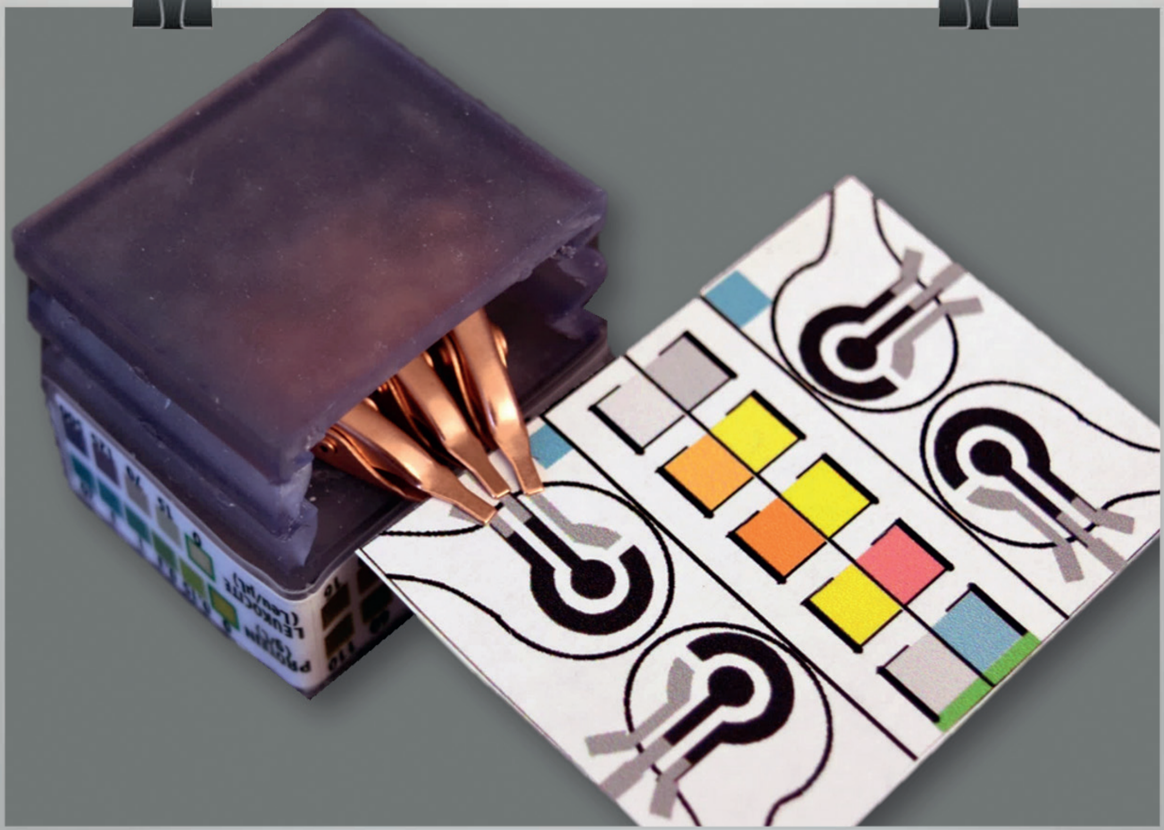
OCTOBER 2017 # 57

the
Analytical Scientist™

Image of the Month



Paper Trails

Researchers have developed a cheap and disposable diagnostic tool powered only by your fingertips. The user taps the triboelectric generator on the bottom of the self-powered paper-based electrochemical device (SPED), and electricity from the tips of the fingers is accumulated in a potentiostat. The user places a fingerprick blood sample on top of the testing region, and a measurement of different analytes, such as glucose or lactic acid, is provided in under 30 seconds. The team envisions the test being used for diagnostics in low-resource settings or by military personnel deployed in remote locations.

Credit: Purdue University photo/Aniket Pal

Reference: A Pal et al., "Self-Powered, Paper-Based Electrochemical Devices for Sensitive Point-of-Care Testing" Adv Mater Technol, 1700130 (2017).

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

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The Power List goes to the movies – inspired by classic western "The Magnificent Seven", originally released in 1960 and rebooted in 2016.

the Analytical Scientist

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Distribution:
The Analytical Scientist (ISSN 2051-4077), and The Analytical Scientist North America (ISSN 2514-7544), is published monthly by Texere Publishing Ltd and is distributed in the US by UKP Worldwide, 3390 Rand Road, South Plainfield, NJ 07080
Periodicals postage paid at South Plainfield, NJ
POSTMASTER: Send US address changes to (Title), (Publisher) C/O 3390 Rand Road, South Plainfield NJ 07080.
Single copy sales £15 (plus postage, cost available on request tracey.nicholls@texerepublishing.com)
Annual subscription for non-qualified recipients £110

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In My View

Report

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Sitting Down With

The Magnificent Scientists

We're back in the saddle for a Power List with a twist.

Welcome to 2017's eagerly anticipated Power List issue! You may have already gathered that there's been a significant change to the list this year. Rather than an overall Top 100, you nominated individuals in 10 categories, all ranked by an international panel of expert judges to produce 10 Top 10s. So, why categorize?

Firstly, we want to celebrate the full spectrum of the analytical endeavour. From the very start, The Analytical Scientist has been motivated by a central goal: to act as a community for the many disparate fields that sit under the banner of analytical science. Separation science and mass spectrometry are wonderful fields – but other areas also deserve attention. By including categories that cover specialties previously under-represented on the list, we're delighted to welcome some new names; about 60 percent of this year's list were not featured in our most recent Top 100 in 2015. Though our chosen few are more diverse than ever in specialty, certain groups are still under-represented – we welcome your thoughts on how we can better bridge the gaps.

Secondly, we are keen to expand our definition of "power" by recognizing that an individual's influence can be measured in many ways (we never pretend that any of our lists are definitive for that very reason). For instance, we felt that it was important to recognize those who go above and beyond to offer the next generation a helping hand – our Mentors. We were all touched by the heartfelt comments from nominators in this category, and narrowing the wonderful selection down to just 10 was particularly tough for the judges.

Finally, we'll admit that we also like to shake things up! From the Top 40 Under 40 to last year's women-only list, we want to keep our celebration of analytical science fresh. Splitting the list provides some alternative insights and new angles; for example, consider how the 14 people who appear in more than one Top 10 are distributed.

No doubt this year's list will attract all the usual excitement, comment and controversy. I'd love to hear your thoughts – the good, the bad and the ugly – at charlotte.barker@texerepublishing.com.

Before I skedaddle, I'd like to close with my sincere thanks to everyone who nominated, our anonymous judges, and the nominees themselves, who provided so many thoughtful, funny and surprising pearls of wisdom – you can read their contributions in full on our website.

Charlotte Barker
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

Giving SEIRA a Boost

New light-trapping sensor increases sensitivity of surface-enhanced infrared absorption spectroscopy devices – by up to 1,000 times

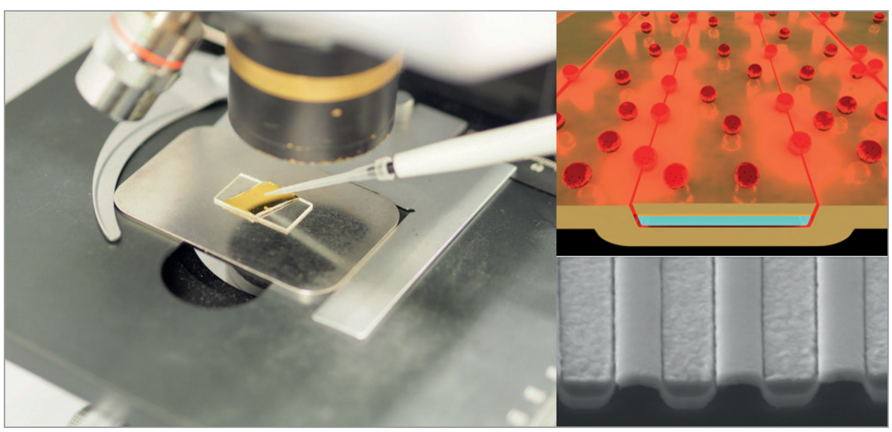
The optical absorption spectra of trace chemical or biological molecules are typically very weak. Now, experts in material science, nano-optics and bio/chemical sensing have developed an optical device that is able to significantly enhance the absorption signal of trace molecules.

The collaborative team's light-trapping structure can squeeze infrared light into sub-5-nm gaps with very high efficiency, resulting in a very strong localized light field. They then demonstrated an application of this "squeezed" light using surface-enhanced infrared absorption (SEIRA) spectroscopy. The sensor, which acts as a substrate for the materials being examined, was found to boost the ability of SEIRA devices to detect molecules at 100 to 1,000 times greater sensitivity than previously reported results.

The device is officially called a "metamaterial super absorber". But how does it work? "The unique sensor consists of two layers of metal with an insulator sandwiched in between," says Qiaoqiang Gan, Associate Professor of Electrical Engineering, State University of New York at Buffalo, USA, and contributing author of the recent paper (1). "Using a fabrication technique called atomic layer deposition, we created a device with gaps less than 5 nm between two metal layers (a human hair is roughly 75,000 nanometers in diameter)." Creating such a small structure is a considerable challenge. "It is extremely difficult to produce uniform sub-5-nm features using current nanofabrication technologies," explains Gan. "The major challenge is practical fabrication over large areas. Building upon atomic-layer-deposition processes, we developed a new scalable nanomanufacturing method, which we are currently using to develop large area structures."

The tiny gaps enable the sensor to absorb up to 81 percent of infrared light, a significant improvement from the 3 percent that similar devices absorb. And, Gan says, when the light is squeezed into such a small volume, its intensity is extremely strong, significantly enhancing its sensitivity in bio/chemical sensing applications, such as sports doping, forensics and art fraud detection.

The ultra-sensitive bio-chip is still at



the R&D stage, but the team are hoping to work on commercialization of the technology. "Our structure still relies on top-down nanomanufacturing methods like optical lithography," says Gan. "If the manufacturing cost barrier can be addressed, we are aiming to deliver a new type of functional biochip for SEIRA as well as SERS sensing applications." *JC*

Reference

1. *D Ji et al., "Efficient mid-infrared light confinement within sub-5-nm gaps for extreme field enhancement", Adv Opt Mater, 5 (2017).*

Calling All Innovators

Nominations are now open for The Analytical Scientist Innovation Awards 2017

The Analytical Scientist Innovation Awards (TASIAs) return for 2017 to showcase groundbreaking technologies, advanced software solutions and innovative instrumentation. So whether you're detecting hazards or ensuring food safety, working in the lab or the field, whether your product is resolutely dependable or completely cutting-edge, now's your chance to enter your technology, instrument or solution for the Top 15 innovations of the year.

Like last year, the great minds behind the top five innovations will each have the opportunity to share the development story in a three-page Solutions article in 2018.

To enter, please email charlotte.barker@texerepublishing.com with the following information:

- Name of innovation
- Launch date
- Brief description (~10 words)
- Detailed description (50-150 words)
- Potential impact (50-150 words)
- One image (if applicable)

The deadline is 3 November, 2017. All nominations will be put to an expert panel, with the winners announced in our December issue.

Read about last year's winners here: tas.txp.to/2016//TASIA

TRI a New Kind of Spectrometer

An inexpensive, smartphone-based device could offer a wide range of point-of-care tests

Everyone's vision of the "laboratory of the future" is different – but most agree that it should be reliable, versatile and efficient. And if those attributes don't come with huge costs or space requirements – even better. Enter the US$550 spectral transmission-reflectance-intensity (TRI)-Analyzer (1), which can perform an array of tests on the spot by harnessing clever optics and the power of a smartphone. But is it the future?

"Several years ago, we completed an early demonstration of a smartphone as a spectrometer. The spectrometer itself was handheld, but to interface with any sort of meaningful biological sample, it needed to be attached to some benchtop optics. The next step was to produce a truly handheld device with everything inside, including the light source and sample interface," says Kenneth D Long, lead author of the paper. To that end, the research team condensed three general optical techniques – transmission, reflection and intensity, each of which uses a different optical path – into a compact package to minimize size and cost. Best of all, the system wasn't designed for a specific test. "So many recent advances in the point-of-care testing realm focus on miniaturizing a test for a single condition. The TRI-Analyzer is a handheld instrument capable of measuring thousands of commercial tests."

The TRI-Analyzer was developed from the ground up. "We wanted to design a device that maximized spectral resolution (and therefore sensitivity) and versatility," explains Long. He and his colleagues began with optical simulations to develop the ideal light path, and then substituted in commercial optical components. First, they designed the custom fiber-optic assembly and the 3D-printed cradle in which the optics are mounted; then, they built a prototype and tested each of the three modalities with basic samples, such as food coloring. "We also wanted to run some proof-of-concept experiments using biological samples from a context where a portable device would be beneficial," says Long. To that end, the team assessed the TRI-Analyzer's performance with an ELISA assay to detect an indicator of pre-term birth (fetal fibronectin protein) and a fluorescent assay to measure phenylalanine, an indicator for phenylketonuria.

The regulation of new medical technologies is stringent, so it will be some time before the TRI-Analyzer is approved for routine clinical use. "The best patient right now would be a cow or horse. Just like people, they catch diseases and are highly mobile. 'Clinic access' is often challenging, and getting results back to patients after laboratory analysis can be difficult when they're out in the pasture. Having a device that could perform a test on-site would obviously be beneficial," says Long.

Personally, though, Long says he is incredibly interested in global health applications. "I'd love to see the TRI-Analyzer used by clinicians in rural or remote places where there might be clinics, but not clinical laboratories. Perhaps a doctor who travels to a dozen clinics on a regular basis could take the TRI-Analyzer with them as a portable lab system instead of collecting clinical samples, sending them off to a lab, and then trying to reconnect with a patient a couple of days later."

