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the Analytical Scientist™

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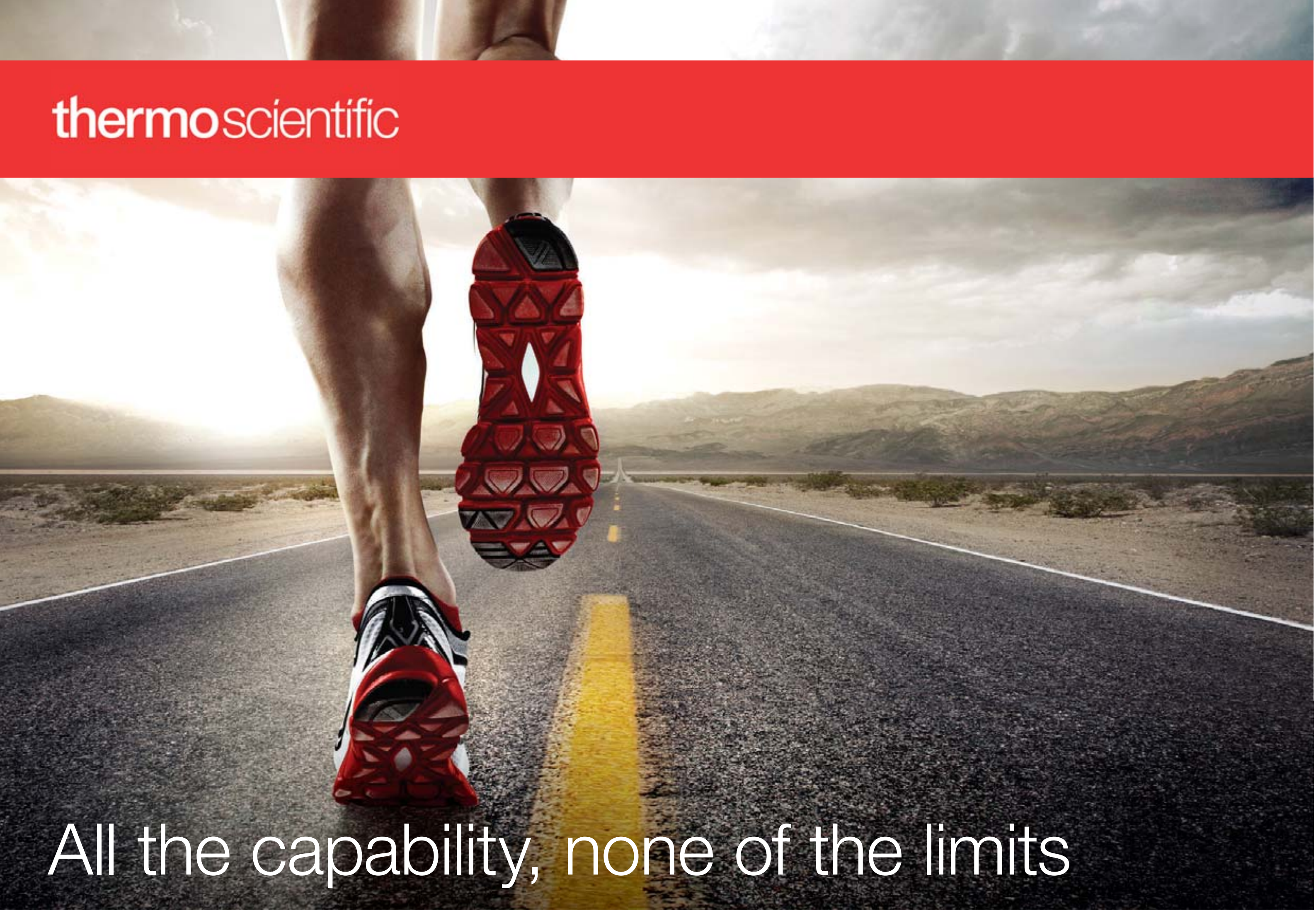

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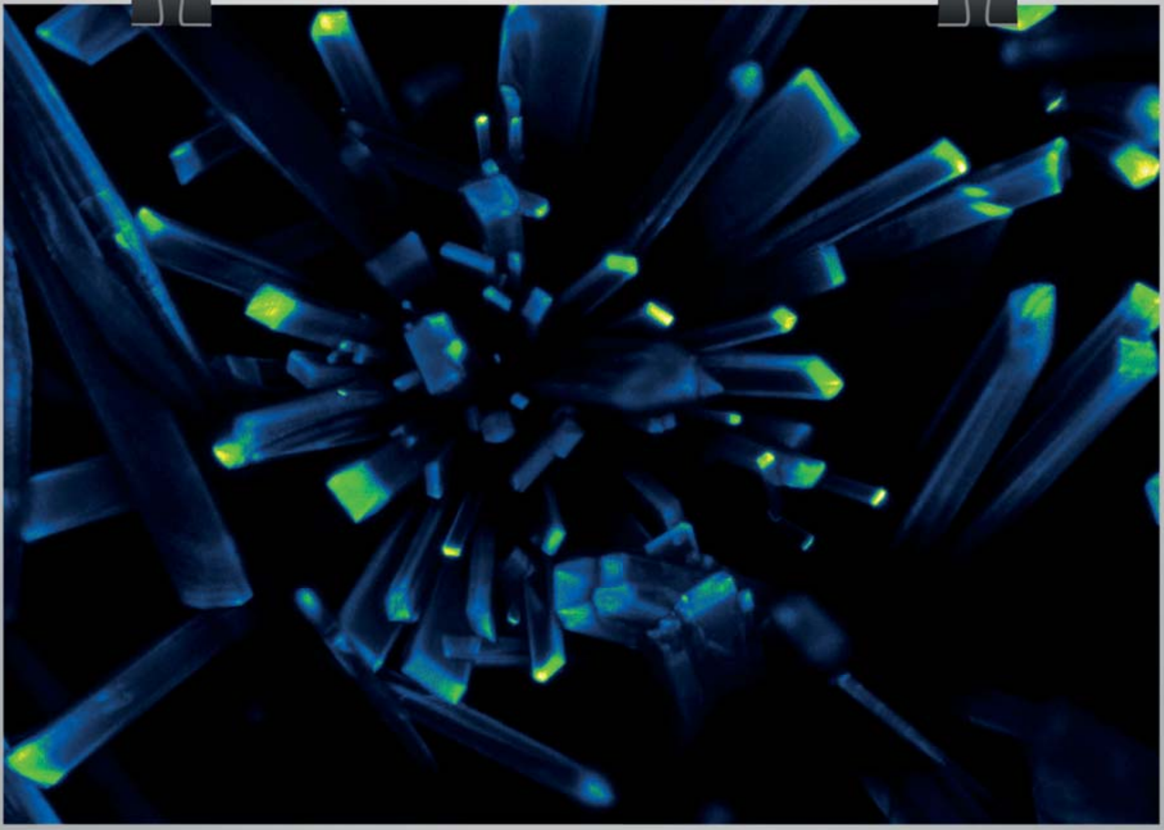
Image of the Month



Crystal Maze

A 2,5-hidroxybenzoic acid matrix-assisted laser desorption/ionization matrix cocrystallized with a fluorescein isothiocyanate-conjugated peptide. The sample was created by Ben Katz, a proteomics specialist at the University of California, Irvine, to improve resolution and lower background noise. Follow Ben on Twitter @ProteinMassSpec.

Credit: Nicole Green, Iowa State University, USA.

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

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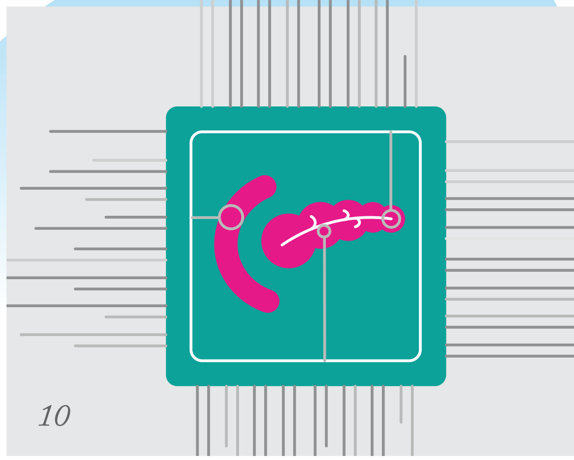
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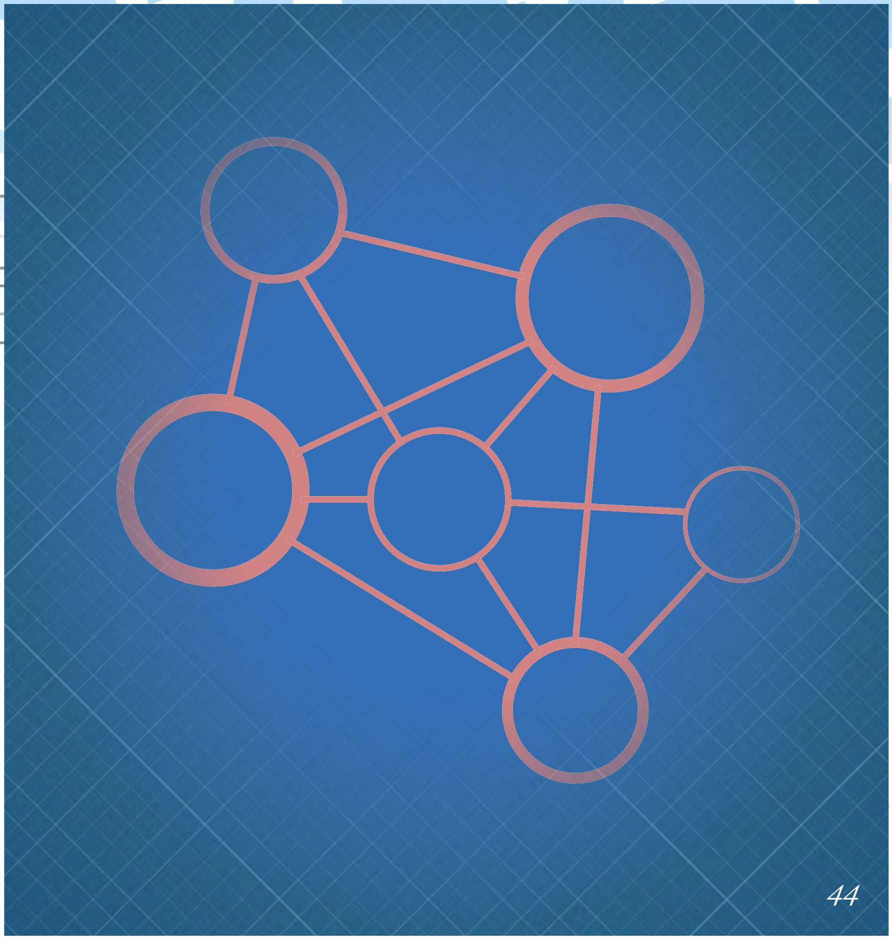
On The Cover

Sometimes the simplest approach is best… The Power List 2019 is here.



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The Power and The Passion

The Power List 2019 highlights the strengths of analytical science – and the community behind it

The Power List 2019 has landed – a celebration of the top 100 most influential figures in analytical science. Curating the list (collecting nominations received from across the globe, working closely with our judging panel, and corresponding with all 100 nominees) has been a lengthy process – but also a privilege. Few fields are supported by a workforce that can lay claim to the level of dedication and passion that our community exudes. Whether speaking of fundamentals or applications, biology, the environment or beyond, it's clear to see that immersion in this field is closely tied to a real belief in its purpose.

And that's likely why the field is so highly connected – and brimming with positivity. As Paul Bohn notes, we have "terrific colleagues all over the world," and this translates not only into prime opportunities for enjoyable and fruitful collaboration, but also into a tightly knit network of support that helps propel each of us forward to tackle the problems ahead.

To thrive, we must move with the times; as such, to quote Caroline West, analytical chemistry is "a dynamic science that changes rapidly." The perpetual progress in our field is highlighted by advances in instrument miniaturization, usability and portability, and the application of artificial intelligence and automation. Increasingly, instrumentation is moving away from labs and into the real world. What's more, the continuous streamlining of the analytical process means that these increasingly portable technologies are providing data that can be interpreted and used in record time.

Of course, all of these endeavors feed into a single end goal (likely the reason we were drawn to science in the first place): to understand our universe and improve lives. For analytical scientists, this mission can take many paths – medicine, agriculture, technology, space exploration, and many more – but, whichever direction we choose, we rarely have to walk alone, instead working within increasingly diverse, passionate and motivated teams. I'm sure Ljiljana Paša-Tolić isn't the only one that would say they love "being part of this great community."

Overall, there are many lessons to be learned from the Power List, but they can be simply summarized for the entire analytical community: we're a busy bunch and we love what we do.

Matthew Hallam
Deputy Editor

Upfront

Reporting on research, personalities, policies and partnerships that are shaping analytical science.

We welcome information on interesting collaborations or research that has really caught your eye, in a good or bad way. Email: charlotte.barker@texerepublishing.com

Tipping the Scales

Alternatives to environment-damaging paint additives may come from an unlikely source: the beauty of bugs

The vibrant orange of a toucan's beak. The emerald green of a turtle's shell. The striking red of a field of tulips. Nature is full of stunning examples of mesmerizing color and beauty – as they say, "nature does it best." Attempts to mimic these tones is an active area of research, gifting today's scientists with an ever-growing library of synthetic compounds for application in food, beverages, paint, cosmetics and beyond.

But, as the high carbon footprint (and toxicity) of many of these pigments becomes more apparent, the demand for more environmentally friendly alternatives grows stronger. Did you know that titanium dioxide – prized for its whiteness – contributes almost 75 percent of a paint can's carbon footprint?

Inspired by such revelations, Andrew Parnell and colleagues set out to find an alternative (1). The *Cyphochilus* beetle, noted for its opaque, white scales, has proven an unusual specimen; its color can be attributed to light scattering (where refraction and reflection of light inside the scale is responsible for its color, shade, tone, and hue) rather than the result of color pigments.

To avoid damaging the beetle's delicate scales, the team used X-ray nanotomography – a non-invasive approach – to study the 3D nanostructure. "The first thing we noticed was that the structure was continuous," says lead author Stephanie Burg. From there, the team generated two hypotheses: firstly, that the structure was likely established at a single point in time during the beetle's development; and secondly, that this process might be easily replicated and reproduced.

To test the latter, the researchers coupled advanced modeling software with liquid-liquid phase separation technology to create a synthetic variant of the scale, comprising a highly reflective (~94 percent) white film. Analysis of the copycat scale made use of scanning electron microscopy, spectroscopic ellipsometry and microspectroscopic measurement, among other approaches. "It turns out that you can get back the exact same response from our model that you get from the beetle scale," says Burg. Now come the challenges inherent to translating these findings into environmentally sustainable products. "We've had some promising preliminary results, but formulation chemistry is a difficult thing to crack," says Parnell.

While tackling that challenge, Parnell has found additional inspiration in the form of *Parides sesostris* – a vibrant-green butterfly. "We're keen to fully grasp this concept of synthetic iridescence by studying a variety of organisms," he says. "A whole plethora of different architectures exist. We are just scratching the surface at present." No pun intended.

In the spirit of collaboration, the group are now putting together a paper that will allow others to manipulate the data obtained from these studies. "We want people to develop their own models, exploring aspects of the problem we haven't looked into," says Parnell.

So why did the beetle evolve to be ultra-white? Parnell has a number of theories – "But that's a puzzle for another day."

