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Image of the Month

The Gouda Old Days

Even die-hard fans of a ripe Stilton may find this a bit hard to swallow – the oldest piece of cheese ever discovered has been found in the tomb of Ptahmes (the Nineteenth Dynasty). The (very) mature cheese residue, a combination of goat/sheep and cow milk, was analyzed using UHPLC/high-resolution nano ESI-MS/MS and radiocarbon dating, and estimated to date from 3200 BP.

Reference. E Greco et al., "Proteomic analyses on an ancient Egyptian cheese and biomolecular evidence of brucellosis", Anal Chem, 90, 9673–9676 (2018).

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

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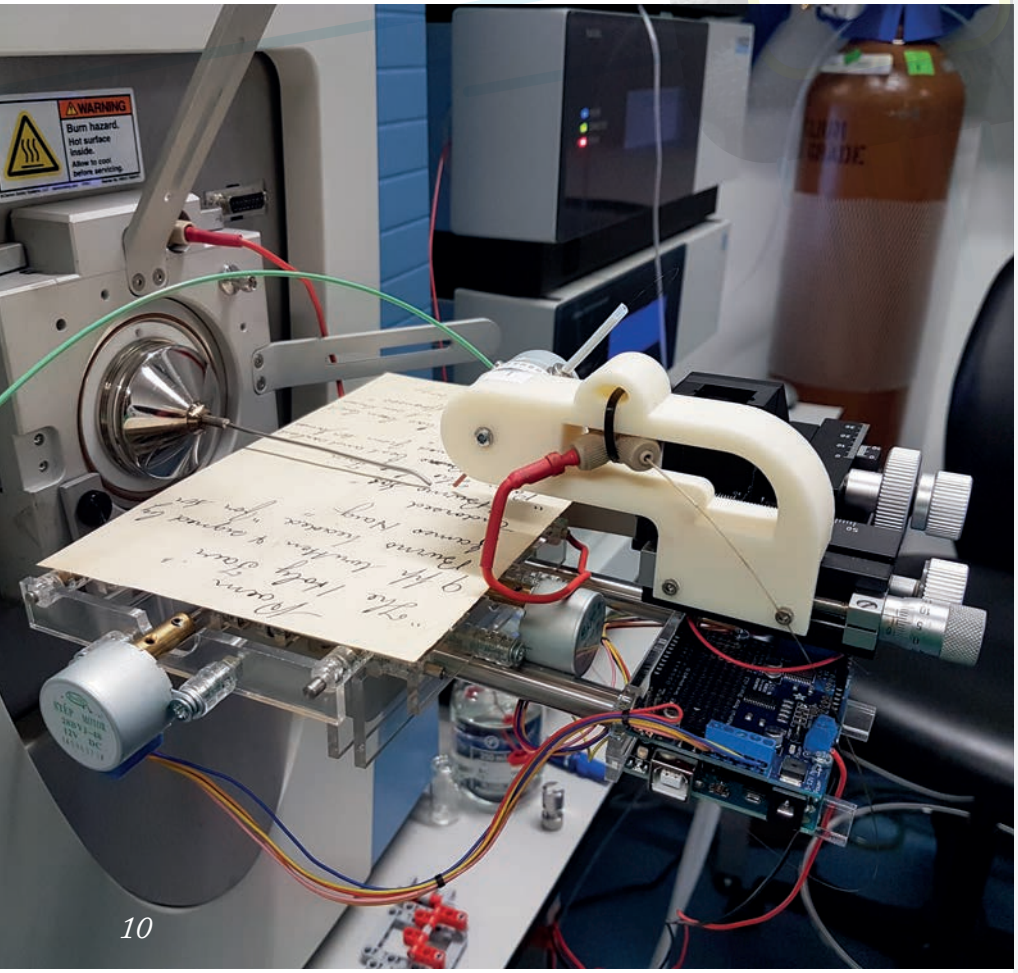