Long and his colleagues hope that the TRI-Analyzer will help free many diagnostic tests from the centralized laboratory. Their ultimate goal? A tool that researchers and clinicians can use to quickly translate both existing and novel biomedical tests from the benchtop to the bedside. Better yet, they anticipate that the decreased logistics of sample collection, shipping, tracking, and follow-up will save time for physicians and laboratory professionals alike.

"I'd hope that we move away from having a separate gadget for each test we want to perform and toward a future where a single device can serve as a more universal portable laboratory capable of measuring many different types of tests," concludes Long. "I hope our work helps nudge the field in that direction." *MS*

Reference

1. *KD Long et al., "Multimode smartphone biosensing: the transmission, reflection, and intensity spectral (TRI)-analyzer", Lab Chip, [Epub ahead of print] (2017). PMID: 28752875.*

From Promotions to PASEF Mass Spec

What's new in business?

In our regular column, we partner with www.mass-spec-capital.com to let you know what's going on in the business world of analytical science. This month, Markes branches out into China, while closer to home, Queen's University Belfast partners up with Waters to launch a Masters program in food safety.

Products

- Bruker introduces timsTOF Pro Mass Spectrometer for PASEF mass spectrometry, plus the D8 Discover Plus XRD System
- SCIEX launches Topaz LC-MS/MS system for CDx in Europe
- PerkinElmer launches QSight 210 MD system for clinical labs

Investments & Acquisitions

- Eurofins to acquire EAG Laboratories for $780m net

Collaborations

- Agilent announces Platinum Sponsorship Agreement with LabCentral
- PerkinElmer and In-Depth Genomics team up for whole genome sequencing diagnostics
- Queen's University Belfast launches joint e-learning initiative with Waters Corporation to tackle food fraud
- Lipotype performs lipid analysis for Flagship VentureLabs

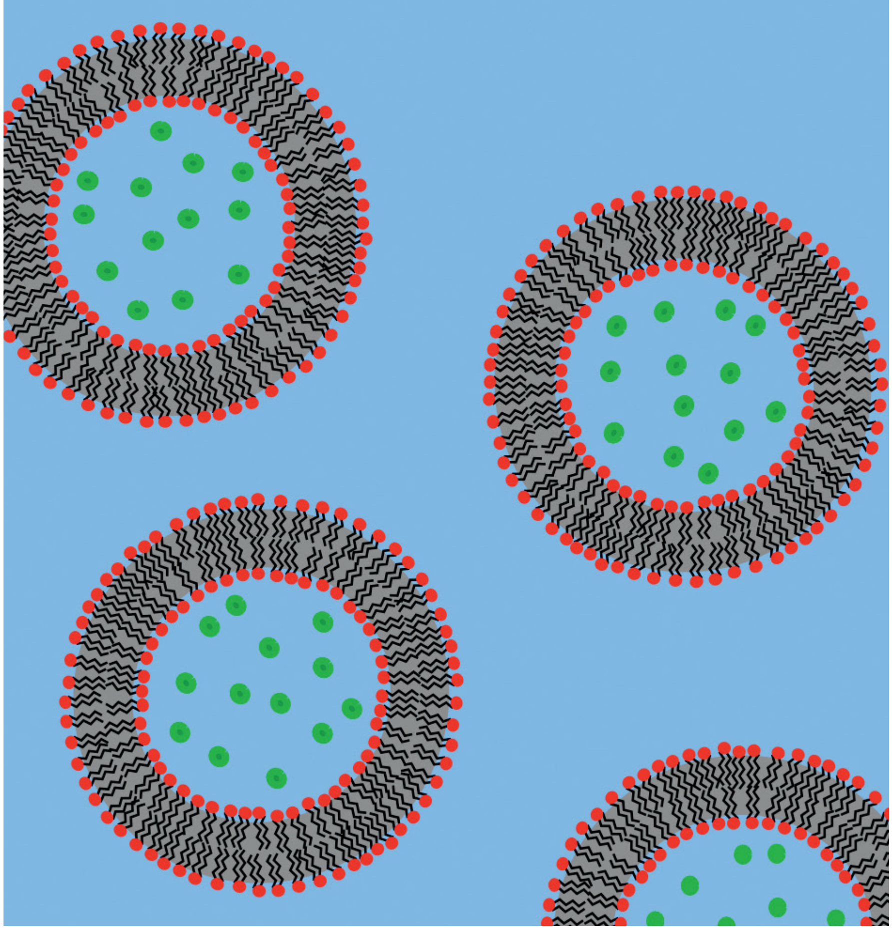
People

- Microsaic Systems promotes Glenn Tracey (pictured) to CEO
- SCIEX appoints Inese Lowenstein as President

Organizations

- Markes International opens Chinese subsidiary in Shanghai

For links to original press releases and more business news, visit the online version of this article at: tas.txp.to/1017/BUSINESS



The Biomarker Breakdown

Could AMD be diagnosed through blood plasma analysis?

It's a classic "chicken and egg" scenario. When retinal diseases like age-related macular degeneration (AMD) strike, early diagnosis and intervention give the best prognosis and visual outcomes. But in reality, retinal disease cannot be diagnosed until structural changes are seen, and some patients only present at ophthalmology clinics when the visual symptoms – and the underlying pathology – are at an advanced stage. Now, a team from Massachusetts Eye and Ear Hospital, Boston, USA, are proposing that metabolomics analysis might hold the key to identifying those at risk during the early stages of disease diagnosis – or even before the disease starts to develop (1).

"Metabolomics has recently been shown to provide biologically informative markers of complex diseases, such as Alzheimer's, so we decided to research the role of metabolomics in AMD to find biomarkers for diagnosis and prognosis in this disease," says Deeba Husain, co-senior author on the corresponding paper (1).

In the study, the team took blood plasma samples from 90 patients with AMD (30 each with early, intermediate and late stage disease) and from 120 patients with normal macular health. The samples were analyzed using ultra high-performance liquid chromatography coupled to tandem mass spectrometry. They found that a total of 87 metabolites, mostly from glycerophospholipid metabolism, differed significantly between patients with AMD and the controls. Of these, 48 were significantly different across the different stages of AMD. "We were surprised to find that glycerophospholipid metabolism specifically seems to have a strong association with AMD – this pathway was highly enriched among the significant metabolites (p=4.7 x 10-9)," says Husain, who believes the results could form the basis of the first blood biomarker for early diagnosis and prognosis of AMD.

But their results aren't just important for diagnosing disease. "The detection of very significant metabolite pathways could lead to finding a new druggable target for treatment," says Husain, "and that could lay the path for personalized medicine in the management of AMD." Next steps for the team include a large multicenter study to validate their findings, as well as a long-term follow-up study to better define the role of glycerophospholipid metabolism in disease progression. *RS*

Reference

1. *I Laíns et al., "Human plasma metabolomics study across all stages of age-related macular degeneration identifies potential lipid biomarkers", PLoS One, 12, e0177749 (2017). PMID: 28542375.*

Funding Tomorrow's Biopharma Pioneers

CASSS announces the inaugural recipients of its new Svec Fellowship for Innovative Studies

The CASSS Frantisek Svec Fellowship for Innovative Studies was created in 2016 to encourage innovative learning opportunities in biopharmaceutical science and technology – and help nurture future leaders in the field.

The first two recipients – Daniela Espinosa-Hoyos and Bert Wouters – have big plans for the funds. Espinosa-Hoyos of Cambridge, USA, will train at The New York Stem Cell Foundation Laboratory, while Wouters, of Amsterdam, the Netherlands, will use his Svec Fellowship for a one-month research stay at the University of Tasmania to work with Brett Paull and Michael Breadmore on 3D printing in analytical chemistry. "I greatly admire how CASSS supports young researchers around the globe, and I will do my very best to make the most out of this research stay," said Wouters.

Applications for the 2018 Svec Fellowship are due by December 31, 2017 and funds will be awarded in the first quarter of 2018. For more information, please visit http://www.casss.org/page/Fellowships.

Planes, Trains and Automobiles

Beyond the Svec Fellowship, CASSS offers a range of grants for students and postdocs, including a Travel Grant program to help students connect to industry. The program provides reimbursement of travel costs to students who present oral or poster presentations at any CASSS scientific meeting. Plus, CASSS will waive conference registration fees.

Applications are accepted year-round, from students and postdoctoral researchers worldwide. For more details, visit http://www.casss.org/page/STG01.

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 edit@texerepublishing.com

The Road to HPLC2018 Part I: Super Separations

As we finalize the program for HPLC2018, I reflect on the advances that are guiding the future of liquid chromatography.

By Norman Dovichi, HPLC2018 Symposium Chair and Grace Rupley Professor of Chemistry and Biochemistry, University of Notre Dame, Indiana, USA,

2018 sees the 47th anniversary of the HPLC symposium, which has grown to become the largest and most visible international conference series dedicated to all aspects of liquid-phase separation science and analysis, including mass spectrometry, chromatography, and electrophoresis. As always, HPLC2018 presents an exciting opportunity to learn of cutting-edge research in separation science. The world's leading experts will deliver presentations on emerging technologies and discuss novel solutions to important problems in pharmaceutical, environmental, and industrial research and development. In addition, vendor workshops and a series of short courses and tutorials will provide outstanding opportunities for newcomers to obtain a solid foundation in the field – and for veterans to update their knowledge. Meanwhile, the exposition will showcase new product launches and innovative products, and the social program will facilitate networking with colleagues from around the world.

Along with the rest of the organizing committee, I am currently in the midst of the exciting, challenging and rewarding task of assembling the conference program. We are delighted to have recruited two outstanding plenary lecturers: Stacey Ma, Vice President at Genentech, will describe the perennially important role of analysis in the pharmaceutical industry, and Richard Smith from the Pacific Northwest National Laboratory will speak on his remarkable recent work on extremely high-resolution ion mobility spectrometry (see tas.txp.to/0717/Smith). The plenaries will set the tone for the rest of the event, in which we aim to cover the most interesting developments from the past year, plus advances that we believe will make a splash in the years to come.

Of course, separations are the primary focus of HPLC2018, and there are a number of areas that deserve special attention. Novel stationary phases with improved properties are continually being developed and commercialized, providing valuable tools for selected analytical problems. Nanoparticle stationary phases provide exciting opportunities for fast and efficient separations. Monoliths enable low backpressure separations, again at high speeds and relatively low pressures. Electrokinetic separations are undergoing a renaissance, particularly when coupled with high-efficiency interfaces with mass spectrometry for metabolomics, glycomics, and proteomic analyses. Finally, multidimensional separations provide powerful tools for the characterization of otherwise intractable samples.

Sample preparation is an important, and sometimes underappreciated, step in analysis. Solid-phase microextraction and other tools can dramatically speed analysis. Perhaps more importantly, they can improve the precision and accuracy of the analysis. And that's why they will also be a focus next year.

Washington, DC provides easy access for the many pharmaceutical companies located in the US Midwest and East Coast, so an important focus of the conference will be on pharmaceutical analysis of small molecules and biopharmaceuticals. To name just two emerging challenges in the industry, continuous flow synthesis of small molecule drugs presents new difficulties for on-line analysis, while the characterization of drug–antibody conjugates is of increasing importance in biopharma.

Proteomics and metabolomics are enabled by chromatographic and electrophoretic separations coupled with powerful mass spectrometric detection. Increasingly complex samples are routinely being analyzed, and issues of throughput and data interpretation are important challenges. The separation of intact proteins is valuable not only for top-down analysis of complex samples but also for analysis of intact antibodies in the biopharma industry. As a new topic, characterization of microbiomes presents interesting and formidable challenges to the bioanalysis community.

Microfabricated separation and sample preparation tools are now commercialized and finding routine use in the laboratory. However, many groups are pushing the state-of-the-art in microfabrication and nanofabrication, which will have a profound impact on separation science. Advances in microfabricated cell culture coupled with on-line sample manipulation and separation provide powerful tools for biology and pharmaceutical analysis.

An interesting new topic in the food and environmental field is cannabis analysis – a real growth industry as certain jurisdictions legalize its medical and recreational uses. Extraction of active components for incorporation into edible products is a surprising application of supercritical fluids. Furthermore, the characterization of psychoactive materials is important, and the identification of pesticide contaminants is of growing interest.

This is the first of a series of short articles in The Analytical Scientist, written by leaders in the field, which will describe important problems and exciting applications in separation science in the run-up to HPLC2018. We hope these articles will provide fodder for discussion at the event, and whet your appetite for the many excellent sessions we are assembling.

HPLC 2018 takes place on 29 July to 2 August in Washington, DC. HPLC2018.org

Out with the Old, in with the New?

Not quite. Tried and tested analytical approaches like ELISA aren't going away in the world of bioprocessing, but modern techniques allow for real-time analysis. Together, they present an orthogonal approach.

By Alex Perieteanu, Director, Biopharmaceutical Services – Life Sciences at SGS Canada.

There have been increasing calls by our global clients for bio-layer interferometry (BLI) – a real-time analytical technique for studying biomolecular interactions – to be incorporated as a routine quality control test in bioprocessing. At the moment, BLI is most commonly used in the research phase for high-throughput target screening, but I believe it is more than applicable for quality control and to ensure that products are consistent and stable from lot to lot. BLI can measure interactions between many different types of molecules, whether a pair of proteins (or multiple proteins), a protein and a small molecule or peptide, or even two different fragments of DNA. Light of a particular wavelength is emitted through a fibre optic probe or biosensor. The probes have a unique chemistry, and multiple different chemistries are available commercially. When a molecule of interest binds to the coated probe, there is a measurable change in the wavelength of the light, giving the ability to monitor on and off binding kinetics in real-time.