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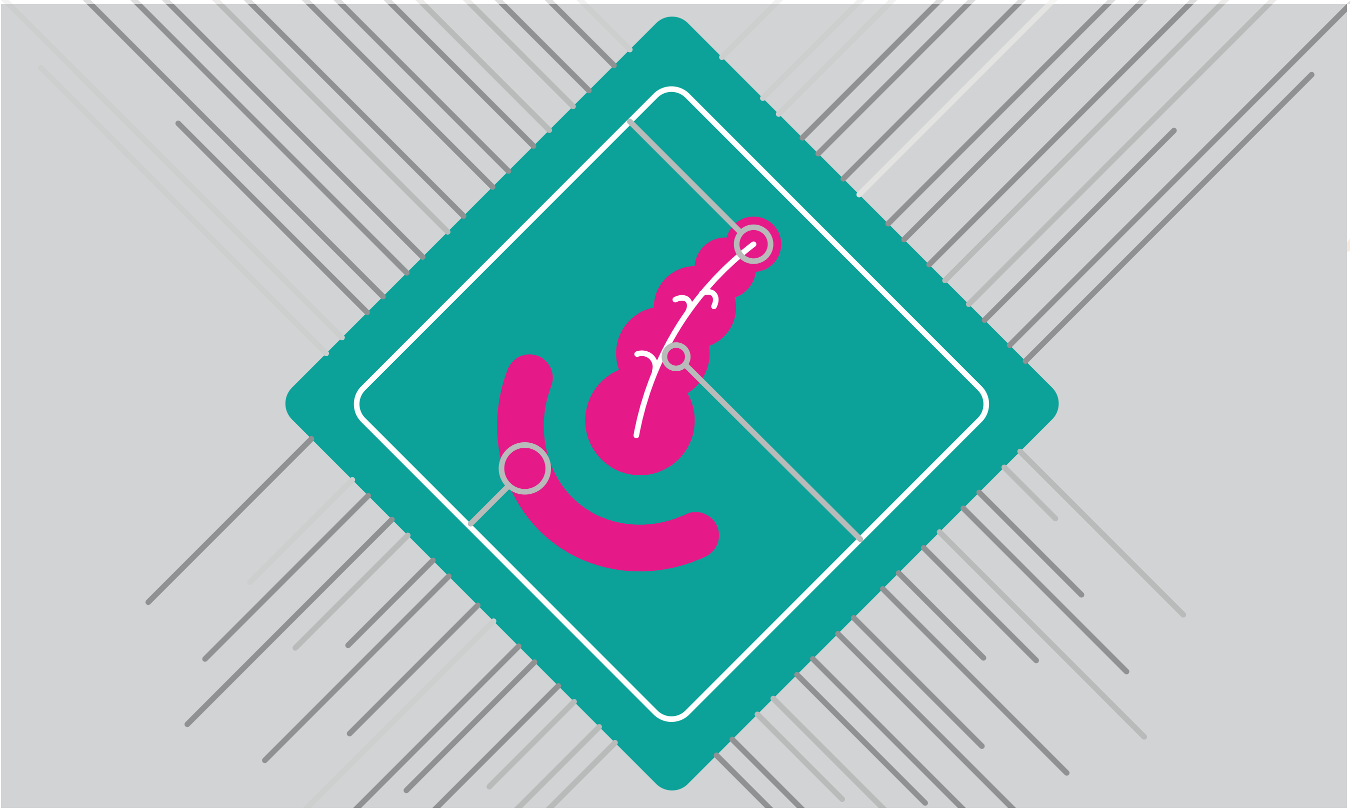

Stimulating and Sensing Insulin Secretion

An "islet-on-a-chip" device could inform beta cell transplantation – and diabetes research as a whole

Diabetes is a global issue of increasing magnitude. In 2017, at least 30 million people in the US had the condition – and another 85 million could be described as "prediabetic" (1). Beta cell transplants represent one therapeutic avenue, but current approaches for confirming the post-transplant functionality of these cells are labor intensive and time consuming, producing data that are difficult to interpret.

Seeking a new approach, Kit Parker and colleagues at Harvard and The University of Florida combined microfluidic technology and stem cell biology to develop an "islet-on-a-chip" device capable of measuring insulin secreted in response to glucose stimulus (2); more specifically, the device is able to continuously sense and quantify insulin secretion by an automated, on-chip immunoassay and fluorescence anisotropy, respectively. "By incorporating microfluidics and optical sensors into a single device, we've been able to acquire reams of information regarding cellular performance and response times in near-real time," says Parker.

"Now that we have a tool, we can begin to develop protocols around quality control – this will help us to know exactly what we are transplanting into the patient," he says. Though the device has hurdles to jump ahead of clinical use, Parker believes it could have an immediate impact on diabetes research: "There is a lot to learn about diabetes using tools like this. This granular understanding of the temporal dynamics of cells is unprecedented, and it's likely that future findings will challenge the established canons in diabetes."

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Explosive Experimentation

A holistic view of fireballs: infrared spectroscopy facilitates the acquisition of continuous chemical data from explosions

What?

Researchers have developed a novel method to study explosions using infrared spectroscopy. Specifically, broadband Swept-wavelength external cavity quantum cascade laser (swept-ECQCL) spectroscopy allows the acquisition of absorption spectra for chemical products produced within explosive fireballs – with the impressive sampling rate of 500 kHz (1).

How?

Directing a laser generated by the swept-ECQCL device through the fireball, the team were able to monitor changes in chemical composition over the first 10 ms post-explosion. Beyond that initial period, and up to the 100 second mark, the team used broadband high-resolution absorption spectra acquired over the spectral range of 2050–2300 cm^{-1} at a 100 Hz rate.

The study examined four types of high-energy explosive during detonation in a purpose-built, blast-resistant chamber. Many products are produced during such explosions, among them carbon dioxide, carbon monoxide, water vapor, and nitrous oxide, and each can be distinguished by its infrared absorption pattern.

Why?

The fleeting nature of detonation presents analytical challenges. Certain probes (for example, thermocouples or pressure transducers) can produce time-resolved data on physical conditions, but provide no chemical information. Meanwhile, laboratory analysis only grants access to accurate chemical profiles of starting materials or end products – leaving a need for guesswork or modeling to fill in the gaps.

In contrast, optical measurement techniques, which can be performed from a safe distance (a crucial benefit in this application), have a sufficiently rapid response – typically limited by the speed of optical detection – and can therefore provide a stream of continuous chemical data as the explosion unfolds.

The team are optimistic that future endeavors – including extending the range of wavelengths studied – will provide insight across a range of disciplines, from crime scene investigation to explosives manufacturing and management.

Reference

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Lotion in the Ocean

The presence of sunscreen compounds in seawater is unlikely to be good for marine ecosystems, but just how bad is the problem?

The benefits of applying sunscreen during a well-deserved beach holiday are widely acknowledged, but the environmental impact of these products is less well known. In addition to UV filters, commercial sunscreens contain a variety of further ingredients, making sunscreen a complex matrix that is difficult to manage both analytically and environmentally. Now, researchers have developed a kinetic model capable of determining the behavior, variability, and contribution of metals and inorganic nutrients from sunscreens to seawater composition. We spoke to Araceli Rodríguez-Romero, one of the project leads, to find out more.

What inspired the work?

The quality of our oceans – home to rich biodiversity and invaluable natural resources – can be affected by excessive human pressures. We are well aware of many pollution contributors – plastic, microbeads, and chemical toxins to name just a few. In recent years, attention has turned towards sunscreens. Organic (oxybenzone, octinoxate) and inorganic (TiO_2, ZnO) UV filters – as well as other innumerable other compounds that are incorporated into sunscreen formulations – are emerging as contaminants of aquatic ecosystems.

Policymakers need to be well informed if they are to implement strategies that protect marine environments, and drive Good Environmental Status. Hence, we wanted to develop a tool capable of modeling the release of metals and inorganic nutrients from sunscreens into marine ecosystems; understanding these risks will be critical for governments concerned with sustainable growth and development in coastal regions.

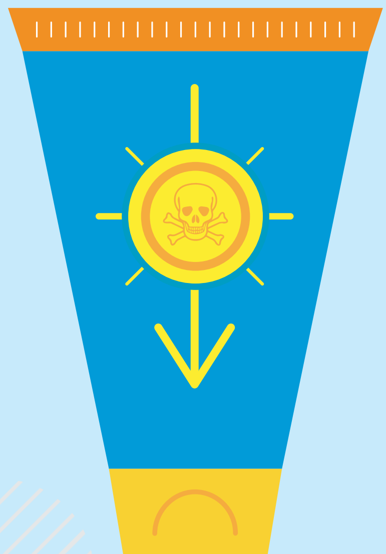
What analytical techniques did you employ?

Using inductively coupled plasma (ICP)-MS after chemical digestion, we determined the metal (aluminum, cadmium, copper, manganese, molybdenum, nickel, lead, cobalt, and titanium) and total phosphorus and silicon content of sunscreens. To determine the quantity of metals released from the sunscreen to the seawater after the experimental exposure, we pre-concentrated seawater samples using a liquid-organic extraction method before analysis – again using ICP-MS. The concentrations of inorganic nutrients in sunscreen and seawater samples were determined using colorimetric techniques in parallel.

We then modeled the data obtained from our laboratory experiments using Aspen Custom Modeler Software.

What did you uncover?

We've been able to explore numerous key variables describing the effects of dissolved trace metals and inorganic nutrients from sunscreen products on marine coastal waters. Release rates (from sunscreen into seawater) were greater under higher UV light conditions for all compounds, with the exception of lead. Notably, titanium and phosphorus were the most readily affected by changes in UV light. As algal blooms in oligotrophic waters such as the Mediterranean Sea are, in part, influenced by an increase of phosphorous, it is clearly of importance to understand the risks associated with sunscreens released into marine coastal ecosystems. We hope that our elemental release model might form the basis of future models that incorporate further chemical and environmental variables.



What are your next steps?

We plan to test our model using other commercial sunscreens – including those labeled as "ecofriendly." We also want to sample coastal waters throughout the day to verify the results obtained in the lab; this will allow us to evaluate the true impact of sunscreens on marine ecosystems. At the same time, we are also working to create and promote a new network dedicated to fostering scientific collaboration between researchers working in the field, the cosmetics industry, and the public and private sectors.

Reference

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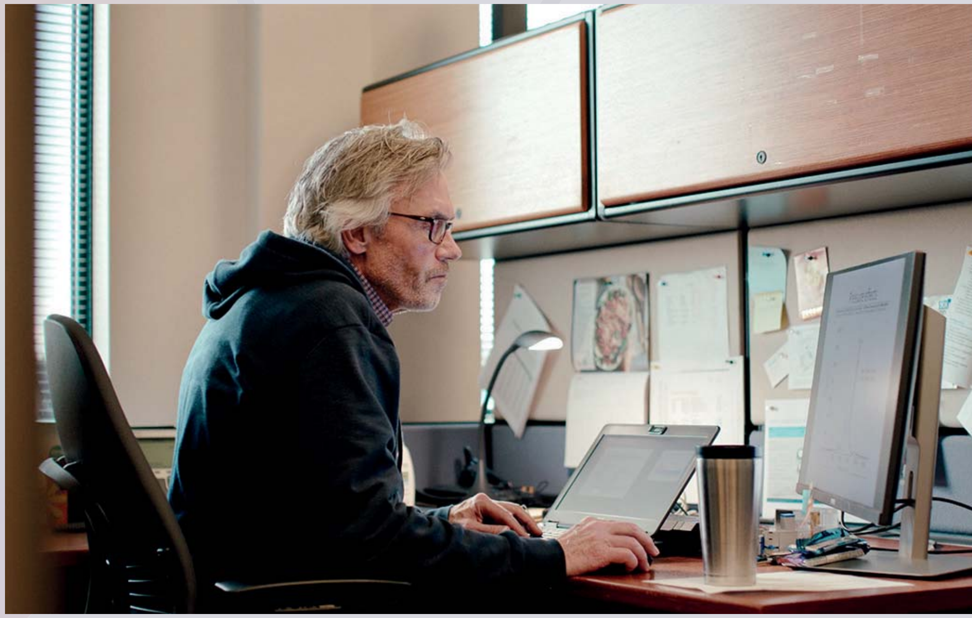
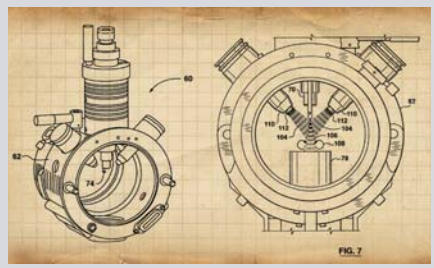
Supercharging Spectrometry

Our analytical capabilities have exploded since the LC-MS revolution of the 1980s – but where will our curiosity take us next?





The release of the first commercial Atmospheric Pressure Ionization tandem quadrupole MS (API III) system from SCIEX at 1989's Pittcon in Atlanta opened the door to pioneering work by enabling the quantification of molecules in liquid-phase samples – work previously possible only in the gas phase. LC-MS subsequently adopted a central role in analytics; Tom Covey, Principal Research Scientist at SCIEX, summarized this revolution in episode one of the Generation Quant series as having "cracked the liquid phase/gas phase dilemma."

Three decades later, key figures in the field returned to Atlanta for ASMS 2019 – some unknowingly retracing the ground where the journey of this vital instrument began, where our ability to perform molecular analyses were forever transformed. From pharmaceutical development to food safety and the wider life sciences, the API III offered solutions to problems that had plagued the field for years. How? By applying an IonSpray source that gave access to both speed and high sensitivity.

> "We were suddenly presented with this new combination of software and hardware that exhibited incredible speed"

"We were suddenly presented with this new combination of software and hardware that exhibited incredible speed – that's why people adopted it," says Liz Thomas, cofounder and CEO of Alderley Analytical. "On a larger scale, this meant that researchers were making faster decisions, and the entire industry was moving more quickly as a result."

SCIEX continues to push the boundaries of quantification to fuel scientific endeavors the world over. The aim: to inform critical customer decisions and make "The Power of Precision" a reality for all. Momentum is building towards this ultimate end goal, with some researchers already harnessing the advanced capabilities of new technology across all applications of MS to improve lives, the environment, and our understanding of science as a whole.

Of course, there is further work to be done, but scientific innovation never stops… And neither do SCIEX. If you'd like to be one of the first to hear about the next big breakthrough from these industry leaders, register your interest at https://bit.ly/2nLQoP9.

In the meantime, the technological feats engineered by the company to date – and a sneak preview of future plans – are shared in Generation Quant (sciex.com/GenerationQuant) – an informative but emotionally charged video that highlights SCIEX's ongoing commitment to the field.

In My View

In this opinion section, experts from across the world share a single strongly-held view or key idea.

Submissions are welcome. Articles should be short, focused, personal and passionate, and may deal with any aspect of analytical science. They can be up to 600 words in length and written in the first person.

Contact the editors at charlotte.barker @texerepublishing.com

Wanted: Native Protein LC-MS

Complex biologic characterization demands a new era of assay technology – the analytical community must seize the opportunity

By Matthew A. Lauber, Waters Corporation, Milford, Massachusetts, USA.

The biologics field is booming and showing no signs of slowing down. As the biotech industry has developed, it has adopted advanced engineering techniques to produce antibody-drug conjugates (ADCs), bispecific monoclonal antibodies and new types of fusion protein scaffolds – and the products are becoming increasingly complex. Yet complexity is no excuse for compromise when it comes to patient safety or lot-to-lot reproducibility, so analytical assays must be up to the challenge of converting complicated biomolecular puzzles into tractable, well-characterized molecules.

There is no one-size-fits-all method for addressing every characterization challenge presented by these new modalities, but it is reasonable to suggest that LC and MS will play a central role. Advances in LC-MS have made it easier than ever to confirm recombinant protein sequences and to investigate product-related impurities. However, LC separations coupled to MS detection have relied largely on denaturing conditions that afford sensitive detection but also restrict our ability to investigate protein conformations and interactions. In short, techniques that couple native separations to MS analysis are needed.

Genuine limitations in reagent and column technologies have long stifled progress. But that's not to say we're not moving forward: for example, Bifen Chen, Ying Ge, and colleagues successfully used volatile salts to directly connect hydrophobic interaction chromatography with a mass spectrometer in 2016 (1). They then applied this method to the interrogation of monoclonal antibody samples (2), highlighting the potential for us to selectively separate intact drug isoforms and immediately access MS information for peak identification. This is particularly beneficial to those looking to characterize cysteine-linked ADCs and bispecific antibodies that would otherwise dissociate under denaturing conditions.

In parallel, Yann LeBlanc and Guillaume Chevreux have started to establish robust, MS-compatible ion exchange separations, including the demonstration that ammonium formate and acetate can be used to carry out salt-mediated pH gradient separations of monoclonal antibodies (3). This seminal work has ushered in a new wave of publications, each describing equally interesting separations – everything from traditional isoelectric focusing to pH gradients supplemented with significant increases in ionic strength (4, 5). But when will these novel methods find their way into routine labs?