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On The Cover

Four Power List finalists "come together" for our Abbey Road-inspired cover

Upfront

the Analytical Scientist

ISSUE 69 - OCTOBER 2018

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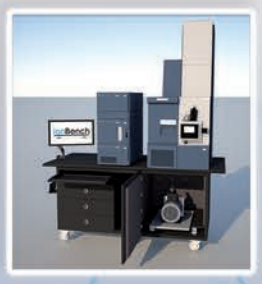

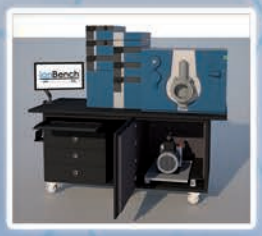

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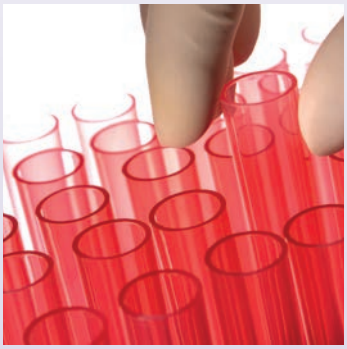

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Analytical Products

Passion, Dedication, Support

Welcome to the Top 40 Under 40 Power List!

For our 2018 Power List, we return to our celebration of the rising stars of analytical science. Starting on page 16, you can read the Fab 40's stories in their own words – and what amazing, inspiring stories they are! Between them they have won major awards, published groundbreaking papers and developed cutting-edge tools – all before the age of 40. So how have they achieved these impressive feats? Are they, like Hollywood actor Mark Wahlberg, adhering to a punishing schedule of 2:30am wakeups and cryo chamber sessions to boost their productivity? When asked for the secret of their success the most common reply was simple: do something that you love, and pursue it with passion.

The answer will come as no surprise to our readers. One of my own great pleasures as an editor is speaking to people who are so passionate about their work. Of course, not every working day is unalloyed joy – many of our Top 40 Under 40 make reference to the inevitable setbacks and disappointments to be found in a career in science. As Matthew Lockett wryly notes, sometimes you have to "love science, even when it does not love you back."

Nevertheless, for these early career scientists, (sometimes unrequited) passion for their field propels them onwards. Gary Patti hits the nail on the head on page 28: "I think obsessed is a good word. It's the feeling of getting halfway through a jigsaw puzzle and then having to stop. There's an irresistible urge to find that missing piece."

As well as passion, curiosity and sheer hard work, success as a young (or old) scientist relies heavily on the support of others. As epigenomic explorer Benjamin Garcia says on page 51, "To become independent and rigorous scientists with the vision to ask and answer important questions, we must be trained and mentored, supported and encouraged." Garcia is now himself a mentor to many – indeed, he says, "When I look back on my career, I will judge myself on the impact I have had on others."

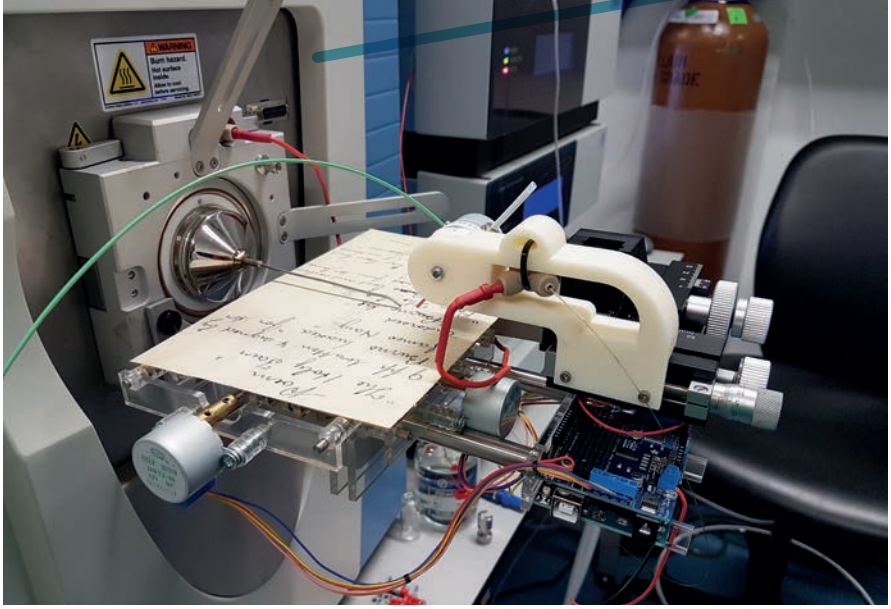
Which brings me to a closing point: as well as congratulating the fantastic 40 themselves, I'd also like to thank their nominators. We, and they, appreciate your efforts to support the next generation of analytical scientists.