BLI's flexibility in experimental design and industrial applicability parallels that of the classical enzyme-linked immunosorbent assays (ELISA). Conceptually, BLI differs from ELISA only in the mode of detection, so ELISA methods can usually be easily transferred to BLI. In practice, the major difference is that the ELISA coating and binding steps are blind, making it difficult to gauge exactly how effective they are; optimization is really only possible based on the end results. BLI, on the other hand, enables a real-time understanding of binding, whether it be during coating or molecular interaction, and is generally more sensitive with a larger dynamic range. The advantage of seeing the binding in real time is that it gives greater insight into the binding kinetics and specificity. With ELISA you obtain the binding affinity (the dissociation constant), but with BLI you don't just get the binding affinity, you generate it through its association and dissociation kinetics – so you not only see what is binding, but how fast.

ELISA's advantage lies in that it doesn't require significant capital expenditure and is a familiar technology. The pharma industry tends to favor tried and tested approaches, and ELISA certainly falls into that category, but BLI really does offer something more and is worth seriously considering. Clearly, ELISA, BLI and other analytical techniques, such as surface plasmin resonance (SPR), have their own particular strengths and weaknesses – and certain applications are simply better suited for different instruments. Speaking from my own experience, I see a slight trend towards the implementation of BLI over SPR, which could be because of perceived barriers to entry with SPR. However, I feel that BLI is highly complementary to SPR. From a business perspective, one might argue that they are competitive in nature but, scientifically speaking, the generation of complementary datasets using orthogonal techniques is always preferred. As such, a strong case can be made for the implementation of both techniques. I would also suggest that it is unlikely that any technique will ever completely take over from ELISA – just as there will always be an important place for a $1 pin prick diagnostic test in addition to an MRI scan.

Analytical technologies have advanced significantly over the last decade, becoming more sensitive and user friendly. It is to the benefit of all us – since we are all patients – to have a range of orthogonal techniques in the analytical toolbox, because the more we can understand products from a functional perspective, the better positioned we are to generate efficacious medicines.

Dwelling on the Fundamentals

The next generation of chromatographers risks losing sight of basic principles

By Victoria F. Samanidou, Laboratory of Analytical Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece.

I was reading an interesting article by Tony Taylor about dwell volume (1) when an uncomfortable thought struck me – how many of my chromatography students would actually understand this?

The article discusses whether the concept of dwell volume is still relevant, given the proliferation of UHPLC, and the fact that extra-column volumes are much reduced.

Taylor writes, "I'm sure most of us are aware that dwell volume is the volume in our HPLC system from the point at which eluent solvents are mixed to the head of the packed bed within the column." Again I pondered: would "most" of us know that?

As chromatographers, we know that resolution relies on selectivity and that dwell volume can affect resolution and selectivity in HPLC methods... But how efficiently can young chromatographers handle selectivity in terms of column chemistry (stationary phase) and mobile phase constituents?

Young scientists may be able to use an Orbitrap LC-MS instrument, both hardware and software. They may be experts in knowing how to collect and interpret data, or how to apply chemometrics. But if one asks a simple question about the basic principles of chromatography, many of them cannot give a decent answer.

The same chromatographers may not know that C18 columns are not all the same, and that manufactures may produce several different types. They may have never paid attention to carbon load or surface area when choosing the analytical column, concentrating only on length, the inner diameter or the particle size.

With regards to mobile phases, do they know why methanol and acetonitrile – although both polar – lead to different eluotropic strength? Does the Snyder solvent selectivity triangle (2) ring a bell? What is the role of TFA, or ammonium acetate in the mobile phase? Why is water not enough? These and many other fundamental aspects too often leave them drawing a blank.

Going back to the initial question – how many know the meaning of dwell volume and how to measure it? How many of them have actually measured it in the instrument they are using? When developing gradient methods and transferring between different high-performance instruments, have they taken into consideration this very important issue?

My point? All HPLC practitioners should be able to answer these types of questions; being able to use highly sophisticated instrumentation in routine analyses is not enough. Not so many years ago, students were at least aware of the theoretical principles of chromatography.

It seems to me that this drop in fundamental knowledge is a reflection of wider changes in education (3). Core education is overwhelmed by the tremendous evolution of technology. The new doors (or rather, the new "windows") that technology opens sometimes lead to a sacrifice of crucial basic education. Undoubtedly, the younger generation rely too much on easy access to knowledge online, and so fail to assimilate the basic principles and theoretical aspects of the techniques they practice.

Virtual reality, virtual knowledge, and finally virtual education, have become part of our lives. My final question: can we stop or reverse the trend, before it is too late? At the very least, we have to give it a try.

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2. *Crawford Scientific, "Going back in time – ternary and quaternary gradients", 2017). Available at: http://bit.ly/2fT1YEr. Accessed October 5, 2017.*
3. *Infogineering, "The difference between data, information and knowledge," (2017) Available at: http://bit.ly/1wrG75E . Accessed October 5, 2017.*

A Question of Efficiency

What exactly do we mean by efficiency? Where can gains be made? How do we know when we've reached an acceptable level? One thing is certain: by being more efficient, we can be more competitive – in business or academia. Introducing "Your Efficiency Challenge!"

We all strive to be more efficient. Why waste time and energy getting a job done? And though measuring efficiency for a simple system or process is relatively straightforward, when we delve deeper into the concept, we find an untameable multifaceted beast. Indeed, when trying to assess (and increase) the efficiency of a complex system with complex processes – an analytical laboratory, for example – we are faced with a somewhat nebulous task, demanding that we focus on one aspect or another, while perhaps neglecting others.

What is "Your Efficiency Challenge"?

The Analytical Scientist has teamed up with Agilent Technologies to run an exciting project over the coming months that begins with your views on efficiency in terms of liquid chromatography and associated workflows. The survey results will help define topics for three lively roundtable discussions and a series of articles that will cover the most important aspects of efficiency. By taking Your Efficiency Challenge, you could also be selected as one of our "challengers," whose responses and questions will serve as case studies for our experts. And the very best will be given the opportunity to join the expert panel discussions. Finally, we'll bring all the insight gained into a compendium – our "Guide to Efficiency."

By looking at the outcomes of the survey, sharing the insights of our experts, and by starting an ongoing discussion on efficiency, we believe that everyone stands to gain.

Experts in efficiency

We spoke with two of our five-strong panel of efficiency experts ahead of Your Efficiency Challenge for some opening 'food for thought.'

"The classical definition of efficiency is the ratio between the output and input. But in analytical chemistry, the output is very often complex in nature; it could be analytical information as measured by number of results and quality of those results," says Wolfgang Kreiss, a Germany-based independent consultant who specializes in the field of laboratory management. "But efficiency could equally be considered the monetary value of the information obtained in an analytical study versus the input of cost and time. In some cases, efficiency simply means delivering the right results on time." Kreiss notes the complexity of potential outputs in analytical laboratories as a confounding factor when attempting to optimize processes and workflows. Because the concept of efficiency spans everything from analytical aspects, such as number of plates or peaks per time, through instrumental aspects (overall analysis speed, ease of use), to the whole laboratory (overall cost per sample), Kreiss says that a holistic view is needed to find inefficiencies.

"We're living in a world that takes a much sharper look at compliance, which means that we must increasingly be able to prove that analytical results are valid," says Kreiss. "In practice, you need instrumentation and software with sufficient speed and processing capacity for statistically valid results – and though the excessive repetition required may not feel efficient, analytical results may hold little or no value if you cannot provide evidence of their validity."

Where would Kreiss begin in an assessment of an analytical laboratory's efficiency? "I would first look at the objective of the lab – after all, the objective defines the 'output' and hence the measure of efficiency. If the lab does routine analysis or process control, I would focus on the instrumentation. Is it standardized across the lab? A circus or museum of instruments is less likely to breed efficiency," says Kreiss. "I would also check the appropriate use of systems – is an advanced system with only one trained operator being used for an analytical task befitting a simpler solution? Or, alternatively, are some operators struggling to meet requirements with instrumentation or software that should be updated?" Efficient interaction between data systems – from the chromatography data system to LIMS to the ERP system – would also be a high priority. "Efficiency is lost very quickly without adequate and direct integration of all necessary software systems," says Kreiss. "It cannot be neglected."

Colinda van Tilburg, Group Leader Analytical Chemistry at Mercachem in the Netherlands, is responsible for method development in an open access analytical department that serves 140 organic chemists, so she fully understands the need for efficiency. "In the contract research world, efficiency is about rapid turnaround of the results that matter; it's also about working 'at the limit' – modern LC systems allow you to get the same result much faster. My belief is that if you have extra speed available, you should use it," says Van Tilburg. "Likewise, repetitive tasks that can be automated should be automated, wherever feasible."

Van Tilburg agrees with Kreiss that efficiency needs to be tackled holistically. And sometimes simple or small changes can have a big impact. "If I'm assessing a new laboratory with efficiency in mind, I take a 'top down' approach. I first look at the infrastructure." Van Tilburg recalls walking into one large laboratory where all the equipment was stacked at the far end.

What is efficiency?

At HPLC 2017 in Prague, we asked a number of analytical scientists a straightforward question: "What does 'efficiency' mean to you?" Responses almost always began with a lengthy pause and ended with a lengthy discussion. Here are some of the answers:

"When I think of efficiency (from an analytical point of view), the first thing that springs to mind is speed – achieving the same task, faster. On the other hand, when it comes to managing a team of 250 people, it's about getting the maximum value for less effort – without driving people to exhaustion!" – Emily Hilder, Director, Future Industries Institute, University of South Australia, Australia.

"Analytically, I think of a stack of theoretical plates that can never really exist. When it comes to managing a lab, efficiency means getting the results out on time and working safely using the correct procedures (among other things)." – David McCalley, Professor in Bioanalytical Science, University of the West of England, UK.

"I think speed is the most important aspect of efficiency from an analytical standpoint – while keeping all of the essential components of the mixture separated, of course. In the lab, daily efficiency has more to do with robust instrumentation and reliable consumables that help you avoid unnecessary repetition and errors." – Gerard Rosse, Associate Director, Structure Guided Chemistry, at Dart Neuroscience, San Diego, USA.

"Efficiency for me means high throughput. But, whatever the situation, it's about utilizing resources in the most effective way." – Andrea Gargano, Postdoctoral Fellow, University of Amsterdam/Vrije Universiteit Amsterdam, the Netherlands.

"Personally, efficiency is something I feel like I often lack! In chromatography, it's something that I constantly strive to achieve, and it relates to separation power per time." – anonymous.

"Analytically, seeing a lot of peaks... In the lab, getting my results on time." – Koen Sandra, Scientific Director, Research Institute for Chromatography, Kortrijk, Belgium; co-founder and R&D Director anaRIC biologics, Ghent, Belgium.

"For a chromatographer, efficiency certainly means the number of theoretical plates. In the lab, efficiency often has a lot to do with the effective flow of information." – Michael Lämmerhofer, Professor, Pharmaceutical Analysis and Bioanalysis, University of Tuebingen, Germany.

"I'm old fashioned so, for me, the plate count is the efficiency. But I know Leonid Blumberg will be upset with me, because it's not really a good measure – performance is not proportional to efficiency. In the lab environment, it depends on the goal; in industry, it's well defined. But in academia, the goal should be to raise students to a certain level, so you may have to accept some inefficiency (reduced number of published papers) as part of a more efficient learning process." – Peter Schoenmakers, Professor and Scientific Director, Van 't Hoff Institute for Molecular Sciences, The University of Amsterdam, the Netherlands.

And finally, at the end of the last day of a long week at HPLC 2017...

"Efficiency means the fastest route back to my hotel... or the next bar..." – anonymous.

What did we learn at HPLC 2017?

i. Efficiency is an important goal for everyone
ii. Efficiency is dependent on the desired outcome, but analytical scientists typically strive for increased throughput.
iii. By discussing efficiency, we can more deeply consider where real gains can be made.

"Nothing was near the door, so everyone had to walk further. That's the first thing I would change in that lab! It's good to see how people actually operate within the infrastructure. Next, I assess how operators are working with the instrumentation. Are the systems easy to set up and use? Is the software intuitive? Finally, I drill down into the analytical methods," says Van Tilburg. "It's also important to look at workflows in their entirety, which enables you to find weak points or bottlenecks. And whatever the laboratory, it's about making the best use of what you have – and should always include the people."

How do you take part in Your Efficiency Challenge?

To fully take part, you should complete the survey. It will only take 15 minutes of your time, but could see your questions being discussed by our team of efficiency consultants – all with proven track records in making gains in efficiency at the analytical, instrumental and laboratory level. At the very least, completing the survey will focus your mind on efficiency – and may spark the motivation needed to make improvements in your own lab.

Are you prepared to take Your Efficiency Challenge? Take part now: tas.txp.to/1017/challenge

HUMANITY IN SCIENCE AWARD

the Analytical Scientist

In partnership with

KNAUER

Richard Jänke

Meet the Winner

Richard Jänke

Richard Jänke from the Global Pharma Health Fund (GPHF) has received the 2017 Humanity in Science Award for "development and continuous improvement of GPHF Minilab™ (www.gphf.org), which represents a breakthrough for the rapid and inexpensive identification of substandard and falsified medicines in low- and middle income countries in Africa, Asia and Latin America".

Richard received his award at a special jubilee reception in Berlin, Germany on October 2, 2017 hosted by KNAUER to celebrate the company's 55th birthday this year. Richard's work will feature in an upcoming issue of The Analytical Scientist.

Could it be you in 2018?

Analytical science has been at the heart of many scientific breakthroughs that have helped to improve people's lives worldwide. And yet analytical scientists rarely receive fanfare for their humble but life-changing work. The Humanity in Science Award was launched to recognize and reward analytical scientists who are changing lives for the better.