Adoption of novel technologies is never easy, but the potential rewards make the venture more than worthwhile. Of course, if we are to develop robust methods that can reproducibly yield easy-to-interpret mass spectra, it will be important to remain scrupulous about reagent quality. And that will require that we learn from those working on high sensitivity trace metal quantitation; here, the most important factor to consider is purity. Certified reagents and high-quality plastics should be used for mobile-phase preparation to avoid the formation of salt adducts. Likewise, the use of different types of volatile salts will require diligent investigation to better understand their effects on electrospray ionization. Nevertheless, by wielding high-resolution, MS-compatible native separations, the field will be able to explore new depths of sample characterization; these new separations may be coupled to the detection of native-like gas-phase conformations using a cyclic ion mobility separator (6), or applied to the detection of large megadalton complexes using charge detection MS (7).

The future of native protein LC-MS is bright, and the ever-evolving complexity of biopharmaceuticals gives just cause for investigators to make fast-paced improvements to emerging approaches. Only time will reveal the upper capabilities of these approaches, but I for one am confident and excited to see where such research takes us.

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Citizen Science and Food Safety

Public food safety testing is in our sights – but we must prepare accordingly to ensure that faith in experts persists

By Michel Nielen, Wageningen Food Safety Research (WFSR), part of Wageningen University & Research, Wageningen, The Netherlands.

Food safety was once considered a given, but the widely reported scandals of recent years have refocused the public's attention and brought to life the reality that food adulteration is an ever-present risk. Accordingly, food analysis acts as a front line of defense against such dangers. But current approaches are only partly effective.

In the September 2019 issue of The Analytical Scientist, Chris Elliott, Hans-Gerd Janssen and I discussed these issues in light of the hot topics to be discussed at RAFA 2019 (1). The consensus: while current approaches offer a high level of protection against food fraud, these services are costly and inefficient. Though we do a good job of detecting non-compliance in about 1 percent of all samples collected, is that a good enough hit rate? If 99 percent of samples are compliant, is the administrative and logistical effort undertaken to assess them wisely spent?

Consider another angle: reducing food spoilage is of the utmost importance across the globe. But how do consumers know if food is good to eat or a danger to health with vague statements on the package such as "best before…." or "may contain…."? The human nose is not always good enough…

I believe that both of these issues could be tackled by the availability of devices that provide near-real-time food quality data acquired at critical points in the appropriate supply chain. In fact, simplified handheld analytical instruments with wireless connectivity and GPS-dependent positioning capabilities would be a valuable asset; such devices could be developed for use by non-experts, who could even use infrared scanners hooked up to their smartphones for instant results. In this arena, near-infrared food scanners, smartphone readers for dipstick immunoassays and even transportable mass spectrometers connected to laptops or tablets are already commercially available.

The advantages of this approach are obvious – as are the disadvantages. At the cost of efficient monitoring, reduced spoilage and a much-widened pool of food testing data, we open the door to the potential use of poor-quality equipment and poorly performed tests to obtain and spread inadequate data via social media, leading to a reduced level of public trust in analytical approaches as a whole. In that sense, the rise of so-called "citizen scientists" – able to produce their own data using devices of which they have little-to-no real knowledge – may harm our field; the opinions of experts may be replaced by those of the next fraud discoverer wielding their fit-for-all monitoring device, with no regard for the quality or method of functioning of the device itself. Charlotte Barker explored the point in her editorial, noting the scope for both risk and potential (2).

Moving forwards, both the food industry and food inspection labs must maintain an in-depth knowledge of the quality and validation status of handheld devices available to the public, and should also continue to identify currently unknown food contaminants through profiling and metabolomics-like workflows; handheld devices will need to be adapted to include these contaminants as soon as they are discovered. Coupled with appropriate training for technicians and researchers, such steps may truly allow the significant shift from benchtop screening to handheld, on-the-go testing.

I estimate that analytical power will reach the hands of the public in as soon as five to ten years. Beyond the food industry, those designing analytical instruments must incorporate quality-by-design principles in their manufacturing processes, leading to foolproof measurements that eliminate (where possible) false-positive and false-negative results with strict quality control features. Thanks to wireless connectivity, poor data may (and should) be automatically flagged by a remote central laboratory expert prior to viewing by the stakeholder to minimize the negative consequences of sharing them.

Perhaps most importantly, however, analytical scientists must further develop their communication with the general public to improve attitudes when dealing with doubts regarding laboratory testing. Though some such doubts may be justified, we are clearly aware that the large majority are not. Allowing the public to share in this faith will be key to the safe implementation of layman food testing – ultimately, improving food safety as a whole.

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Around the World in 80 Assays

Analytical chemistry is an essential global network – here's my advice on how to navigate this exciting world and build a successful international career

By Naidong Weng, Head of Bioanalysis and Pharmacokinetics US East Coast, Discovery Sciences, Janssen, Philadelphia, New Jersey, USA.

Analytical chemistry is key to advancing human well-being. From identifying novel therapeutics to supporting the fight against climate change, pivotal decisions rely on the data generated by analytical scientists. As a result, we operate in a global field, and establishing an international career is a necessity for the majority of scientists entering analytical chemistry today.

Though we may not be completely aware of it, we constantly operate in a global fashion. The data an analytical scientist generates in China might be used as part of a regulatory filing for novel medicines as far away as Australia, Brazil or Italy; as the old adage goes, "all roads lead to Rome." There's more than one pathway you can follow to establish yourself internationally in this field, but I'd like to share a few pieces of advice that have helped me in my career.

When opportunities to get more involved in global projects present themselves, whether it be as a manager or simply a member of the team, one must give serious consideration to their involvement and seize the opportunity where appropriate. Such opportunities come with a degree of responsibility, and analytical scientists must deliver the promised data to a high standard in a timely manner – strong

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technical contributions and collaboration are key elements for success.

Joining a professional association can also provide us with valuable experience and allow us to expand our network, which subsequently affords the opportunity to learn from seasoned professional leaders. In China, there is the Chinese American Chromatography Association and Chinese American Society for Mass Spectrometry, volunteer-based, non-profit organizations that focus on helping members to develop their professional careers. Both organizations provide excellent opportunities for young scientists to get involved in their respective fields by contributing to various sub-committees.

Because of the critical nature of analytical data in such a spread of research areas, the guidelines that act to harmonize our methods of working (such as the ICH guidelines on quality, safety, efficacy, and mixed topics) are crucial. Getting involved with the workstream teams that contribute to these guidelines is a great way for you to quickly grasp global and regional regulations, and to also interact with even more scientists in the same space. Of course, bearing in mind cultural differences in such partnerships is essential from the beginning of your career to the end. We cannot assume that we automatically know and appreciate another's culture; always try to put yourself in another's shoes before making assumptions in the scientific community.

Peer-reviewed publications and presentations at meetings ensure that one's presence doesn't go unnoticed in the scientific community, and, though it's valuable to publish papers in high-impact analytical chemistry journals like Analytical Chemistry, publications in journals targeted to specific analytical areas also represent an effective way to communicate your research. Volunteering to review for analytical chemistry journals is another approach by which you can build your scientific credentials; reviewing other scientists' work can help you build connections with journal editors – many of whom are renowned experts – and help you become a better author and researcher.

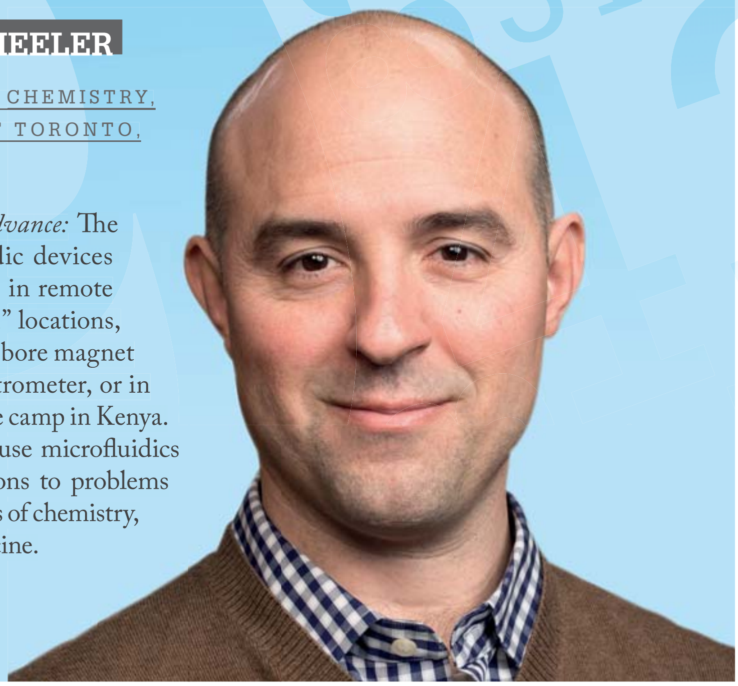
Success is always lying in wait for prepared minds, and each of us must seek out this success on our own path. I do, however, hope that my own experiences might help the budding analytical scientists of tomorrow; our field is making waves across the globe – and one day you will, too.

THE POWER LIST

THE POWER LIST 2019 100
the Analytical Scientist

The Power List is back once again to celebrate the achievements of the most influential figures in analytical chemistry – nominated by our readers and whittled down by our judges to the final 100. From protecting the environment to developing pioneering new technology, our high-octane hundred are making their mark on the analytical sciences – and the world. The top 20 are ranked, while the rest of the list appear alphabetically.

AARON WHEELER



PROFESSOR OF CHEMISTRY, UNIVERSITY OF TORONTO, CANADA.

Exciting recent advance: The use of microfluidic devices to solve problems in remote or "hard-to-reach" locations, such as inside the bore magnet of an NMR spectrometer, or in an isolated refugee camp in Kenya.
Research goal: To use microfluidics to develop solutions to problems spanning the fields of chemistry, biology and medicine.

ADAM WOOLLEY

PROFESSOR, BRIGHAM YOUNG UNIVERSITY, USA.

Career highlight: Working with a diverse group of excellent students and colleagues, and being able to watch their continued professional development.
The future: I see two key yet diverging directions: miniaturization and simplification through tools like integrated microdevices, paper microfluidics, 3D printing and point-of-care diagnostics, and sophisticated analytical instrumentation that yields ever-increasing amounts of information with improved detection limits.

ACHILLE CAPPIELLO

PROFESSOR OF ANALYTICAL CHEMISTRY, UNIVERSITY OF URBINO, ITALY.

Career highlight: Being a scientist today means operating on an international level, where industry and academia work in synergy. I took my first steps into the field of LC-MS interfacing under Professor Klaus Biemann at MIT, equipped with state-of-the-art organic MS equipment.
Research goal: To make use of simpler and faster LC-MS, and to increase the accessibility of LC-MS.
Nominator comment: "It's easy to nominate Cappiello for this award due to his extensive publication history, and contributions to the fields of LC, MS and LC EIMS."

ALEJANDRO CIFUENTES

PROFESSOR, LABORATORY OF FOODOMICS, SPANISH NATIONAL RESEARCH COUNCIL, SPAIN.

Research goal: Our lab investigates food safety, quality and bioactivity, and we are now working on the application of transcriptomics, proteomics and metabolomics alongside green processes for bioactive compound extraction to identify substances useful in the fight against Alzheimer's disease.
Best part of the job: We frequently need to collaborate with other groups and laboratories from institutions across the world, and the publications we produce together are a greatly enjoyable part of the work.

ALEXANDER MAKAROV

PROFESSOR AND DIRECTOR OF RESEARCH, LIFE SCIENCE MASS SPECTROMETRY, THERMO FISHER SCIENTIFIC, GERMANY.

Career highlight: It may not have felt this way at the time, but the commercial launch of the very first Orbitrap mass spectrometer (LTQ Orbitrap) is a definite highlight.
The future: MS is growing in a way akin to the civil aviation industry – commercially oriented, highly automated, regulated and specialized, and slow to change, but also indispensable in modern society.
Eureka moment: I've had many; when I finally understood how to inject ions into the Orbitrap analyzer for one, or more recently finding out why the ions of intact viruses could survive in the trap for abnormally long periods.

ANDRÉ DE VILLIERS

PROFESSOR, STELLENBOSCH UNIVERSITY, SOUTH AFRICA.

Career highlight: The opportunity to interact, work with and learn from leading scientists.
Exciting recent advance: The rapid development of 2D-LC, particularly comprehensive 2D-LC, is very exciting. Many challenges remain, but dedicated instrumentation and an established theoretical framework mean it's a great time to work in this field.

ANDREW DEMELLO

PROFESSOR OF BIOCHEMICAL ENGINEERING & CHAIR OF THE INSTITUTE FOR CHEMICAL AND BIOENGINEERING, ETH ZURICH, SWITZERLAND.

Research goal: The development and application of smart microfluidic tools, such as ultra-high-throughput imaging flow cytometers able to perform high-resolution cell imaging from body fluids at rates approaching half a million cells per second.
Eureka moment: I'm not sure I've had too many of those, but I will always remember the early winter morning when Adam Woolley and I got our initial results from the first lab-on-a-chip device.

AMANDA HUMMON

ASSOCIATE PROFESSOR, THE OHIO STATE UNIVERSITY, USA.

Research goal: My group uses MS to explore the colon cancer proteome and phosphoproteome. We are developing imaging MS approaches to examine molecular distributions in spheroids.
Best advice received: Early in my career, Norman Dovichi warned me that dealing with the rejection and criticism inherent to the work can be tough. After a proposal rejection, he said to me: "Be like a duck, let it roll off your back." With that in mind, I try not to take criticism personally, but use it as a way to improve my science instead.

BARBARA LARSEN

SENIOR TECHNOLOGY FELLOW, DUPONT NUTRITION AND BIOSCIENCES, DENMARK

Passionate about: In short, fitness for purpose – whether you are elucidating a structure or quantifying product impurity, it's critical to provide the best analytical data possible with appropriate sensitivity and accuracy.
Research goal: Our work focuses on applying proteomics to understand cellular processes at various stages of fermentation. By combining omics data with a systems approach, we can improve the fermentation process by increasing the number of functional cells and reducing the time needed to produce the end product.

Nominator comment: "Bodenmiller led the development of imaging MS."

BERND BODENMILLER

DIRECTOR OF THE DEPARTMENT OF QUANTITATIVE BIOMEDICINE, UNIVERSITY OF ZURICH, SWITZERLAND.

Exciting recent advance: The breath-taking pace of development in the field of multiplexed and multiscale imaging.
Eureka moment: Seeing the first tissue image generated by imaging mass cytometry.
Research goal: To develop experimental and computational methods to explore tissue ecosystems with spatial resolution.

BONNER DENTON

GALILEO PROFESSOR OF CHEMISTRY & PROFESSOR OF GEOSCIENCES, UNIVERSITY OF ARIZONA, USA.

Career highlight: My group introduced high-performance array detectors (charge-coupled detectors and charge injection detectors) to the world of analysis, revolutionizing most arenas of low-light spectroscopy.
Exciting recent advance: We have focused on pushing the array detector revolution into MS, while also pursuing improved ion analyzer technologies.
Nominator comment: "Time to bring some real 'power' to the Power List by celebrating the powerhouse that is Bonner!"

CAROL ROBINSON

PROFESSOR, UNIVERSITY OF OXFORD, UK.

Exciting recent advance: In the past year we have observed the ejection of protein complexes directly from membranes – something I never thought I would see.
Eureka moment: When I first saw the GroEL tetradecamer fly through the mass spectrometer.
Best part of the job: Seeing something for the first time, and subsequently trying to understand what it means!

CAROLINE WEST

ASSOCIATE PROFESSOR, UNIVERSITY OF ORLÉANS, FRANCE.

Career highlight: I feel rather too young to have one! But I do see it ahead of me.
Research goal: To improve the understanding of separation processes in LC and supercritical LC.
Best part of the job: The diversity of topics. I always tell my students that whatever your interests are (sports, health, astronomy, cosmetics or just about anything else) you can always find a related area of analytical chemistry. It's also a dynamic science that changes very rapidly – I could never get bored of it.

CATHERINE CLARKE FENSELAU

DISTINGUISHED UNIVERSITY PROFESSOR EMERITUS, UNIVERSITY OF MARYLAND, USA.

Best advice received: My Dean once bumped into me in the elevator and told me that I should never again come to work at the medical school wearing green shoes.
Research goal: To exploit MS in the biomedical sciences with ingenuity and dedication.
Eureka moment: When our MS experiments successfully revealed that acyl-linked glucuronides can alkylate proteins.
Best part of the job: We get to play in everybody else's sandbox, so to speak, which brings many opportunities.