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



Burns After Reading?

Metabolomic analysis of Burns manuscripts sorts the facts from the fakes

A team from the University of Glasgow, UK, performed a chemical analysis on documents purportedly written by Scottish poet, Robert Burns – and developed a method to identify the genuine manuscripts. Comparison of the ink spectra using HRMS allowed them to create an authenticity map to distinguish the authentic versions – but not without a few analytical (and practical) issues along the way.

The project was the result of a multidisciplinary collaboration between Karl Burgess (Head of Metabolomics) and Gerry Carruthers (Professor of Scottish Literature and a Burns expert). "Gerry was looking for someone who could use a chemical analysis technique to distinguish real from faked Burns manuscripts, and my PhD student recommended me," says Burgess. "At the same time, I was trying to recruit someone to do surface analysis mass spectrometry, and James Newton came on board. The rest is history!"

They started off with DESI-MS. "James spent his first year building a robotically controlled DESI (desorption electrospray ionization) source, optimizing it, and faking Burns documents to provide samples that we could test to destruction. DESI turned out to be relatively insensitive, and we would have had to fold the documents up to fit them onto the source," says Burgess. Liquid extraction surface analysis (LESA) also required them to fold the documents, but the quality of the spectra convinced the team to find a workaround. "We ended up using manual LESA, pipetting a couple of microliters of solvent onto the document by hand before transferring it to the Advion NanoMate for direct infusion mass spectrometry (DIMS)," says Burgess. This simple method meant they were able to take a bottle of solvent, some tips, a pipette and a bag of tubes to a library or collection, and sample documents on site.

The first problem they encountered, Burgess says, ultimately had one of the best outcomes of the project. "We wanted a positive control for the inks and we mentioned this to our collector–collaborator, who brought us a hand-written book from the 17th century, describing the production of lots of liquids – including inks (as well as carbonized ivory, stale beer and wasp galls)," he says. "James then used the recipes to make the inks."

Now they have a working method, the team want to build a database of hundreds of documents, so that they can put other authors' works into context.

Reference

1. *J Newton et al., "Minimally destructive atmospheric ionization mass spectrometry authenticates authorship of historical manuscripts", Sci Rep, 8, 10944 (2018). DOI:10.1038/s41598-018-28810-2.*

Microchips and Advanced Microscopy

Business in brief: What's going on in analytical science?

Products and launches

- HORIBA has launched the Duetta, a compact fluorescence/absorbance spectrometer that performs non-destructive, non-contact analysis.
- Agilent's 870 Laser Direct Infrared imaging system claims to speed up analysis times from "hours to minutes."
- SCIEX announced new applications for CESI-MS (capillary electrophoresis with electrospray ionization) in September, including the proteomics and metabolomics fields.
- Thermo Scientific launched their ISQ_EM system – offering a mass range of 10-2000 m/z .

Collaborations

- Bruker has expanded its collaborations with Bioinformatics Solutions Inc, Evosep and the Max Planck Institute for Biochemistry, Germany.
- PharmaFluidics has entered into a partnership agreement with Thermo Fisher Scientific. This will allow the company to combine their own µPAC technology with Thermo's mass spectrometers.