Has your own work had a positive impact on people's health and wellbeing? Details of the 2018 Humanity in Science Award will be announced soon.

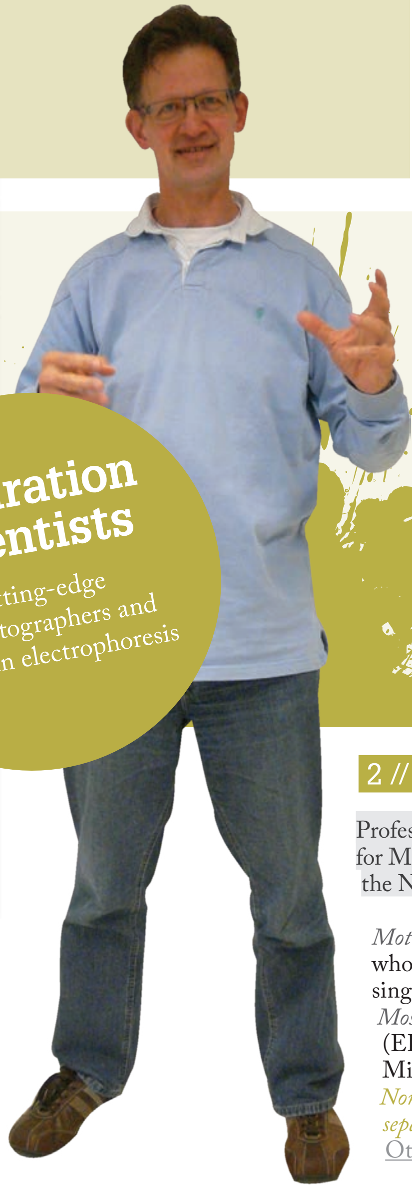
@Humanityaward Humanity in Science Award

www.humanityinscienceaward.com

FROM THE PEOPLE WHO BROUGHT YOU
THE POWER LIST 'TOP 100' AND '40 UNDER 40'

THE MAGNIFICENT TENS

After 2016's celebration of women in analytical science, we return to the Top 100 for 2017. But there's a twist. This summer, we asked you to nominate scientists in ten categories – from the stars of separation science, to omics explorers, to the mentors training the next generation. Here, we present the 10 Top 10s of analytical science.



Separation Scientists

Cutting-edge chromatographers and experts in electrophoresis

1 // Gert Desmet

Full Professor and Department Head, Vrije Universiteit Brussel, Belgium.

Career highlight
Scientifically, my work on shear-driven chromatography and the development of the kinetic plot method. Professionally, my appointment as Associate Editor to Analytical Chemistry and receiving an ERC Advanced Grant.
Other categories: Mentors, Leaders

2 // Peter Schoenmakers

Professor and Scientific Director, Van 't Hoff Institute for Molecular Sciences, The University of Amsterdam, the Netherlands.

Motivation Working with excellent young people, who keep asking challenging questions every single day.
Most exciting current project Definitely the STAMP (ERC) project – Separation Technology for A Million Peaks.
Nominator comment: "Continually forging the future of separation science."
Other categories: Leaders

3 // Robert (Bob) Kennedy

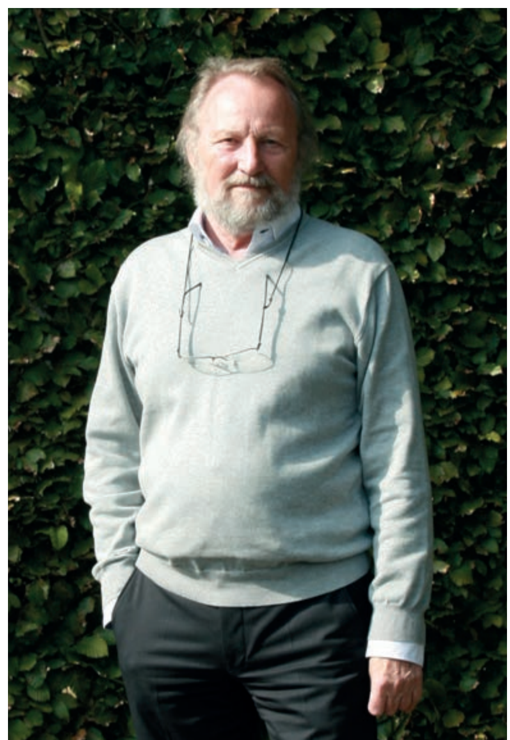
Hobart H Willard Distinguished University Professor of Chemistry; Professor of Chemistry, Chair-Chemistry, College of LS&A; Professor of Pharmacology, Medical School, University of Michigan, Ann Arbor, USA.

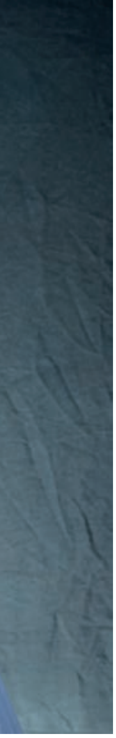
Why analytical science?
I liked the idea that an analytical chemist can contribute to many different areas, such as biology, environmental studies and forensics. That versatility and practicality, grounded in physically oriented chemistry, was very appealing.
Other categories: Mentors, Leaders

4 // Pat Sandra

Emeritus Professor, Organic Chemistry, Ghent University; Founder and President, Research Institute for Chromatography, Kortrijk, Belgium.

Most successful collaboration
As I was both an academic and an entrepreneur, my answer is twofold. Scientifically, my collaboration with the pharmaceutical industry was the most rewarding. Technologies and methods could be developed that had a direct impact on pharmaceutical R&D as well as on QC. On the other hand, collaboration with instrument manufacturers was very successful – some of our ideas were implemented in state-of-the-art analytical instrumentation, such as stir bar sorptive extraction (Twister).
Other categories: Leaders





5 // Jim Jorgenson

W. R. Kenan, Jr. Professor of Chemistry, University of North Carolina at Chapel Hill, USA

Career highlight
Imagining the possibilities of doing separations by capillary electrophoresis with potentials of 30,000 volts – and then seeing that idea turn into a reality – was every bit as exciting as I imagined.
The joy of separation science
I love the challenge of developing new approaches for the separation and analysis of complex mixtures. The work is not only intellectually stimulating but also highly practical and important.

6 // Luigi Mondello

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

Most exciting current project One of our most recent advances is the construction of a nano-LC system coupled to EI-MS detection, extending the advantages of GC-MS to LC-amenable compounds. It combines the benefits of miniaturized analytical instruments with the unique features of EI-MS spectra for molecular fingerprinting.
Hero of separation science Since the beginning of my scientific career, I have always looked up to Pat Sandra's stellar achievements in the field of separation science, and regarded him as an idol.
Nominator comment: "A pioneer in the field of multidimensional chromatography."

7 // Daniel W. Armstrong

Robert A. Welch Distinguished Professor, Department of Chemistry and Biochemistry, University of Texas at Arlington, USA.

Why analytical science?
I was always interested in science. However, I quickly found that to effectively investigate any interesting problem, one had to have the right tools and techniques – and often these didn't exist or were inadequate. It became apparent to me that the invention, development and understanding of such innovative approaches was often more elegant than the problems they were used to solve.
Nominator comment: "Continued ground-breaking contributions to all aspects of separation science; especially in the area of chiral separations."
Other categories: Mentors

8 // Janusz Pawliszyn

Professor, Department of Chemistry, University of Waterloo, Ontario, Canada.

The limits of separation science
We have definitely not reached the limits in the area of sample preparation. We are still in the midst of development and acceptance of microextraction technologies. There are great opportunities to contribute to fundamental understanding of separation processes involved in sample preparation, as well as to develop new approaches leading to improvements in this critical step.

9 // Milton L. Lee

H. Tracy Hall Professor Emeritus, Department of Chemistry and Biochemistry, Brigham Young University, Provo, Utah, USA.

Advice to my younger self
Put more effort into developing collaborations. I have done a pretty good job of this during my career; however, I could have started earlier and been more effective. Involving others in research increases creativity and productivity because of the different skills and insights that are brought together.
Nominator comment: "Milton Lee has been contributing for more than 40 years to the fields of GC, LC and SFC, and has earned a strong reputation among separation scientists."

10 // Dwight Stoll

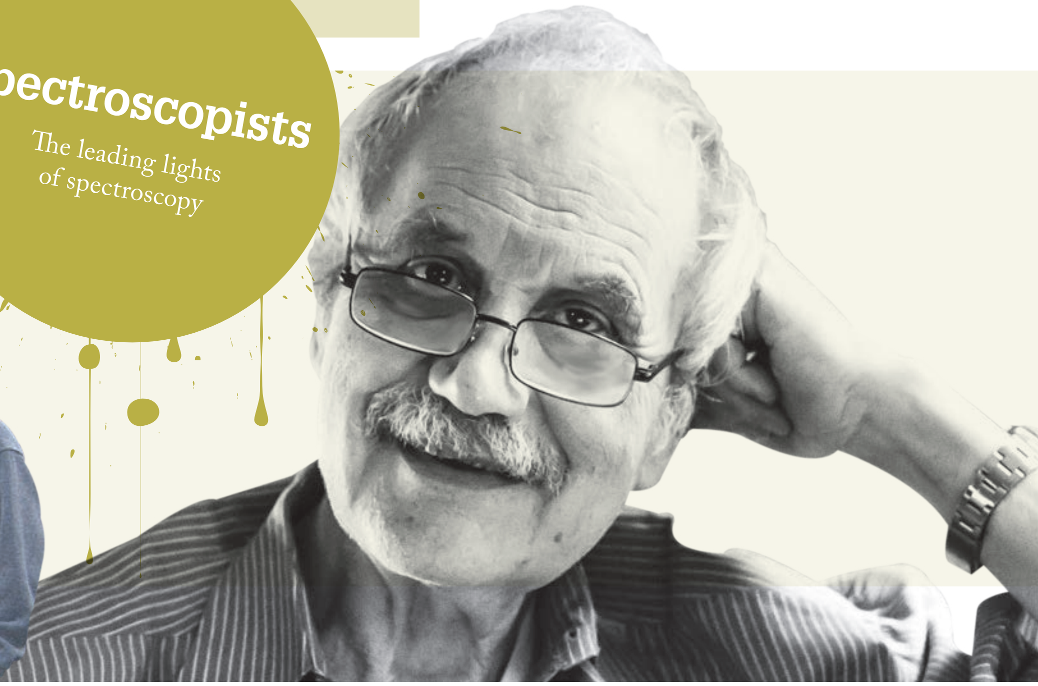
Associate Professor and Co-Chair in Chemistry, Gustavus Adolphus College, Department of Chemistry, St. Peter, Minnesota, USA.

Most exciting current project
Earlier this year we kicked off a big new project in my lab, focused on the development of 2D-LC for biopharmaceutical and related applications. There is so much technology innovation happening around tools for biomolecule analysis – from column technology to mass spectrometry. We will leverage these technologies in 2D-LC methods that will deliver unprecedented performance for the analysis of complex materials, ranging from monoclonal antibodies to oligonucleotides

and lipid mixtures. While my laboratory at Gustavus is the home of the project, we are forming deep collaborations with investigators in both industry and academia.
Nominator comment: "He is a scholar, a deep thinker, a superb motivator of undergraduate students, and a creative, focused separation scientist. As a leader in the emerging field of multidimensional LC separations, Dwight's influence will be felt for decades."

Spectroscopists

The leading lights of spectroscopy



1 // Gary M. Hieftje

Distinguished Professor and Robert & Marjorie Mann Chair in Chemistry, Indiana University Bloomington, USA.

Advice to my younger self
Don't follow trends but carve your own path. Work hard, be enthusiastic, have fun – and sleep less.

Why is spectroscopy so exciting?
Spectroscopy, defined in its broadest terms, is one of the most flexible, informative, and powerful methods of scientific observation and characterization.

Nominator comment: "Gary is not only one of the leading figures in the field but also an amazing mentor."

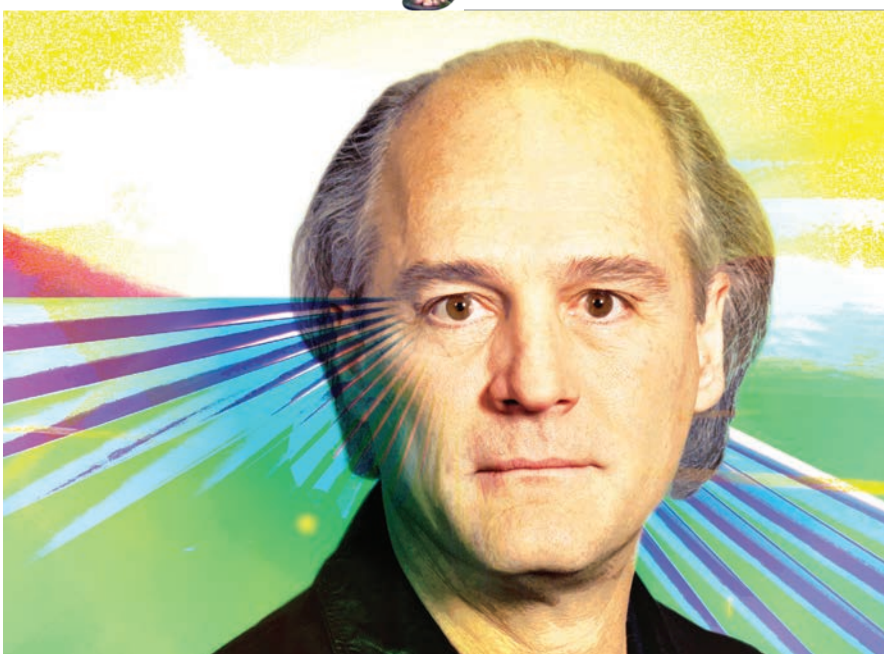
2 // Nico Omenetto

Research Professor, Department of Chemistry, University of Florida, USA.