CHARLOTTA TURNER

PROFESSOR OF ANALYTICAL CHEMISTRY AT LUND UNIVERSITY & CHAIR OF THE ANALYTICAL CHEMISTRY DIVISION OF THE SWEDISH CHEMICAL SOCIETY, SWEDEN.

Career highlight: Receiving my first research grant in Sweden as the "wild card" among those receiving the Igvar Carlsson Award in 2006, and receiving the Svante Arrhenius Award for my research on green analytical chemistry in 2017.
Research goal: Contribute to sustainable development by enhancing the value of renewables like lignin, seaweed and food waste.
Nominator comment: "Lotta serves on a number of committees – such as the Euroanalysis conference series – and made (inter)national headlines by freeing her doctorate student and his family from an Islamic State warzone."

CHARLES WILKINS

DISTINGUISHED PROFESSOR OF CHEMISTRY AND BIOCHEMISTRY, UNIVERSITY OF ARKANSAS, USA

Career highlight: Development of the first Fourier Transform Ion Cyclotron Resonance mass spectrometer, which played a key role in commercialization of the technique.
Best advice received: To explore new areas that others have not – this has led me in a number of novel directions in my research life.

CATHERINE COSTELLO

WILLIAM FAIRFIELD WARREN DISTINGUISHED PROFESSOR & DIRECTOR OF THE CENTER FOR BIOMEDICAL MASS SPECTROMETRY, BOSTON UNIVERSITY, USA.

Research: Establishing the structures of biopolymers to understand structure–activity relationships and their influence in biological processes related to health, growth and development and disease.
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."

CHRISTY HAYNES

ASSOCIATE HEAD OF THE DEPARTMENT OF CHEMISTRY & DISTINGUISHED MCKNIGHT UNIVERSITY PROFESSOR, UNIVERSITY OF MINNESOTA, USA.

Exciting recent advance: My group's first nanomaterial design project for agricultural applications is coming to fruition (literally)! We've been designing nanoparticles to controllably transform and release nutrients that promote healthy crop growth following uptake by a plant.
Best part of the job: You're only limited by how widely you read and your imagination. Analytical chemists can impact a wide range of fields, because being able to measure something means that you can make progress towards understanding it.

DAMIEN ARRIGAN

PROFESSOR OF ANALYTICAL CHEMISTRY, CURTIN UNIVERSITY, AUSTRALIA.

The future: We're heading towards single-molecule analysis using smaller electrodes (interfaces) in electroanalytical research.
Best part of the job: I still get a kick out of seeing our newest papers in print and seeing my students transform into experts.

Nominator comment:
"Arrigan is an excellent example of a leading figure who puts others' interests before his own."

DAVID MCCALLEY

PROFESSOR OF BIOANALYTICAL SCIENCE, UNIVERSITY OF WEST ENGLAND, UK.

Career highlight: Being invited to attend the Festschrift conference held in honor of Lloyd Snyder in Ellecom, The Netherlands, in 2001, where I met many of the researchers responsible for establishing the foundations for modern LC.
Best advice received: After defending my thesis in a viva-voce examination at the University of Bristol, LS Bark advised me to recognize that the most important piece of equipment in the lab was not the latest ultra-high-resolution linked chromatograph-mass spectrometer, but a well-maintained analytical balance.
Nominator comment: "The elusive combination of a great scientist with perfect stage presence; he's the 'must see' event at any conference."

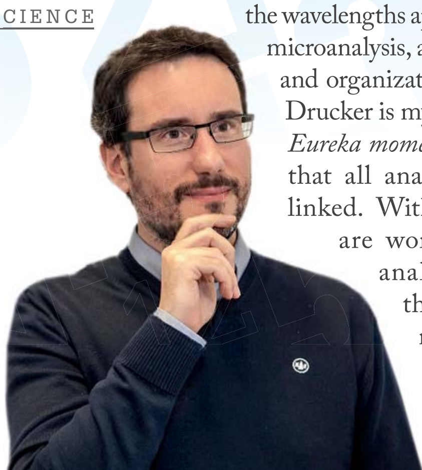
CORAL BARBAS

DIRECTOR OF THE CENTRE FOR METABOLOMICS AND BIOANALYSIS (CEMBIO), SAN PABLO CEU UNIVERSITY, SPAIN.

Research goal: We develop strategies to obtain reliable identifications and measurements of metabolites in response to changes such as disease state, diet and receipt of treatment.
Eureka moment: I began my research career in pharmaceutical analysis, and was sceptical when moving to metabolomics. I was studying a group of infected mice in my early days and one was misclassified; when a representative from the animal husbandry pointed out that one of the animals wasn't infected, I looked at the screen and immediately exclaimed that it must be number 8. All of the animals were ordered on screen by their degree of infection, and I became a believer in metabolomics at that moment!

DAVIDE BLEINER

EMPA MATERIALS SCIENCE & TECHNOLOGY, LABORATORY FOR ADVANCED ANALYTICAL TECHNOLOGIES, SWITZERLAND.



Best advice received: There is no such thing as fundamental or applied science, only useful or useless.

Research goal: My interests lie in shortening the wavelengths applied in laser ablation microanalysis, as well as in leadership and organizational practices (Peter Drucker is my hero).
Eureka moment: When I realized that all analytical methods are linked. With this in mind, we are working on a "green" analytical instrument that combines hybrid multidimensional techniques in one approach.

DAVY GUILLARME

SENIOR LECTURER AND RESEARCH ASSOCIATE, UNIVERSITY OF GENEVA, SWITZERLAND.

Career highlight: When I entered the field of biopharmaceutical protein characterization by chromatographic techniques and their linking to MS in 2011; I think this was the perfect time, and my enthusiasm continues today.
Research goal: To improve the quality and safety of biopharmaceutical drugs by developing innovative analytical tools.

DETLEF GÜNTHER

PROFESSOR AND VICE PRESIDENT FOR RESEARCH AND CORPORATE RELATIONS, ETH ZURICH, SWITZERLAND.

Career highlight: My students.
Exciting recent advance: The reference-free quantification (size and number) of nanoparticles.
Research goal: Improving our understanding of fundamental analytical processes in the hope of impacting research into real-world problems.

DUNCAN GRAHAM

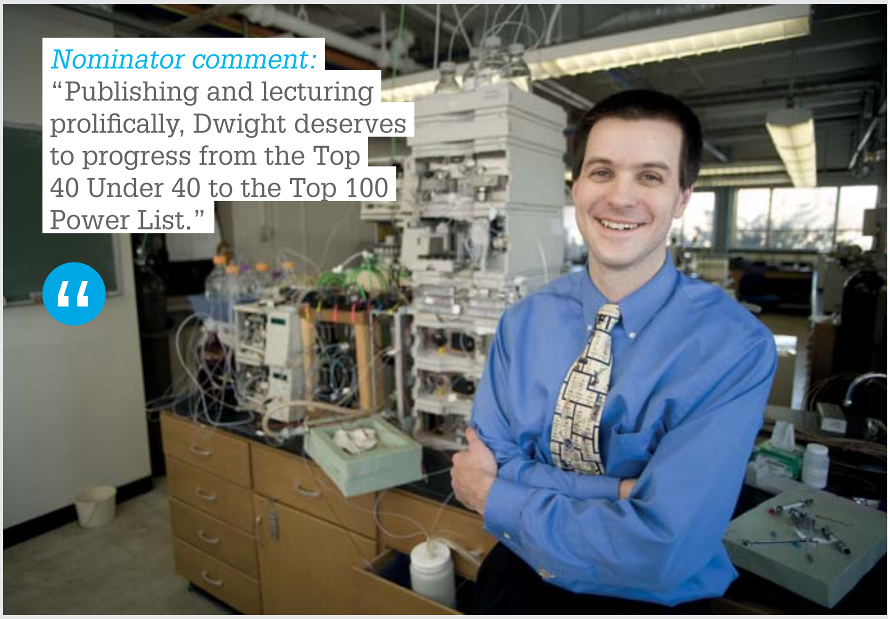
DISTINGUISHED PROFESSOR & HEAD OF THE DEPARTMENT OF PURE AND APPLIED CHEMISTRY, UNIVERSITY OF STRATHCLYDE, UK.

Best advice received: While sitting in a rowing boat on freezing waters off the coast of Gothenburg, I asked the late Rick van Duyne how many genuinely new ideas I should have as an academic. He said he'd had two, maybe three, genuinely new ideas in his career, and to try not to force them.
Best part of the job: The great science and great company; I have a lot of fun doing this job, and that's what life should be about!

DEIRDRE CABOOTER

ASSOCIATE PROFESSOR, UNIVERSITY OF LEUVEN, BELGIUM.

The future: The demand for multidimensional techniques is increasing; I anticipate further software developments concerned with analysis and data interpretation, and also technique optimization.
Best part of the job: Getting to do what I love every day and hoping it can make a difference. Not to mention the great community!



Nominator comment: "Publishing and lecturing prolifically, Dwight deserves to progress from the Top 40 Under 40 to the Top 100 Power List."

DWIGHT STOLL

PROFESSOR, GUSTAVUS ADOLPHUS COLLEGE, USA.

Research goal: Producing innovative technologies and approaches to improve the effectiveness, accessibility and usability of 2D-LC.

The future: Consumers are thirsty for increasingly automated instrumentation due to difficulties in finding and retaining separations experts in some fields, which leads to the need to work towards more highly automated schemes.

ERIN BAKER

ASSOCIATE PROFESSOR, NORTH CAROLINA STATE UNIVERSITY, USA.

Best advice received: Publishing a paper on the advances and limitations of a method is extremely important for the scientific community to know what areas require development, and to avoid wasting time and money reinventing the wheel.

Research goal: My group uses analytical techniques and omics to measure molecular changes in our bodies and answer questions such as how a given toxin induces metabolic changes and causes disease.

EVAN WILLIAMS

PROFESSOR OF CHEMISTRY, UNIVERSITY OF CALIFORNIA, USA.

The future: New advances are constantly happening in MS across a number of different disciplines; for example, mass measurements of intact viruses (up to hundreds of megadaltons) are now possible.

Best part of the job: I enjoy developing new instruments and methods to measure the previously unmeasurable – the resulting joy of discovering something completely new is incredible.

EMILY HILDER

DIRECTOR OF THE FUTURE INDUSTRIES INSTITUTE, UNIVERSITY OF SOUTH AUSTRALIA, AUSTRALIA.

Best advice received: You learn more by asking questions than looking for answers.

The future: We are able to separate complex, multicomponent mixtures, but analyzing the ever-increasing amount of data generated remains a challenge; the application of machine learning and artificial intelligence in separation science represents an exciting opportunity for us to realize the full potential of these techniques.

Nominator comment: "A thought leader in the field, great separation scientist and a role model for women in analytical scientist. And a good person to boot!"

FRANCES LIGLER

LAMPE DISTINGUISHED PROFESSOR OF BIOMEDICAL ENGINEERING, UNC-CHAPEL HILL & NC STATE UNIVERSITY, USA.

Career highlight: Induction into the National Inventors Hall of Fame in 2017.
Eureka moment: This summer, it took a 7-year-old at Camp Invention 30 seconds to solve a technical problem that had stymied me for over a decade – that was definitely a "wow" moment.
The future: Increased capacity for out-of-lab measurements, and improved capability regarding long-term, continuous monitoring.

FABRICE GRITTI

PRINCIPAL CONSULTING SCIENTIST, WATERS CORPORATION, USA.

Career highlight: Receiving the Joseph Franz Karl Huber Lecture Award at HPLC 2019. The Award is given to scientists who have made major contributions to the advancement of HPLC, and it was a privilege to be put on a pedestal alongside past recipients like Attila Felinger and Gert Desmet.
Exciting recent advance: Witnessing the rise of 3D printing technology in analytical laboratories to design more robust and better performing columns or devices for multidimensional LC.

GARY SIUZDAK

PROFESSOR & DIRECTOR OF THE SCRIPPS CENTER FOR METABOLOMICS, THE SCRIPPS RESEARCH INSTITUTE, USA.

Career highlight: Developing "activity metabolomics" through XCMS/METLIN, thus enabling the discovery of metabolites able to modulate phenotype. Beyond biomarker discovery and gaining mechanistic insight, this metabolomic capability is now being fully appreciated.
Best part of the job: Free "molecular spirits" from Endless West – please send more!
Nominator comment: "A metabolomics scientist with unique vision and numerous recent accomplishments, including the growth of METLIN to over half-a-million molecular standards!"

GÉRARD HOPFGARTNER

PROFESSOR OF ANALYTICAL SCIENCES AND MASS SPECTROMETRY, UNIVERSITY OF GENEVA, SWITZERLAND.

Research goal: Provide MS tools and solutions for identifying and quantifying molecules in complex samples to better understand biological systems.
Best part of the job: The broadness of the field; an analytical scientist needs to have keen theoretical understanding, the creativity to forge future advances, and the application skills to gain insight into real-world samples.

GONGKE LI

PROFESSOR AND DIRECTOR OF THE INSTITUTE OF ANALYTICAL SCIENCES, SUN YAT-SEN UNIVERSITY, CHINA.

The future: We are developing in situ, in vivo and online sample preparation techniques that are showing promise and may simplify studies of trace composition in complex systems (such as chemicals altering human mood) in the future.
Exciting recent advance: A breakthrough in complex sample preparation for trace analysis of toxic components, which was awarded The Natural Science Award by the Ministry of Education.
Nominator comment: "One of the leading women in analytical science in China. She has an excellent publication record and is increasingly visible on the international stage."

GOVERT SOMSEN

PROFESSOR OF BIOMOLECULAR ANALYSIS AND ANALYTICAL CHEMISTRY, VRIJE UNIVERSITY AMSTERDAM, NETHERLANDS.

Career highlight: I started my career in an era of booming bottom-up proteomics, but our first peaks were questionable and people thought we were crazy. Now, after persistent development, we can assign hundreds of proteoforms of a single protein in just one run!

Best advice received: When going for my first job interview my father said "don't oversell, just be yourself." He was right, because the people that matter are those good at recognizing important qualities without you having to show them off.

HUWEI LIU

PROFESSOR, PEKING UNIVERSITY, CHINA.

Career highlight: Teaching my students, and also developing new technologies and methods in chromatography and MS for applications ranging from explosive detection to food analysis and diagnosis.

Best advice received: Be a good person first and a good scientist second.

GUOWANG XU

PROFESSOR OF APPLIED CHEMISTRY, CHINESE ACADEMY OF SCIENCES, CHINA.

Research goal: To address the technical challenges associated with MS-based metabolomics, such as comprehensive coverage, throughput and unambiguous structural determination for unknown metabolites.

Exciting recent advance: We developed leading platforms for complicated sample analysis with significantly increased peak capacity and identification ability; a kit we developed based on LC-MS analysis to measure serum glycocholate is now approved for use in Chinese clinics.

JANE HILL

ASSOCIATE PROFESSOR OF ENGINEERING, DARTMOUTH COLLEGE, USA.

Research goal: To discover, validate and translate into the clinic breath biomarkers for infectious disease diagnosis.

The future: Larger clinical validation studies, and miniaturized analytical systems for bedside use.

Best part of the job: Forging a new group in the area of volatile metabolomics, and working with numerous wonderful trainees.

Nominator comment:
"If I were a student today, I'd be enrolling in her lab!"

JARED ANDERSON

PROFESSOR, IOWA STATE UNIVERSITY, USA.

Career highlight: Seeing the students we train go on to build their own scientific careers – no matter what stage they leave us at, it's always exciting to watch them move forwards.
Best part of the job: We are able to solve challenging problems with great societal implications. These challenges are rarely solved by working alone, which creates an engaging, supportive and collaborative environment.
Nominator comment: "A leading mind in sample preparation and chromatography. His work on novel applications using ionic liquids, especially in the bioanalytical realm, will lead a paradigm shift in purifying and preserving biological samples."