Company and people updates

- The National Institute of Health has awarded US $1.5m to Vanderbilt University to support their aim to map the human body at the cellular level using MS imaging.
- Waters has appointed two new members to its Board of Directors. CEO of Waters, Chris O'Connell, said: "Linda Baddour offers deep strategic insights…Gary Hendrickson brings a wealth of global leadership and governance experience."
- Nestor Zaluzec (senior scientist at US DOE Argonne Laboratory) has been recognized for his contributions to advanced microscopy – by being named an inaugural Fellow in the Legends Class of the Microanalysis Society.

For links to original press releases, visit the online version of this article at: tas.txp.to/1018/BUSINESS.

Source of Light – and Inspiration

A new center for electron bio-imaging was officially opened by one of the three Nobel Prize winners behind the cutting-edge technology at its heart

Courtesy of Diamond Light Source.

While the world hurries to congratulate the 2018 Nobel Prize winners, we're still celebrating Richard Henderson, who, along with Jacques Dubochet and Joachim Frank, won the 2017 Nobel Prize in Chemistry "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution (1)." Why? On September 12, 2018, Henderson officially opened Diamond Light Source's electron bio-imaging centre (eBIC) in Cambridge, UK. The event coincided with the announcement of a partnership between Diamond and Thermo Fisher Scientific, which adds two new microscopes and professional cryo-EM services specifically for the pharmaceutical industry.

The additional capacity makes eBIC one of the largest cryo-EM sites in the world – a true nod to the technology's fast-growing significance in structural biology. Rich Whitworth, Content Director of The Analytical Scientist, was given the opportunity for a brief one-on-one with the Nobel laureate.

Forgive the obvious question, but how did it feel to win "the prize" in science?

Obviously, it's a great honor. The Nobel Foundation has a great impact on the world, and it really raises the profile of science a great deal. However, I have to say, we were not entirely surprised – and I'll tell you two amusing stories that got me thinking… First, in 2013 or so, when we started to get really good results with cryo-EM, my students kept asking me, "Do you think you will get a Nobel Prize for this?" I answered by saying it was "a bit of a lottery." Second, on the Thursday afternoon at the end of our 2016 annual cryo-EM meeting, the closing pantomime sketch featured a "wheel of fortune" that could predict the next Nobel Prize winner; because it was a cryo-EM meeting, five of the six spots on the wheel were dedicated to "Cryo-EM," the sixth slot was reserved for "CRISPR/CAS 9." In the sketch, the wheel was spun several times, but the arrow always landed on "CRISPR-Cas9," much to everyone's amusement. No Nobel Prize for cryo-EM! Of course, as it turns out, cryo-EM did win a year later…

You've been working on cryo-EM for many years – has progress been as rapid as you expected?

It's been much slower than we thought. Scientists, generally speaking, are optimists. If you're a pessimist, you probably shouldn't do research because you'll always expect to fail – perhaps try the insurance industry. I was originally in X-ray crystallography and then electron crystallography, and then, about 20 years ago, I decided that single-particle cryo-EM had a great future. We started experimenting and we thought we'd have it all done by the end of the year – that was 1997 or so. But there were all sorts of problems that had to be tackled one by one. The microscopes and the computer programs certainly improved over the years, but it was the development of new detectors around five years ago that really took us over the hump. Today, it's much better than it was five years ago, and in another five years it will be better still. It will be faster, the data will be better, and it will provide higher resolution with less effort. It's really quite a positive atmosphere at the moment in this area of structural biology.

Do you think cryo-EM will supplant X-ray crystallography for structural biology?

I don't think it will fully supplant current methods, but it will become the number one choice in some cases – particularly when it comes to structures with difficulties; for example, issues with stability, purity, or conformational heterogeneity. The synchrotron-based experiments will continue – they allow us to collect 300 datasets per day, whereas with cryo-EM it's currently one. But the technology will improve, and I see no reason why we can't get to 300. In the coming years, we will know the structure of virtually every molecule in biology that we're interested in. But there will still be plenty to do. If we could design one drug to activate and one drug to inhibit every one of those molecules, we'd be in a very powerful position.

