) has allowed a team of researchers at the University of California San Diego and Stanford University to chemically map the development of maize roots. This technique reveals a range of distribution patterns amongst small molecules across the stem cell differentiation in the root. From this discovery, scientists can form a roadmap to improved processes for agriculture, food production, and climate resilience.

Credit: UC San Diego (2023)

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QUOTE OF THE MONTH

"Innovators possess an inquisitive nature, constantly asking why, how, and when questions. They exhibit a strong curiosity and an unwavering desire to seek answers, even if they are unknown or challenging to obtain. Their mind does not stop until they have the answer. They approach problems with the mindset of efficiently finding experimental solutions when deemed necessary."

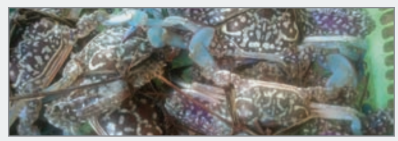
Pieter Dorrestein. See page 15.

Credit: UCSD Communications

Crustacean Creations

How crab shells could be used for biodegradable components in spectrometers

Seafood is delicious (sorry, vegetarians), but it also creates large amounts of solid waste; namely, crustacean shells. While working on an alternative use for crab shell waste, a team of researchers in the Philippines found a somewhat unlikely application: diffraction gratings – an essential component within spectrometers.



Credit: Efren Gumayan

Chitosan was extracted from the crab shells in crushed powder form and used to make bioplastic diffraction gratings through a replication process known as soft lithography. By analyzing the chitosan grating replicas with atomic force microscopy and diffraction experiments, researchers proved that the nanoscale groove structures are comparable to those made of silicone – providing a greener alternative.

Co-author Efren Gumayan says: "Once we've optimized the process, we could create green and cost-effective light-weight spectrometers."

As scientists across the world call out for more affordable, more sustainable, and more portable testing devices, will the crab have the last laugh? Probably not.

References available online

In My View

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

In *Our* View: The Grand Challenge

Twelve of this year's Power Listers answer one crucial question: what is the biggest challenge facing analytical science in 2023 – and beyond?

Scott McLuckey: There is a lack of recognition of measurement science at the molecular level as an intellectual pursuit in its own right. Progress in all of the molecular sciences obviously requires measurements, but the prevailing view among both scientists (outside of analytical chemistry) and funding agencies is that the measurement already serves the need.

Though many scientists will agree that many of our greatest discoveries and developments were made without a motivation to solve the measurement problems to which they are now applied, there is still a push to stick with a universally understood phrase: "necessity is the mother of invention." The laser was not developed with either femtosecond spectroscopy or reading bar codes in grocery checkouts in mind. Mass spectrometry was not developed to identify post-translational modifications of proteins. Magnetic resonance was not developed to locate tumors. Simply by looking at the subjects awarded with Nobel Prizes, we can see examples directly related to measurement science that emerged from origins quite distant from their ultimate impact.

Gary Hieftje: Excessive concentration on applications and chasing the most recent "hot" problem instead of emphasizing fundamental research and the development of novel instruments and methods. The latter will build the field and break ground for the future.

Albert J.R. Heck: The administrative burden and social-political agendas of today often interfere – preventing scientists from focusing on science. We need to foster fundamental research, ensuring that scientific talent can focus on their craft to improve the world for future generations to come.

Aebersold Rudolf: I see two big challenges facing the field right now. First, science policy and the ensuing trends in science funding have shifted from the investigation of fundamental principles towards generating rapid and tangible benefits for society. This is readily apparent in the life sciences, where large sums of research funding are allocated to translational research and where funding for developing new analytical methods or for studying fundamental principles of living systems across the incredible breadth of species is hard to come by. The consequence is the starvation of the innovation engine that eventually fuels translation.

The second challenge is the use of the flood of data generated by many analytical techniques to generate new knowledge. In the life sciences, the quality, breadth and volume of data that can be generated from minute amounts of sample is astounding. To create new knowledge from the data, computational tools have to be developed to explore the full richness of the data and new paradigms are required to explain the results. As an example, statistical associations are frequently used to detect connections within large datasets. New conceptual and computational approaches will be required to detect causal relationships between associated events.

Deirdre Cabooter: We need to ensure that students are sufficiently trained in the fundamentals, so they can adequately troubleshoot and truly understand what they are doing and for what reason. I am a little worried about some evolutions taking place in our education system at the moment, where there seems to be an increasing interest in developing soft skills at the cost of the basics. Of course, soft skills are important as well, but I think these can more easily be developed at a later stage when you're already active in a professional environment. It becomes much harder to catch up on the basics at later stages.

Chuck Lucy: High costs of purchasing and maintaining instruments is limiting students' hands-on experience. Miniature and portable instruments are helping with affordability, but it's an enduring challenge. Undergraduate research and industrial internships offer students the chance to play with instruments, gain confidence, and discover their passions. It's up to us to open our labs to our students.

Thomas J. Wenzel: From an educational perspective, it is incredibly challenging to find the time and resources to work with faculty members to create an active learning environment across all subjects. The effectiveness of active learning is critically dependent on the qualities of the instructor, but, unfortunately, there are many instructors that have very little experience in active learning. Beginners often need time and feedback from skilled practitioners to refine their effectiveness.

Jeremy Nicholson: For me, it's irreproducibility in science. Irreproducibility undermines scientific integrity by casting doubts on the accuracy and validity of research. It wastes resources as researchers invest time and funding into efforts that cannot be built upon or validated. This challenge has far-reaching implications for policy decisions, medical treatments, and technological advancements. Publication bias arises when only positive results are published, skewing the scientific knowledge base and impeding progress.

Moreover, replication crises in biomedical research raise concerns about the robustness of scientific findings. A lot of modern biomedical science is multidisciplinary and at the top end requires the integration of physical, mathematical, and biological sciences – this is a challenge to referees and journal editors, meaning that there is increased effort required to check if analyses are accurate or even appropriate. As an associate editor of a major journal, I see manuscripts making impossible claims based on statistically underpowered studies using poorly executed experiments and without appropriate validation on a daily basis. These problems can be found in the world's top journals (and far more often than you might think). Of course, this is driven by the ever-increasing demand to publish and raise grant funding in the background of an increasingly impatient world. However, we as scientists are responsible for delivering appropriate and data and models to serve societal demands. If we fail to do that, we are invalidating the thing that sets science apart from all other subjects: the pursuit of fundamental and objectively demonstrable truths.

Roy Goodacre: It's well documented that there is a reproducibility crisis in science – some of these issues are highlighted in "A manifesto for reproducible science" (1). The authors in this paper conclude that a staggering "85 percent of biomedical research efforts are wasted, while 90 percent of respondents to a recent survey in Nature agreed that there is a 'reproducibility crisis'." This may be dated information, but nothing has really changed.

In chemical analysis, the truth of our measurements should be immutable. For the analytical science field, this is usually represented by mass, abundance, and identity. As analysts, we should be prepared to stand by our data and our reasonings should be evidence-based. In metabolomics, there are significant challenges in metabolite identification. My team's opinion piece on this topic was published earlier this year (2), which further pushes this ideology – ensuring metabolite identifications are based on common sense, facts, and evidence.

Elena Ibañez Ezequiel: Sustainability is the biggest challenge today. We can have new equipment that is more accurate and sensitive, which can be used for studying different fields such as medicine, food, pharma, environment, etc., but we need to be aware of the need for developing greener procedures that can ameliorate the huge threats we have in front of us, such as climate change and sustainability.

Anthony Gachanja: A major challenge in science today is inclusivity for all – including major limitations in availability of facilities for scientists in developing countries. Without the ability to experiment and interact with scientific ideas, it is difficult to explore new territories. Science across YouTube is fantastic – providing opportunities to indulge firsthand, but lab work is still essential for that Eureka moment within research studies. Setting Centers of Excellence is a great step forward – setting up science camps for different grades of learners will keep the fire of science exploration burning.

Koen Sandra: There are multiple challenges revolving around the building complexities and logistics of our field. Therapeutic and prophylactic modalities are more complex, and it's becoming increasingly difficult to optimally handle and interpret the tons of information that our instruments generate on a daily basis. Costs continue to rise and there is a pushing concern for sustainability, yet while we continue to struggle to find skilled chromatographers and mass spectrometrists, our issues will continue. We need more hands on deck with critical mindsets – not just users of the dazzling analytical techniques available on the market.

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1. *MR Munafò et al, "A manifesto for reproducible science," Nat Hum Behav (2017). DOI: 10.1038/s41562-016-0021.*
2. *G Theodoridis et al, "Ensuring Fact-Based Metabolite Identification in Liquid Chromatography–Mass Spectrometry-Based Metabolomics," Anal Chem, 95, 8, 3909–3916 (2023). DOI: 10.1021/acs.analchem.2c05192.*

the Analytical Scientist

POWER LIST

The Analytical Scientist Power List returns to celebrate the successes of the field's leading lights! In the spirit of our recent 10-year anniversary, nominees were assessed for their excellence and impact over the past decade – across four categories: Inventors and Trailblazers, Leaders and Advocates, Connectors and Interdisciplinarians, and Mentors and Educators. We've limited nominees to a single category to create a list of 100 (25 per category) each with a ranked Top 10, but we recognize that many – if not most – of the individuals on this year's list deserve recognition for efforts across several areas. This is to be expected; after all, when you say "analytical scientist," what should come to mind if not: "innovator," "trailblazer," "leader," "advocate," "connector," "interdisciplinarian," "mentor," "educator"…

INNOVATORS *and* TRAILBLAZERS

#1 ALEXANDER MAKAROV

Director Global Research LSMS, Thermo Fisher Scientific, Bremen, Germany; Professor of High-Resolution Mass Spectrometry, Utrecht University, The Netherlands; and Fellow, Royal Society, UK

Qualities of an innovative thinker? A combination of phantasy and erudition to think outside of the box but not far enough to drown in the ocean of unrealizable ideas…

Making the most out of your invention… The most important thing is to create a team behind your invention! This is one of the main reasons for me to stay in industry: a multi-talented and a very versatile extended team that allows one to bring ideas into thousands of laboratories.

Picking a problem… It is always difficult and error-prone to decide which battles to fight – and, like in any battle, you need a bigger strategic goal to guide your direction, but also resources and capability to tackle the immediate challenge.

Biggest challenge facing the field? When it comes to mass spectrometry, I think that the generally insufficient rate of hardware miniaturization and commoditization is limiting expansion of this otherwise excellent technique!

#2 CAROL ROBINSON

Director, Kavli Institute of Nanoscience Discovery, University of Oxford, UK

Qualities of an innovative thinker? Not to be constrained by existing dogma. Just because something is predicted not to work, it doesn't mean it will never yield anything interesting. Early in my career, the widely held view was that proteins in the gas phase of a mass spectrometer would invert such that their hydrophobic core would be exposed. This is now clearly not the case. Had we not doubted this dogma, we might never have tried to fly protein complexes in a mass spectrometer.

Making the most out of your invention… I am often motivated by the issues that surround me. From COVID-19 to cancer, depression to dementia – these are conditions that have affected us all, whether directly or indirectly, and that makes me more determined to bring our tools to bear to try to bring new understanding and provide new insights.

#3 R. GRAHAM COOKS

Henry B. Hass Distinguished Professor of Chemistry, Purdue University, USA

Biggest challenge facing the field? A lack of appreciation of the intricacies of analytical science by other disciplines (especially chemists) who see it as little more than an exercise in measurement using commercial instrumentation. Like modern day pharaohs, the organic synthetic chemist commands – "measure it!" – without pausing to recognize the ingenuity that went into the slaves' work of conceiving the method, building the instrumentation and achieving useful performance criteria. The "measure it" request at the end of that multi-year process is often a simple application, but the process that allows it is a unique combination of new scientific insights and skillful technology.

Book for scientists? "Thing Knowledge: A Philosophy of Scientific Instruments" by Davis Baird. The book presents a formal epistemology of instrumentation, arguing that the conception of a new instrument is an act of fundamental science as the resulting device embodies all later applications, which merely represent applied science. This view is a corrective to the increasingly dogmatic opinion that only hypothesis driven research has intrinsic scientific value.

#4 JEREMY NICHOLSON

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

Qualities of an innovative thinker? There is no single quality that leads people to be innovators, that's why innovation is difficult to do and especially to teach. Scientific curiosity is a fundamental quality that drives an innovative thinker to explore and seek knowledge. leading to the discovery of new connections and possibilities. This usually works best in individuals with diverse educational and scientific backgrounds where a lot of unusual connections are already latent in their thought processes. Off-the-wall or non-linear thinkers usually have a renegade streak in them that leads to the rejection of traditional patterns of thought, to challenge assumptions, and explore unconventional ideas. Innovation often requires revolution and that results in opposition from traditionalists and linear thinkers. Thus, tenacity is also a crucial quality for innovators, as it enables them to continue in the face of challenges, learn from their failures, and stay focused on their goals until the rest of the world is ready to receive and understand their message. However, being too far ahead of the curve is always tough.

#5 CHAD MIRKIN

Director, International Institute for Nanotechnology & George B. Rathmann Professor of Chemistry, Professor of Chemical and Biological Engineering, Northwestern University, USA

Qualities of an innovative thinker? There are many. It is essential to be inquisitive, work hard, and work intelligently. Also, don't forget to enjoy the process. Don't be afraid to take risks or make mistakes; failure is a part of learning and growing.

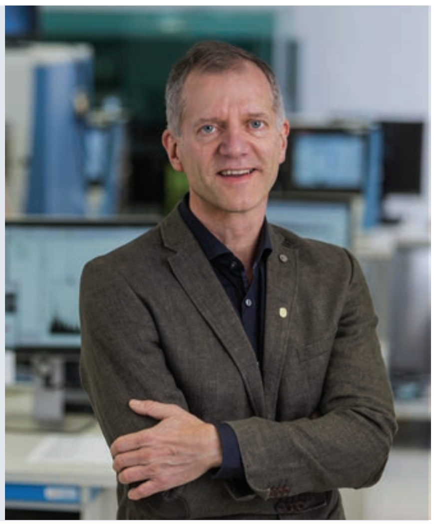
Making the most out of your invention… Be exceptionally critical. Identify a path to an invention to solve a problem that is worth solving and produce a product people will buy. If you wouldn't buy it, likely no one else will or should.

Picking a problem… In my group, we follow the science. Our approach is grounded in the scientific method, which allows us to explore new areas fearlessly. Fundamentally, we pursue ideas that are intellectually stimulating and that will open new avenues in science and ones that have great potential to lead to tools and processes that will benefit society.

#6 MATTHIAS MANN

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

In another life… I might be a computer person, specifically developing algorithms and analyzing data – preferably multi-dimensional proteomics data. One of my typical jokes: "I much prefer programming to working."