JENNIFER BRODBELT

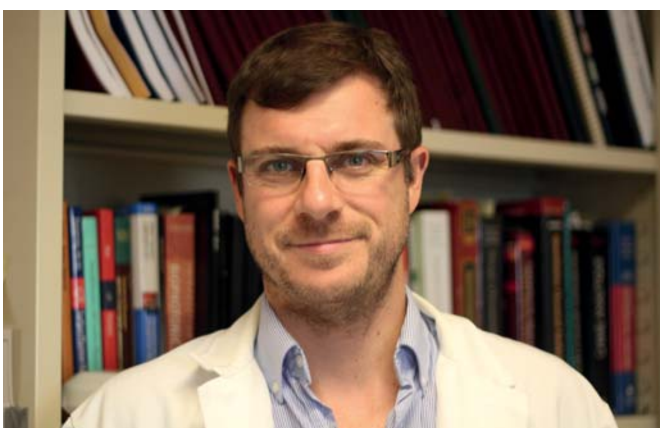
ROLAND PETTIT CENTENNIAL CHAIR PROFESSOR IN CHEMISTRY AND CHAIRPERSON, UNIVERSITY OF TEXAS, USA.

Best advice received: Your graduate students are your most important resource; cultivate a group culture that encourages innovation and collaboration, and your research program will flourish.
Research goal: To develop new MS strategies for characterizing biological molecules. We accomplish this by developing and utilizing photodissociation as an innovative method to activate and dissociate ions and yield informative fragmentations.

JEAN-FRANCOIS MASSON

PROFESSOR, UNIVERSITY OF MONTREAL, FRANCE.

Career highlight: The support of my family is a definite highlight. They travelled over 4,000 kilometers to attend my PhD defense, and my 4-year-old son attends whatever seminars of mine he can.
Eureka moment: I was an elite ice hockey player while growing up in Canada, and had a eureka moment in realizing the similarities between chemistry and hockey. In chemistry, however, you get better with age, rather than worse, and are more likely to make a living off your passion!



JIM LUONG

FELLOW, ANALYTICAL SCIENCES, CORE R&D, THE DOW CHEMICAL COMPANY.

The future: In chromatography, I anticipate advances in multi-hyphenation techniques, and improvements in selectivity and inertness of stationary phases, ultra-trace detection with selective detectors, metal 3D printing and miniaturization.
Best part of the job: The role of an analytical scientist has many exciting facets, from detective work on practical solutions to instrument design and development – the options are limitless.

JUSTIN GOODING

CO-DIRECTOR OF THE AUSTRALIAN CENTRE OF NANOMEDICINE & CO DIRECTOR OF THE NEW SOUTH WALES SMART SENSING NETWORK, UNIVERSITY OF NEW SOUTH WALES, AUSTRALIA.

The future: Chemical and biological sensing is heading in three directions simultaneously: conceptually, we are beginning to develop quantitative sensors; from an engineering perspective, we are increasingly able to integrate sensors with further technologies; and economically, we are moving towards cheaper sensors, like paper.
Research goal: To develop new measurement technologies that allow us to answer previously unanswerable questions.

JOSEPH LOO

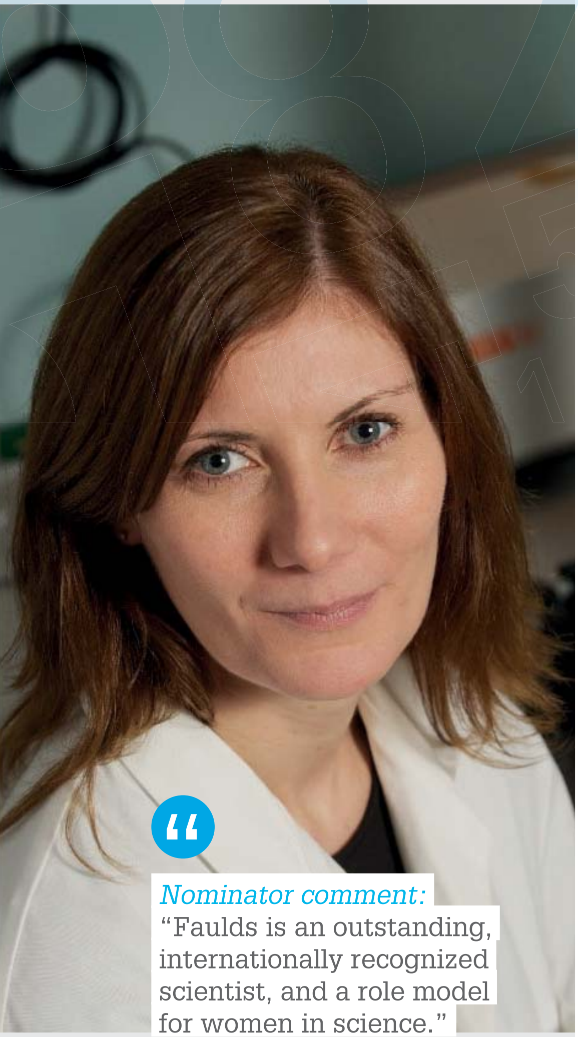
PROFESSOR, UNIVERSITY OF CALIFORNIA LOS-ANGELES, USA.

Eureka moment: My eureka moment came at the beginning of my career. I was trained to "break" molecules for analysis, so when developing ESI-MS for protein characterization it seemed natural to me to attempt to "break" the large protein molecules to sequence the fragments. After realizing I could generate gas-phase protein fragments and interpret the fragments against expected sequences, I saw that this could be further developed. Today we call this top-down MS, or proteomics… Little did I know I'd still be working on the same topic nearly 30 years later.

JOSEPH WANG

DISTINGUISHED PROFESSOR, UNIVERSITY OF CALIFORNIA, USA.

Career highlight: Mentoring numerous talented students and postdocs, who have gone onto become leading scientists across the globe.
Best advice received: Keep searching for the best, don't give up, and have fun!
The future: On-body, non-invasive, real-time diagnostics will replace analysis at centralized labs.



Nominator comment: "Faulds is an outstanding, internationally recognized scientist, and a role model for women in science."

KAREN FAULDS

PROFESSOR, HEAD OF BIONANOTECHNOLOGY AND ANALYTICAL CHEMISTRY, UNIVERSITY OF STRATHCLYDE, UK.

The future: Raman spectroscopy and SERS are transitioning into use as biomedical tools to study diseases and pathogens – in future, they will be used for diagnosis and treatment monitoring.
Research goal: To improve peoples' lives or the environment. My ambition is to develop approaches that will allow early disease detection, facilitating faster and more specific medical interventions that improve outcomes and reduce cost.

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.

KELLY ZHANG

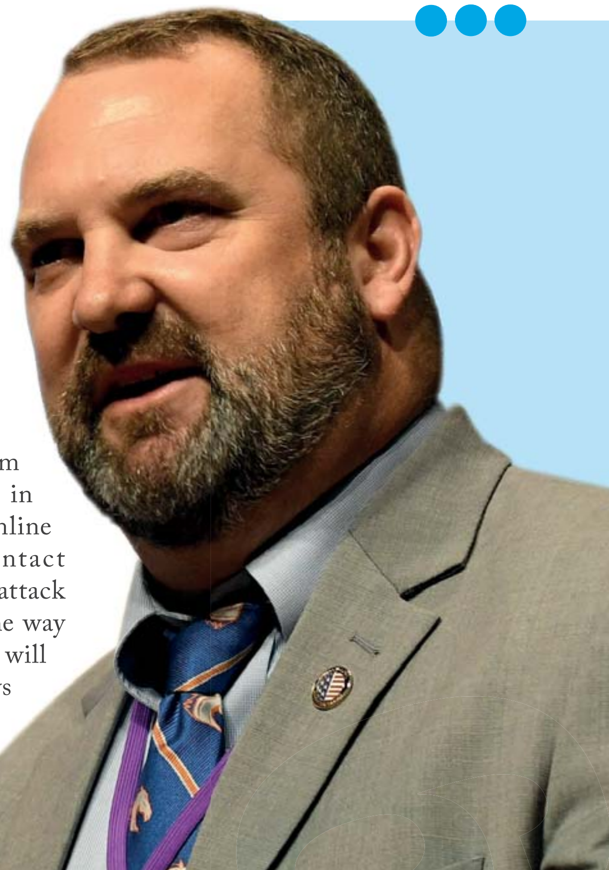
PRINCIPAL SCIENTIST, SMALL MOLECULE ANALYTICAL CHEMISTRY, GENENTECH, USA.

Research: Working with cross-disciplinary teams to move novel therapies from research into the clinic.
Nominator comment: "Kelly is a member of the permanent scientific committee for HPLC and is an acting organizer for HPLC 2020 in San Diego."

KEVIN SCHUG

PROFESSOR & SHIMADZU DISTINGUISHED PROFESSOR OF ANALYTICAL CHEMISTRY, UNIVERSITY OF TEXAS, USA.

Best part of the job: You're always on a learning curve because of the ubiquitous need for measurements, and there are both fundamental and applications-based questions to answer.
Exciting recent advance: I'm very excited about our success in developing methods for the online comprehensive 2D-LC of intact proteins. If we can eventually attack mixtures of intact proteins in the way we approach small molecules, this will enable the development of assays useful in many areas.



LANE ALLEN BAKER

PROFESSOR OF CHEMISTRY, INDIANA UNIVERSITY, USA.

Best advice received: If the big thing you're worried about right now won't matter in five years, then it probably isn't that big of a thing.

The future: Electrochemical measurements, especially electrochemical imaging, will benefit from quicker, more sensitive and truly nanoscale measurements, opening the door to the creation of imaging platforms that allow us to "visualize" chemistry, biology and material science in new ways.

LJILJANA PAŠA-TOLIĆ

LABORATORY FELLOW & DEPUTY FOR TECHNOLOGY, ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY, PACIFIC NORTHWEST NATIONAL LABORATORY, USA.

Best advice received: Success is liking yourself, what you do, and how you do it.

Best part of the job: I love being part of this great community, and advancing technologies needed to answer questions central to biology, health, the planet and people. It's great fun.

LIVIA EBERLIN

ASSISTANT PROFESSOR, UNIVERSITY OF TEXAS AT AUSTIN, USA.

The future: Ambient ionization MS has come a long way in recent years, especially for clinical applications. I expect that these methods will move closer to doctors and patients, eventually leading to routine use to accelerate diagnosis and clinical decision making.

Research goal: I'm passionate about research surrounding the interface between chemistry and medicine – my group is focused on developing innovative MS technologies to solve clinical problems, such as cancer diagnosis.

LINGJUN LI

DISTINGUISHED PROFESSOR OF PHARMACEUTICAL SCIENCES AND CHEMISTRY, UNIVERSITY OF WISCONSIN-MADISON, USA.

Career highlight: Discovering novel neuropeptides from hypothalamic extracts and subsequently deciphering their functions. Also, receiving the prestigious Biemann Medal from the American Society for Mass Spectrometry.

Exciting recent advance: We've made continued progress in developing novel chemical tags for high-throughput omic analyses; we have begun studying glycosylation patterns during the progression of Alzheimer's disease using such approaches.

LUIGI MONDELLO

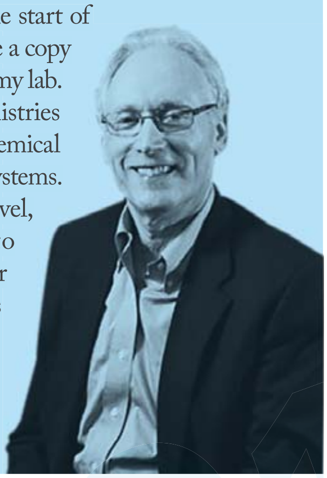
FULL PROFESSOR OF ANALYTICAL CHEMISTRY, UNIVERSITY OF MESSINA, ITALY.

Career highlight: Landmark developments in comprehensive chromatography revolutionized the community over a decade ago; my highlight is having being a central contributor to improving the power and accessibility of these technologies.
The future: I foresee the wider acceptance of multidimensional and comprehensive chromatography as these methods become more robust and reliable, and the benefits of their hyphenation with MS will be better exploited.
Nominator comment: "His rigorous and innovative methods will inspire the next generation of scientists in both academia and industry."

MARK MEYERHOFF

PHILIP J ELVING PROFESSOR OF CHEMISTRY, THE UNIVERSITY OF MICHIGAN, USA.

Best advice received: "Don't major in minor things" – I read this in a paperback at the start of my academic career, and now give a copy of the book to undergraduates in my lab.
Research goal: Finding new chemistries to devise highly selective electrochemical and optical sensors and sensing systems. We are also investigating novel, low-cost approaches to produce nitric oxide for medical applications without the need for gas tanks.



MELISSA HANNA-BROWN

GLOBAL EXTERNAL TECHNOLOGY & COLLABORATIONS LEAD, PFIZER PHARMACEUTICAL SCIENCES & CAMS EXECUTIVE CHAIR, UK.

Recent exciting advance: Standing up as the executive chair to launch CAMS (the Community for Analytical Measurement Science) together with UK government officials and industry leaders across different sectors; CAMS is an industry-led consortia network focused on bringing coherence to our community in the UK and Ireland.
Research goal: I work in the pharmaceutical industry, where measurements enable medicine discovery, development and manufacturing. In particular, my role at Pfizer involves coordinating with the external ecosystem to accelerate development lifecycles and get new treatments to patients faster.

MICHAEL BREADMORE

PROFESSOR & DIRECTOR OF THE AUSTRALIAN CENTRE FOR RESEARCH ON SEPARATION SCIENCE, UNIVERSITY OF TASMANIA, AUSTRALIA.

Career highlight: The commercial release of GreyScan – the world's first inorganic explosive trace detection system – in late 2018.
Best advice received: Do something hard and important. If it works, it's brilliant; if it doesn't, you still get a good paper.
Best part of the job: Waking up every day faced with questions to which there is no answer yet.

MICHAEL LÄMMERHOFER

PROFESSOR OF PHARMACEUTICAL (BIO-) ANALYSIS, INSTITUTE OF PHARMACEUTICAL SCIENCES, UNIVERSITY OF TÜBINGEN, GERMANY.

Career highlight: Achieving professorship at my institute; a full professorship is the ultimate goal of an academic career, bringing with it lots of duties and responsibilities, but also the freedom to follow your own ideas.
Best part of the job: It involves a lot of interdisciplinary science, which gives our work additional value and makes the field extraordinarily interesting and diverse.

MICHAEL ROPER

PROFESSOR, FLORIDA STATE UNIVERSITY, USA.

Career highlight: Watching my students excel by obtaining exciting results, graduating and getting great jobs.
Best part of the job: Solving problems by lending our expertise to scientists across multiple fields carries a great feeling with it, and makes me think that our field will always have a place.
Nominator comment: "Roper's work studying cellular dynamics in microfluidics systems is an excellent example of how analytical systems can advance biological studies."

NANCY ALLBRITTON

KENAN DISTINGUISHED PROFESSOR & CHAIR OF UNC/NC STATE JOINT DEPARTMENT OF BIOMEDICAL ENGINEERING, UNIVERSITY OF NORTH CAROLINA, USA.

Research: Leading a multidisciplinary team of chemists, physicist, engineers and materials scientists to develop new assays and technologies for single-cell biochemical analysis, cell sorting and cloning, and recapitulating organ-level function.
Nominator comment: "A key driver of single-cell analysis using CE-based methods – she has pioneered the interface between analytical chemistry and bioengineering."

PAUL CREMER

J. LLOYD HUCK PROFESSOR IN NATURAL SCIENCES, PENNSYLVANIA STATE UNIVERSITY, USA.

Eureka moment: The many discoveries we make through serendipity, such as our observation that ortho-rhodamine and para-rhodamine dye behaviours differ as a function of pH; we used the former to build a biosensor platform.
The future: Vibrational spectroscopy has been dominated by nonlinear spectroscopies like SFG in recent years, but now Raman and infrared approaches have also demonstrated utility. Our ability to combine such techniques means the future looks bright – it's an exciting time to be a vibrational spectroscopist!

PERDITA BARRAN

DIRECTOR OF THE MICHAEL BARBER CENTRE FOR COLLABORATIVE MASS SPECTROMETRY, MANCHESTER INSTITUTE OF BIOTECHNOLOGY, UNIVERSITY OF MANCHESTER, UK.

Career highlight: I have two: building ion mobility mass spectrometers with enormous capabilities for structural analysis, and diagnosing Parkinson's Disease from simple skin swabs.
Exciting recent advance: In our group, I'd have to say our work in Parkinson's diagnosis. But in the world of biological MS, probably the increased relevance of lipids as disease biomarkers.

Nominator comment: "The ultimate ambassador for analytical science."

PETER SCHOENMAKERS

VAN'T HOFF INSTITUTE FOR MOLECULAR SCIENCES, UNIVERSITY OF AMSTERDAM, NETHERLANDS.