For more about Diamond Light Source and eBIC, visit www.diamond.ac.uk

Reference

1. *https://www.nobelprize.org/prizes/chemistry/2017/summary/*

No Sex Please, We're Copperheads!

Mass spec "venomics" analyzes the deadliness of asexually produced snakes

Who?

A team from the Liverpool School of Tropical Medicine, UK, and the Evolutionary and Translational Venomics Laboratory, Spain, have analyzed the venom of snake offspring in a recent study (1).

What?

The researchers were looking specifically at copperhead snakes conceived via facultative parthogenesis (FP) – where the mother reproduces without fertilization – to ascertain whether sexless reproduction might negatively impact the potency of venom (negative if you're not their prey, that is).

Why?

Previous studies have shown that FP in jawed vertebrates can result in a lack of genetic diversity, which typically leads to lower evolutionary fitness. What's more, as it was only observed in captivity, it has been considered a "reproductive error" (1) rather than a viable mode of procreation. So you might expect FP to have a negative impact on a genetically complex survival trait like venom composition.

How?

They collected the venom of four snakes born in captivity to wild-collected females. They then used 2D gel electrophoresis to gain a proteomic profile and LC-MS/MS to compare and analyze the samples, looking specifically at toxicity and coagulopathic effect.

Findings?

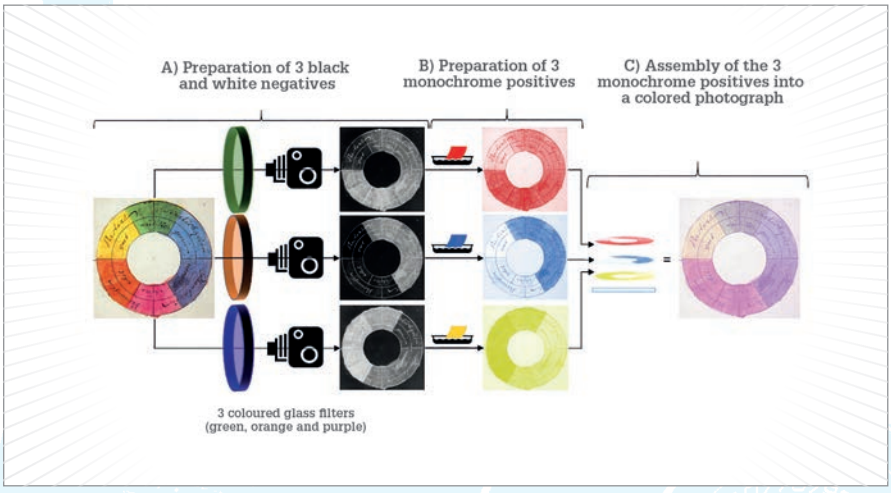
FP was found to have little impact on the chemical complexity of the copperheads' venom – in fact, there was a high degree of similarity with the venom sampled from each snake's mother. The researchers believe this finding reinforces the viability of FP "as a potentially important mode of reproduction."

Reference

1. *JJ Calvete et al., "Venom complexity in a pitviper produced by facultative parthogenesis", Sci Rep, 8, 11539 (2018). DOI: 10.1038/s41598-018-29791-y*

Photos in Focus

Using synchrotron spectroscopy to work out the chemistry behind 200-year-old photographs – and raise the profile of a long-neglected artist



Pioneering photographer Ducos du Hauron developed the general principle of three-color carbon printing (1).

Marine Cotte works in the European Synchrotron Radiation Facility, Grenoble, France, where her job is to support researchers in their scientific endeavours. A colleague asked for Cotte's help to analyze some fragments of a photograph produced by pioneer of color photography, Louis Ducos du Hauron.