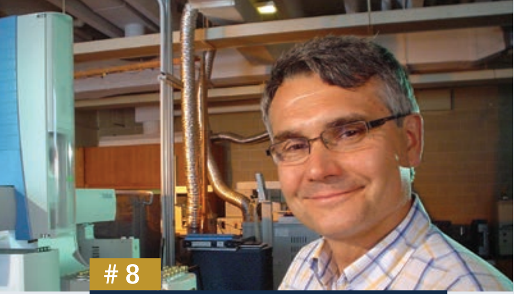
#7 JAMES W. JORGENSON

William Rand Kenan Professor of Chemistry, Emeritus, Department of Chemistry, University of North Carolina at Chapel Hill, USA

Qualities of an innovative thinker? Imagination – thinking "outside the box." This needs to be coupled with good judgment, to weed out the interesting but impractical ideas, which will otherwise dilute your productivity.

Making the most out of your invention… Teaming up with talented and experienced people who can develop, polish, produce and successfully market your invention. A wonderful idea or invention is just a seedling which requires expert assistance to nurture into full bloom.

Picking a problem… Tackle problems that people really need to have solved. Try to avoid developing a solution in search of a problem. Talk to your colleagues, and read the scientific literature broadly, to gain an appreciation of the important problems.



#8 JANUSZ PAWLISZYN

University Professor, Canada Research Chair, Department of Chemistry, University of Waterloo, Canada

Making the most out of your invention… Find the "killer application" – the application that is not addressed well by current technologies.

Biggest challenge facing the field? Designing portable devices to facilitate on-site, bedside, and in-vivo applications.

Missing from the toolbox? Simple rapid screening devices. Instrument companies are focusing on development of high performance expensive instrumentation for solving scientific challenges leading to important discoveries, however, analytical chemists also need smaller, low cost devices capable to perform high throughput, hopefully on-site determinations.

Controversial opinion? Non-experts should not run analytical chemistry courses.

#9 J. MICHAEL RAMSEY

Minnie N. Goldby Distinguished Professor of Chemistry, University of North Carolina at Chapel Hill, USA

Qualities of an innovative thinker? Curiosity – how can we solve this problem for which there is not an existing solution or how do we better solve a problem for which there is already a solution?

Making the most out of your invention… Perseverance – pushing through invention and demonstration of a new concept and then translating the technology into a commercial product. Achieving the translational part of this trajectory typically requires patenting of the fundamental concepts of your invention. Translation can be achieved through various paths such as licensing of patents to an existing company or founding and financing a company focused on development of your invention.

#10 RON HEEREN

Distinguished Professor, Maastricht University; Director, M4i, The Maastricht MultiModal Molecular Imaging institute; Member of the Dutch Academy of Arts and Sciences, The Netherlands

Qualities of an innovative thinker? Approach the world as if no boundaries on what is possible exist. Or stated differently, think in possibilities and not in restrictions. As soon as you think in restrictions, you limit your own possibilities to move beyond the state-of-the-art. This quality is amplified if combined with a healthy dose of curiosity regarding the world around you. Many innovations also occur serendipitously and unexpectedly following a surprise discovery or meeting with a colleague that asks an unexpected question that triggers you to think out of the box.

Making the most out of your invention… Collaboration, collaboration, collaboration! The translation of innovations into an applied domain requires the involvement of domain experts and people that complement one's own expertise to maximize impact. Making the most out of an invention/innovation is, just like the research itself, teamwork.

Book for scientists? The immortal life of Henrietta Lacks by Rebecca Skloot.

ERIN BAKER

Associate Professor, Chemistry Department, the University of North Carolina at Chapel Hill, USA

Picking a problem… To truly dive into a problem, you must love the area you are working in. There have been many times I have wanted to apply for a proposal because it seemed like a good chance for funding, but when I searched inside myself, I knew I could not really put my all into that research area. Therefore, I have passed on certain opportunities to really focus on studies I can be passionate about.

Missing from the toolbox? Many mass spectrometrists would love a soft, high-sensitivity ionization source that works for a wide range of molecules and has less ionization suppression than electrospray ionization. This would enable much higher throughput studies for complex samples, while also providing in depth analyses for more molecules.

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

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!

Advice? Work hard, collaborate with people with different expertise and enjoy yourself.

DAVID E. CLEMMER
Distinguished Professor of Chemistry & Robert and Marjorie Mann Chair, Indiana University, USA

Picking a problem… When I began my laboratory, I had very clear ideas about what I would work on. But, if I'm honest, I didn't know where they would lead. As my laboratory became more established it attracted a number of very talented students and postdocs. Usually, we began with a discussion of what they might work on and then returned after running experiments with data that took some time for me to understand. Often by the time that they presented the work to me they had a pretty good feeling for it. Essentially, the longer that it took me to understand it, the more likely it was that we worked together on the ideas into the future. Those experiments that went as planned were also important. But, we found ourselves testing the ideas that we didn't expect and this became what we were working on. Early on I worried about us spending our time in this way. Looking back, I'm not sure why this bothered me. It was that result that we couldn't quite pin down that required a new type of measurement.

PURNENDU (SANDY) DASGUPTA
Hamish Small Chair, University of Texas at Arlington, USA

Instrument you couldn't live without? A high-resolution digital microscope.

In another life… The near-impossible – trying to make a living writing poetry!

Advice? Think differently, but be patient. And don't be too hard on yourself. Nothing is that important. Have fun!

PIETER DORRESTEIN
Professor, Skaggs School of Pharmacy and Pharmaceutical Sciences, and Director, Collaborative Mass Spectrometry Innovation Center, the University of California at San Diego, USA

Qualities of an innovative thinker? Innovators possess an inquisitive nature, constantly asking why, how, and when questions. They exhibit a strong curiosity and an unwavering desire to seek answers, even if they are unknown or challenging to obtain. Their mind does not stop until they have the answer. They approach problems with the mindset of efficiently finding experimental solutions when deemed necessary. These thinkers recognize that the information taught in classes, found in literature, or presented in textbooks is a snapshot of knowledge at a particular time. They understand that human interpretation is involved, and that knowledge is subject to change. They approach existing knowledge with a critical mindset, always seeking to challenge, expand, and improve upon it.

Credit: UCSD Communications

LIVIA S. EBERLIN
Associate Professor, Department of Surgery, Baylor College of Medicine, USA

Making the most out of your invention… I think the secret is having a true passion for how your invention could change the status quo or solve a significant problem that is dear to you. Having the long term vision of what you invention can accomplish fueled by a personal passion for what you invented produces a deep perseverance and commitment for making it successful. I've been experiencing this with the MasSpec Pen technology that we invented in my lab – we truly love the technology and we know that it could bring incredible benefits to patients battling cancer, and the tangibility of that reality has helped us work through many challenges and tackle complicated clinical studies with the utmost commitment and passion to making it a reality in medical practice.

FABRICE GRITTI

Principal Consulting Scientist, Waters Corporation, USA

Qualities of an innovative thinker? To be able to bridge unsolved critical practical problems from today and all disciplines of fundamental physics and chemistry.

Making the most out of your invention… Any invention or innovation must be exposed to the application field at an early research stage for direct feedback in order to refine its development and guarantee its successful impact.

Biggest challenge facing the field? One important challenge concerns the huge amount of data to be collected and processed by the artificial intelligence algorithms used to boost accuracy, speed, and performance of future analytical tools.

Book for scientists? Quantum Electrodynamics: The Strange Theory of Light and Matter by Richard Feynman demonstrates that the most sophisticated theory in science can be understood by the layperson using everyday language, humoristic tone, and simple visuals.

FRANCES S. LIGLER

Eppright Chair and Professor of Biomedical Engineering, Texas A&M University, USA

Making the most out of your invention… Identify the customer with the most pressing problem that can be solved using your invention. Make sure that the development of the invention into a commercial/sharable product is done in such a way that the intended customer can use it to solve his problems in the simplest, most effective, fastest, and least expensive way possible. If your exact invention is surpassed during the development process, glory in the realization that you sparked an even better innovation!

CHRIS POHL

Technology Consultant, CAP Chromatography Consulting, USA

Qualities of an innovative thinker? The single most important quality in a truly innovative thinker is the ability to identify cases where consensus opinion is incorrect. There are many examples in science and in my own career where the consensus understanding of how something works or the inherent properties of a given material has been proven to be incorrect. The ability to see possible holes in the consensus opinion is critical when it comes to developing novel approaches to solving problems previously considered impossible.

In the background, two of Pohl's heroes, Thomas Edison and Albert Einstein.

JOEL M. HARRIS

Professor of Chemistry, University of Utah, USA

Making the most out of your invention… For me, the impact of my innovations have been greatly enhanced by collaborations. These relationships arise out of attending talks at meetings outside of my area, meetings with colleagues and visitors in my department to discuss research ideas, and occasionally someone coming with a measurement problem they have been unable to solve. The resulting conversations have provided a great mix of new science, questions that are unanswered, and opportunities for our measurement ideas to generate discoveries in areas beyond my own research experience.

RICHARD D. SMITH

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

Qualities of an innovative thinker? I think it is the step that follows the birth of the idea, concept, or invention, and achieving an effective balance between having confidence in it, and simultaneously being open to challenges to it, both from yourself and from others as it matures.

Most exciting development or trend? To me, the most important emerging development across our field is the effective integration of different data types, and particularly those involving larger and larger data sets.

ZOLTAN TAKATS

Professor of Analytical Chemistry, Department of Surgery & Cancer, Faculty of Medicine, Imperial College London, UK

Nominator comment: Professor Takats is an acclaimed inventor in the area of "ambient mass spectrometry" having produced breakthroughs in desorption electrospray ionization (DESI), rapid evaporative ionization mass spectrometry (REIMS) and the highly innovative iKnife that can be used by surgeons to see whether whether a tissue being removed is cancerous or not. This invention resulted in his election to the Fellowship of the Academy of Medical Sciences in 2021.

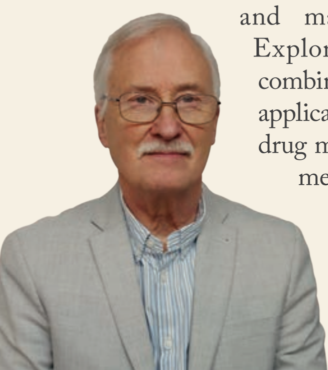
IAN WILSON

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

Qualities of an innovative thinker? If I were Mark Twain, I would probably say something like "laziness combined with intelligence and ambition" – such a person will find the quickest and simplest way to achieve their aims… But I'm not a truly innovative thinker like Mark Twain was!

Picking a problem… These days the problems tend to find me! Otherwise, I find that looking at one or two past problems that couldn't be solved with technology available at the time, provides some interesting opportunities.

Most exciting development or trend?? For me, it's the combination of highly efficient LC linked to ion mobility and mass spectrometry. Exploring what this combination can do with applications in omics and drug metabolism will keep me very busy for the next few years…



RICK YOST

Professor Emeritus, Analytical Chemistry, University of Florida, USA

Qualities of an innovative thinker? Persistence. If yours is a truly innovative, revolutionary idea, then many (most?) experts in the field will tell you that it won't work. That's probably a good sign that the idea is worth pursuing!

Missing from the toolbox? First, an LC system with the separation power of capillary GC that's easy to use. No matter how many "U"s you add in front of HPLC, we are still far away from routine LC separation that rivals capillary GC. And then I want an ionization technique for LC that is as universal and democratic as electron ionization (EI).

KELLY ZHANG

Distinguished Scientist and Director, Genentech

Qualities of an innovative thinker? I believe innovation happens at intersections. Collaborating with scientists from different disciplines helps me and my team to turn roadblocks into opportunities and come up with creative solutions.

Missing from the toolbox? There is a lack of analytical technologies that can holistically characterize complex samples. Different technologies and sample preparations are required to characterize one sample, but each technology can only provide a piece of the information, and often the original sample gets disrupted or altered during sample preparation and/or the process of analysis. This is especially challenging when dealing with complex drug modalities.

LEADERS *and* ADVOCATES

#1 VICKI WYSOCKI

Professor, Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio, USA

Raising the field's profile… I'm always puzzled when I meet scientists who don't seem to understand that analytical science is a field of research. Part of the problem is universities that don't provide structures that value analytical science – with divisional structures that don't include analytical science at all. Over the years, I've attended topical conferences where attendees come up to me and ask what molecules or disease I work on. They seem surprised that mass spectrometry instrument and method development could be considered a field of study! Fortunately, funding agencies and industry value analytical science. The fact that my graduating PhD students always have multiple job offers is telling – there is high demand for scientists who understand the value of measurement science.

Missing from the toolbox? I am hopeful that in the future, we will integrate the data from multiple tools much better than we've been able to. The key is creative computational work that brings data from disparate techniques together. Although there is concern about the role of artificial intelligence in our future, I can't wait to see the advances that can be made with modern analytical science when we apply modern computational approaches to our measurement science data and other available data, including personal and health care data sets.

#2 GERT DESMET

Full Professor and Department Head, Vrije Universiteit Brussel, Belgium

Raising the field's profile… I may be naïve, and this is certainly controversial, but I think that sailing under a new flag such as "chemical measurement science" rather than "analytical science" could rid us of the false image of nitpickers and dry sticks that we sometimes bear and might again enthuse the young. What we do is extremely spectacular (measuring the presence of molecules at the ppt level or even below, identifying a complex wine by its chemical fingerprint, detecting upcoming illnesses in the preclinical stage…) but we are not selling it well enough. Some of our fellow chemists consider us a service technology, but our measurements and the progress this field has made are crucial. So, we have all the reasons to be proud and a thorough rebranding might be a way to give us back this proudness.

#3 JONATHAN V. SWEEDLER

James Eisner Family Endowed Chair of Chemistry, Professor of Bioengineering, Neuroscience, Physiology and Medicine, University of Illinois at Urbana Champaign, USA

Attracting talent… There are many talented undergraduate students interested in the research that analytical chemists perform. What is not to like about chemists that work on real world problems related to health and disease, environmental science and many other important areas? The same is true for graduate students. Analytical chemistry traditionally has not had problems convincing graduate students to study our field. For me, the issue is not a lack of interest but making sure that our field remains attractive throughout their careers. For a professor, I can reframe this: how do we keep the interest of our students and postdoctoral associates? I have noticed a few research groups that have multiple students change fields, and others that keep the students interested in the analytical sciences. The common theme in the latter is that everyone enjoys their research and education. If we, as mentors and leaders, spend our time complaining – about funding, about research, about competitors – then those we mentor have the takeaway message that we don't like our jobs. Why should they stay involved in analytical chemistry? I am not suggesting that we hide the truth. While we all have aspects of our jobs that are less exciting and fun, I greatly enjoy the profession and I want to communicate my enjoyment to my students. If we stay excited and let students know why analytical chemistry remains a fulfilling field, we will not lack talented scientists.