Best advice received: If your results confirm your expectations, it is comforting; if they are not what you expect, it is interesting.
Eureka moment: For chromatographers, thinking "outside the box" implies thinking "outside the column."
Best part of the job: We work to provide accurate, factual and repeatable information – we leave it to the other scientists to speculate.

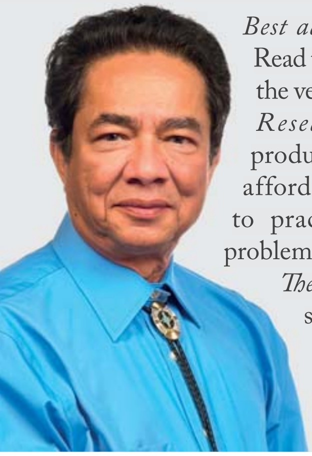
PHILIPPE SCHMITT-KOPPLIN

PROFESSOR, DIRECTOR OF THE RESEARCH UNIT ANALYTICAL BIOGEOCHEMISTRY & HEAD OF THE COMPREHENSIVE FOODOMICS PLATFORM, GERMANY.

Research goal: Describing unknown yet important small molecules and their interactions in biotic and abiotic processes using orthogonal analytical tools.
Eureka moment: Realizing the lack of metabolic and small molecule diversity among complex living systems when compared with abiotic chemosynthetic environments, such as in outer space or extreme terrestrial environments (hydrothermal systems, for example). It makes our species seem small in the universe.

PURNENDU DASGUPTA

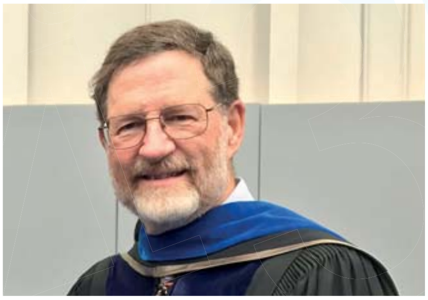
PROFESSOR & HAMISH SMALL CHAIR IN ION ANALYSIS, UNIVERSITY OF TEXAS ARLINGTON, USA.



Best advice received: Read the very old, and the very new.

Research goal: To produce simple and affordable solutions to practical analysis problems.

The future: We will see a transition from small to smaller.



RICHARD YOST

PROFESSOR & HEAD OF ANALYTICAL CHEMISTRY, UNIVERSITY OF FLORIDA, USA.

The future: When I started at the University of Florida some 40 years ago, MS was not a widely accepted technique. Organic chemists used it to confirm they had synthesized the correct compound, natural product chemists used it to find novel compounds in a given organism, and physicists and physical chemists used it for fundamentals. Today, MS may well be the dominant technique in our field, and there's no indication it's slowing down!

ROHIT BHARGAVA

FOUNDER PROFESSOR OF ENGINEERING AND CHEMISTRY & DIRECTOR OF THE CANCER CENTER, UNIVERSITY OF ILLINOIS, USA.

The future: It's an exciting time for optical chemical imaging via infrared and Raman vibrational spectroscopies. An abundance of new ideas, theoretical advances, instrument configurations and applications mean that the field is poised for unprecedented growth.

Research goal: To develop better chemical imaging technology from first principles-based theoretical analyses.

Nominator comment: "A pioneer of infrared spectroscopic imaging. He has provided numerous seminal studies, and continues to set the standard to this day."

RON HEEREN

DISTINGUISHED PROFESSOR OF MOLECULAR IMAGING, UNIVERSITY OF MAASTRICHT, NETHERLANDS.

Exciting recent advance: Breakthroughs in imaging resolution and throughput with technologies that have improved our sensitivity by orders of magnitude – data-dependent imaging, MALDI-2 and spatial resolution are great examples.

Research goal: To generate and use complex molecular information from tissue samples to improve the precision of clinical decision making at the fundamental, instrumental and applied levels.

ROY GOODACRE

PROFESSOR OF BIOLOGICAL CHEMISTRY, UNIVERSITY OF LIVERPOOL, UK.

Career highlight: This summer I woke up on the sand of a river bank in northern Australia and was transported by helicopter to an inland escarpment, where we used a portable point-and-shoot Raman spectroscopy device to investigate the chemistry of pigments used in aboriginal rock art – pretty cool and exciting stuff!

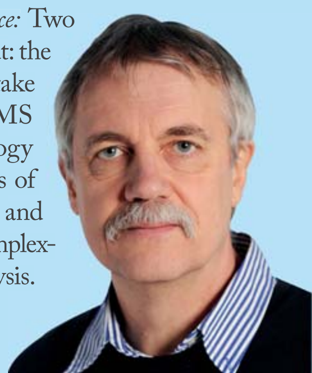
Best advice received: I was once told "early to bed, early to rise, work hard and advertise" with regards to conferences. Today I've adapted this to "late to bed, early to rise, work hard and advertise" and I think it's worked rather well.

RUEDI AEBERSOLD

PROFESSOR OF MOLECULAR SYSTEMS BIOLOGY, ETH ZURICH & FACULTY OF SCIENCE, UNIVERSITY OF ZURICH, SWITZERLAND.

Career highlight: Witnessing and contributing to the amazing technological development of MS-based proteomics, from the inception of the field to present.

Exciting recent advance: Two developments stand out: the rapid advance and uptake of SWATH/DIA MS as a central technology for proteomic analysis of large sample cohorts, and the development of complex-centric proteome analysis.



RYAN BAILEY

ROBERT A. GREGG PROFESSOR OF CHEMISTRY, UNIVERSITY OF MICHIGAN, USA.

The future: Smaller, faster, and cheaper! It's great to see microscale analytical tools penetrating mainstream clinical diagnostics, and as smaller technologies provide increasing amounts of information, analytical scientists will have to work closely with bioinformaticians to transform high-density data sets into actionable disease signatures.
Research goal: To create microscale analytical technologies to extract high levels of information from limited biological samples.

SARAH TRIMPIN

PROFESSOR, WAYNE STATE UNIVERSITY, USA.

Research: Developing fundamental understanding of newly discovered methods that raise questions for ionization methods in MS.
Nominator comment: "She has taken a brave approach to studying the fundamentals of newly discovered methods for molecule transfer, regardless of size or volatility, from the solid state in a small molecule matrix to gas-phase ions for MS analysis."

SUSAN LUNTE

RALPH N. ADAMS PROFESSOR OF CHEMISTRY AND PHARMACEUTICAL CHEMISTRY, DIRECTOR OF THE RN ADAMS INSTITUTE FOR BIOANALYTICAL CHEMISTRY & DIRECTOR OF THE CENTER OF MOLECULAR ANALYSIS OF DISEASE PATHWAYS, UNIVERSITY OF KANSAS, USA.

Career highlight: Becoming Ralph N. Adams Professor of Bioanalytical Chemistry; Buzz Adams was an incredible scientist and human being, and it's a great honor to have a professorship and run an institute in his name.
Best part of the job: Analytical chemists are collaborators by nature so there are always exciting new measurement problems to solve.

SUSAN RICHARDSON

ARTHUR SEASE WILLIAMS PROFESSOR OF CHEMISTRY, UNIVERSITY OF SOUTH CAROLINA, USA.

Career highlight: The opportunity to collaborate with incredible toxicologists and epidemiologists in my research; as a chemist, I can only go so far in solving the health issues surrounding drinking water disinfection byproducts.
Exciting recent advance: Finally "cracking the code" in identifying new brominated sulfonate disinfection byproducts formed by the reaction of hydraulic fracturing wastewaters with chlorine.

XIAOHONG FANG

PROFESSOR, CHINESE ACADEMY OF SCIENCES, CHINA.

Research: Development and application of bioanalytical and biophysical technologies to analyze biomolecular interactions and reactions at the single-molecule level.
Nominator comment: "Xiahong Fang is an outstanding scientist, and valued editor of Analytical Chemistry."

TAKEHIKO KITAMORI

PROFESSOR, UNIVERSITY OF TOKYO, JAPAN.

Career highlight: Becoming Dean of the School of Engineering in 2010, and Vice President in 2012.
Eureka moment: I saw that a chromatic aberration on an old microscope enabled the true thermal lens optical configuration; a small channel fabricated onto a glass slide during creation of the thermal lens microscope then turned out to be the world's first pressure-driven microfluidic device.

YOSHINOBU BABA

PROFESSOR, NAGOYA UNIVERSITY, JAPAN.

Research: Development and application of bioanalytical and biophysical technologies to analyze biomolecular interactions and reactions at the single-molecule level.
Nominator comment: "Baba is a pioneer in microfluidics."

YING GE

PROFESSOR, UNIVERSITY OF WISCONSIN-MADISON, USA.

Research goal: To develop innovative technologies to understand cardiac disease, identify new molecular targets for diagnosis, and ultimately provide novel treatments for heart failure.
Eureka moment: I conceived the idea to develop a photo-cleavable surfactant for top-down proteomics in 2011; a talented postdoc (Tania Guardado) and a brilliant graduate student (Kyle Brown) subsequently synthesized a photo-cleavable anionic surfactant for this application.
Nominator comment: "Ge is conducting cutting-edge research that is making waves in the fields of MS, separations, proteomics and (eventually) personalized medicine."

ZOLTAN TAKATS

PROFESSOR, IMPERIAL COLLEGE LONDON, UK.

Research: Takats is a pioneer in the field of ambient MS and led the development of several mass spectrometric ionization techniques.

"

Nominator comment:
"His work in DESI and imaging is of the utmost importance."

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GARY HIEFTJE

DISTINGUISHED PROFESSOR EMERITUS AND MANN CHAIR OF CHEMISTRY, INDIANA UNIVERSITY, USA.

Career highlight: Producing 70 doctorates, 25 MS recipients, 29 postdocs and 29 undergraduate researchers. Unlike scientific developments, which often have a finite duration, the mentoring of students and co-workers is bound to have a lasting influence.
The future: Novel instrumentation will continue to make an impact as we move forward. In the words of Sir Humphry Davy: "Nothing begets good science like the development of a new instrument."
Nominator comment: "A world leader in atomic and molecular MS, instrument development, and teaching."

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SUSAN OLESIK

PROFESSOR, OHIO STATE UNIVERSITY, USA.

Career highlight: We used a GC column that was a part of the Cassini-Huygens probe to sample the atmosphere of Titan, Saturn's biggest moon.
Exciting recent development: We discovered a way to improve the detection limits for K-Ras proteins, which act as biomarkers for various human cancers.
Nominator comment: "She is an innovator, discreetly forging her own path in separation science."

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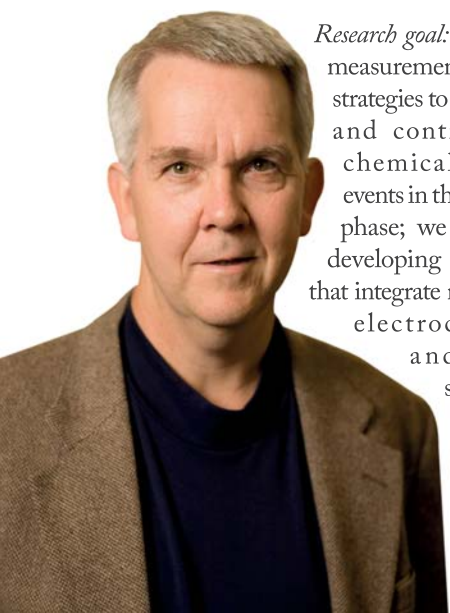
PAUL BOHN

ARTHUR J. SCHMITT PROFESSOR OF CHEMISTRY AND BIOMOLECULAR ENGINEERING, PROFESSOR OF CHEMISTRY AND BIOCHEMISTRY, & DIRECTOR OF THE ADVANCED DIAGNOSTICS AND THERAPEUTICS INITIATIVE, UNIVERSITY OF NOTRE DAME, USA.



Research goal: To develop measurement tools and strategies to characterize and control single chemical reaction events in the condensed phase; we do this by developing approaches that integrate nanoscience, electrochemistry and optical spectroscopy.

MILTON LEE

EMERITUS PROFESSOR OF ANALYTICAL CHEMISTRY, BRIGHAM YOUNG UNIVERSITY & CHIEF SCIENCE OFFICER, AXCEND LLC, USA.

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Research goal: My research has moved towards small, portable chromatographic instrumentation, most recently producing a hand-portable micro/nanoflow capillary liquid chromatograph.
Best advice received: When I started at Brigham Young University some 40 years ago, I was advised to look for opportunities for collaboration. Taking this advice, I've had the pleasure to work with colleagues in environmental biology, developmental biology, microbiology, plant science, chemical, mechanical and electrical engineering, physics, and so on.
Nominator comment: "Milton has made consistent contributions to separation science in many fields, and is a pioneer in the development of new technologies and instruments."

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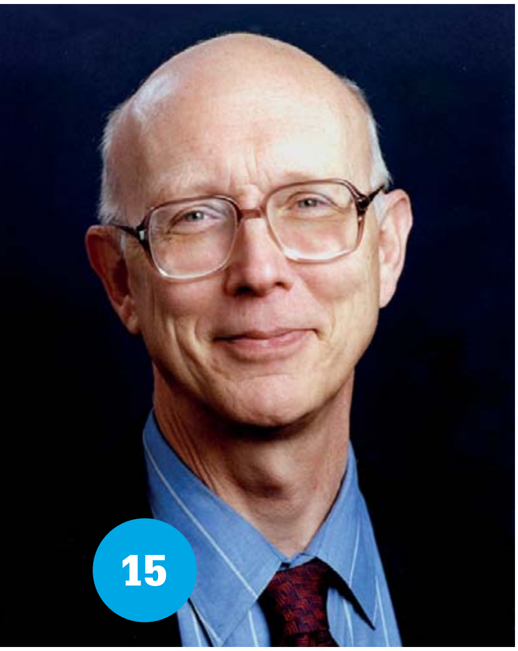
MARY WIRTH

W. BROOKS FORTUNE DISTINGUISHED PROFESSOR, PURDUE UNIVERSITY, USA.

Research: 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.



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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.

Nominator comment: "George deserves a place on the list for his contributions to microfluidics and low-cost assay development."

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VICKI WYSOCKI

PROFESSOR AND OHIO EMINENT SCHOLAR AT THE DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY & DIRECTOR OF THE CAMPUS CHEMICAL INSTRUMENT CENTER, OHIO STATE UNIVERSITY, USA.

Research goal: To develop better ways of measuring large protein and nucleoprotein complexes by MS.
Best advice received: A few years before John Fenn won the Nobel Prize, he told me to "never look back, never second guess." This happened as I moved from one position to another, but any time I started to doubt I'd made the right choice I thought of his advice and kept moving forward.
Nominator comment: "Vicki has a huge impact in fundamental analytics and fragmentation technologies; UVPD and SID were pioneered by her and her group."

NORMAN DOVICHI

GRACE-RUPLEY PROFESSOR OF CHEMISTRY AND BIOCHEMISTRY, UNIVERSITY OF NOTRE DAME, USA.

Nominator comment: "Dovichi was an early adopter of CE in the 1980s, developing the sheath-flow cuvette for LIF coupled to CE for single-molecule detection and pioneering CE-LIF sequencing methods for DNA in the early 1990s. He then developed a robust interface for CE-MS and recently prepared CE to investigate the microbiome – an innovative and enabling technology. What's more, he's mentored hundreds of postdocs during his career, many of whom are now professors across the world."