"I first used infrared microscopy, which allows you to scan two-dimensional regions, define the pixel size and then move from one pixel to another, acquiring an infrared spectrum at each pixel. In this way you can ascertain the molecular composition, as well as see where the molecules are distributed," Cotte says. "Synchrotron infrared microscopy turned out to be very efficient for the identification of organic components, such as gelatine, celluloid, resin, oil, and so on."

Cotte also used X-ray microscopy to work out the elements of composition, and in particular, to identify the pigments. "Ducos du Hauron's books showed he didn't use the same pigment at the beginning of his career as he did later on," she explains. "By identifying the pigments, we could work out a kind of 'chronological marker'; for example, we could identify Prussian Blue pigment by the presence of iron." The next step was to identify the technique used for printing, and for this they used X-ray fluorescence spectroscopy to distinguish different oxidation states. The presence of chromium suggested carbon printing.

Despite his contribution to the photography field, Ducos du Hauron never enjoyed commercial success. "I had not heard of him – barely anyone had – until recently, but his work has become important to me," says Cotte. "He was really passionate, spending 40 years constantly trying to improve, not to make a profit, but simply to develop a technique that anyone could use." Some museums are exploring the idea of exhibitions to coincide with the anniversary of his death, which, Cotte hopes, will give Ducos du Hauron some visibility. "Hopefully the museums – and our scientific research – will finally give him some of the recognition he deserves," she says.

Reference

1. *M Cotte et al., "Rediscovering Ducos du Hauron's color photography through a review of his three-colour printing processes and synchrotron microanalysis of his prints", Angew Chem Int Ed, 57, 1-6 (2018). DOI: 10.1002/anie.201712617.*

Don't Have Your Fake or Eat It

The fight against fake pharma continues: researchers at Colorado State have developed a straightforward way to detect counterfeit antibiotics – using a simple color-changing paper test. Researcher Charles Henry tells us more

What was the inspiration behind the test?

For the last decade, I've been working with other scientists in the developing world, and have learned much about how healthcare works – or doesn't work – in those countries. This piqued my interest in developing low-cost tests that could improve healthcare for people living in those areas. At the same time, Kat Boehle (1) and I were working on a test for anti-microbial resistance. The test detects bacteria by measuring an enzyme (betalactamase) involved in antibiotic resistance – using the bacteria's own resistance machinery against it. Kat

and I realized we could use that same enzyme to detect antibiotics using a test that was both unique and low-cost.

How does the test work?

The user simply dissolves the antibiotic in water, before adding the sample to the device. It then travels down a channel with dried nitrocefin, rehydrates the substrate, and is transported to the detection zone where betalactamase is stored. If the antibiotic is not present or is diluted, the betalactamase will react with nitrocefin, causing the device to turn from yellow to red. However, if the antibiotic is genuine, it will outcompete the nitrocefin to bind with betalactamase, resulting in no color change (remaining yellow).

The test also incorporates a pH indicator – necessary since fillers commonly used in falsified drugs can alter the pH of the solution and affect the validity of the test. If the test turns red, or the pH indicator suggests that the solution is acidic or alkaline, the user should avoid using the drug.

How do you envision it being used in the field?

We envision the test being used primarily by individuals. We are hoping that by making the test inexpensive and user-friendly, patients can take charge of their own health by identifying falsified antibiotics. Also, scientists who study falsified and substandard antibiotics around the world currently have to gather samples in the field and transport them to a central laboratory for expensive and laborious testing – so the test could save time and money in research too.

What are your plans for the future?