#4 PAT SANDRA

Founder and Scientific Advisor, RIC group; Emeritus Professor Ghent University, Belgium

The decade's most important development? The range of developments in mass spectrometry has been enormous in the last decade and has introduced analytical performance in all areas and for all disciplines that were unthinkable ten years ago.

Most exciting development or trend? As an emerged trend, I would like to mention the growing awareness of and interest in the importance of good sample preparation. More and more automated systems (robots) for different matrices and targets are described in the recent literature and are offered commercially. Much better precision, accuracy, reproducibility, ruggedness and instrumental performance are achieved by reducing or even eliminating human actions in the sample preparation step. Moreover, by optimizing and miniaturizing the sample preparation step, an important contribution is also made to the greening of analytical chemistry.

#5 EMILY HILDER

Interim Head, Advanced Strategic Capabilities Accelerator, Department of Defence, Australia

Attracting talent… We need to actively encourage greater diversity and inclusion. Greater diversity and inclusion means both opening the field to many more talented scientists and also widening our perspective to what talent is. This brings increased creativity, innovation and new ways of thinking, as well as a much bigger field of talent!

Book for scientists? All scientists – actually not just scientists – should read "Latitude" by Dava Sobel. It's not just a story of great scientific discovery, of adventure and persistence, but it demonstrates the power of science, data and accurate measurement to change the world for the better. All told through a fabulous story.

#6 JENNIFER VAN EYK

Professor, Advanced Clinical Biosystems Research Institute; Director, Precision Biomarker Laboratories; Founder and Director, Smidt Heart Institute, Cedars-Sinai Medical Center, USA

The decade's most important development? Proteomics! The power of proteomic approaches is that they bring the best of both hypothesis-driven and hypothesis-generation research together. Proteomics technologies allow you to ask key questions, but the data provides a larger set of information about the cell, tissue or body fluid. Although one can focus on specific proteins or pathways, it is impossible to ignore the broader system responses. This ensures that one does not try to fit the data into a preconceived box, but instead pushes one to contemplate the remarkable complexity of biology and how little we still know.

#7 DAVY GUILLARME

Senior Lecturer and Research Associate, School of Pharmaceutical Sciences, University of Geneva, Switzerland

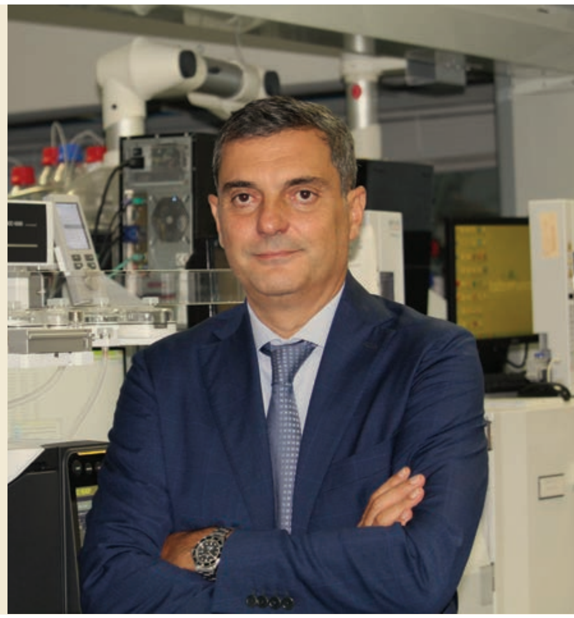
Biggest challenge facing the field? One of the biggest challenges facing analysts today is data processing. With today's much more powerful, faster and more sensitive instruments, we are faced with a veritable tsunami of data that we need to be able to process quickly so that this stage does not become the bottleneck of analytical methods. The new generation of scientists is much better prepared for data analysis, whereas scientists who graduated in the 20th century sometimes feel overwhelmed in this area. Indeed, this science is evolving very rapidly, and this trend is likely to accelerate with the use of machine learning and artificial intelligence.

#8 LUIGI MONDELLO

Full Professor of Analytical Chemistry; Chemical, Biological, Pharmaceutical and Environmental Sciences Department, University of Messina, Italy

Attracting talent… Broadly speaking, more opportunities should be put in place, for researchers to progress in their careers and to benefit from funding. But analytical science should be promoted as one of the most technologically advanced and interdisciplinary branches of chemistry, offering effective tools to face global challenges in security, nutrition, and human well-being. Finally, the numerous careers in the field should be spread in terms of their variety, characteristics, and opportunities.

Biggest challenge facing the field? The ever-increasing levels of regulation across all sectors of analytical science have resulted in the need for increased sample throughput and laboratory productivity. In the search for smaller environmental footprints, instrumental configurations shaving off the solvent and energy consumption of traditional analytical methods will shape the future of separation science – hopefully!



#9 JOHN YATES III

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

Raising the field's profile… We need to hammer on the fact that our lives are touched by analytical science in everything we do. It keeps our water, food and air safe, it helps us diagnose disease, and it helps drive innovations and discoveries.

Book for scientists? I've got two: The Entrepreneurial State: Debunking Public vs. Private Sector Myths, by Mariana Mazzucato; and Where Good Ideas Come From: The Natural History of Innovation, by Stephen Johnson. The first book puts forth the idea that only governments have the stamina and patience to fund high-risk, long-term research – not venture capitalists or industry. The second book studies the process of innovation with both examples and stories. Innovations are often the product of past experiences and prepared minds.

#10
BENJAMIN GARCIA

Raymond H. Wittcoff Distinguished Professor, Head of the Department of Biochemistry and Molecular Biophysics, Washington University in St. Louis, USA

Raising the field's profile… I feel this will come if we as analytical chemists deliberately attend more non-analytical chemistry type conferences and meetings. We all go to the analytical conferences to see the latest approaches or technology, but that is somewhat preaching to the choir. Going to other conferences such as ASBMB, AACR or cell biology conferences will continue to promote and honestly educate other non-analytical scientists about how our new technology can be beneficial for their research or patient health, etc. Specifically, in my field (mass spectrometry), there are scientists outside the field that only view MS as an identification technique for proteins or metabolites. They have no clue about all that mass spectrometry can do for structure biology, clinical analysis, etc. We have to make a real effort as an analytical field to attend non-analytical conferences consistently.

RUEDI AEBERSOLD

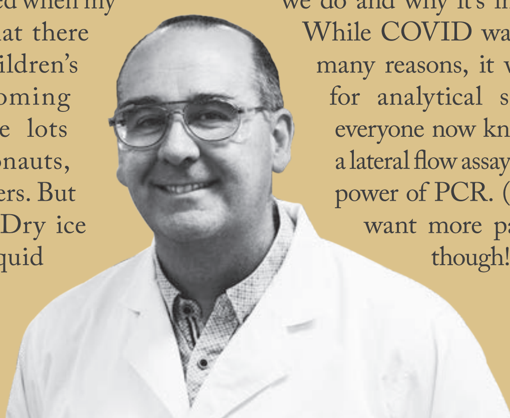
Professor of Molecular Systems Biology, Institute of Molecular Systems Biology, ETH Zürich, Switzerland

Raising the field's profile… "When you cannot measure it, when you cannot express it in numbers, your knowledge is of a meager and unsatisfactory kind" is a quote attributed to Lord Kelvin. In essence it states that at the root of scientific investigations are data, frequently generated by analytical science and technology. This notion is reinforced if we follow advances in many fields of research including chemistry, physics, atmospheric science and the life sciences. In recent years the impact of analytical sciences in the life sciences has been particularly impressive. Advanced fluorescent imaging techniques were the basis for sequencing the genome, cryoEM single particle analysis indicates the structure of biomolecules at atomic resolution and mass spectrometric techniques have made great inroads towards the exploration of the many layers of information of the proteome. Following Lord Kelvin's quote the profile of analytical science could therefore be raised by highlighting not just the performance metrics of analytical methods but rather their contributions to shaping the understanding of the world we live in.

MICHAEL BREADMORE

Professor of Chemistry, University of Tasmania, Australia

Attracting talent… Engaging children at an early age is the absolute best thing we can do… I discovered when my kids were younger that there aren't many good children's books about becoming scientists. There are lots about doctors, astronauts, builders and train drivers. But not many scientists. Dry ice and detergent and liquid nitrogen ice cream go a long way with a five-year old.



Raising the field's profile… We need to be prepared to communicate to everyone at a level they can understand what we do and why it's important. While COVID was bad for many reasons, it was great for analytical science – everyone now knows what a lateral flow assay is and the power of PCR. (We don't want more pandemics though!)

CATHERINE E. COSTELLO

William Fairfield Warren Distinguished Professor & Director of the Center for Biomedical Mass Spectrometry, Boston University, USA

Nominator comment: Costello is a life-long pioneer in MS and glycoanalysis, past president of ASMS, HUPO and IMSF, and is actively engaged in promoting the careers of young scientists. In glycobiological MS she defined the oligosaccharide fragmentation nomenclature.

ELENA IBAÑEZ EZEQUIEL

Research Professor, Foodomics Laboratory, Institute of Food Science Research (CIAL-CSIC), Spain

Attracting talent… One of the most important issues is making talented researchers aware of the importance of analytical chemistry in all aspects of science. It cannot be considered as a mere tool, but rather a complete discipline that contributes to the advancement of science, knowledge, and society.

Missing from the toolbox? I think what is missing is a massive use of green metrics in analytical chemistry. Wouldn't it be impressive if all the analytical equipment, protocols and systems had tools installed that would determine the greenness of any analytical methodology?

LISA JONES

Professor and Chancellor's Associates Endowed Chair in Chemistry and Biochemistry, University of California San Diego, USA

An inspirational leader? Jenny Van Eyk! The scale that she does research on is amazing. Her focus on personalized medicine is admirable because this is so difficult. She is always at the forefront of the field – whether that be in automation, instrumentation, or bioinformatics. Her ability to do that in multiple areas is exceptional. And on top of that, she is a very nice person. She is always willing to take time to talk about my research plans or help me with issues that I am having. She is so supportive of women in mass spectrometry.

Biggest challenge facing the field? I think a challenge for the field is the perceived lack of biological importance of analytical measurements. Analytical methods are often looked at as just tools used to support the more important biological science. There is a lack of respect in some ways for what analytical measurements bring to science.

CHRISTINA JONES

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

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

NEIL KELLEHER

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

Advice for someone starting out? When I started my career in science, I didn't necessarily have a strategic plan; I had no great advisors and no one in my family worked in science. But I did have unbridled enthusiasm and tons of raw energy. And I think that that is something people tend to forget. Be enthusiastic! Be energetic! Another hugely important trait for people starting out is self-belief. There are many things that erode your self-efficacy and career persistence. We have set up a system of peer review that is not always constructively critical; sometimes it's just critical. But that's just the way it is, so don't let it get you down!

MICHAEL LÄMMERHOFER

Professor of Pharmaceutical (Bio-)Analysis, Institute of Pharmaceutical Sciences, University of Tuebingen, Germany

Raising the field's profile… Spread out to the public and tell the people the impact of analytical sciences on our society. There is no water quality, no food safety, no pharma product quality, no clinical diagnostics, personalized medicine, biomedical research, no doping control, and no safe environment without analytical sciences. It opens doors for gaining new insights into hitherto undiscovered realms and dimensions.

STEVEN J. LEHOTAY

Lead Scientist, USDA Agricultural Research Service, Eastern Regional Research Center, USA

Raising the field's profile… One way to raise the profile of analytical science is to give analytical scientists a raise! Doctors, lawyers, teachers, engineers, and many other professionals need certification to work in their profession, and if analytical chemists and/or analysts would also have to meet certain knowledge and performance standards to do their jobs, then they should also receive more pay. For years, many laboratories have been hiring untrained technicians at the lowest pay possible, which causes those with the ability to conduct higher-quality analytical chemistry to work in other fields. This is not a new idea, but hire higher talent with higher pay!

KIM PRATHER

Distinguished Professor & Distinguished Chair in Atmospheric Chemistry, Scripps Institution of Oceanography, USA

Research: Developing and conducting measurements for aerosol chemistry – aerosols occur in our environment in many forms and have profound effects on the climate and health, but are relatively poorly studied.

MICHELLE REID

Co-Founder, The Coalition of Black Mass Spectrometrists, USA

Heroes/mentors? 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.

MARJA-LIISA RIEKKOLA

Professor of Analytical Chemistry, Head of the Laboratory of Analytical Chemistry, Department of Chemistry, University of Helsinki, Finland

Pivotal moment: When the Faculty Council of University of Helsinki selected me, the youngest and only woman among ten competitive applicants to the position of full professor of analytical chemistry. The final decision was based mainly on the independent scientific assessment reports written by four highly respected and well-known international professors.

MARIO THEVIS

Forensic Chemist and Professor for Preventive Doping Research, German Sport University Cologne, Germany

Attracting talent… Make the relevance of research and a (potential) subsequent application of an analytical approach or technology transparent and comprehensible to the talented scientists – this is vital for motivating such individuals to commit to the field.

Most exciting development or trend? A particularly fascinating field of research in analytical chemistry has become the investigations into exposomics. Here, various facets combine to paint an extremely complex picture, and joint efforts of all analytical science sections are required to support understanding and, eventually, influencing future directions.

Biggest challenge facing the field? In the light of the complexity of cause-and-effect questions, a major challenge appears to be the deducing of casualties from analytical data. Interdisciplinarity seems to be of even greater importance now than ever before.

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.

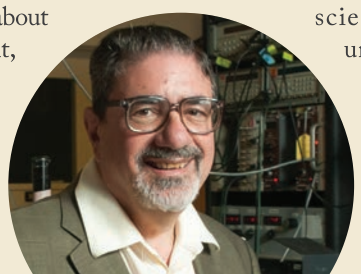
RICHARD N. ZARE

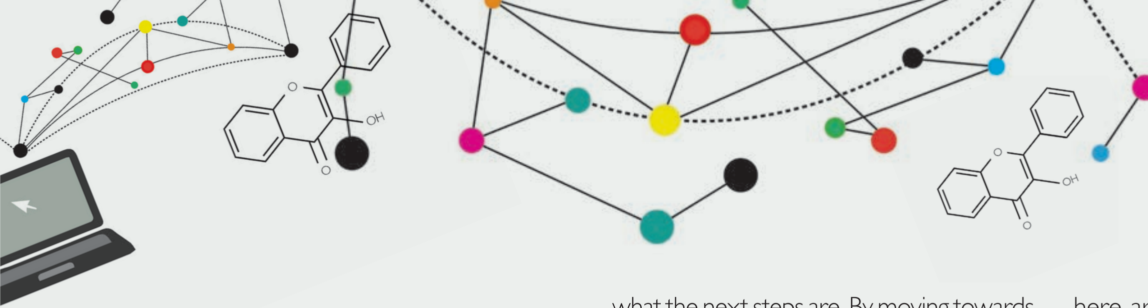
Marguerite Blake Wilbur Professor of Natural Science, Department of Chemistry, Stanford University, USA

Raising the field's profile… Emphasize that measurement is at the heart of all experimental work, that what we regard as truth is based on observation, and that a measurement with no estimate of its uncertainty does not constitute an acceptable measurement. Analytical chemistry is about chemical measurement, and in that sense so many more researchers are doing analytical chemistry than is commonly appreciated.