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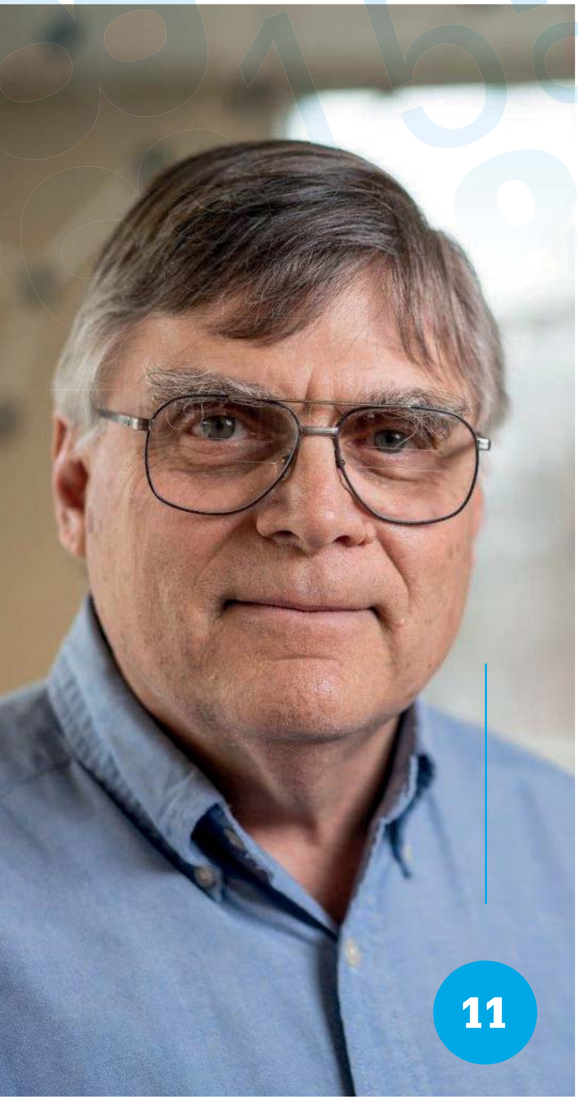
NEIL KELLEHER

PROFESSOR, NORTHWESTERN UNIVERSITY, USA.

Research: Kelleher's group has three primary focuses: top-down proteomics, natural products biosynthesis and discovery, and chromatin biology. These interests have led to success in driving technological development and the application of MS to problems lying at the interface of biology and chemistry.



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DAVID CLEMMER

DISTINGUISHED PROFESSOR & ROBERT AND MARJORIE MANN CHAIR OF CHEMISTRY, INDIANA UNIVERSITY, USA.

Best advice received: Not advice I've received per se, but I do like the statement "Measure what is measurable. Make measurable what is not." – Galileo Galilei.
Exciting recent advance: Charge detection MS, particularly as carried out by the labs of Martin Jarrold, Evan Williams and Philippe Dugourd, has come a long way; the technique measures the ionic charge number, and mass/charge, making it possible to measure the mass of very large particles for the first time.

9

JANUS PAWLISZYN

PROFESSOR, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF WATERLOO, CANADA.

Career highlight: I've focused on developing green technologies in analytical chemistry, such as approaches for sample preparation that facilitate the solvent-free integration of sampling with extraction.
Best advice received: "Do not follow the beaten track – explore your own ideas."

JOEL HARRIS

DISTINGUISHED PROFESSOR OF CHEMISTRY, UNIVERSITY OF UTAH, USA.

Career highlight: Conducting quantitative chemical analysis at the limit of imaging and counting individual fluorescently-labelled molecules; we have used this method to observe the affiliation of signalling proteins with lipid membranes and the kinetics of DNA hybridization.
Exciting recent advance: In the past year, my colleague Eric Peterson has adapted single-molecule imaging to observe the hybridization reactions of unlabelled DNA – our venture into "dark matter" reaction kinetics.

DANIEL ARMSTRONG

R. A. WELCH DISTINGUISHED PROFESSOR, UNIVERSITY OF TEXAS AT ARLINGTON, USA.

Exciting recent advance: Developing the first GC-MRR instrument, and showing that it can have improved selectively than HRMS and/or NMR.
Best part of the job: Seeing the results of your research being used by others to solve important problems.
Nominator comment: "Armstrong continues to improve pharmaceutical and environmental research, and – ultimately – our own lives. He is an amazing mentor who has guided hundreds of scientists."

8

GERT DESMET

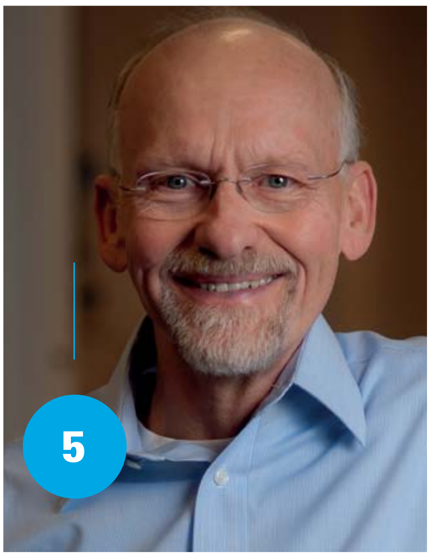
FULL PROFESSOR & DEPARTMENT HEAD, VRIJE UNIVERSITEIT BRUSSEL, BELGIUM.

Career highlight: On the scientific side, my work on shear-driven chromatography and development of the kinetic plot method; on the professional side, my appointment as Associate Editor to Analytical Chemistry and receipt of an ERC Advanced Grant.
Best advice received: My PhD supervisor and then department head told me to "stay away from university politics as best you can and focus fully on the research. If you're research is successful, you'll get things achieved without having to lobby for them anyway."
Nominator comment: "When I have a separation question, I do what everybody does… I ask Gert Desmet!"

JAMES JORGENSON

PROFESSOR, UNIVERSITY OF NORTH CAROLINA, USA.

Career highlight: The development of CE, with our first publications appearing in 1981.
Eureka moment: When we realized that, in the case of CE, the faster we can migrate sample components, the better resolved they will be – seldom can we do something both faster and with a better outcome!
Nominator comment: "A continual innovator in separation science, with major contributions to nano-LC and UHPLC. His focus on fundamentals has pushed forward the Human Genome Project, forensic DNA analysis and LC-MS proteomics."



RICHARD SMITH

BATTELLE FELLOW & CHIEF SCIENTIST, PACIFIC NORTHWEST NATIONAL LABORATORY, USA.

Research: The development and application of advanced methods, instrumentations and informatics capabilities to biological research, particularly proteomics and metabolomics.
Nominator comment: "Smith has led the way in many important MS developments."

JOHN YATES

ERNEST W. HAHN PROFESSOR, THE SCRIPPS RESEARCH INSTITUTE, USA.

Exciting recent advance: We are making great progress towards developing methods for 3Dproteomics and the application of these methods to studies of Alzheimer's disease and cancer.
Eureka moment: We were working on an integrated LC/LC method 25 years ago that combined strong cation exchange and reversed phase particles in the same column. There was an "oh wow" moment when we flowed the 80 percent acetonitrile buffer across and column and observed that peptides were retained on the SCX phase.

ROBERT KENNEDY

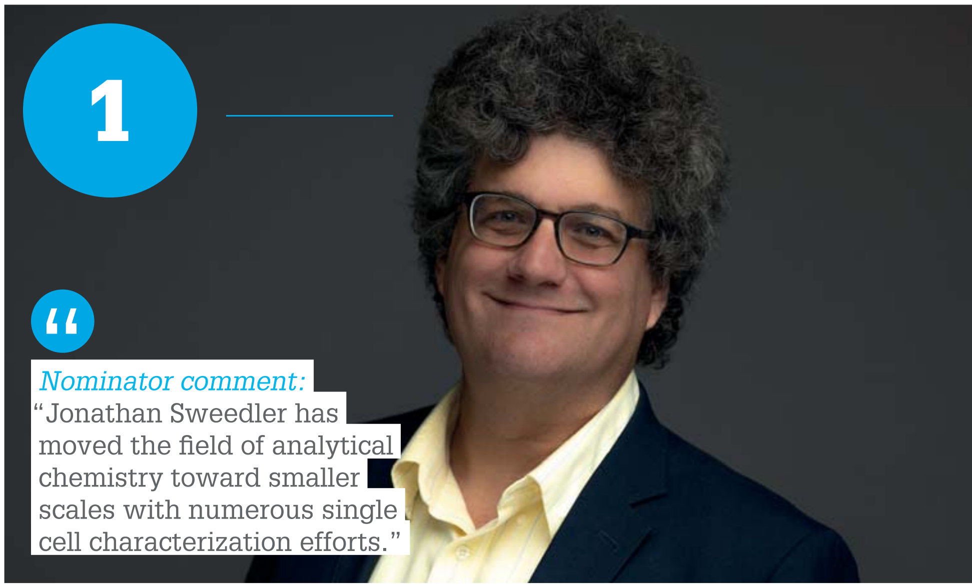
HOBART WILLARD DISTINGUISHED PROFESSOR OF CHEMISTRY, UNIVERSITY OF MICHIGAN, USA.

Career highlight: When my student Lan Huang was first able to measure insulin secretion from single cells using a microelectrode it was incredibly exciting. I had tried to do the same experiment myself, but Lan did it much better than me – through this I learned the power of excellent students. A close second highlight happened around the same time, when Nikki Schultz demonstrated the first immunoassay by CE – this kickstarted a long string of papers on affinity interactions by CE.
Best advice received: This advice was not given to me personally, but Ralph Adams used to keep a quote by P. Handler in his lab that I will paraphrase: "Each scientist owes it to his or herself and society to address the largest question for which the tools are ready and they are the right person."
Best part of the job: My favorite thing about being an analytical scientist is that it is necessary in so many fields, and so it's possible to contribute to multiple areas of science.
Nominator comment: "A recent Martin Medal winner, Robert Kennedy is a continued leader in chemical separations and analytical neuroscience."

GRAHAM COOKS

HENRY BOHN HASS DISTINGUISHED PROFESSOR, PURDUE UNIVERSITY, USA.

Career highlight: Working with graduate students and postdocs, 50 of whom have gone on to faculty positions.
Best advice received: "If you worry about tenure, you don't deserve it."
The future: MS is in the early stages of expansion from analysis to chemical synthesis and materials preparation.
Research goal: Exploration of the "four corners" of MS: instrumentation, fundamental ion chemistry, societally relevant applications and connecting with undergraduates.
Eureka moment: The development of a system that screens 6,000 reactions an hour.
Best part of the job: The freedom to wander across the landscape of science and still be at home in analytical chemistry.



Nominator comment:
"Jonathan Sweedler has moved the field of analytical chemistry toward smaller scales with numerous single cell characterization efforts."

JONATHAN SWEEDLER

JAMES R. EISZNER FAMILY ENDOWED CHAIR IN CHEMISTRY, DIRECTOR OF THE SCHOOL OF CHEMICAL SCIENCES & PROFESSOR OF NEUROSCIENCE, PHYSIOLOGY, MEDICINE AND BIOENGINEERING AT THE BECKMANN INSTITUTE, UNIVERSITY OF ILLINOIS, USA.

Research goal: I have two overarching goals. The first is to create and improve a range of technologies for probing brain chemistry, and the second is to use this technology to understand memory, thought and behaviour in animals ranging from comb jellies to slugs to humans. I'm excited about our recent efforts to probe neurotransmitters, metabolites and lipids in tens of thousands of brain cells, providing us with an unprecedented view of cell-to-cell heterogeneity.
Career highlight: I really enjoy working with talented undergraduate students, graduate students and research scientists, and watching them grow into outstanding scientists.
Best part of the job: The short answer: it's fun! We help advance our understanding of health, work towards curing diseases, and improve our knowledge of the environment. Being an expert in measurement science opens up doors to a broad range of research careers.

Solutions

Real analytical problems
Collaborative expertise
Novel applications

METLIN at 500K

Tandem MS identification as the 21st century standard for small molecule and metabolite identification

By Gary Siuzdak

The Problem

As metabolomics took off in the early 2000s, it became increasingly clear that GC-MS data was hampered by its 1950s-era electron ionization – using a single designated ionization energy with the need for derivatization – and a focus on molecules that are stable enough to survive the GC oven. An alternative was needed – one that could harness the emerging power of MS/MS techniques.

Background

For decades, GC-MS was the dominant metabolite and small molecule identification technology, despite its drawbacks. This dominance was primarily due to the impressive size of its chemical libraries; for example, NIST's library of GC-MS mass spectra, which contained information for over 270,000 individual compounds.

The 2002 Nobel prizes celebrated developments in the now ubiquitous electrospray ionization (ESI). ESI allows for the observation of a broader range of molecules due to its non-destructive nature. Yet, though these newer ESI tandem MS approaches were adopted quickly in metabolomics and proteomics, they were not universally adopted in studies of metabolites and chemical entities because no comprehensive tandem MS databases existed. That is, until a series of three papers (1-3) documenting breakthroughs using METLIN (a cloud-based and freely available ESI tandem MS library) found themselves challenging the dominance of GC-MS.

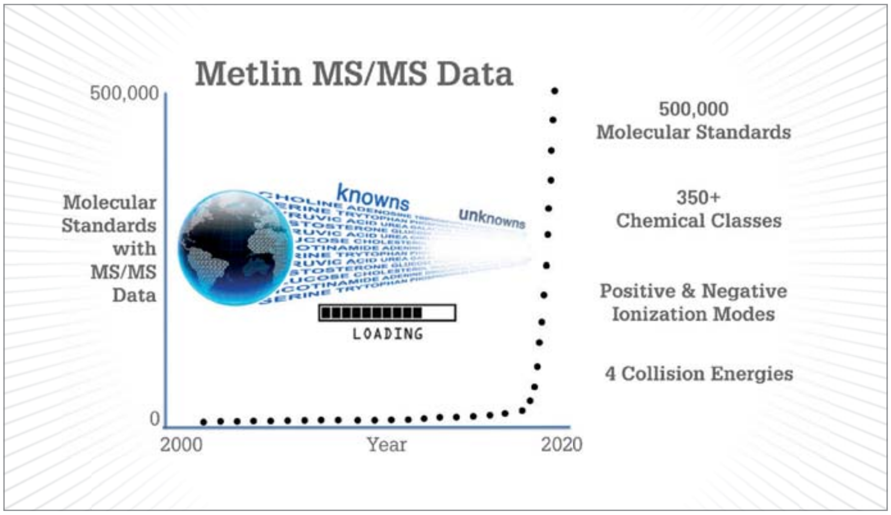
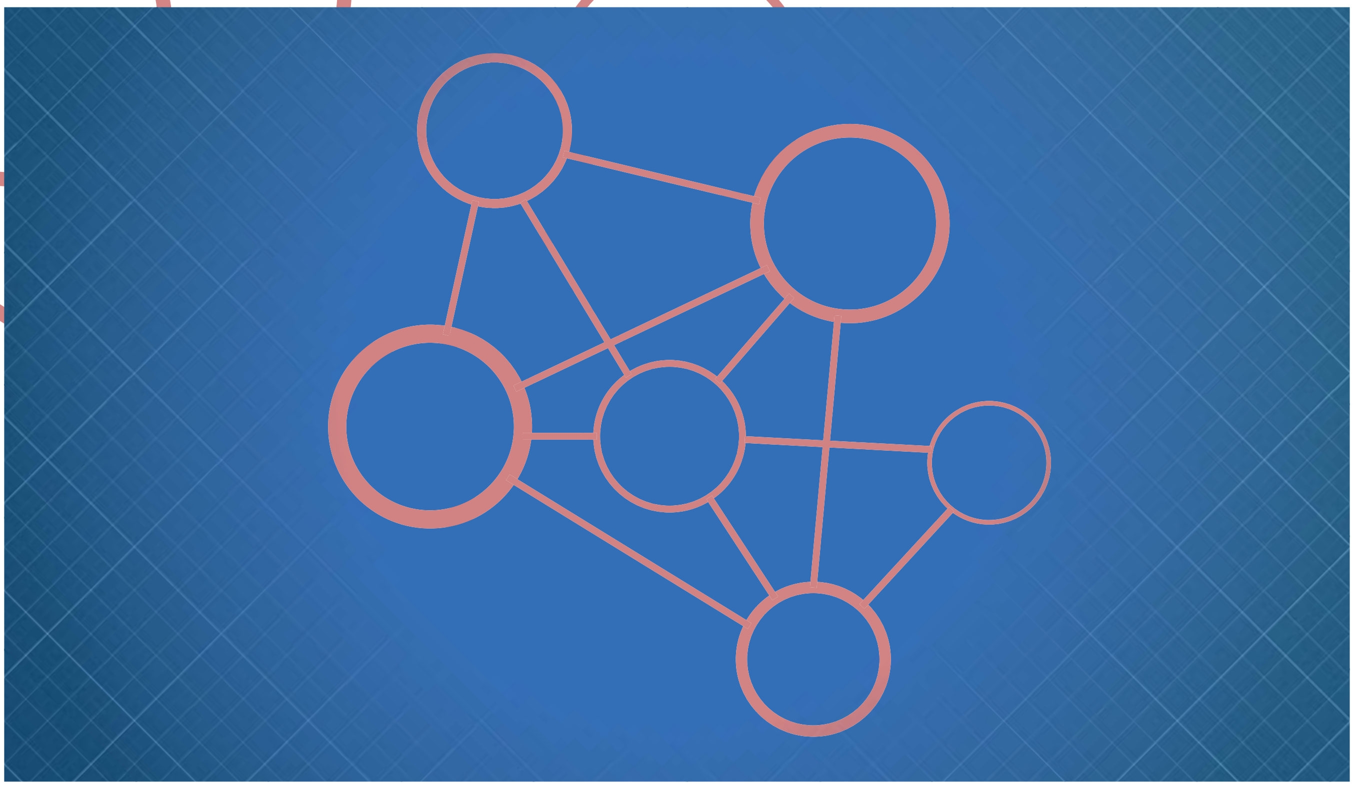


Figure 1. METLIN growth to multi-level data on over 500,000 molecular standards since its origins in the early 2000s.