Biggest surprise
In 1994, a phone call inviting me to take the co-editorship of Spectrochimica Acta Part B.

My hero of spectroscopy
Kees Alkemade, a physicist involved in fundamental work on flame spectroscopy, with a genuine interest in analytical aspects. I learned from him to always "look around the corner" for unexpected discoveries.

Nominator comment: "A lifetime of contributions to analytical spectroscopy, especially in the applications of lasers and as Editor of Spectrochimica Acta."



3 // Richard (Rick) Russo

Senior Scientist, Lawrence Berkeley National Laboratory, California, USA.

Most important lesson
When you want to move ahead "outside the box", the system is likely to say no. Better to ask for forgiveness than approval!

The next big breakthrough in spectroscopy
I see growing interest in biomedical imaging and the use of hyphenated technologies like LA-ICP-MS/LIBS/LAMIS for measuring every element/isotope in a sample, with spatial resolution.

4 // Alfredo Sanz-Medel

Emeritus Professor of Analytical Chemistry, University of Oviedo, Spain.

Most successful collaboration
My collaboration with medical doctor Jorge B. Cannata on aluminum toxicity in renal failure patients, which elucidated the mechanisms behind dialytic dementia disease and how it can be reversed. Today, the problem is virtually nonexistent in Spanish hospitals. It was a rewarding experience and marked the beginning of my tendency to collaborate closely with medical doctors (to study ocular diseases, cancer, and more).

Why is spectroscopy so exciting?
Even after so many years, my interest in spectroscopy remains enormous because it provides such varied, profound and powerful analytical tools to study isotopes, elements, small molecules, big molecules, biomolecules and, more recently, nanoparticles, nanostructures and nanobiomolecules.

5 // Peter Griffiths

Emeritus Professor of Chemistry, University of Idaho, USA.

Most important lesson
Friendship and collaboration with other scientists in my field is far more important than cut-throat competition.

My heroes of spectroscopy
Foil Miller, Professor Emeritus of the University of Pittsburgh, who passed away this year at the age of 100, was a good experimental spectroscopist and an amazing teacher of spectroscopy. Bruce Chase (University of Delaware) has a more in-depth understanding of the theory and practice of vibrational spectroscopy than anyone else I know. The other attribute that I admire in Bruce is that he always seems to have fun in what he does, whether in or out of the lab.

6 // Bernhard Welz

Professor, Universidade Federal de Santa Catarina, Brazil.

Research
Atomic absorption spectrometry, inductively coupled plasma mass spectrometry, and their application to environmental and oil and coal analysis.
Nominator comment: "Nominated for his lifetime contributions to analytical sciences in Germany and later in Brazil."

7 // Ramon Barnes

Professor Emeritus of Chemistry, University of Massachusetts, USA.

Biggest surprise
Feeling the excitement of making a research discovery surprised me.

What makes spectroscopy so exciting?
Spectroscopy is among the fundamental frontiers of science, and its applications in plasma spectrochemistry achieve ever-new solutions to problems in fields from earth sciences (geochemistry, high-resolution isotopic analysis) to medicine (metal speciation, mass cytometry).

8 // Kay Niemax

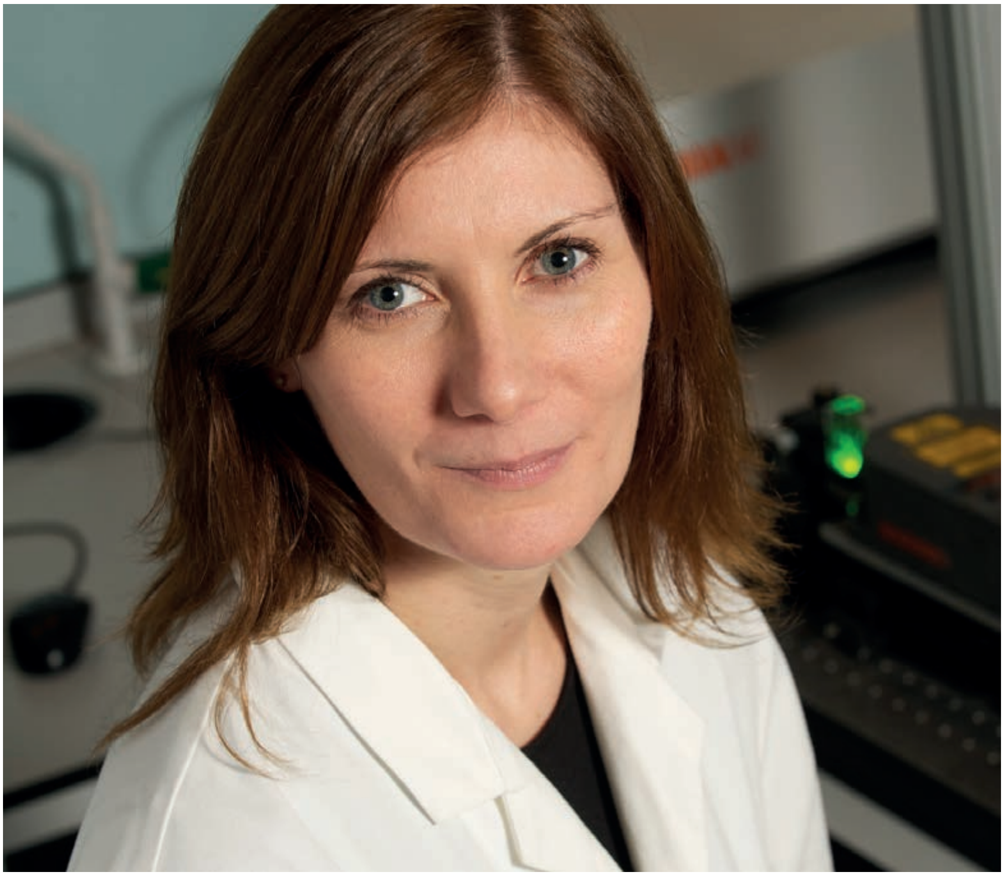
Emeritus Professor of Physics, Technical University of Dortmund, Wilhelm-Ostwald-Fellow of the Federal Institute for Materials Research and Testing, Berlin, Germany.

Most exciting current project
Studying ionization of highly excited Rydberg-atoms in thermal vapors, and – together with colleagues at Lawrence Berkeley National Laboratory – the interaction of metallic nanoparticles with molecules in the gas phase.
Luckiest break
My career change from fundamental atomic and molecular spectroscopy to analytical spectroscopy after 15 years in research.

9 // Ralph Sturgeon

Emeritus Researcher, National Research Council, Canada.

Proudest moment
An NRC Outstanding Achievement Award I received in 2009 was most appreciated, as it came as a result of the support of the Chemical Metrology Group that I had been leading for the past decade.
The next breakthrough in spectroscopy
I'd like to believe that, whatever it is, it will stem from development of analytical instrumentation that directly contributes to the betterment of our health. Mass spectrometry and biophotonics are ripe for development.



10 // Karen Faulds

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

Motivation
I have always been motivated by research that has real-world applications and implications – in particular, developing ways to improve the diagnosis and treatment of disease using optical spectroscopy.

Advice to my younger self
Never give up and always have confidence in yourself.

My hero of spectroscopy
C. V. Raman, of course! My research focuses on the use of Raman and surface-enhanced Raman and C.V. Raman won the Nobel prize in physics in 1930 for the observation of light scattering, which became known as the Raman effect.

Mass Spectrometrists

Masters of mass spec

1 // R. Graham Cooks

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

Career highlight
Working with PhD students and postdocs. On the technical side... Many things, starting with MS/MS for complex mixtures and going through MRMs, matrix-assisted ionization, miniature mass spectrometers and now accelerated solution-phase reactions in droplets. All great fun.
Nominator comment: "Cooks' research has transformed the field of mass spectrometry. His recent work on ambient ionization opens up unique opportunities to bring mass spectrometers into every doctor's office."
Other categories: Inventors

2 // Alexander Makarov

Director, Global Research Life Science Mass Spectrometry, Thermo Fisher Scientific, Germany.

Most successful collaboration
A decade-long collaboration with Matthias Mann in the field of bottom-up proteomics, plus – since 2012 – a collaboration with Albert Heck (Utrecht University) that has resulted in great extension of the mass range of Orbitrap mass spectrometry and its application to structural biology.
Other categories: Inventors

3 // Alan G. Marshall

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

Most successful collaboration
With Melvin Comisarow when we were both at University of British Columbia, culminating in the invention and early development of Fourier-transform ion cyclotron resonance mass spectrometry.
The joy of mass spectrometry
It's universal – every molecule has mass, and every different chemical formula has a different mass. Thus, we can resolve and identify more chemically different species than any other technique.

4 // Carol Robinson

Royal Society Research Professor, Chemistry, University of Oxford, UK.

Research
Gaining new insight into protein structure, function and interactions by means of mass spectrometry.
Nominator comment: "A real role model."

5 // Richard Smith

Battelle Fellow and Chief Scientist, Biological Sciences Division, Pacific Northwest National Laboratory (PNNL), Washington, USA.

Motivation
The desire to contribute to society by developing separation and mass spectrometry technologies that are applicable to routine applications, particularly in areas of biological and biomedical importance. I love the range of challenges, from understanding how and why things work, to team development efforts that may span years to make the new technologies useful and robust.
Other categories: Inventors

6 // Ron Heeren

Director of Maastricht MultiModal Molecular Imaging Institute (M4I), Distinguished Professor and Limburg Chair at Maastricht University, the Netherlands.

Career highlight
Building M4I and establishing translational clinical molecular imaging. On a more scientific level, the development of Timepix-based detection systems (originating from CERN) for protein imaging mass spectrometry was an amazing highlight.
Where is mass spectrometry headed?
To the clinic, where molecular identities, molecular localization and dynamics can be monitored at different diagnostics levels both in vivo and ex vivo.

7 // Zoltan Takats

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

Biggest game changer
I think it was the development of MALDI 2 by Klaus Dreisewerd's group. This technology has the true potential to change the entire MS imaging and high-throughput MS fields.
Nominator comment: "The invention of DESI and the iKnife puts him right at the cutting edge."
Other categories: Inventors

8 // Ruedi Aebersold

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

Proudest moment
A surprise symposium held on my 60th birthday. Many former students and postdocs, collaborators and mentors came to discuss their work and enjoy time together. It was exciting to see that some of the concepts, techniques, ideas and working styles our lab developed over the years are being continued in unexpected directions, and form the basis of so many successful careers.
Other categories: Omics Explorers, Leaders

9 // John Yates III

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

Most exciting current project
We are working on a cystic fibrosis project that is leading to some very interesting insights into why the mutant protein doesn't work.
Other categories: Omics Explorers, Leaders

10 // Catherine E. Costello

William Fairfield Warren Distinguished Professor, Boston University, Massachusetts, USA.

Research
Development and application of MS-based methods to study glycobiology, protein post-translational modifications and folding disorders, cardiovascular and infectious diseases, and bioactive lipids.

Giants of Nano

Microfluidics and nanoscale science

1 // Chad Mirkin

Director, International Institute for Nanotechnology; George B. Rathmann Professor, Chemistry; Professor, Chemical and Biological Engineering, Biomedical Engineering, Materials Science & Engineering, and Medicine. Northwestern University, Illinois, USA.

Career highlight
The discovery of spherical nucleic acids, which are being used extensively in materials science, biology, and medicine. The discovery also culminated in my receipt of the Dan David Prize from Israel last year, which highlighted the enormous effort made by so many outstanding researchers who have trained in my laboratories over the past two decades.
Nominator comment: "Most cited chemist in the world in the past decade and the inventor of dip-pen nanolithography, recognized by National Geographic as one of the top 100 scientific discoveries that changed the world."

2 // J. Michael Ramsey

Goldby Distinguished Professor of Chemistry, University of North Carolina at Chapel Hill, USA; Scientific Founder, Caliper Life Sciences; Scientific Founder, 908 Devices Inc.; Scientific Founder, Genturi Inc.

Why analytical science?
I was fortunate to have a good high school chemistry teacher and I have always been fascinated by machines and instruments. My curiosity has led to a life contemplating novel ways to measure and characterize chemical species.
The next 10 years
I hope to see an expanding interest in the development of micro- and nano-fabricated technologies for elucidating chemistry and biochemistry. I also hope that I cannot currently imagine the technologies that emerge over this period!
Other categories: Inventors

3 // Andreas Manz

Professor, Microfluidics for the Life Sciences, Systems Engineering Department, Saarland University; Senior Scientist, KIST Europe, Saarbrücken, Germany.

Motivation
Crazy new ideas, new combinations of things.
The next 10 years
I would be happy if microfluidics could become as common as screws and nuts in a workshop.

4 // Shuming Nie

Grainger Distinguished Chair in Engineering, Professor of Bioengineering, Chemistry, Electrical and Computer Engineering, Member of the Beckman Institute, the Micro/Nanotechnology Lab, and the Institute for Genomic Biology, University of Illinois at Urbana-Champaign, USA.

Advice to my younger self
If I were to start all over again, I would focus on the development of cutting-edge analytical technologies, and the application of these technologies to address major chemical and biomedical problems.
Proudest moment
Twenty years ago, when my student Steve Emory and I discovered "hot" nanoparticles that were able to amplify the efficiency of surface-enhanced Raman scattering (SERS) by 14–15 orders of magnitude.

5 // Mary Wirth

W. Brooks Fortune Distinguished Professor, Analytical Chemistry, Purdue University, USA.

Research
Using nanotechnology to modernize the materials used for lab tests and for the discovery of the biomarkers that are the targets of lab tests.