The decade's most important development? I think it will turn out to be the importance of machine learning in aiding chemical analysis, although I do not believe that this point of view is widely appreciated at this time.

Biggest challenge? Simply put, gaining more respect for analytical science's importance to understanding nature.





Making Digitalization Work for Everyone

Balancing the needs of experimental and data scientists can pull organizations in different directions. Fortunately, there are digital technologies that suit both camps.

By Richard Lee, Director, Core Technology and Capabilities, ACD/Labs

Analytical labs today often have an army of scientific instruments, running 24/7 and generating an immense amount of data. Organizations recognize that there are opportunities to leverage that data to generate additional insights – and there's a lot of excitement about the possibility of AI and machine learning. But there are also significant challenges.

Lab instruments are often sourced from multiple vendors, each reliant on its own proprietary data format, which creates a lack of interoperability. There are also differences in terms of the data disposition: data generated by one system may be locked into a database, requiring extraction, whereas other systems generate discrete data files. Tackling these issues allows the development of machine learning algorithms, AI frameworks, or other applications for further use downstream. But to get there, data scientists need a representation of the data, abstracted from the individual experiments. They also need remote access, usually via cloud storage.

On the other hand, an organization's experimental scientists want immediate access to highly interactive data so they can figure out whether their experiment worked and what the next steps are. By moving towards cloud storage, not only are organizations spending a lot of money, but they may be creating some inefficiencies for scientists. Instead of being able to grab data straight from the instrument, they're having to wait for files to download from the cloud – which may take quite some time for high-resolution imaging data, for example.

These two equally valid use cases for analytical data pull organizations in different directions – and finding the right balance can create real headaches. Fortunately, there are technologies available to help organizations make their data work for both camps.

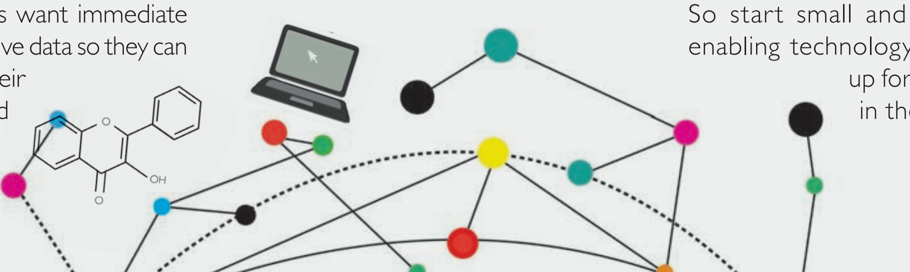
There are now a number of cloud storage providers that have their own object stores – a data storage architecture for storing unstructured data – which organizations can use to store their analytical data. Vendor software can then access that data and pull it back into their own applications via an application programming interface (API). Abstracted data can also reside in data warehouses, which can be leveraged by data scientists for machine learning algorithms.

We're also seeing the rise of browser-based technologies, which can allow experimental scientists to access their data on demand in a way they're used to (everyone uses browsers like Google Chrome or Microsoft Edge on a daily basis). ACD/Labs' Spectrus JS allows scientists to process and interpret their analytical data from any browser, for example.

Automation technology is also making a difference for analytical scientists by stitching together datasets from multiple different techniques and experiments, telling a compelling chemical story. Key here are universal data formats, such as ACD/Labs' spectrus format. Raw data files can be imported directly to the Spectrus environment and scientists can access their data through the instrument software, process it as they normally would with a single interface, and query by metadata or chemical structures. Processed data files can also be imported into the Spectrus platform, allowing scientists to continue using instrument software they're used to while being able to assemble and store data from different vendors and techniques together in a scientifically searchable repository. Data scientists can also access the same normalized, contextualized data via an API for machine learning algorithms. Right now, we have a Windows client, but we're moving towards browser-based access – and that's very exciting.

Overall, there are technologies available to address the major challenges facing organizations as they embark on their digital transformation journey. I also know that it can be difficult to know where to start, which makes taking those first crucial steps that much harder. My main message? Don't wait. There are gains to be made today. And there are initiatives to develop standard data formats for all analytical data, which are fantastic (though we're a long way from ratification). Find a workflow that could see some immediate benefit from digitalization – an area where you know there will be a measurable impact – and start there. You can then expand based on that initial pilot program. I'd also suggest investing in data management and storage, making sure it's all in one place, properly tagged, and accessible to everyone. This approach puts you on the first step on the ladder so that you're ready to benefit from AI in the future.

The utopian potential of digitalization is exciting, but it can also be paralyzing. So start small and simple, embrace enabling technology, and set yourself up for success – now and in the future.



CONNECTORS *and* INTERDISCIPLINARIANS

#1 ALBERT J.R. HECK

Chair, Biomolecular Mass Spectrometry and Proteomics, Utrecht University; Scientific Director, Netherlands Proteomics Center

A problem interdisciplinarians should tackle? Understanding how the human brain works, which I feel requires much more research at the cellular and molecular level. Spatial and single cell multi-omics and single molecule approaches should meet with more classical molecular and structural biology approaches – maybe with further assistance from deep-learning technologies.

The secret to a successful interdisciplinary collaboration? A successful interdisciplinary collaboration should be a multi-directional process. Educate and be educated, present and listen, and trust each other as experts in your chosen field. I have enjoyed the process of learning from collaborators – gaining knowledge in fields such as stem cell biology, immunology, electron microscopy, imaging, cardiovascular diseases, and virology. I believe these experiences have made me a better mass spectrometrist.

#2 PAUL HADDAD

Emeritus Distinguished Professor, School of Natural Sciences, University of Tasmania, Australia

The secret to a successful interdisciplinary collaboration? I believe that interdisciplinary collaborations flourish when scientists are prepared to move outside of their traditional narrow areas of expertise and take the time to understand other disciplines. This takes considerable effort and time but true interdisciplinary collaboration only occurs when a mutual understanding of different perspectives exists.

The decade's most important development? The development of Quantitative Structure-Retention Relationships technology – whereby the retention time of a compound can be predicted accurately based only on knowledge of its chemical structure. This technology has become particularly important in the elimination of false positives in non-targeted metabolomics using LCMS.

#3 SUSAN RICHARDSON

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

A problem interdisciplinarians should tackle? A chemist alone is unable to understand which drinking water disinfection by-products (DBPs) are the most important to focus on. Interdisciplinary work can help us find a solution.

The secret to a successful interdisciplinary collaboration… Understanding the needs of each discipline involved in your work. For example, toxicologists need more materials than chemists and need to perform more replicates – requiring adjustments to extraction techniques. Being open to compromises is key to making the process work. It's also important to work with someone that you trust. I've been blessed through my career to collaborate with some wonderful people across a variety of disciplines (from engineers to epidemiologists), who have been tremendous colleagues.

#4 PAUL MAYEWSKI

Director, Climate Change Institute, University of Maine, USA

Attracting talent… We need to show young people that scientists and explorers are real people too – most of whom probably never thought they'd end up working in their current area! By showing the next generations that they can combine their interests and hobbies, we can encourage them to seek opportunities and explore what the field holds.

#5 DUNCAN GRAHAM

Professor, Associate Principal & Executive Dean of Science, Faculty of Science, University of Strathclyde, UK

The secret to a successful interdisciplinary collaboration? Taking the time to understand the language and expectations of the others in areas different to your own. There also has to be a common desire to work together and recognition that it's a synergistic partnership and not a transactional service provision to enable someone else to progress.

Fostering interdisciplinary working… Boundaries are more blurred than ever and I see analytical scientists responding well to challenges. When I was president of the Royal Society of Chemistry's analytical division and also on the Cancer Research UK's science committee, we held a workshop bringing together analytical scientists and cancer researchers. This allowed the challenges in the cancer field to be presented then new collaborations formed to address these challenges. More opportunities like this opens opportunities for collaboration.

#6 ROY GOODACRE

Professor of Biological Chemistry, Institute of Systems, Molecular and Integrative Biology, University of Liverpool, UK

A problem interdisciplinarians should tackle? One challenge I would like to see solved is the generation of computational models of mammalian systems. Many people are already striving to develop the so-called "Digital Human." If we had a biology model of a system that encompasses integration and communication within cellular, organ, multi-organ, and whole animal processes, we could understand biochemistry and physiology in more detail. These advances could allow us to predict treatments for pathophysiological processes, understand the aging process, and perhaps predict how exposure to chemicals and varying environments affects this interconnected model of "life" over decades to different exposomes. This would be a game changer for medicine.

#7
ANDREW DEMELLO
Professor of Biochemical Engineering in the Department of Chemistry and Applied Biosciences at ETH Zurich, Switzerland

Most exciting development or trend?? The analytical chemistry community has excelled at generating new tools that allow us to generate high-quality chemical and biological information on very short time scales. Microfluidics is an excellent example.

Missing from the toolbox? I don't think we have yet developed a complete suite of downstream tools that are able to fully extract information. We're not far off, and I hope that we will soon have a range of ultra-sensitive, fast and information-rich detectors able to detect complex samples at sub-nM concentrations.

#8
MILTON LEE
Emeritus Professor of Analytical Chemistry, Brigham Young University; Chief Technology Officer, Axcend; USA

Fostering interdisciplinary working? More professional encouragement and recognition for interdisciplinary efforts would incentivize collaborative work. We could achieve this by valuing well-designed collaborations more for research grant proposals – increasing the number of awards for collaborative teams rather than individuals. Most scientific achievements are accomplished with team efforts and we should reflect this in our support across the field.

#9
LLOYD M. SMITH
Professor of Chemistry, University of Wisconsin-Madison, USA

A problem interdisciplinarians should tackle? I'm very interested in the technical challenge of comprehensive proteoform analysis in biological systems. Proteoforms are the different molecular forms of proteins, reflecting genetic variations, RNA splicing processes, and post-translational modifications. As the primary effectors of function in biology, it is crucial to understand and monitor the nature and regulation of these many protein forms, and their changes in response to perturbations. It is remarkable that so much still remains to be done to reveal the hidden protein-level secrets of biology despite the increasing sophistication of biomolecular analysis tools.

#10
DANIEL W. ARMSTRONG
R.A. Welch Distinguished Professor, Department of Chemistry and Biochemistry, University of Texas at Arlington, USA

The secret to successful interdisciplinary collaboration? There is no secret, just a decision: you can either remain isolated, self-acquiring knowledge and raising funds (which can be a costly and lengthy process), or you can collaborate with individuals/groups from different fields to increase productivity, decrease costs, and help you reach solutions at a faster pace. Working amongst others also broadens your overall knowledge, which could be applied to future research projects. When interdisciplinary projects work – which is often – problems are solved, publications are produced, and everyone is happy.

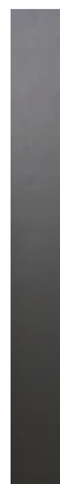
RICHARD VAN BREEMEN
Professor of Pharmaceutical Sciences, Oregon State University, USA

Biggest challenge facing the field? Deciding how the next generation of mass spectrometrists focus their effort as the field of biomedical mass spec reaches maturity. Some academics have been advising their students to pursue other fields as the history of mass spec suggests we should be entering a new era.

Most exciting development or trend? I'd like to believe that there will be an upcoming era of mass spec worthy of academic study and scientific investigation – which could be dominated by medical application areas. We're already seeing this addition in operating theaters, which could be the start of a new era of medical mass spec.

ZONGWEI CAI
Chair Professor, Department of Chemistry, Hong Kong Baptist University, China

Nominator comment: Zongwei builds multidisciplinary teams with researchers from biomedicine including cancer, cardiovascular disease, and virus fields.



LUTGARDE BUYDENS

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

The secret to a successful interdisciplinary collaboration? Diversity in all aspects facilitates a broad and open-minded approach to various problems. Diversity in expertise, gender, and cultural backgrounds are all important assets to a successful interdisciplinary collaboration.

Biggest challenge facing the field? Finding young analytical scientists with a strong analytical chemistry education to join a diverse team and address complex challenges that require interdisciplinary approaches.

KAREN FAULDS

Professor and Head of Bionanotechnology and Analytical Chemistry, University of Strathclyde, UK

A problem interdisciplinarians should tackle? I think every big problem the world is facing HAS to be tackled through interdisciplinary work – from climate change and poverty to earlier diagnosis and treatment of disease. All challenges can be addressed by bringing people with different expertise together (and actually listening to them!) rather than working in silos.

Fostering interdisciplinary working… We need to find different ways of bringing people together across a variety of disciplines to share their science and allow cross fertilization of ideas.

Biggest challenge facing the field? Cost of living is causing a highly negative effect on people deciding to do PhDs. If this drop continues, we could be facing further skills gaps in analytical science with less people trained in interdisciplinary research.

JEAN-FRANÇOIS (JEF) FOCANT

Full Professor, Chemistry Department, Faculty of Sciences, University of Liège, Belgium

A problem interdisciplinarians should tackle? We know that most cancer survival rates increase with early diagnosis, and such early-stage cancer screening can only be attained in an interdisciplinary fashion. Medical scientists must develop their knowledge of cancer development stages and the expected biological signals of cancer proliferation; analytical chemists must master sensitive and selective detection methods of relevant pathophysiological information for screening; and data scientists need more complex data sets, especially with the implementation of AI. Although this sounds simple on paper, setting up a collaborative venture of this nature is far from easy.

The secret to a successful interdisciplinary collaboration? Friendship and honesty.

AMANDA HUMMON

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

The secret to a successful interdisciplinary collaboration? I think the key to successful interdisciplinary collaboration is having different research areas compliment each other and respect the expertise of other groups. Our current collaboration with a team of pulmonologists is a good example of this. Our team brings analytical measurement strategies to the table, whereas the pulmonologists bring expert knowledge in lung function and disease. These distinct research areas create a complimentary, productive, and enjoyable collaboration.

HANS-GERD JANSSEN
Senior Scientist, Compositional Analysis, Unilever Science & Technology, Wageningen; Part-time Professor, Recognition-based Analytical Chemistry, Wageningen University; The Netherlands

Fostering interdisciplinary working… Help people understand that working with other disciplines doesn't mean you're failing with your own technique. Of course, we should always strive to improve our methods and the reach of their capabilities, but we should not see collaborative work as a negative. New insights and progress occur when different techniques meet.