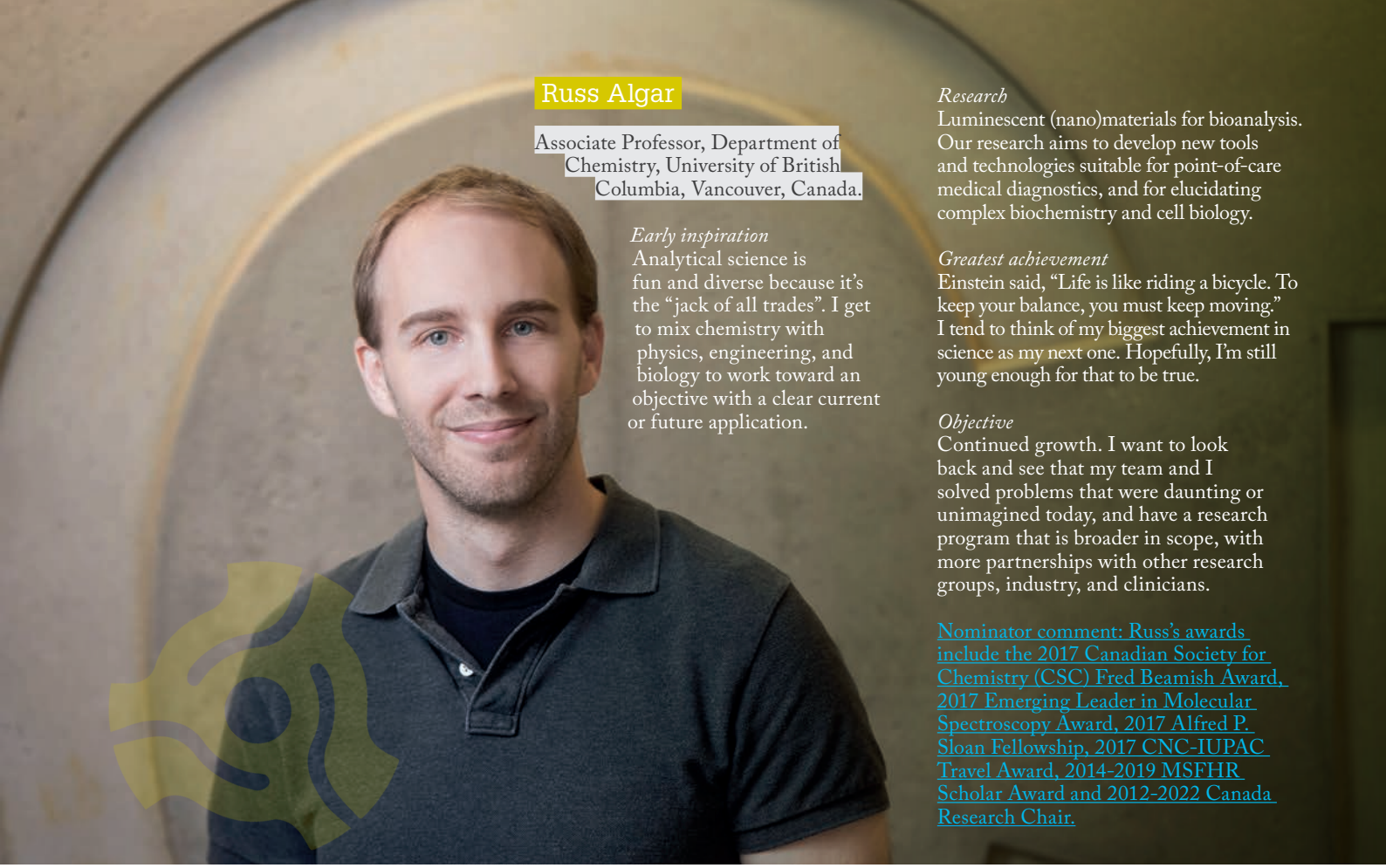
First, our current device needs some additional optimization, particularly when dealing with acidic fillers (such as aspirin) that stabilize the reaction, making it hard to distinguish falsified drugs. Additionally, we would like to develop a cell phone application or portable Raspberry Pi program for users who want to quantify the active ingredient – instead of the simple "yes or no" answer that is currently in place.

Reference

1. *KE Boehle et al., "Paper-based enzyme competition assay for detecting falsified β-lactam antibiotics", ACS Sens, 3, 1299–1307 (2018). DOI: 10.1021/acssensors.8b00016.*

THE FAB *forty*

The Top 40 Under 40 Power List returns to celebrate the gifted young scientists making waves in analytical science. Here we present the rising stars of the field (in alphabetical order), as nominated by our readers and shortlisted by our independent judging panel.