6 // George Whitesides

Woodford L. and Ann A. Flowers University Professor, Department of Chemistry and Chemical Biology, Harvard University, Massachusetts, USA.

Research
NMR spectroscopy, organometallic chemistry, molecular self-assembly, soft lithography, microfabrication, microfluidics, and nanotechnology.
Other categories: Leaders

7 // Paul Alivisatos

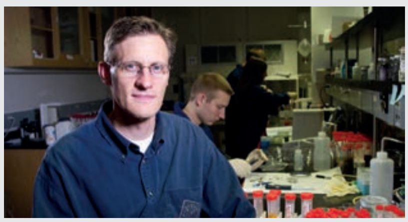
Samsung Distinguished Professor of Nanoscience and Nanotechnology; Professor of Chemistry and Materials Science & Engineering, University of California, Berkeley, USA.

Research
Understanding and exploiting the properties of nanomaterials for technological applications.

8 // Adam T. Woolley

Professor, Brigham Young University, Utah, USA.

Luckiest break
My first US government grant (Department of Defense). The program officer initially told me he wouldn't be able to fund it, and suggested I withdraw the proposal. About a week later he called and told me he had received my withdrawal letter, but that he had a new plan to try to get it funded: he asked me to submit a revised budget (about 10 percent higher!) and got it funded.
Nominator comment: "Outstanding scientist and nice fellow."



9 // Christy Haynes

Elmore H. Northey Professor of Chemistry, University of Minnesota, USA.

Advice to my younger self
Many scientists, especially during their early years of training, fear that they aren't smart or creative enough to be successful. Don't spend any of your energy worrying about this.
The next 10 years
I hope that nanotechnology will be in use for a variety of proactive applications in sustainability, enhancing our use of clean energy, making it possible to have cleaner water and air worldwide, and helping overcome shortages in our global food supply.

10 // Andrew deMello

Professor of Biochemical Engineering, Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences ETH Zürich, Switzerland.

Most successful collaboration
New technologies are only as good as the problems that they solve, and our collaborations with end users (whether chemists, biologists or medics) have almost always proved the most fulfilling and successful. For example, our recent collaborations with Maksym Kovalenko's group at ETH Zurich have allowed us to create a new suite of microfluidic tools to design and build bespoke functional materials – something we could never have imagined or achieved alone.
Nominator comment: "deMello is a world leader in microfluidic technology, who has made many seminal contributions to the field, including important advances in synthetic processing, droplet-based microfluidics, ultra-high sensitivity detection in small volumes and systems for point-of-care diagnostics."

Pharma Pioneers

Stars of small molecule and biopharmaceutical analysis

1 // Ian Wilson

Professor, Chair in Drug Metabolism and Molecular Toxicology, Department of Surgery & Cancer, Faculty of Medicine, Imperial College London, UK.

Motivation

A major driver is the sheer pleasure in finding things out – why bother with Sudoku when biology provides real puzzles to solve? Another is the hope that something I find out will make a difference.

Advice to my younger self

Stop messing about and get on with it – the time goes quicker than you could ever imagine.

2 // Koen Sandra

Scientific Director, Research Institute for Chromatography, Kortrijk, Belgium; co-founder and R&D Director anaRIC biologics, Ghent, Belgium.

Key trends in pharmaceutical analysis

We have noticed a clear trend in addressing analytical needs more and more towards biological products. As a result, our focus has shifted from small chemical entities to antibody formats, such as monoclonal antibodies, bi-specifics, antibody–drug conjugates and fusion proteins. Furthermore, immune, cell and gene therapies are the way of the future. All of these add to the complexity of the analytical work, meaning that techniques like 2D-LC will become more widely applied, and LC-MS will find an entry in routine environments.

Nominator comment: "One of the leading scientists today in the field of biopharmaceutical characterization."

3 // Neil Spooner

Spooner Bioanalytical Solutions Ltd and School of Life and Medical Sciences, University of Hertfordshire, Hertfordshire, UK.

Proudest career moment

Definitely setting-up my own business. Would people be willing to pay me to do what I love? Thankfully it has exceeded my wildest dreams!

The future of bioanalysis

More automation. More outsourcing. Increased consolidation of CROs. Increasing and exciting analytical challenges through novel molecular constructs and, of course, microsampling/patient centric sampling.

4 // Davy Guillarme

Senior Lecturer in the School of Pharmaceutical Sciences, University of Geneva/University of Lausanne, Geneva, Switzerland.

Luckiest break

I started my career with the development of analytical methods for small molecules. In 2012, we decided to evaluate the possibilities of chromatographic approaches (including LC, 2D-LC and LC-MS) for the analysis of protein biopharmaceuticals. Looking at the pharmaceutical market in 2017, I think we took a good decision at the right time.

5 // Deirdre Cabooter

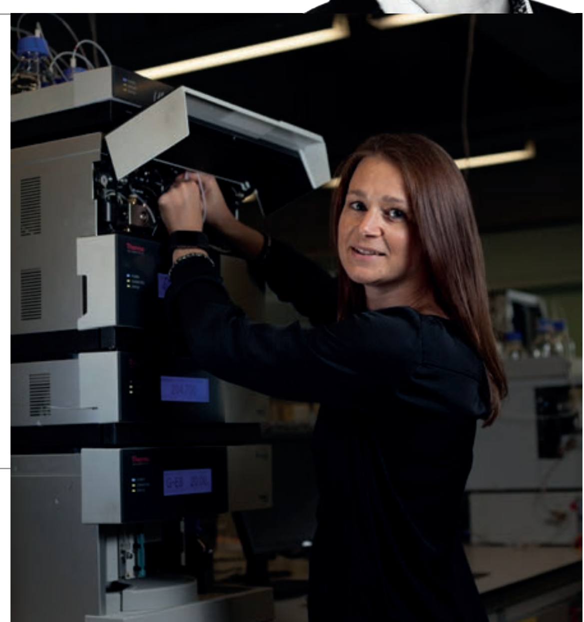
Associate Professor, Department of Pharmaceutical and Pharmacological Sciences, University of Leuven, Leuven, Belgium.

Most exciting current project

I'm very excited about a new project we are about to embark on to automate method optimization for multidimensional analysis.

Advice to my younger self

Work hard and be persistent, but don't forget to relax from time to time!



6 // Jean-Luc Veuthey

Professor, School of Pharmaceutical Sciences, University of Geneva, Switzerland.

Research
Development of analytical techniques for the analysis of pharmaceutical drugs and drugs of abuse in different biological matrices.

7 // William Hancock

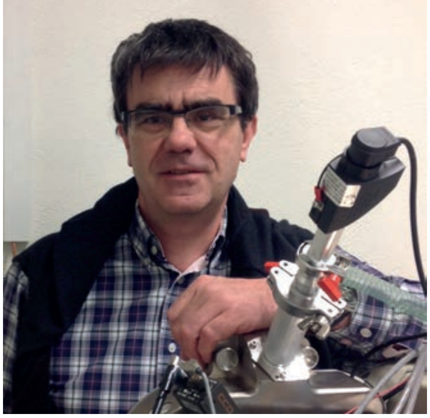
Founding Editor-in-Chief, Journal of Proteome Research (retired); Bradstreet Chair in Bioanalytical Chemistry, Northeastern University, Massachusetts, USA.

Career highlight
The development of HPLC methods for peptide mapping, as well as the analysis of rDNA-produced therapeutic proteins.
What's next?
My current interests are focused on the development of biosimilar drugs (FDA Advisory Committee) and the challenges of the supply of protein therapeutics to lower and middle income countries for the treatment of non-communicable diseases – for example, insulin for diabetes.

8 // Melissa Hanna-Brown

Technology & Innovation EU Lead, Pfizer Global R&D, Sandwich, UK and Department of Chemistry, University of Warwick, UK and President Analytical Division, Royal Society Chemistry, UK.

Why pharmaceuticals?
My role focuses on finding innovative analytical technologies and strategies that can accelerate "molecule to medicine" development. I'm inspired on a daily basis, because of the impact I know it can have on patients' lives.



9 // Gérard Hopfgartner

Professor in Analytical Sciences and Mass Spectrometry, Department of Analytical and Inorganic Chemistry, University of Geneva, Switzerland.

Proudest career moment
My team's paradigm shift in the early 1990s in bioanalysis – moving from liquid chromatography with classical detectors such as UV or fluorescence, to liquid chromatography with tandem mass spectrometry detection to support drug discovery and development.

10 // H. Thomas Karnes

Professor Emeritus, Editor of Journal of Chromatography B, School of Pharmacy, Virginia Commonwealth University, USA.

Research
Regulatory biorelevant drug release and the use of luminescence, chromatography, mass spectroscopy, immunoreactors and microfluidics for drug analysis.
Nominator comment: "Recently retired, Karnes is an expert in the field of bioanalytical chemistry. He was a great teacher on the use of bioanalytical techniques, method development and validation."

Omics Explorers

Uncovering the secrets of life through genomics, proteomics, lipidomics, metabolomics, and more

1 // John Yates III

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

Challenges ahead for omics
Integration of the data. It's complex so we need better approaches to combine the data for better insights.
Other categories: Mass Spectrometrists, Leaders

2 // Gary Siuzdak

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

Most exciting current project
Metabolomics activity screening (MAS); this project is taking metabolomics beyond biomarker discovery and towards identifying biologically active endogenous metabolites that can be used to intentionally modulate phenotype.
Why metabolomics?
Metabolites are the most downstream components in the biochemical cascade and therefore are closest to the phenotype. Thus, metabolomics can be used to identify metabolites for phenotype modulation; I believe this is where the real power of metabolomics lies.

3 // Ruedi Aebersold

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

Why omics?
In the 1990s, I worked at the Department of Molecular Biotechnology at the University of Washington in Seattle, which was one of the leading genomics departments at the time. In that environment and working on protein analytics, it was an obvious question to ask – could we come up with techniques that would, at some point, allow us to study the proteome in a comprehensive manner? We have been pursuing this goal ever since.
Other categories: Mass Spectrometrists, Leaders

4 // Jennifer Van Eyk

Director, Advanced Clinical Biosystems Research Institute, Director of Basic Science, The Barbra Streisand Women's Heart Center, Co-Director, Cedars Sinai Precision Health, The Erika Glazer Endowed Chair in Women's Heart Health, The Heart Institute, Department of Medicine, Cedars-Sinai Medical Center, California, USA.

Biggest surprise
How truly gifted and remarkable people are.
Challenges ahead for omics
Bringing discovery to patient care, which requires us to have a shared vision – to reduce barriers, engage new approaches and find new paradigms at every step along the way.
Nominator comment: "A visionary leader in the field of clinical proteomics. She deserves recognition for the creative and transformational approach she is forging for the application of multiple omic sciences to address clinically meaningful problems."

5 // Joshua D. Rabinowitz

Professor, Chemistry and Integrative Genomics, Princeton University, New Jersey, USA.

Research
The Rabinowitz lab aims to achieve a quantitative, comprehensive understanding of cellular metabolism. Ongoing research includes technology development, metabolic regulation in microbes, biofuel production, metabolic impact of infection and cancer cell metabolism.

6 // Norman Dovichi

Grace-Rupley Professor of Chemistry and Biochemistry, University of Notre Dame, Indiana, USA.

Luckiest break

The first was when I took a postdoctoral fellowship in the physical chemistry group at Los Alamos Scientific Laboratory with Dick Keller, to work on gas-phase spectroscopy. Keller's lab was in a building that required security clearance, and my clearance was delayed by four months. In the meantime, I managed to make a second home for myself with the biophysics group – among the world's leaders in flow cytometry. This experience with flow cytometry proved seminal for the development of our capillary array electrophoresis DNA sequencer.

7 // David Wishart

Professor, Departments of Biological Sciences and Computing Science, University of Alberta, Canada.

Most important lesson

A few hours in the library or a few minutes on the Internet can save you (and your students) weeks of futile work in the lab.

Challenges ahead for omics

Most people would say it's the data challenge, but I think omics researchers have to show that omics research can lead to real benefits in everyday life.

Nominator comment: "Pioneer of metabolomics in Canada, who established HMDB and related databases to advance metabolomics worldwide."

8 // Oliver Fiehn

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

Motivation

I am motivated by novel discoveries – when a breakthrough technology opens new doors to avenues that people thought were impossible to travel! Metabolomics is one such "impossible" road, and I am glad many people are now exploring it. Read more at tas.txp.to/1017/Fiehn.

Other categories: Mentors

9 // Jeremy Nicholson

Professor of Biological Chemistry, Director of the MRC-NIHR National Phenome Centre Head of the Department of Surgery and Cancer, Faculty of Medicine, Imperial College London.

Advice to my younger self

Concentrate your efforts on developing technologies that will meet future and emergent healthcare challenges. Help create new, analytically driven pathways to clinical decision making. Avoid intellectual narcissism at all costs – it's not about you!

Nominator comment: "Inventor of metabonomics, inspiration behind the UK National Phenome Centre."

10 // David Muddiman

Jacob and Betty Belin Distinguished Professor of Chemistry and Founder and Director, W.M. Keck Fourier Transform Mass Spectrometry Laboratory, North Carolina State University, USA.

What's next for omics?

The more we learn the more we realize we need to integrate omics data. From proteoform biology, to glycomics, lipidomics, metabolomics, and fluxomics – to really understand biology, it is absolutely imperative that we measure these networks of biological information to really understand the "complete" picture of the system under investigation.

Public Defenders

Scientists protecting people and planet

1 // Mario Thevis

Professor for Preventive Doping Research, Director – Institute of Biochemistry/Center for Preventive Doping Research, German Sport University Cologne, Germany.