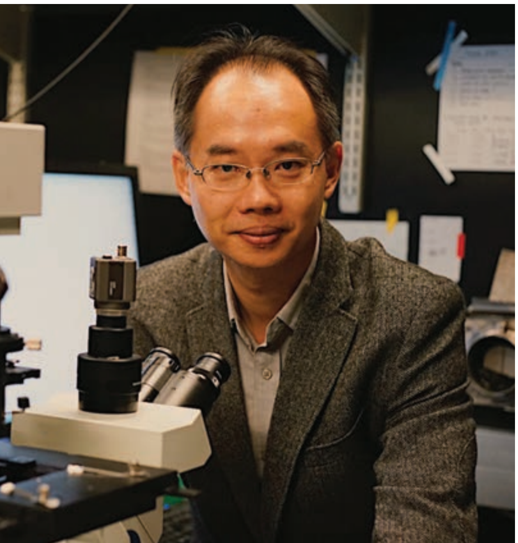
Missing from the toolbox? The analytical toolbox is currently full of highly specific tools with a very narrow application field. We're missing a more generic tool with a broad coverage of analytical problems – a method that allows us to manage incoming questions rapidly without having to make changes (for example, change chromatographic columns, install another MS ion source, or re-optimise settings).

PAULINE LEARY
CBRNE Subject Matter Expert, Noble, USA

Nominator comment: We're continually impressed with the depth of Pauline's spectroscopic understanding and dedication to the spectroscopy field. She is also extremely generous in sharing time and knowledge with colleagues, students, and innovators of spectroscopic technologies and instrumentation.

MARCELLO LOCATELLI
Associate Professor of Analytical Chemistry, Department of Pharmacy, University "G. d' Annunzio" Chieti-Pescara, Italy

The secret to a successful interdisciplinary collaboration… The success of an interdisciplinary collaboration lies in the ability to come together as equals at the table, and discuss data integration to achieve the most accurate representation possible. It is crucial to constantly question and critically evaluate everything, particularly one's own data, in order to maintain a scientific perspective. Establishing harmony among experts, fostering trust and friendship, and creating an environment where individuals can freely express their thoughts and ideas without being hindered by their hierarchical positions is also essential.



WEI MIN
Professor of Chemistry, Columbia University, USA

The secret to a successful interdisciplinary collaboration? Understanding the language and logic of your collaborator as much as possible. Your work is much more efficient if your thoughts are synthesized without a hurdle. I often try to read a collaborator's recent technical papers to absorb their ideas.

Biggest challenge facing the field? Democratizing cutting-edge techniques to make them more accessible. There is still a large gap between the developers and the end user.

Missing from the toolbox? The integration between optical techniques and omics techniques. Though they are well developed in separate fields, more value can be generated if this integration can be bridged.

JESSICA E. PRENNI

Professor, Department of Horticulture and Landscape Architecture, Colorado State University, USA

The secret to a successful interdisciplinary collaboration? The secret is simple: good communication and mutual respect. I believe almost all areas of science can benefit from interdisciplinary collaboration. Plus, collaborative science is way more fun!

Fostering interdisciplinary working… One of the challenges, especially in academia, is that the existing structures for evaluating performance do not always value collaborative science. Changing this framework could go a long way to encouraging and enabling collaborative science.

KOEN SANDRA

CEO and Co-owner, RIC group; Visiting Professor, Ghent University; Belgium

The secret to a successful interdisciplinary collaboration? "If you want to go fast, go alone. If you want to go far, go together." One of our core values as a company is "stronger together" – we have no room for big ego's. I have yet to meet that multi-disciplinary know-how-to-do-it-all superhero. Even if that person did exist, humility is still the true key to success. Partnerships that lack trust and respect draw us away from our core values are doomed to fail.

KEVIN SCHUG

Professor and Shimadzu Distinguished Professor of Analytical Chemistry, University of Texas at Arlington, USA

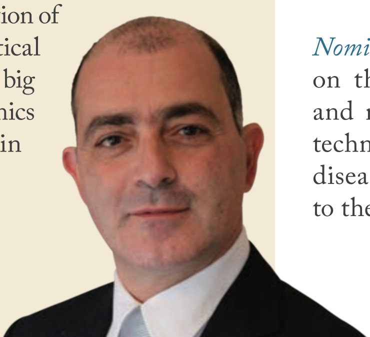
Biggest challenge facing the field? Universities in the US are shifting away from hiring analytical chemistry faculty with formal credentials. This issue is worsened by a thriving job market in the industrial sector, where analytical chemists with PhDs tend to find employment. Additionally, there is a limit on funding for analytical chemists in academic institutions. I have worked to fill this funding gap in my own research by collaborating with industry partners – though virtually all of my students have been taking jobs in industry. With less focus on pushing boundaries in analytical measurements in academia, less students will be exposed to the wide range of analytical technologies available – making the competition for classically trained analytical chemists more fierce when applying for industry jobs.

GEORGIOS THEODORIDIS

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

Most exciting development or trend? There is a strong trend in bringing LC-MS technology into the clinical lab. I'm sure that the biochemical lab of the future will look very different – moving away from the current arsenal (assays) and towards LC-MS(MS).

A problem interdisciplinarians should tackle? Understanding the biochemistry of non-communicable diseases with the application of advanced analytical technologies and big data mining. Omics fields are key in such aspects.



MARY WIRTH

Retired W. Brooks Fortune Distinguished Professor, Purdue University, USA

Nominator comment: Focusing on the interface between chemistry and medicine, Wirth aims to create technology for the earlier detection of disease through simple lab tests prior to the onset of symptoms.

MENTORS *and* EDUCATORS

1 PETER SCHOENMAKERS

Full Professor, Analytical Chemistry Group, University of Amsterdam, The Netherlands

Nominator comment: Without Peter, many young scientists (from bachelor students to young professors) would not be where they are. He is THE mentor version 4.0 – always present to actively help the younger generation. I have never seen someone put so much time, energy, and enthusiasm into shaping the next generations of scientists like Peter does.

2 ROBERT KENNEDY

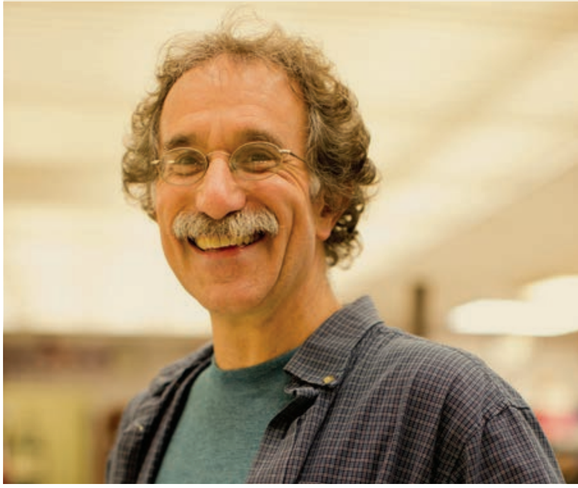
Professor of Chemistry and Pharmacology, Department of Chemistry, University of Michigan, USA

Qualities of a successful mentor or educator? Genuine interest in the student/mentee. I think if you are interested in your students and mentees as people, everything else that you need such as enthusiasm, willingness to support, and putting their interest first will flow from it. You should also find out what motivates them, which is the first step to finding the right projects and type of study.

3 THOMAS J. WENZEL

Charles A. Dana Professor of Chemistry, Emeritus, Bates College, USA

Attracting talent... Practicing analytical scientists often work on interesting and complex problems, usually as part of a team. However, the traditional educational approach at an undergraduate level emphasizes individualism – rarely giving students the opportunity to work on meaningful problems they can relate to. Designing courses where students work in teams on interesting problems provides a more attractive representation of analytical science.



4 CHARLES (CHUCK) LUCY

Professor Emeritus, University of Alberta, Department of Chemistry, Canada

Attracting talent... We need to show students and the public that analytical sciences serve humanity and the environment – from testing the safety of drinking water, to checking blood glucose to manage diabetes. Above all, analytical science seeks the truth to the remarkable degree that chemical measurements can reveal. In a time of fake news and alternative facts, seeking the truth is an attractive pursuit.

5
CHRISTY L. HAYNES
Department Head and Distinguished McKnight University Professor of Chemistry, University of Minnesota, USA

A mentor or educator who inspired you? I had a graduate student mentee that really inspired me – acknowledging me in her thesis “You truly believed I deserved to be here and worked tirelessly to nominate me for awards, accolades, and supported my dreams outside of science. You said my name in rooms where it mattered.” I think about this regularly, and it reminds me how important it is to keep mentees in the conversation.

Attracting talent… Broadening the definition of analytical chemistry and welcoming people working at all interfacial boundaries. We should also be conscientious of developing an analytical chemistry community that recognises traditional and non-traditional scientific input. Adding more diversity allows the opportunity for new solutions to important issues that are currently getting too little attention.

6
SUSAN OLESIK
Dow Professor and Chair, Department of Chemistry and Biochemistry, The Ohio State University, USA

Qualities of a successful mentor or educator? A successful mentor and educator must listen first and guide second.

Attracting talent… We must show young students the importance and positive impact that analytical science brings to many people’s lives and the world as a whole.

Biggest challenge facing the field? We’re not attracting and retaining enough talent to sustain the field. We must work hard to fix this issue.

7
PHILIP MARRIOTT
Professor of Chemistry, Monash University, Australia

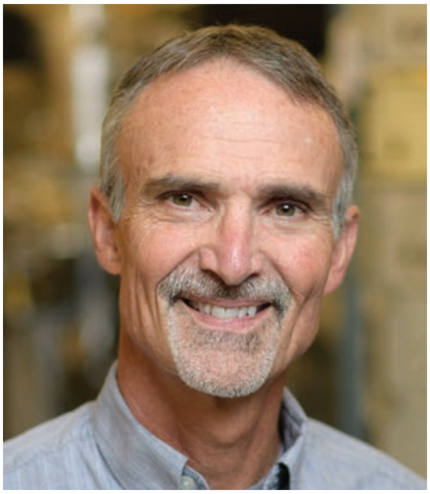
The decade’s most important development? There is an ever-increasing trend towards collaboration across disciplines, which is key in developing all areas of science. With analytical science playing a key role in these collaborations, we have the measurement capabilities to solve big emerging problems across various disciplines. Understanding the importance of analytical science is key to answering questions within biology, health, environmental science, and other crucial fields. True collaborative efforts can multiply the outcomes of our research.

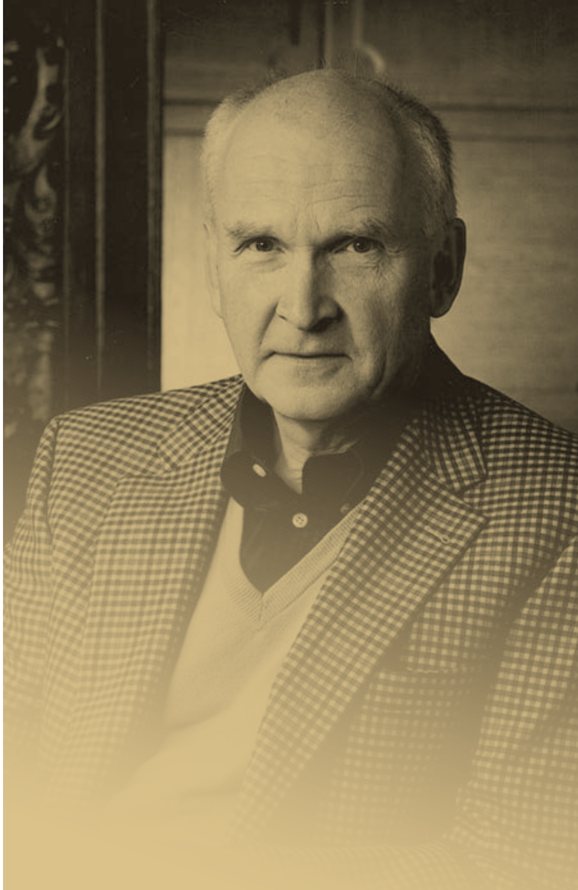
#8
VALÉRIE PICHON
Professor, Sorbonne University; Director, Laboratory of Analytical, Bioanalytical Sciences and Miniaturization (LSABM), École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris (ESPCI Paris); France

Biggest challenge facing the field? I believe that the future lies in the development of smaller, faster, cheaper, and greener analytical devices – with an especially large impact on personalized medicine. However, the challenge is twofold. These green tools must remain efficient to provide the expected response. The analysis should evaluate the environmental impact of its approach on a global scale, considering factors beyond the tool itself.

#9
SCOTT MCLUCKEY
John A. Leighty Distinguished Professor of Analytical Chemistry, Purdue University, USA

Qualities of a successful mentor or educator? The culture of an education group is particularly important in enabling each member's individual development – which is influenced by the dynamic personalities within the group. However, the mentor or leader of the group has a dominant influence on group culture (e.g., competitive vs. cooperative). With this responsibility, it is important to remain vigilant in maintaining an atmosphere that best facilitates personal development and to clearly articulate and model the expectations. If the mentor does this well, older students will reinforce positive values and strongly contribute to education goals – including problem solving and teamwork skills.





#10
WOLFGANG LINDNER
Professor Emeritus, Analytical Chemistry, University of Vienna, Austria

Biggest challenge facing the field? Analytical sciences have an enormous impact in almost all fields of chemistry and bio-sciences, but its standing is often underrated. Analytical values always need to be discussed in the full context of the question, yet analytical chemists are often not fully integrated in the decision making process.

JENNIFER BRODBELT
Professor of Chemistry, University of Texas at Austin, USA

Qualities of a successful mentor or educator? The knack for motivating people with different mindsets and attributes. Each student or trainee has a different set of goals and life experiences, and figuring out how to guide them to maximize success and achievements is challenging. No single roadmap will work for everyone.

Biggest challenge facing the field? Most analytical instrumentation has become a black box. The ability to build, modify, and trouble-shoot instruments has become increasingly difficult.

DEIRDRE CABOOTER

Professor, Department of Pharmaceutical and Pharmacological Sciences, University of Leuven, Belgium

Attracting talent… We need to stress the importance of separation sciences across a variety of fields: environmental, food, clinical, pharmaceutical, chemical, cosmetic… A skilled analyst has so many opportunities! We have to stop seeing ourselves as a tool at the service of these disciplines and take pride in all the ongoing developments that improve and increase the output generated in these fields.

Most exciting development or trend? Artificial intelligence to rationalize, speed up, and automate the analytical workflow.