The Solution

METLIN had humble beginnings back in 2002 – tens of molecules were slowly acquired if and when standards became available. As you can imagine, the tandem MS data was accumulated at a glacial pace. Skip forward to February 2019: METLIN bypassed the NIST GC-MS database mark with tandem MS fragmentation data for 300,000 molecular standards. In August 2019, it reached the milestone of 500,000 standards (see Figure 1), encompassing vast metabolic and chemical diversity (see Figure 2). There are experimental data for each molecule in both positive and negative ionization modes, each generated at four different collision energies. Originally designed to facilitate the field of metabolomics, METLIN has now leapfrogged into the broader field of small molecule chemical analysis, including organic chemistry, pharmaceuticals, toxicology, exposure research, and drugs of abuse.

The feat was made possible by a group of highly talented Scripps Research staff



with innovative ideas and the drive to see them through. H. Paul Benton and Aries Aisporna combined their efforts to address the critical informatic challenges, which included transferring the standards' physical information to the MS instrumentation, as well as automating the identity (and data) transfer to METLIN, and – most importantly – automated data curation. Elizabeth Billings, Emily Chen and Winnie Heim designed a preparation approach that maximizes sample transfer and ESI tandem MS data acquisition. Winnie has also played a key role in the collection of retention time and tandem MS data, and manually curating compound data that did not pass the automated curation step – not a trivial endeavor at this scale.

With a success rate of approximately 80 percent, the platform is robust – but it is far from perfect, with around 20 percent of molecules not providing sufficient precursor ionization or suffering isolation window contamination, among other problems. To reach 500,000, we've had to analyze over 600,000 molecular standards (at the time of writing), with over 100,000 molecules not passing our automated and manual vetting.

Central to the integrity of any library is the use of standards. As we know all too well, the wrong identification can send our collaborators off on a "wild goose chase" for months – if not years. And though the size of the library is important, the dominant factor in moving ESI tandem MS identification forward is access to standards (just as in GC-MS data). METLIN is projected to grow its tandem MS database to over a million validated molecular standards in 2020, allowing the community to finally move out of the 1950s. Given the obvious benefits of metabolite and chemical entity identification, and the possibility for unknown identification through H. Paul Benton's original similarity searching (4, 5), METLIN represents an overdue transition to the 21st century that – when complementing GC-MS – is allowing small molecule identification to become significantly more comprehensive.

Beyond the solution

METLIN's growth will have far-reaching implications, firstly by increasing the ease and reliability of molecular identification exercises, but also by providing researchers with countless further opportunities to exploit the housed data. It is worth noting that METLIN is 30 times bigger than alternative standards databases and is a refined resource that has been widely used for over a decade. It's certainly come a long way since 2002… But we aren't finished yet! A number of further developments are planned, including:

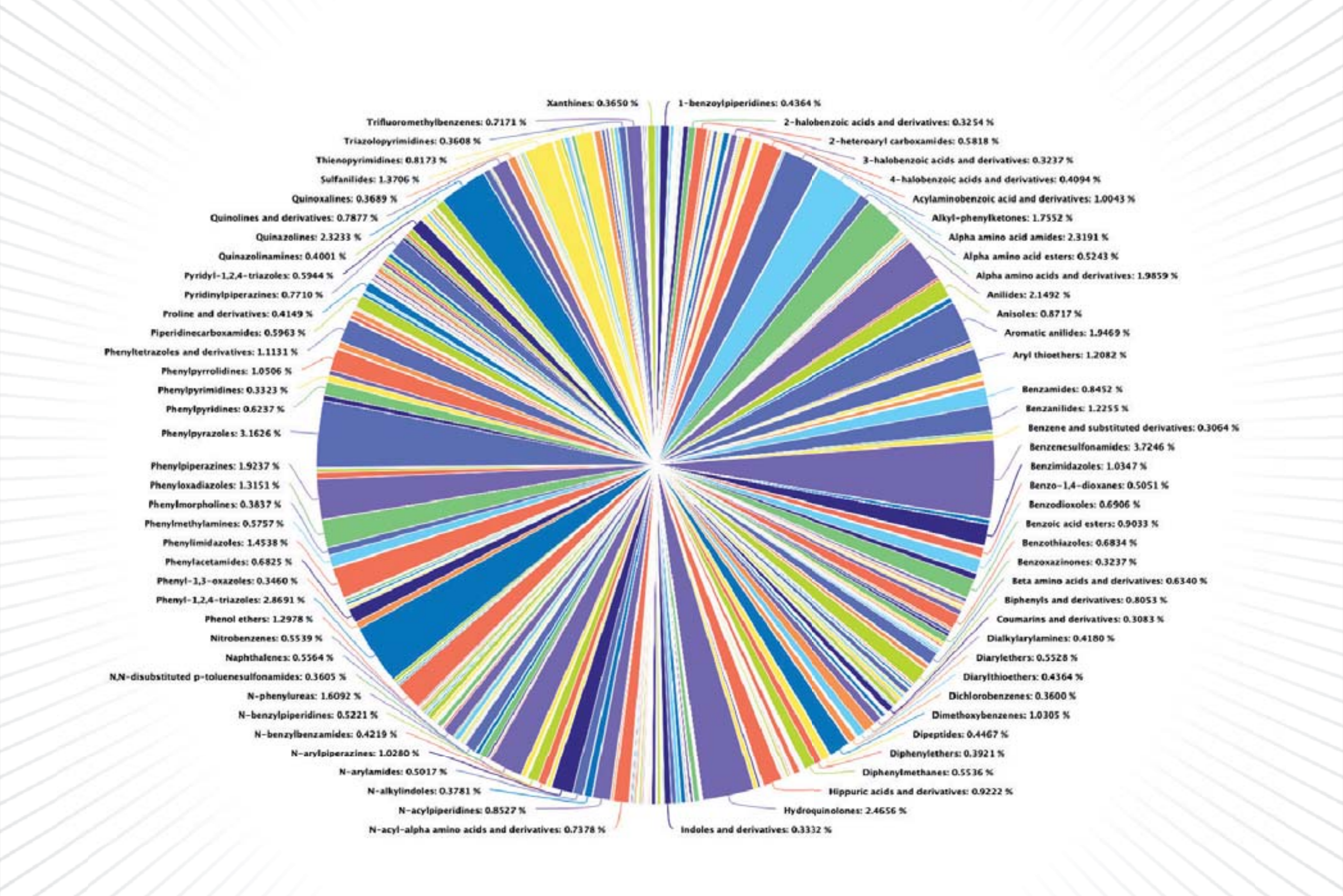


Figure 2. The chemical diversity represented within METLIN based on functional groups.

- the development of similarity searching for unknown identification (1, 4),
- use of METLIN's retention time data to facilitate machine learning predictive algorithms,
- introduction of hydrophobicity filtering from retention time data to improve molecular identification,
- molecular structure determination from MS/MS data by machine learning approaches,
- automated generation of multiple reaction monitoring parameters for quantitative analysis (6),
- endogenous and exogenous activity annotations (5),
- and MS/MS-based pathway mapping (7).

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Quantitative Analysis of Copolymers using a Pyroprobe

Quantitative analysis of poly(styrene-isoprene) copolymers including RSDs and a calibration curve using a CDS Model 6150 Pyroprobe

By Karen Sam

Analytical pyrolysis is a powerful tool for the qualitative analysis of polymers. The analysis usually starts from a simple pyrogram match to an existing pyrolysis database to identify the polymer chemical structure. If multiple polymers are identified, a quantitative method is often adopted by comparing peak areas of the pyrolysis products to determine each polymer ratio. In this application, styrene-isoprene block copolymers, which are large-volume, low-cost, commercial thermoplastic elastomers, are analyzed by following this approach.

Experimental Parameters

Block copolymer standards styrene-isoprene at 14, 17 and 22 percent (styrene to copolymer weight ratio) were obtained from Sigma Aldrich. Solutions of each copolymer standard were prepared in tetrahydrofuran to 1 mg/mL. A 5µL aliquot of each weight percent copolymer solution was added to a Drop-In-Sample Chamber (DISC) tube, then pyrolyzed to a setpoint of 600°C using a CDS 6150 Pyroprobe.

Pyoprobe

Setpoint: *600°C 30 seconds*
DISC Interface: *300°C*
Transfer Line: *300°C*
Valve Oven: *300°C*

GC-MS

Column: *5 percent phenyl (30m x 0.25mm)*
Carrier: *Helium 1.25mL/min, 75:1 split*
Oven: *40°C for 2 minutes*
10°C/min to 300°C
Ion Source: *230°C*
Mass Range: *35-600amu*

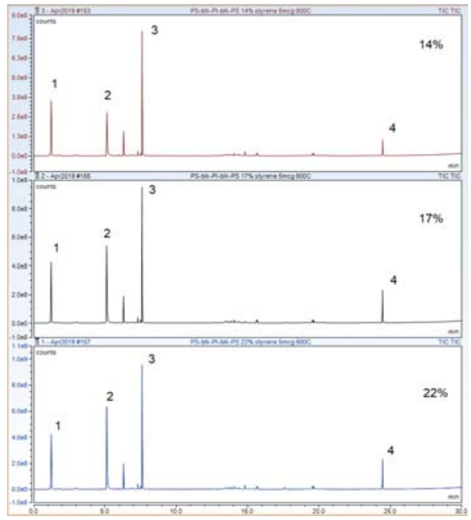

Figure 1. Poly(styrene-isoprene) copolymer pyrogram with 14 percent (top), 17 percent (middle), and 22 percent (bottom) styrene. Peak 1: Isoprene monomer, Peak 2: Styrene monomer, Peak 3: Isoprene dimer, Peak 4: Styrene trimer

Styrene: Isoprene Dimer	
	Area Ratio
Rep 1	0.85
Rep 2	0.86
Rep 3	0.87
Rep 4	0.87
Rep 5	0.86
Rep 6	0.84
Rep 7	0.87
RSD	1.13%

Table 1. 7 runs of styrene monomer to isoprene dimer ratios of 17% styrene-isoprene copolymer

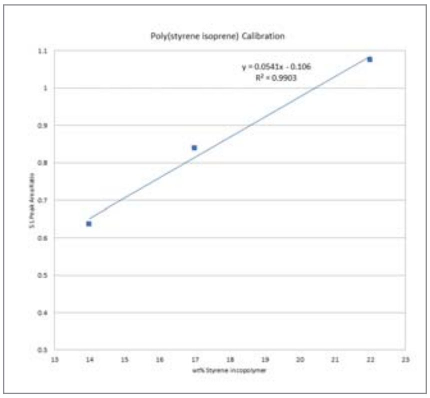

Figure 2. Styrene monomer to isoprene dimer ratio vs styrene weight percent in copolymer

Results and Discussion

Figure 1 shows pyrograms of poly(styrene-isoprene) copolymers containing 14, 17, and 22 weight percent styrene.. When pyrolyzed, polystyrene is principally broken down to monomer (Peak 2 in Figure 1) and trimer (Peak 4 in Figure 1). As the styrene weight increases in the copolymer, so does the area of the peaks from polystyrene (Peaks 2 and 4) in relation to the peaks from polyisoprene (Peaks 1 and 3).

Considering the signal to noise ratio and the simplicity of algorithm, the highest peaks from styrene monomer (Peak 2) and isoprene dimer (Peak 3) were chosen for quantitative analysis. Area ratios of these two peaks were plotted against the weight percent of styrene in each of the standards in Figure 2, which shows a linear calibration with an R2>0.99. The reproducibility study was also carried out from seven sample runs on the 17 percent styrene standard. An RSD of 1.13 percent is obtained in Table 1.

The linearity and RSDs demonstrate that the latest version of the Pyroprobe from CDS is adept at the quantitative analysis of copolymers.

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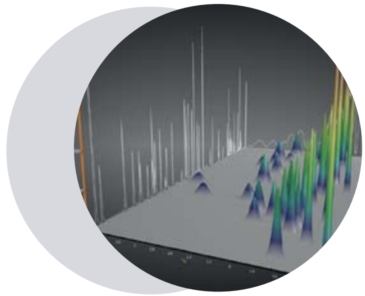

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Leading the Charge

Sitting Down With… Carol Robinson,
Professor of Chemistry, University of Oxford, Oxford, UK

How did your career in science begin?

I've always loved chemistry, but never thought about going to university as a child because nobody in my family had done it before. I eventually got a job as a technician and worked in several laboratories, which only nurtured my interest further. At Pfizer, I was encouraged to take part in day release studies, through which I eventually earned my chemistry degree and found myself wanting to conduct further research. This soon led me into my PhD in the use of MS – a technique that I've always had a fascination with – for peptide sequencing at Cambridge University. The process of fitting spectra to structures to solve problems excites me – it's like a giant jigsaw puzzle. I focused on peptides because proteins were of huge interest at the time, especially neuropeptides and their roles in nerve signaling.

You took a significant career break after your PhD…

I did – and it was considered a very unusual thing to do. Many people doubted that I would return to research because it would be so difficult, but I was determined to try. When I did return, it was no straightforward task – I applied for various posts and eventually had to take a more junior position in which I had next-to-no input into the research taking place. As the research advanced, however, I developed many of my own ideas and came to a point where I knew that I really wanted to investigate protein folding and interactions.

How has your work developed since then?

It's come on leaps and bounds – I've been researching molecular states through ion mobility MS, and I've particularly enjoyed the challenge of getting membrane proteins to "fly" in different ways in detergent, nanodiscs and the membranes themselves. Right now, I'm focusing on studying the complexity of a number of natural targets in the gas phase: lenses, mitochondria and plasma membranes, to name a few. At first, nobody expected gas-phase protein analysis to work, so each new nugget of information we obtain feels validating, and I'm confident that we will continue to surprise ourselves in this area in the future as the technology continues to expand. These days, the possibilities are more or less limited only by your imagination.

"These days, the possibilities are more or less limited only by your imagination."

You were the first female Chemistry Professor at Oxford and Cambridge – did these achievements feel like milestones to you?

They did – and I felt a lot of pressure because I thought maybe other women might not follow in my footsteps if I didn't succeed. I felt a huge responsibility to show that women can flourish in this field, and I would say that I have achieved that. Today, the ratio of male to female professors is more even, and it's great to see so many women on the programs for key conferences and so on, but – of course – there is still some way to go. To any women considering entering this field, I say go for it! It's a fantastic career with endless opportunities, and a little confidence can go a long way. In fact, if I could give my younger self any advice, it would be to have more confidence: you're capable of much more than you realize.

What would you say is your greatest achievement?

I've received many awards over the years, but (not to embarrass my children) I always say that being a mother is my greatest achievement.

What's most enjoyable about being a scientist?

Definitely observing something for the first time – there is nothing that can prepare you for that excitement. But, as I get older, I also love to see how the careers of my students take off; it's great to hear from them, catch up on what they're doing now, and hear that I helped them to achieve what it is they wanted from their careers. The best thing about science is that there is always a new breakthrough on the horizon – and the excitement that follows when it eventually rears its head.

Can you tell us of a recent breakthrough that gave you that feeling?

We published a paper in Science last year that documented the study of biological molecules directly from membranes. The study used vesicles formed from intact membranes; these vesicles expelled complexes that had never been seen before, so we were able to analyze these for the first time in terms of their interactions within the native membrane. It was incredible because we always thought that it would be far too complicated to achieve and interpret, but now we're able to conduct many studies in this way. I'm sure many more such breakthroughs will come with the arrival of our new mass spectrometer, which we helped to develop – watch this space!


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