Most exciting current project
Exploring alternative strategies for drug testing that reduce the burden of sample collection without compromising the quality of the analytical result.
Most rewarding moment
Providing the analytical data that helped answer important questions in complex and difficult cases. There have been a few cases where the unexpected was eventually proven and, while rare, they have always justified the effort of critical follow-up.

2 // Julie Schappler

Lecturer, Group of Analytical Sciences, School of Pharmaceutical Sciences, University of Geneva, Switzerland.

Proudest moment
Being runner-up of the Humanity in Science Award in 2015 for our low-cost CE device. The international analytical community was recognizing our work, and our project was entering a new and bigger stage.
Nominator comment: "Julie Schappler is involved in a humanitarian project aimed at fighting counterfeit medicines and sub-standard drugs in emerging countries with low-cost capillary electrophoresis."

3 // Michael Breadmore

Professor, Australian Centre for Research on Separation Science (ACROSS), School of Physical Science, University of Tasmania, Australia.

Proudest moment
Every time one of my students graduates.
Advice to my younger self
Dream big, aim high, publish quality.
Working for others
We have been working for over a decade on GreyScan – a new instrument to improve rapid screening for inorganic explosives at airports and other mass transit locations. When it eventually gets deployed it will improve the safety of world travel.

4 // Steven Lehotay

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

Career highlight
Development and transfer of analytical methods to meet real-world needs are the highlights of my career, and QuEChERS in partnership with Michelangelo Anastassiades and others has been most prominent.
Nominator comment: "A dedicated civil servant and analytical chemist. When many of his classmates were pursuing careers in industry or academia, Steve always wanted to work in government for the sake of making a difference in the public service sector."

5 // Elena Ibanez

Research Professor, Foodomics Laboratory, Bioactivity and Food Analysis Department, Institute of Food Science Research (CIAL, CSIC), Madrid, Spain.

Luckiest break
I always say that finding a place where you can really be yourself and put your ideas in practice is the luckiest break you can have. I found mine in the creation of the Foodomics group together with Alejandro Cifuentes. From that point I started believing the African proverb: "If you want to go fast, go alone. If you want to go far, go together."

6 // Kim Prather

Distinguished Chair in Atmospheric Chemistry, Director of the Center for Aerosol Impacts on Chemistry of the Environment, Department of Chemistry and Biochemistry and Scripps Institution of Oceanography, University of California, San Diego, USA.

Motivation
Making a difference for our planet. Our research on aerosol impacts on clouds can help explain why we are seeing a sudden increase in weather-related disasters.
Most rewarding moment
Discovering that dust from 12,000 miles away in Africa (and ocean microbes) affects snowfall over California.

7 // James P. Landers

Commonwealth Professor, Departments of Chemistry, Mechanical Engineering and Pathology, University of Virginia, USA.

Biggest surprise
That I have been fortunate enough to have the success that I have. Coming out of a small mining town in the far reaches of northern Ontario, Canada, the odds of my becoming a professor at one of the premier public universities in the US were not good.
Why forensics?
I always had an affinity for biochemistry, but engineering and making "mousetraps" also fascinated me. The research in my program has a unique melding of both of these, and that combination makes me want to come to work every day.
Nominator comment: "Landers is working at the cutting edge to advance and expedite forensic testing. For example, his lab saw a major unmet need for readily deployable forensic kits – and worked to contribute rapid multiplex DNA amplification using an inexpensive microdevice for human identification via short tandem repeat analysis. This creative invention and active translation is a hallmark of his research."

8 // Lourdes Ramos

Research Scientist, Department of Instrumental Analysis and Environmental Chemistry, Institute of Organic Chemistry, Scientific Research Council (CSIC), Madrid, Spain.

Career highlight
I prefer to focus on long-term achievements like contributing to the development of fast and green analytical methodologies, or improving our knowledge about the presence and fate of legacy and non-regulated pollutants in the environment, and the early identification of unknown microcontaminants.

9 // Christopher Mulligan

Associate Professor, Analytical Chemistry, Department of Chemistry, Illinois State University, USA.

Working for others
My research team is focused on providing those who are tasked with keeping us safe (like law enforcement and first responders) with tools to help them perform their duties more effectively. By leveraging portable MS technologies and ambient ionization methods, we seek to provide them with chemical information on-demand, in a platform that is simple, reliable, economical and court-admissible.
Nominator comment: "Of note is that Mulligan conducts his research with undergraduate and Masters level students, training these future forensic scientists through rare and unique research experiences."

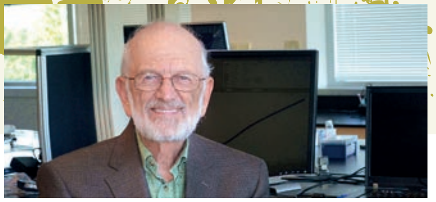
10 // Eric Reiner

Senior Mass Spectrometry Research Scientist, Ontario Ministry of the Environment and Climate Change, Canada.

Research
Analysis of dioxin-like and other persistent toxic organics, including halogenated flame retardants, perfluorinated compounds and industrial chemicals using advanced analytical techniques.
Nominator comment: "A leader in environmental forensics."

Inventors

Clever minds whose breakthroughs are shaping analytical science



1 // R. Graham Cooks

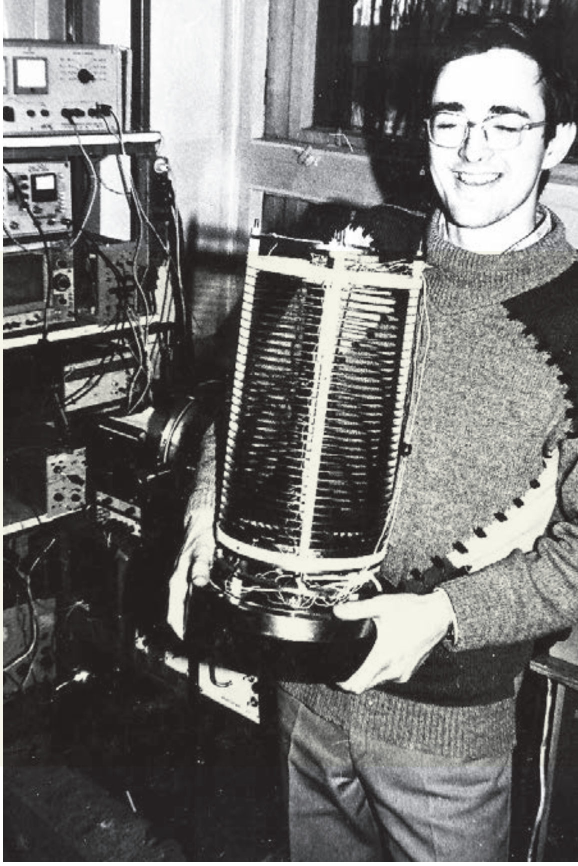
Henry B. Hass Distinguished Professor, Chemistry, Purdue University, Indiana, USA.

Game changers in mass spectrometry
For some of us it is ambient ionization, for others the Orbitrap mass analyzer. For others, ion soft landing and surface-induced dissociation.
What makes a successful inventor?
Unhappiness. Unhappiness with the status quo, including yourself. The same properties that make for successful poets.
Other categories: Mass spectrometrists

2 // J. Michael Ramsey

Goldby Distinguished Professor of Chemistry, University of North Carolina at Chapel Hill, USA; Scientific Founder, Caliper Life Sciences; Scientific Founder, 908 Devices Inc.; Scientific Founder, Genturi Inc.

Greatest invention
The early inventions covering electrokinetic control of material transport in microfluidic networks stand out, and were the basis for Caliper. But our inventions surrounding miniaturized ion traps, which led to the discovery of high-pressure mass spectrometry (908 Devices) were equally rewarding.
Other categories: Giants of Nano



3 // Alexander Makarov

Director, Global Research Life Science Mass Spectrometry, Thermo Fisher Scientific, Germany.

What's next?
We are working on making Orbitrap mass spectrometry faster, more sensitive and easier to own and apply.
Other categories: Mass Spectrometrists

4 // Zoltan Takats

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

Advice to my younger self
Stay in one place and focus on science instead of moving on every few years.
What makes a successful inventor?
Testing all seemingly crazy ideas.
Other categories: Mass Spectrometrists

5 // Richard Smith

Battelle Fellow and Chief Scientist, Biological Sciences Division, Pacific Northwest National Laboratory (PNNL), Washington, USA.

Greatest invention

The recent development of structures for lossless ion manipulations (SLIM), which provide a broadly flexible "ion chemistry workbench". I am particularly proud of the second-generation SLIM, which use traveling waves to move ions, and have allowed us to fabricate compact ultra-long path devices – achieving the elusive combination of ultra-high resolution and ultra-sensitive ion mobility separations in conjunction with mass spectrometry.

Other categories:
Mass Spectrometrists

6 // Chris Pohl

Vice President, Chromatography Chemistry, Thermo Fisher Scientific, USA.

What's next?
I'm working on a new anion exchange synthesis method that produces extraordinary selectivity for ions of different net charge. I am exploring the range of possibilities to see if we can make a material that will not retain ions unless they are monovalent.

Technology breakthroughs
The advance that I find most exciting is the recent development of pillar array technology. For the first time, it appears possible to develop chromatographic structures with independent control of both feature size and permeability, which opens the possibility of exceedingly long columns with acceptable backpressure.

Nominator comment: "Ion chromatography would not have developed as the versatile technique we know without Chris's contributions."

7 // Purnendu (Sandy) Dasgupta

Hamish Small Chair in Ion Analysis, Department of Chemistry and Biochemistry, University of Texas at Arlington, USA.

Motivation
Curiosity, with eventual utility as the propellant.

Proudest moment
Every time I hood the latest PhD recipient. Each one is a greater accomplishment than the last – they are cumulative!

Nominator comment: "Sandy Dasgupta is a visionary and has contributed significantly to wide-ranging areas, including arsenic detection, perchlorate detection, dried blood spot analysis, and ion chromatography."

8 // Bernd Bodenmiller

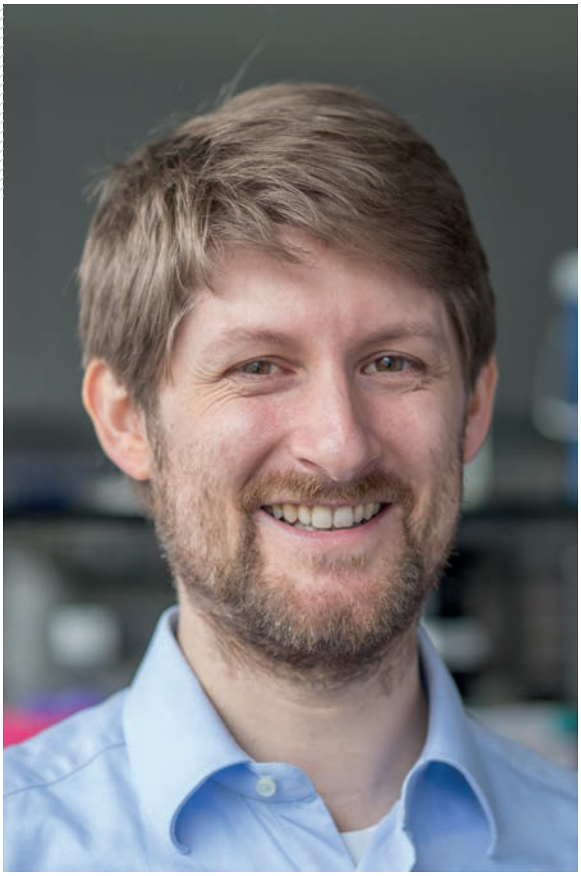
Assistant Professor for Quantitative Biology, Institute of Molecular Life Sciences, University of Zurich, Switzerland.

Most important lesson
That a highly motivated and synergistic team composed of brilliant people can move mountains.

Biggest surprise
To see that imaging mass cytometry worked almost immediately.

What's next?
We are developing novel experimental and computational approaches for imaging mass cytometry and applying it to study the tumor ecosystem.

Nominator comment: "Bernd Bodenmiller led the development of imaging mass cytometry, which is rapidly spreading and already used for the study of many diseases."



9 // Klaus Witt

Senior Technology Lead, R&D, Liquid Phase Separations Business, Agilent Technologies, Germany.

Motivation
Appling technology to make this world a better one. During my career I met three very influential persons: Dave Packard, Bill Hewlett and Steven Jobs. Each of them gave me valuable advice, which I still use in daily work.
Nominator comment: "Klaus Witt is the leading inventor of 70 granted patent families for Hewlett-Packard/Agilent. In my view, he is one of the most productive inventors in the HPLC instrument industry."

10 // Shane Tichy

R&D LC/MS Single and Triple Quadrupole Manager, Agilent Technologies, Santa Clara, California, USA.

Proudest moment
My proudest accomplishment is the Ultivo Triple Quadrupole LC/MS mass spectrometer. I still remember the day – February 8, 2016, a Monday – when we observed signal on our newly built breadboard prototype for the first time. The team and I were overjoyed.

Mentors

Supervisors, colleagues or teachers inspiring the next generation of scientists

1 // Susan Olesik

Dow Professor and Chair, Department of Chemistry and Biochemistry, The Ohio State University, USA.

Advice to my younger self
Trust yourself and reach for the sky.
Who are your own mentors?
Isiah Warner was an outstanding mentor to me.
Nominator comment: "Susan Olesik pioneered the field of enhanced-fluidity liquid chromatography – now commonly used by the pharmaceutical industry. Two recent awards highlight the breadth of her accomplishments in both high-impact research and extraordinary advocacy for public understanding of science – the Award for Chromatography and the ACS Helen M. Free Award for Public Outreach, conferred by the American Chemical Society."