PETER CARR

Distinguished University Teaching Professor, Department of Chemistry, University of Minnesota, USA

Qualities of a successful mentor or educator? Making an effort to stay abreast of developments in a wide array of fields, not just what's happening in your own scientific backyard. Over the years, I've adopted and applied ideas from biochemists, physical organic chemists, and chemical engineers to analytical chemistry goals. Having a wider pool of knowledge to draw from can provide hugely beneficial when educating students – and also proves the importance of interdisciplinary collaboration. Working on your own analytical science skills and improving as a scientist will also improve your teaching skills.

PAOLA DUGO

Professor of Food Chemistry, University of Messina, Italy

Qualities of a successful mentor or educator? Listening to your students, understanding their needs, and offering your availability when necessary.

Book for scientists? Basic Gas Chromatography by Harold M. McNair and James M. Miller is a starting point and a must read for separation scientists.

OLIVER FIEHN

Director, NIH West Coast Metabolomics Center; Paul K & Ruth Stumpf Endowed Professor in Plant Biochemistry, UC Davis Genome Center, USA

Qualities of a successful mentor or educator? Making as much time as possible for mentees.

Attracting talent… Money! Salaries are far too low in academia – which is encouraging researchers to flee to industry en masse.

Missing from the toolbox? Better software to estimate FDR for compound identifications and molar concentrations.

Controversial opinion? Metabolomics and lipidomics don't need further developments. The data provided by service companies is sufficient.

ANTHONY GACHANJA

Professor of Analytical and Environmental Chemistry, Jomo Kenyatta University of Agriculture and Technology, Kenya

Qualities of a successful mentor or educator? To be a mentor, you need to be a good listener, have patience, and be able to put yourself in the mentee's shoes. It's important to understand their current situation, level of exposure, knowledge bank, and what resources are available to them. By aligning with them, you're in a position to give guidance for their scientific career. Sharing your knowledge and contacts can also boost their progression.

The decade's most important development? The development of high-resolution measurements of mass and magnetic resonance, which is cross-cutting for all areas of science. To retain talented scientists into the future, such facilities must be made accessible everywhere – including resource starved counties. Scientists across the world should have the same opportunities to contribute to solving world problems.

FACUNDO M. FERNANDEZ

Regents' Professor and Vasser-Woolley Chair in Bioanalytical Chemistry, Associate Chair for Research and Graduate Training, School of Chemistry and Biochemistry, Georgia Institute of Technology, USA

Qualities of a successful mentor or educator? To listen to the mentee and try not to apply a universal solution to their needs. Each person is unique and so are their needs.

Attracting talent… What inspires me about analytical chemistry is that it has a direct application to solving real life problems, in addition to basic scientific questions. By showcasing this impact we will inspire future generations of scientists to follow a similar path than we have.

Missing from the toolbox? Analytical chemistry needs to be democratized. We can achieve incredible measurement feats, but the price of instruments is costly – increasing the divide between scientists that have access to high instrumentation and those that do not. We need to lower the cost of instrumentation without sacrificing performance. The driving force in instrumentation should be societal impact and widespread use alongside profitability.

DANIEL HARRIS
Michelson Laboratory, United States Navy,
China Lake, California

Nominator comment: For over four decades Daniel Harris has written the "gold standard" of analytical chemistry textbooks, used by about half of North American students and many more around the world through its numerous translations. He is not only concerned about the students in the class, but also considers what they need to know when they start graduate school or their first job. It's not surprising that many analytical chemists continue to have their copy of QCA within reach years if not decades after they finish their analytical courses.

MATTHEW LOCKETT
Associate Professor, Department of Chemistry
and Lineberger Comprehensive Cancer Center,
University of North Carolina at Chapel Hill, USA

Qualities of a successful mentor or educator? Empathy. Innovation is an energy-intensive process that requires focus and time and everyone requires different approaches to sustain motivation and creativity. Life can and does get messy – requiring us to redirect our efforts to maintain our health and well-being. Supportive environments promote innovation while minimizing the perceived weakness of asking for help.

GARY HIEFTJE
Distinguished Professor Emeritus, Department of
Chemistry, Indiana University, USA

Qualities of a successful mentor and educator? Enthusiasm. If the advisor or educator isn't excited about the research or teaching subject, how can the mentee be?

Attracting talent… Analytical science is often viewed as the servant of other disciplines. We need to raise the stature of our field by highlighting basic discoveries and new inventions that open up entirely new avenues of scientific investigation. As Sir Humphry Davy once said, "Nothing begets good science like the development of a good instrument."

BHAVIK PATEL
Professor of Clinical and Bioanalytical Chemistry, School of Applied Science & Centre of Stress and Age-Related Diseases, University of Brighton, UK

Attracting talent… This should be easily achieved given how cool analytical chemistry is! As analytical chemistry educators, it is our responsibility to inspire the future generation – reaching out to schools to showcase the important role analytical scientists play within society. It is important that we amplify and provide opportunities for talented early career analytical scientists to showcase their work.

Biggest challenge facing the field? Our approach towards developing the future generation of analytical chemists has not moved with the times – the curriculum is quite static. We must ensure creative processes are developed for the delivery and assessment of analytical sciences. This will boost the employability of graduates and prepare them for a diverse range of careers.

RENÃ A.S. ROBINSON
Principal Investigator and Professor of Chemistry, Dorothy J. Wingfield Phillips Chair, University of Pittsburgh, Pennsylvania, USA

Qualities of a successful mentor or educator? Humility.

Missing from the toolbox? One-click data analysis tools that can manage massive datasets from collection to information. Wouldn't it be great to click a single button to learn new discoveries and gain biological implications from complex datasets?!

VICTORIA SAMANIDOU
Professor of Analytical Chemistry, Aristotle University, Thessaloniki, Greece

Attracting talent… By empowering, encouraging, and acknowledging the abilities and efforts of scientists, we can invite interest to our field – showcasing the most significant section of chemistry and the wide range of applications it brings to many scientific fields. Additionally, we must ensure that no discrimination is allowed in the lab. Science is for everyone – the inclusion of diverse genders, races, nationalities, sexual orientations, and identities is indisputable. Analytical techniques should also be accessible for individuals with visual or other impairments using the suitable educational material. This allows talented students among disabled groups to be included in research teams.

Missing from the analytical toolbox? A universal sample preparation technique compatible with all matrices, analytes, and techniques.

Credit: Yannis Tsouflidis

FRANK SVEC
Professor, Department of Analytical Chemistry, Faculty of Pharmacy, Charles University, Czech Republic

Attracting talent… The talent acquisition process must begin as early as possible so students can understand that no advanced society can function without science. When we talk about analytical chemistry, it is important that students see our enthusiasm for the field. Lectures should be inspiring and interesting projects should be shared with students to spark their curiosity. It also wouldn't hurt to send students to conferences, allowing them to see icons that they may have only known from publications, converse with professionals, and see for themselves what is currently happening in the field.

ISIAH M. WARNER
Boyd Professor and Emeritus Philip W. West Professor Analytical & Environmental Chemistry, Howard Hughes Medical Institute Professor, Louisiana State University, USA

Nominator comment: Isiah is one of the top recognized mentors in the US. The LSU chemistry graduate program is the nation's largest producer of African-American chemistry PhDs, largely due to Isiah's efforts in encouraging and mentoring these students.

Improving Drug development

The Intabio ZT system couples imaged capillary isoelectric focusing (icIEF) to mass spectrometry – overcoming a 30-year biopharmaceutical development bottleneck in charge variant analysis

At ASMS 2023, SCIEX announced the launch of its new system for intact protein and charge variant analysis: the Intabio ZT system. Here, Kristen Nields, Senior Scientist at The Janssen Pharmaceutical Companies of Johnson & Johnson, discusses common bottlenecks in the drug development pipeline, the importance of charge variant analysis and the benefits of the integrated mass analysis workflow provided by the Intabio ZT system.

What does your group do at Janssen?

We develop new modalities for different therapeutic areas. Once a biotherapeutic is deemed viable, it's handed over to us for in-depth characterization. We look at disulphide bond reductions, biophysical properties (such as charge heterogeneity), mass analysis, size exclusion and so on before going through cell line selection. We then take the data, along with bioreactor data (such as titer, cell density and cell growth), and we pick a top clone. The top clone then goes into a master cell bank for the production of clinical material, which allows the development team to create efficient and scalable upstream and downstream processes for manufacturing.

Please explain the importance of charge variant analysis in the drug development pipeline.

Part of characterizing a protein involves examining its charge heterogeneity – post-translational modifications affect the charge on both the acidic and basic sides of the protein. It is important to understand a protein's charge profile and how to control it before upstream process development. The levers you pull to increase titer can impact charge heterogeneity, which then becomes locked in at harvest downstream and cannot be removed. In short, charge variant analysis is important for establishing a valid release method.

What are common bottlenecks in the current workflow?

The major bottleneck is method validation for imaged capillary isoelectric focusing (icIEF), which is the primary technique used for charge variant analysis. Why? Because the smallest process changes can alter the acidic or basic isoforms of the protein, affecting the peak areas and rendering the initial assay invalid. When this happens, a comprehensive investigation under good manufacturing practice guidance is required.

Determining the identity of the acidic peak using icIEF alone is challenging, and it can take 1 or 2 months to reach purification at the required levels for progression of clinical testing. This process leads to significant downtime, product holds, extensive quality control efforts and the potential need to engage with regulatory agencies to resolve the issue.

How does the Intabio ZT system address these challenges?

On the front end, it's a typical icIEF system, so all the front-end components stay the same. This means existing validated icIEF methods can be directly applied to this system, so you will achieve the same charge profile. And that's crucial because introducing new technologies for products that are in phase III development or already approved can create significant regulatory challenges, including side-by-side testing for up to 5 years to demonstrate comparability.

Once the sample comes off the microfluidic icIEF chip, it enters the mass spectrometer, where you can analyze the acidic and basic peaks in real time and identify each peak.

This new integrated workflow is a real game changer, serving as an intact protein multi-attribute methodology in the field of mass analysis. The Intabio ZT system gives you a real-time online icIEF-UV/MS profile, which allows us to investigate the composition of each peak. This results in fewer investigations and faster identification compared to the alternative approach, which required fractionation and subsequent peptide mapping in the hopes of finding agreement with the icIEF-UV profile.

For years, we biochemists and chemists have wanted to know what's under those peaks, and now we can find out – in real time – and that's exciting!

What does this "game changer" mean for drug development?

Ultimately, the Intabio ZT system will help ensure faster biopharmaceutical product characterization and process development – a huge bottleneck in biopharma – to reduce drug development timelines.

APPLICATION SPOTLIGHT:

Aromatic Analysis

An understanding of whiskey aroma profiles can lead to a better understanding of different whiskey products, but comparing various similar but complex chromatograms can be complicated and time-consuming. ChromaTOF® Sync takes the challenge out of the comparison by compiling and aligning analyte information across the entire sample set, highlighting statistically significant similarities and differences.

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

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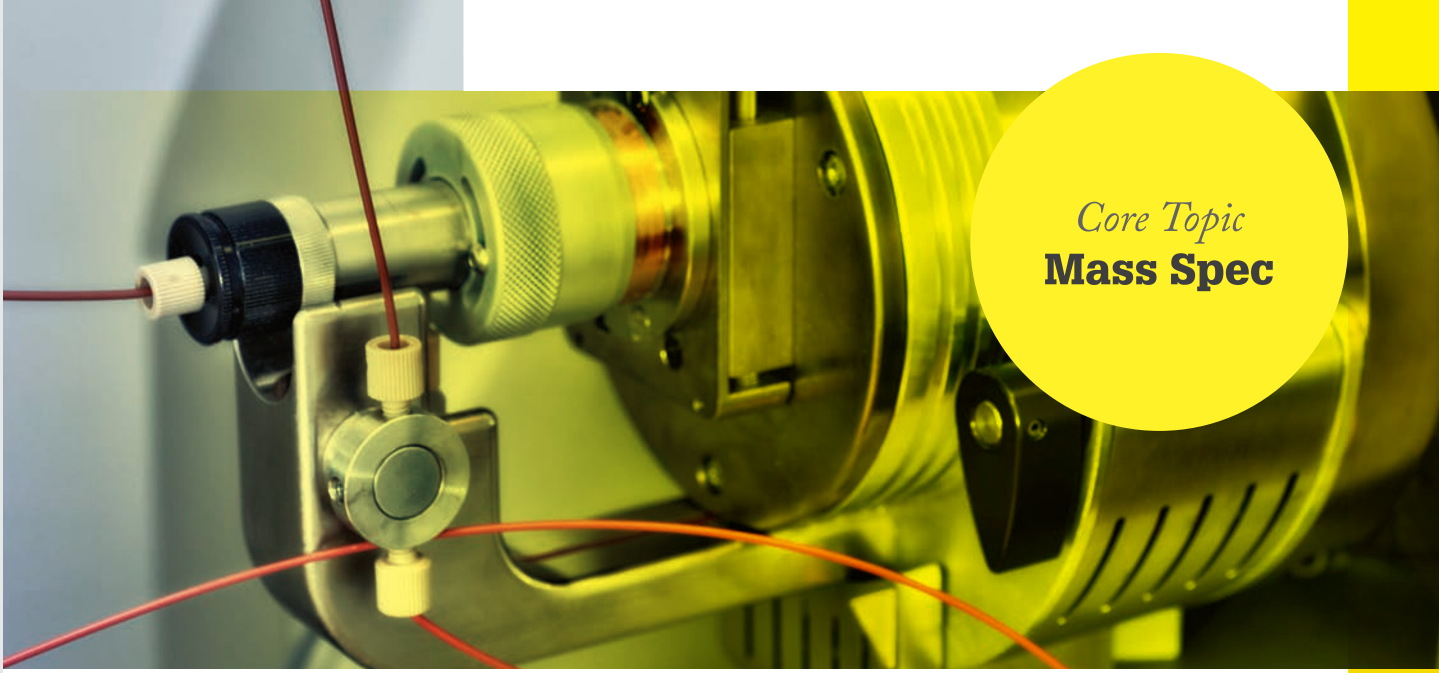


Credit: Shutterstock

Core Topic
Mass Spec

A sign of life? Saturn's moon Enceladus is one of the best candidates for life elsewhere in the solar system. Enceladus harbors an ocean of liquid water beneath its icy surface – like Europa and Titan – and jets that shoot water vapor into space. NASA's Cassini flew by and took a sample of the plume ice sprayed out of the subsurface ocean and analyzed it using Cassini's Cosmic Dust Analyzer, which includes a time-of-flight mass spectrometer. Recently, researchers announced that resulting spectra included phosphorus – a key building block for life.

What's your proteome age? The concept of "biological age" has emerged in recent decades – the idea being that age can be predicted from physiological markers and may differ from a person's chronological age. But which markers? An international team of researchers used a combination of mass spec and small RNA sequencing to quantify proteins and miRNAs, respectively, that changed in abundance with age. They then used the data to develop age-predictive models. They found that proteins yielded the most accurate model, followed by miRNA, and that using both together improved predictions.

Scent of a woman – or a man. The profile of scent compounds from a person's hand can be used to predict their sex, according to research from Florida International University, USA. The team used headspace-solid phase microextraction-gas chromatography-mass spectrometry (HS-SPME-GC-MS) to analyze the volatile scent compounds present on the palms of 60 individuals – half male and half female. The analysis successfully predicted a person's sex with a 96.67 percent accuracy rate. The researchers hint at forensic applications, given that trace amounts of evidence can be deposited on everyday objects through touch interactions.

Ohio's mass spec Mystery Machine. On February 3, 2023, a train carrying numerous hazardous chemicals derailed in East Palestine, Ohio, USA. Following a controlled burn of some of the hazardous cargo, residents reported headaches and respiratory, skin, and eye irritation. To monitor air quality, researchers drove a cargo van around the area for two days in late February. This Mystery Machine contained a proton transfer reaction-mass spectrometer, which revealed that average concentrations of benzene, toluene, xylenes, and vinyl chloride were below minimal risk levels for intermediate and chronic exposures; but levels of acrolein were up to six times higher than the local rural background. Nontargeted analyses identified levels of additional unique compounds above background levels. Jinkies!

References available online

IN OTHER NEWS

Informed by mass spec data, researchers develop diagnostic tool to visualize protein biomarkers of well-developed sperm to determine if surgical sperm extraction may be successful for certain infertile men.

Researchers from Sichuan University, China, use ultraviolet photoionization time-of-flight mass spectrometry to assess exhaled breath of kidney transplant recipients.

Southern University of Science and Technology, China, researchers develop fully automated and integrated workflow for high-throughput proteomics sample preparation and drug target identification.

Julia Laskin and colleagues use nanospray desorption electrospray ionization (nano-DESI) mass spectrometry to image low-abundance eicosanoids, lipid mediators of inflammation, asthma, fever, pain, hypertension, and stroke.

(Still) Pushing the Limits of Mass Spec Miniaturization

Discussing the multidisciplinary engineering challenge that is developing increasingly small mass spectrometry instruments with 908 Devices CEO and co-founder Kevin J. Knopp

We last spoke with Kevin Knopp, CEO and co-founder of 908 Devices back in 2014, after 908 Devices' handheld mass spectrometer (the MX908) – a world first – took the top spot in our inaugural innovation awards.

How has the instrument landscape changed over the past decade? Which applications are the team at 908 Devices excited about today? And what are the limits to mass spec miniaturization? We caught up with Knopp at ASMS 2023 to find out.

Refresh our memory… What was the inspiration behind 908 Devices?

Myself and a handful of other co-founders – some of whom worked together at a previous company – saw a need for what we thought of as high-quality trace detection. We really became enamored by the concept of taking mass spectrometry – arguably the gold standard of chemical and biochemical analysis – out of the lab to that point of need.

We wanted to democratize the notion of mass spectrometry. There is a whole side of the industry trying to push the envelope in terms of sensitivity and speed. You see these big, high-horsepower, heavy, supercomputer-style mass spectrometers – which are wonderful and necessary – but there's an unmet need for simpler solutions where you can expand the user base of these tools. There are tons of laptop and tablet users that just need to run their samples without having to send it off to a lab.

That's the road we've been on for over 11 years – finding new ways to do mass spec on a smaller scale, while also optimizing sample preparation on the front end and AI and machine learning on the back end.

Have your priorities shifted over the past decade?

We started off in the forensics space with our first handheld mass spectrometer – and it continues to be used to combat the opioid crisis and to detect counterfeit pharmaceuticals. We keep track of the number of pills, for example, that are being detected and seized each quarter with the MX908 technology, which is really exciting and rewarding – especially when you consider that six out of every ten pills contains a lethal dose of fentanyl, according to the DEA.

Over the years, we've expanded into biopharma and bioprocessing. Biopharma manufacturers want to be able to measure and control their key process parameters – amino acids, metabolites, and so on – at-line. And that's why we launched the REBEL cell culture media analyzer. But there's still some manual sampling that's required, which we'd like to eliminate through on-line connections. In August 2022, we acquired TRACE Analytics with this in mind. And earlier this year, we launched MAVEN, a device for on-line monitoring and control of glucose and lactate in cell culture processes.

A big focus for us at the moment is critical quality attributes – post-translational modifications, charge variant analysis, native analysis – and making a system that removes the complexity of chromatography. We've got this simple chip-based solution – ZipChip – that you can take out of the box and use without having to do any method development.

Finally, we're excited about the emergence of multiomics and remote sampling. We're working with researchers at Duke University to conduct multiomic analyses from a single sample containing 20 microliters of dried blood using our prototype microfluidic chips in our ZipChip device. For context, our multiomics approach combines metabolomics, top-down and bottom-up proteomics, and peptidomics to better understand what's happening at the

molecular level. Given the nature of personalized medicine, sample volumes matter, and ultimately such a complete analysis could potentially be performed at the single cell level.

What are the main technical challenges associated with pushing the limits of miniaturization?

I remember seeing a cartoon from the 1980s that showed someone in the future with a laptop-sized mass spectrometer – larger than the devices we've got today. So it's interesting to think about what might be possible in the future. But we certainly haven't reached a limit.

Looking at the theoretical curves, you can operate closer to atmospheric pressure while maintaining resolutions by increasing frequencies of the drive. So that puts a lot of pressure on your electronics and other parts of the system. Fundamentally, it's about creating a balance with multiple levers to pull. You need a small and power-efficient pump that has the flow rate you need, then you need to make an ionizer that's also small and efficient, as well as a trapping structure that will handle the higher pressures. There are many factors in play.

It becomes a multidisciplinary engineering challenge, where you're taking the mechanics, fluid handling in some cases, electronics (analog and digital), and putting them together in close proximity while also being smart about how you operate to maintain speed. That's where the software and algorithms come in.

But there is a roadmap to keep making things smaller. We see a path to a device that's half the size they are today – and I'm sure we'll be able to see the next step once we get there.

How do you tackle the multidisciplinary nature of the problem?

This is the biggest challenge. Even when you've figured out, from a mechanical engineering perspective, how to put things within close proximity of each other so that your pumping system can operate efficiently at the required pressures and flow rates, there's more work to do. You have to start thinking about potential applications, which means data interpretation software.

You need to involve experts in electronic design and software algorithms. You must also work closely with customers to find out what they really need – be that from the perspective of an operator working on in-field drug testing where true positive and false positive rates are important to someone working in bioprocessing where accuracy and precision for specific analytes are key.

What commercialization lessons have you learned?

It can be a long road from the initial idea through to commercialization. Persistence and perseverance are key. You also have to listen to the market – what do they really want? You might not like the answer, but there needs to be an appetite for your invention. The engineering, mechanics, and the science of creating the product is half of the work – the other half is on the commercial side. So that means marketing, investing in sales professionals, publishing application notes, building your brand, and so on. It's quite an endeavor in itself. You can control physics, but humans are humans – you have to persuade hearts and minds to adopt a new way of thinking and doing things.

What other trends are you seeing in terms of instrument innovation?

We're seeing an increasing number of faster – supercomputer-style mass specs – from some of the big players. But there's a lot of room for improvement on the chromatography side too, where method development can slow down the overall analysis. Our Science Founder, Mike Ramsey, often says that we could cut down analysis times from seven or eight minutes to less than one minute.

This move towards faster mass spec is really exciting when you start thinking about where we can go in terms of high-throughput proteomics and metabolomics.

What do you see as the killer applications for miniaturized mass specs over the next 5–10 years?

There's certainly a lot of opportunity remaining in the markets we're playing in today, such as forensics, bioprocessing, and multiomics. Within bioprocessing, I'm excited about the emergence of cell therapies. With autologous cell therapy, such as CAR T, you're talking about one batch per patient. I've been to several cell therapy conferences recently. And some of the players in this space are taking more conventional instrumentation and adding robots to make big pods, which is an interesting approach. Other companies are looking at it more fundamentally, asking how we might be able to make small-volume bioreactors integrated into the transfection process and informed by analytics. I see miniaturized, on-line mass specs fitting in here.

AI is a hot topic right now…

We've spoken about using miniaturized mass specs to harness data from a large molecule or cell therapy manufacturing process. But the next step is figuring out what to do with that information to tweak the process and increase yields – this is where AI or machine learning could come in to make predictions and offer feedback with regard to what you should be changing; for example, adding a particular supplement or sugar in a few hours based on the available data. But you need the data in the first place. So as these AI-based models emerge, the demand for inputs into those models will increase – which is where, once again, the analytics and on-line sensors come in.

Credit: Shutterstock

Core Topic

Spectroscopy

A bubbling LIBS application. Underwater LIBS has shown promise for oceanic applications, but the fundamentals of laser-induced plasma in water aren't well understood. To learn more, researchers examined the role of laser-induced plasma and cavitation bubble interactions underwater. Fast imaging and shadowgraph techniques revealed the temporal evolution of the bubble and plasma, detecting a severe pulse-to-pulse fluctuation in the latter. This was attributed to a transition period, characterized by instant decline of pressure in both elements.

No labels attached. Researchers from Texas A&M University, USA, have developed a thermostable Raman interaction profiling (TRIP) technique to study molecular structure and protein–ligand dynamics. The researchers successfully characterized antigen–antibody and protein–drug complexes in real time, while retrieving highly reproducible and accurate Raman signals. This cost-effective and label-free approach demonstrated higher speed than other methods, such as X-ray scattering, suggesting future applications in the pharmaceutical industry.

What Raman says. Common analytical techniques for therapeutic protein identification are efficient, but require extensive sample preparation and removal of samples from their containers. To overcome these challenges, scientists applied a Raman spectroscopy-based approach – involving a bioprobe and chemometrics – to monoclonal antibody (mAb) identification. The team were able to rapidly and noninvasively identify three different mAbs, demonstrating Raman spectroscopy's potential in biopharmaceutical analysis.

Beauty lies within… The unique history of Arabian-Nubian Shield gemstones was revealed by scientists employing a trio of spectroscopic techniques. Chemical composition was studied with laser-induced breakdown spectroscopy (LIBS), suggesting that iron content and other elements such as copper influence the color of the stone – a distinct characteristic of its origin. Crystalline structure, another indicator of its source, was identified via Raman spectroscopy, distinguishing gems from Egypt and Jordan. Finally, fourier transform infrared (FTIR) spectroscopy was employed to generate signature water peaks that differentiate synthetic from natural gems.

References available online

IN OTHER NEWS

Laser-induced breakdown spectroscopy (LIBS) coupled with sorting algorithms shown to improve waste characterization and management processing after accurately identifying 80 different waste samples.

Attenuated total reflection-Fourier transform infrared (ATR-FTIR) spectroscopy reveals that high levels of organic pollutants in plastiglomerates are damaging coastal ecosystems in Indonesia.

Researchers demonstrate the usefulness of Raman spectroscopy for exploring cultural heritage artifacts by analyzing the yellow coloring in Buddhist paintings from the late Joseon dynasty (17th–19th centuries).

NASA Mars Perseverance Rover's deep ultraviolet (DUV) Raman and fluorescence spectrometer reveals evidence of diverse organic material on Mars.

Ten Year Views: With Vassilia Zorba

Lasers, plasmas, Mars, and more lasers…

To commemorate our 10th anniversary, we're reflecting on the field of analytical science – speaking with leading figures and friends of The Analytical Scientist to understand how far the field has come over the past decade, what lessons have been learned, and where we go from here. In this installment, Vassilia Zorba, Group Leader for Laser Technologies Group at Lawrence Berkeley National Laboratory, and Associate Adjunct Professor in Mechanical Engineering at the University of California, talks us through the benefits of laser implementation in analytical science – and what the future holds for spectroscopy…

In your opinion, what has been the most significant development in spectroscopy over the past 10 years?

It's difficult to pin down just one, as there have been so many great developments during that time. There have been some interesting advancements in nonlinear optics and their integration in the field of analytical chemistry. Specifically, the use of nonlinear ultrafast laser-matter interactions in the laser plasma formation regime, which has been instrumental in addressing issues like improving spatial and depth resolution. We've also made advances in our ability to propagate pulsed laser beams and deliver energy at long distances. With this development, we're now able to suppress diffraction, which allows us to concentrate pulsed laser energy to a target at a remote location. This discovery has been a critical component in our ability to generate plasmas for remote spectroscopy applications.

Another pivotal moment has to be the ChemCam mission to Mars. This was a very challenging problem to tackle and ChemCam's success has been extremely beneficial for the field of laser-induced breakdown spectroscopy (LIBS). This tremendous milestone has demonstrated the amazing possibilities of LIBS as well as introducing its capabilities to a wider audience. We've seen the flexibility of the technique and what can be achieved – which has encouraged many researchers to use LIBS in their work. Seeing such advancement in technology is always an exciting moment.

What are some of the key applications for lasers?

Energy conversion and storage are significant application areas – laser spectroscopy allows us to understand variations of chemical composition in solar cells and Li-ion batteries. Researchers have also been looking at biomedical imaging with laser spectroscopy, including LIBS.

Personally, I favor the recent direction towards all-optical isotopic techniques, which unlock completely different types of applications. The development of the laser ablation molecular isotopic spectrometry (LAMIS) technique in particular has opened up new horizons in terms of what is possible for many different areas in biomedical and environmental research. When it comes to nuclear security, the ability to detect isotopes optically is incredibly important for measuring the levels of enrichment in nuclear safeguards and forensics. Isotope ratio mass spectrometry has shown the tremendous information we can gather regarding when or where something was made – based on high precision measurements of Isotopic ratios. Transitioning even a few of these isotopic ratio measurement capabilities from mass spectrometry to laser spectroscopy can be a real game-changer for rapid analysis in the field. It all comes down to the level of precision; for some applications, laser spectroscopy can already do very well – for others requiring very high levels of precision we're not quite there yet, but we're getting closer!

What about your own work with next-gen laser tools?

In the past, I worked on the utilization of ultrafast LIBS to analyze lithium ion batteries with high resolution. This involved using three-dimensional imaging to look at the composition of

"I have two main goals. The first is to fuse advanced optics and nonlinear concepts with analytical spectroscopy to improve current capabilities in cross cutting applications. The second involves training the next generation of scientists to drive further progress in the spectroscopy field."

minor elements in complex matrices. Additionally, by looking at interfacial layers as thin as 50 to 100 nanometers, we can understand how chemical reactions during battery charging can affect the macroscale battery performance after electrochemical cycling.