2 // Harold McNair

Professor Emeritus, Analytical Chemistry, Virginia Tech, Virginia, USA.

What makes a good mentor?
One who realizes how much he or she was mentored by parents, teachers, fellow students and friends. All of us, particularly me, benefited from this mentoring, and my attitude is: please pass it on!
Nominator comment: "Harold has been a mentor for so many chromatographers through the years, whether for his students at Virginia Tech, or attendees at the more than 100 short courses he organized and delivered throughout the last 35 years. It is estimated that he has taught more than 10,000 chromatographers through these courses. More importantly, his charismatic nature, his style of open inquiry and inquisitive research, and his caring nature have made him a mentor to emulate. I try to run my own research group the same way that I learned from him."

3 // Robert (Bob) Kennedy

Hobart H Willard Distinguished University Professor of Chemistry; Professor of Chemistry, Chair-Chemistry, College of LS&A; Professor of Pharmacology, Medical School, University of Michigan, Ann Arbor, USA.

Proudest moments
Being named on the Power List; every time a student graduates with a nice dissertation and the start of a new career; and figuring out how to measure insulin secretion from single cells.
Nominator comment: "A number of The Analytical Scientist's Top 40 Under 40 Power List were either former students or departmental colleagues of Bob's, evidence of his significant impact."
Other categories: Separation Scientists, Leaders

4 // Peter Carr

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

Proudest achievement
Our studies of the basic thermodynamics and intermolecular interactions governing phase equilibria, which lie at the heart of separation science.
Best advice I ever received
To stay abreast of developments in a wide array of fields, not just what was going on in my own scientific backyard. This notion has led me to adopt and apply ideas from biochemists, physical organic chemists and chemical engineers to the goals of analytical chemistry.

5 // Daniel W. Armstrong

Robert A. Welch Distinguished Professor, Department of Chemistry and Biochemistry, University of Texas at Arlington, USA.

Proudest moment

It can be gratifying when you publish something that few seem to know or care about, and then a few years later it has major scientific impact; for example, chiral separations, ionic liquids in separations and MS, and D-amino acids in biological systems. However, I am proudest when my former students and postdocs do well in their careers.

Best advice I ever got

I received two pieces of "wisdom" from my PhD advisor. First, if you publish fast enough, you don't have to worry about competition. Second, there are a lot of very bright people in this "business," but only a few will actually matter.

Nominator comment: "Professor Armstrong is an exceptional supervisor and scientist, who constantly goes the extra mile for his students."

Other categories: Separation Scientists

6 // Isiah M. Warner

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

Motivation

I enjoy helping people achieve their goals and find their path in life.

Nominator comment: "The LSU graduate program in chemistry is the nation's largest producer of African-American PhDs in chemistry, largely due to the efforts of Isiah in encouraging and mentoring these students. His outstanding mentoring achievements have been recognized by his receipt of a Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring in 1998, the 2000 AAAS Mentor Award for Lifetime Achievement, and others."

7 // Gert Desmet

Full Professor and Department Head, Vrije Universiteit Brussel, Belgium.

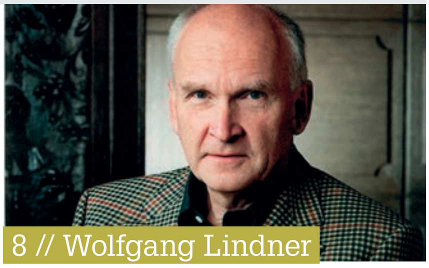
Advice to my younger self

My only recipe was working very hard in a collaborative spirit, and that more or less brought me automatically from my little corner in the lab to the Department Head's office.

What makes a good mentor?

A good mentor is a motivator and stimulator, but first and foremost someone who puts himself on the same level as his mentees and is always open to criticism from them.

Other categories: Separation Scientists, Leaders



8 // Wolfgang Lindner

Professor Emeritus, Analytical Chemistry, University of Vienna, Austria.

Advice to my younger self

Stay curious in all directions. Get a solid fundamental background in your field. Do not make easy compromises. Find a unique scientific niche. Make post-doc and sabbatical stays abroad, but not in exactly the same field, thus broadening your knowledge and views in many very valuable ways. Try to be an entrepreneur and believe in yourself; it makes you more independent and less open to attacks.

9 // Oliver Fiehn

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

What makes a good mentor?

I try to listen carefully to the wishes and dreams of my scholars and students, and find a way to help them. I also give them many opportunities, from finding research funds for them, to meeting interesting people.

Other categories: Omics Explorers

10 // Anthony Gachanja

Professor, Department of Chemistry, Jomo Kenyatta University of Agriculture and Technology (JKUAT), Kenya.

Motivation

The deep desire to see analytical science skills develop in Africa to a level equivalent to other parts of the world. This knowledge is critical for the development of the African continent in all sectors, including agriculture, medicine, environment, security and infrastructure.

What makes a good mentor?

They should understand the landscape of the subject well, be deeply inspired from within, and must feel and see the depth of the subject area.

Nominator comment: "Anthony is a leading light for African science – as well as being an excellent researcher, he is passionate about enabling analytical science in Africa and empowering the next generation of researchers."

Leaders

Analytical champions influencing the progress of measurement science

1 // Gert Desmet

Full Professor and Department Head, Vrije Universiteit Brussel, Belgium.

Where is analytical science heading?
Analytical science is the enabling technology to discover all the key processes in our body and brain. There is so much that humanity still doesn't know, and this will continue to drive progress to ever more comprehensive, fast and sensitive measurements for many more decades to come.
Other categories: Separation Scientists, Mentors

2 // John Yates III

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

Where is mass spectrometry headed?
Single cell analysis!
What makes a good leader?
Leading by example.
Other categories: Mass Spectrometrists, Omics Explorers

3// Peter Schoenmakers

Professor and Scientific Director, Van 't Hoff Institute for Molecular Sciences, The University of Amsterdam, the Netherlands.

Challenges ahead for analytical science
The education of a new generation of scientists who are capable of using and understanding the ever more complex techniques and instruments available (and the application domain they work in). Underqualified users are using instruments as black boxes, which creates great risks.
Nominator comment: "He is the face of analytical science in Europe and has spent much of his time training the next generation."
Other categories: Separation Scientists

4 // Robert (Bob) Kennedy

Hobart H Willard Distinguished University Professor of Chemistry; Professor of Chemistry, Chair-Chemistry, College of LS&A; Professor of Pharmacology, Medical School, University of Michigan, Ann Arbor, USA.

What makes a good leader?
Being a good listener, so that one understands what the real issues are. Being open to the ideas and wisdom of others. Having the energy to persist in getting things done.
Nominator comment: "Bob has influenced the progress of a wide range of analytical tools, including CE, LC, MS, in vivo measuring, and electrode sensors."
Other categories: Separation Scientists, Mentors

5 // Ruedi Aebersold

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

Where is proteomics heading?
I believe that the most transformative contributions of proteome analytical techniques to biology and medicine will come from three areas. First, the fast, robust, low-cost quantification of hundreds of proteomes at a high degree of reproducibility to support comparative studies, such as clinical cohorts, perturbation matrices of cells or population-based studies. Second, the determination of the organization and structure of proteins in cells and tissues in the form of complexes and functional modules. Third, the biologically meaningful integration of proteomics data with other types of omics data.
Other categories: Mass Spectrometrists, Omics Explorers

6 // Jonathan Sweedler

Editor-in-Chief, Analytical Chemistry; James R. Eiszner Family Endowed Chair in Chemistry and Director of the School of Chemical Sciences, University of Illinois at Urbana-Champaign, USA.

Proudest moment
Being selected as the Editor of Analytical Chemistry. The opportunity came as a surprise and was not in my career plans at the time. So far, being Editor has been a lot of fun!

Advice to my younger self
Though research ideas and results are important, success also depends on developing strong writing skills; these are not innate and improve with training and practice. Thus, at every opportunity, work to improve both your scientific and proposal writing proficiency. Your success can depend on these abilities.

7 // Richard Zare

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

Most successful collaboration
The multitude of collaborations with my coworkers, without whose efforts so little would have been actually accomplished.

Luckiest break
Marrying my wife and having three wonderful daughters who have supported me, as I have sometimes neglected them to devote myself to my career.

What makes a good leader?
A person who can listen to others, show empathy with different points of view, and is not afraid to make a firm decision when needed.

8 // Pat Sandra

Emeritus Professor, Organic Chemistry, Ghent University; Founder and President, Research Institute for Chromatography, Kortrijk, Belgium.

Advice to my younger self
Never think that you have it all figured out – keep on learning. As Einstein famously said, "Once you stop learning, you start dying." I was often so involved in my own work, that I missed opportunities to progress faster in my research by not following hot topics in other disciplines.

Nominator comment: "A key researcher in the analytical field. He has never hesitated to assume the leadership position, as an organizer of scientific symposia (Riva) or from a societal point of view (the dioxin incident in Belgium)."

Other categories: Separation Scientists

9 // Emily Hilder

Director, Future Industries Institute, University of South Australia, Australia.

Career highlight
Establishing the ARC Training Centre for Portable Analytical Separation Technologies (ASTech), and the opportunities created for students and researchers.
Advice to my younger self
Slow down a bit, and enjoy the journey.
What makes a good leader?
Traits I associate with good leaders are an ability to really listen and learn from others (and admit when they are wrong), being able to make decisions and providing a supporting environment where others can feel safe to fail.
Nominator comment: "Emily Hilder is already recognized in Australia and beyond as a leader that others want to follow. She is the most inspiring mentor, not just to her own team, but to other young scientists all over the world."

10// George Whitesides

Woodford L. and Ann A. Flowers University Professor, Department of Chemistry and Chemical Biology, Harvard University, Massachusetts, USA.

Other categories: Giants of Nano

For more advice and insight from our magnificent nominees, visit tas.txp.to/POWER2017.

Opening Doors With Omics

Sitting Down With… Oliver Fiehn, Director, NIH West Coast Metabolomics Center, Paul K & Ruth Stumpf Endowed Professor in Plant Biochemistry, UC Davis Genome Center, California, USA.

What was your route into science?
I was always interested in understanding how things worked; I was curious and serious, and asked a lot of questions – not what you would call an "easygoing" child! In high school, I discovered that I had a passion for chemistry. When I finished my PhD in 1997, I wanted to go into industry, but there was high unemployment in the sciences in Germany at that time – 2,000 graduate chemists for every few hundred industry positions. I got a postdoc position at the Max-Planck Institute in Potsdam and came to find metabolomics particularly fascinating. After a short time, I became group leader. So that was my trajectory – a chain of reactions…

What fascinated you about metabolomics?
On my first day, my boss said, "Don't ignore the small peaks." Abundance doesn't equate to importance; compounds at very low concentrations, such as hormones, can have huge effects – as can high abundance compounds like glucose. That's the concept of metabolomics – looking at the whole picture, trying to understand what it means and unraveling biological technologies along the way. It is asking an open-ended question, which always leads to new discoveries and opens doors. And it is simply a lot of fun!

How has the field changed in the last 20 years?
In the beginning, we were mainly hunting low-abundance peaks (or peaks in general) and didn't think that much about quantification, harmonization and standardization. Then, ten years ago, we started the Metabolomics Standards Initiative. Now, we can feed metabolomics data into databases, and compare and contrast findings across studies. Any one study doesn't tell you the truth; you have to find multiple lines of evidence and compare them in meta-analyses – that's how you figure out the functions of different compounds. The field has become more serious these days, more established, and – I hope – more useful for clinical and biomedical research.

Could you give an example of the modern approach?
My group found diacetylspermine – an acetylated version of spermine – in blood for the first time ever, and discovered that it is indicative of people who will get lung cancer within the next six months. We carried out two independent clinical trials, each with 300 people, and found very high significance. Of course it needs to be replicated in further cohorts, but it was an important finding.

Another significant discovery was the so-called FAHFA lipids, by Barbara Khan at Harvard. This is a new class of compounds that influences and directs insulin sensitivity and insulin resistance, so is important in metabolic syndrome, and in the development and progression of diabetes. Again, more research needs to be done – that's the case with all scientific discoveries; after the initial excitement, you need to dig deeper.

You manage a big group…
I am director of the West Coast Metabolomics Center, a consortium of different laboratories at UC Davis. I directly manage two of those labs; one is my own research lab, where we work with postdocs, visiting and project scientists, PhD students and cheminformatics specialists. The second is a service laboratory, with 13 full-time staff who manage the 17 mass spectrometers, and process over 25,000 samples a year, for more than 400 studies. These are two different entities, but both are important. I would never call the service lab team technicians; they are scientists, dedicated to pursuing analytical chemistry in a rigorous manner, and ultimately trying to help people. It is a shame that it's so hard to publish method validation work in analytical journals – they only want new methods, not robust ones, which is strange to me. Analytical chemistry methods have to be proven and validated to be robust.

"It's the best job in the world – and I'm very grateful to society for allowing me to do it."

How does working as a scientist in California compare to Germany?
The culture is more "thriving" here; it is more vibrant, open-minded and energetic. We have absolutely fantastic scientists at Davis, and I love working here – it's fabulous.

What is your biggest source of inspiration?
I am a member of the Molecular and Cellular Biology Department, and my lab is located in the Genome Center, so I am surrounded by biologists. I'm also member of the Comprehensive Cancer Center in Davis. It means my inspiration comes from actual biological and medical questions. For example, we recently received a grant from Columbia University to research chronic fatigue syndrome. I think if we take analytical chemistry seriously, we can really have an impact on people's lives. That's what drives me.

What are you most thankful for in your career?
My freedom. I can follow my own ideas – I'm my own boss, and I can pursue my vision and favorite topics in metabolomics. It's the best job in the world – and I'm very grateful to society for allowing me to do it.