More recently, I've been looking into applications in nuclear security and nonproliferation. By using ultra-fast laser tools and advanced optics, we can propagate a pulsed laser beam over long distances for remote sensing from solids. There are multiple forms of interesting spectroscopic information we are only now able to unveil as some of the technology components are becoming more mature. A lot of work goes into manipulating beam propagation and phase wavefront – for example, using laser filaments or orbital angular momentum beams to deliver a high amount of energy across a remote distance. The pulsed laser energy must be high enough to form a plasma from a solid sample so we can extract elemental and isotopic information.

You mentioned lithium ion batteries – how can analytical science help us here?

In the semiconductor industry, we know that there is very tight control in standardization of the process – for example, fabrication is performed under clean room conditions. However, this is not the case for battery manufacturing – which means that batteries can often work successfully despite the presence of impurities or compositional variations.

But when it comes to large format applications, such as electric vehicles, we need to better understand the composition of raw materials to be able to control the macroscale battery performance. Once you start charging a battery, electrochemical reactions take place which adds a layer of complexities. Understanding composition and mapping variations of composition as a function of space and depth can give electrochemists clues to making better batteries. This includes battery components such as anodes, cathodes, solid state electrolytes, and interfacial layers formed on battery electrodes.

What is most exciting to you about the future of spectroscopy?

A new concept that has been introduced in the laser-metal interaction community, which is called cold ablation or ablation cooling. Thanks to tremendous developments in laser technology, we have the capability to produce gigahertz (GHz) bursts of femtosecond laser pulses – these are nanosecond-spaced series of pulses of femtosecond duration. Recent research looked into the mechanisms of GHz burst ablation with femtosecond pulses for the first time, and the results showed significant differences to traditional femtosecond plasmas – both in terms of expansion of the ablation ejecta and what we do on the surface. I think this is a very exciting direction to go into – and it offers possibilities for improving our spatial and depth resolution even more as well as improving our analytical performance as a whole.

What would you personally like to achieve in the next 10 years?

I have two main goals. The first is to fuse advanced optics and nonlinear concepts with analytical spectroscopy to improve current capabilities in cross cutting applications. The second involves training the next generation of scientists to drive further progress in the spectroscopy field. Specifically, I want to make the field more appealing for students by giving them a taste of the possibilities within spectroscopy.

What advice do you have for someone who is new to the field of analytical science?

Perseverance is the number one thing to learn. It's also useful to keep an open mind about learning and fusing different concepts – even those from other disciplines. Research is becoming more interdisciplinary, and by incorporating a diversity of ideas and principles from chemistry, physics, and engineering, you could unlock a multitude of possibilities. Overall, being prepared to work hard and not being afraid to expand your scientific horizons will help you advance in your career and contribute to the field.

Vassilia Zorba is Group Leader, Lawrence Berkeley National Laboratory, Berkeley, California, USA.

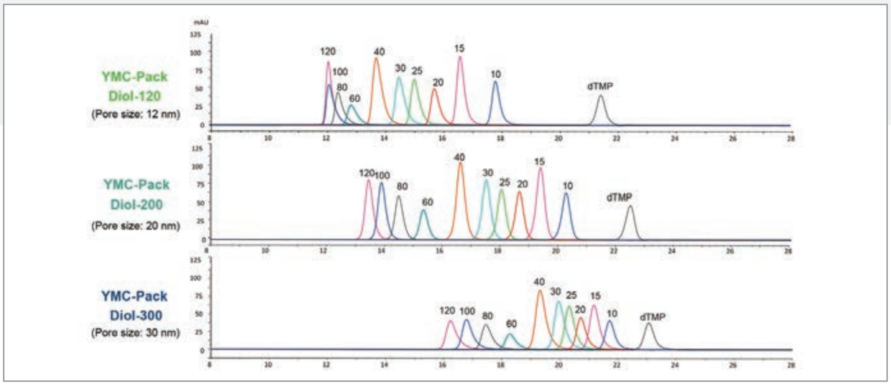


Figure 1: SEC analysis of ssDNA of 10–120mer length using YMC-Pack Diol columns with different pore sizes.

Pore Size Selection for Separation of Oligonucleotides by YMC-Pack Diol Columns

Oligonucleotide length usually ranges from 12–25mer. However, the demand for longer oligonucleotides with lengths up to 200mer is increasing. These extremely long oligonucleotides are used in a variety of molecular biology applications, including site directed mutagenesis.

Separation of oligonucleotides by size exclusion chromatography (SEC) is a valuable alternative to the standard methods: ion pair reversed phase liquid chromatography (IP-RP) and anion exchange chromatography (AEX).

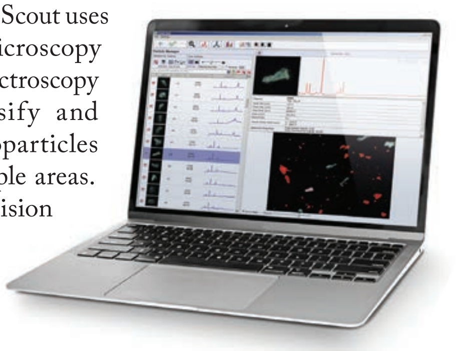
Three different columns of the YMC-Pack Diol series with distinct pore sizes were tested for their ability to separate DNA of various lengths. Single-stranded DNAs (ssDNA) with lengths ranging from 10–120mer were compared to double stranded DNA (dsDNA) with lengths of 10–300mer as well as to proteins of different sizes.

YMC-Pack Diol-120 (12 nm) was best suited for shorter oligonucleotides (10–40mer), whereas YMC-Pack Diol-200 (20 nm) showed the best resolution for oligonucleotides of medium size (30–80mer). Longer oligonucleotides of 60-120mer in length were separated most effectively by YMC-Pack Diol-300 (30 nm).

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

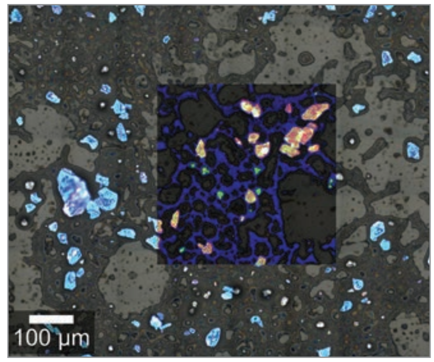
WITec ParticleScout – Automated Raman-based Microparticle Analysis Tool

WITec ParticleScout uses white-light microscopy and Raman spectroscopy to find, classify and identify microparticles over large sample areas. Its speed, precision and user-friendliness can benefit researchers in environmental science, microplastics research, pharmaceutical development, geology, food science, and many other fields.

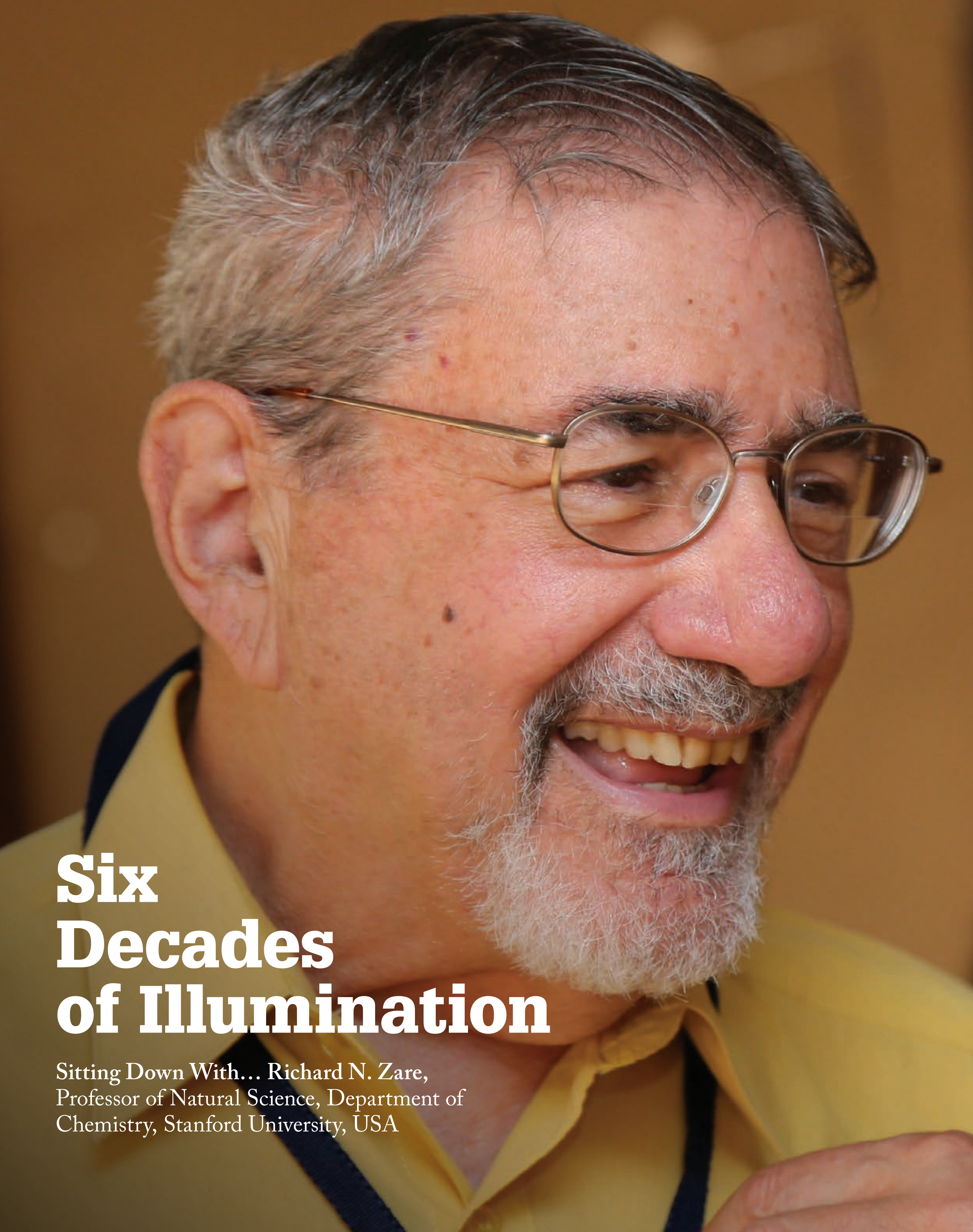


ParticleScout's advanced software routines sort particles by physical attribute and acquire their Raman spectra. Focus stacking that keeps large particles in focus and full integration with the TrueMatch Raman database management software are without equal in the marketplace.

ParticleScout also features integration time optimization to reduce total measurement time, vignetting correction, smart zoom, sample illumination options, smart separation of adjacent particles, multiple sample area targeting, and quantitative report formatting to present data using table, bar graph histogram and pie chart templates for ease and clarity.



Explore WITec ParticleScout: https://raman.oxinst.com/products/software/particlescout



Six Decades of Illumination

Sitting Down With… Richard N. Zare,
Professor of Natural Science, Department of Chemistry, Stanford University, USA

How did your fascination with chemistry begin?

As a child, I was full of questions – asking why things were the way they were. In kindergarten, I remember asking my teacher what holds up the stars, and I was frustrated because she didn't give me a satisfactory explanation. I knew that light bulbs were in the ceiling, but I didn't understand how the lights from the stars were held in the sky.

My father failed chemistry in graduate school and I think that may be one reason why I gravitated towards it, despite his protests. In fact, my parents said that it would only lead to unhappiness, but I was enamored by the chemistry books lying around the house – sneaking them into my bedroom at night and reading under the covers with a flashlight.

They wouldn't let me have a chemistry set, so I went to the pharmacy (which these days would be similar to a drugstore) and asked for powdered charcoal, potassium nitrate, and sulfur. The pharmacist asked if I knew what I was doing, to which I said yes – despite setting the basement of my house on fire while meddling with magnesium in the upcoming months and years. But I loved playing around with chemistry and learning how and why reactions occurred.

You received your PhD in 1964 and are still full time faculty. Have you seen much change as a researcher and professor over the past 60 years?

I think students are just as smart and creative today as they've always been. However, distractions – television, social media, and so on – have negatively impacted people's attention span. Everyone's looking for sound bites of information, as opposed to spending a reasonable amount of time researching a topic. There also isn't a lot of interest in math anymore. As a whole, I'd say I have seen surprisingly little change. That being said, I've been very lucky during my career to work with some wonderful people – both advisors and students.

You've collaborated on various projects over the years – can you explore a few of the outcomes?

I'm a big advocate for multidisciplinary work – bringing people together with different expertise from different fields is where the biggest breakthroughs occur. In these situations, you're able to do things together that would be impossible separately – and everybody wins.

For example, I've worked with a medical doctor in China on a health related research project. The regulations for collecting data samples are much more relaxed in China than they are here in the US, so this collaboration granted me access to many different types of medical samples that I wouldn't have had in solo projects.

I've also recently been in collaboration with Basheer Chanbasha, a professor of chemistry at King Fahd University of Petroleum and Minerals in Saudi Arabia, to explore nitrogen fixation. We're actually able to take nitrogen from the air and turn it into ammonia or urea using water microdroplets striking a catalyst. The outcomes of this are very exciting. There is a long way to go before this might be commercialized, but if we could push this process, we could be looking at something very different to the Haber-Bosch process for producing ammonia.

Please tell us about laser induced fluorescence – and what you accomplished…

When I was a graduate student, I worked with Dudley Herschbach while he was pioneering crossed molecular beams. The experiments looked particularly hard, so I got involved with the theory of molecules – using a mercury lamp to excite vapors of the iodine molecule and make I2 fluoresce.

The laser was discovered in my lifetime and people didn't know what to do with it. I decided to use it as a source to excite fluorescence of molecules. Some rather influential people at the time told me to forget it, but I continued to push further because I knew there was potential.

With more work I discovered that you can capture fluorescence with a photodetector by exciting a sample with a laser. This optical spectroscopic technique is now known as laser induced fluorescence (LIF), and is regularly used to analyze gasses, liquids, and solids..

With LIF, we became the first people to see a single molecule in a solution at room temperature. This was a great achievement that I don't believe got enough promotion at the time – but it was a breakthrough for the field nonetheless. I knew the future possibilities from LIF were going to be great.

What motivates you – and what keeps you on track?

I think what initially drove me was an attempt to please my father and show my worth as a scientist. Though as I've worked my way through the field, I think it is a combination of curiosity and the pleasure I receive in sharing new knowledge with others – I believe a lot of others in this line of work will share this sentiment.

Communicating this excitement with others and learning to look at the world differently is an extraordinary thing. In a sense, I think science and art are much more related than people often give credit. As a painter, you'd be frustrated if no one else saw your work, regardless of how much you enjoy creating art. Similarly, when I discover something about nature, I want to share this information with others. For me, it's about being curious and interacting with others to share exciting knowledge.