Russ Algar

Associate Professor, Department of Chemistry, University of British Columbia, Vancouver, Canada.

Early inspiration
Analytical science is fun and diverse because it's the "jack of all trades". I get to mix chemistry with physics, engineering, and biology to work toward an objective with a clear current or future application.

Research
Luminescent (nano)materials for bioanalysis. Our research aims to develop new tools and technologies suitable for point-of-care medical diagnostics, and for elucidating complex biochemistry and cell biology.

Greatest achievement
Einstein said, "Life is like riding a bicycle. To keep your balance, you must keep moving." I tend to think of my biggest achievement in science as my next one. Hopefully, I'm still young enough for that to be true.

Objective
Continued growth. I want to look back and see that my team and I solved problems that were daunting or unimagined today, and have a research program that is broader in scope, with more partnerships with other research groups, industry, and clinicians.

Nominator comment: Russ's awards include the 2017 Canadian Society for Chemistry (CSC) Fred Beamish Award, 2017 Emerging Leader in Molecular Spectroscopy Award, 2017 Alfred P. Sloan Fellowship, 2017 CNC-IUPAC Travel Award, 2014-2019 MSFHR Scholar Award and 2012-2022 Canada Research Chair.

Robbyn K. Anand

Assistant Professor, Department of Chemistry, Iowa State University, Ames, USA.

Early inspiration
Despite a keen interest, I faced many obstacles in pursuing a career in science, including being actively discouraged from it based on my gender. This resistance only increased my determination, and now one of the most satisfying parts of my job is leading events that promote diversity in science.

Greatest achievement
My group recently developed a fully integrated process for parallel single-cell analysis in a device amenable to point-of-care use. The ability to interrogate tissues at the single-cell level has radically changed how disease is understood, and making that capability widely accessible is a major step towards personalized medicine.

Scientific heroes
My graduate advisor, Richard M. Crooks, for mentoring young scientists with sustained and focused intent. There are many attributes that make a scientist great, but what creates a legacy is active investment in others.

Advice
Embrace failure. While a student, I tried improvisational acting, and what I learned was revolutionary. Allowing yourself to take risks and to pose new ideas inevitably leads to failure. Learn from it and move on. "The master has failed more times than the beginner has even tried." – Stephen McCranie.

Nominator comment: "Robbyn has demonstrated immense creativity in the way she marries electrochemical methods such as dielectrophoresis with separation systems. Her group is focused on developing wearable devices capable of hemodialysis to assist those who suffer from kidney failure – and developing microfluidic platforms in which cancer cells can be captured and analyzed."

Andrew Ault

Assistant Professor, Department of Environmental Health Sciences, Department of Chemistry, University of Michigan, Ann Arbor, USA.

Research
My group and I develop spectroscopic and microscopic methods that enable study of the chemistry of atmospheric aerosols. We focus on individual particles (10-1,000 nm) containing thousands of compounds and with viscosities ranging from liquid to glassy.

Greatest achievement
Developing the first analytical methods to measure the acidity of atmospheric aerosols, both spectroscopically and colorimetrically, with more methods in the pipeline! These novel approaches are transforming our understanding of aerosol acidity, which drives haze and smog formation globally, but has traditionally been deemed too difficult measure.

Objective
My hope in the next decade is for improved predictions of aerosol impacts on global health and climate through greater understanding of aerosol chemistry. This will be enabled by rapid improvement in spectroscopy and mass spectrometry of aerosols, and my goal is to play a major role!

Prediction
Methods that enable spectroscopic analysis of complex samples under environmental conditions at spatial resolution not easily accessible in the past (<100 nm). For example, photothermal infrared spectroscopy is rapidly advancing and will enable vibrational spectroscopy of far smaller particles, materials, and biological systems than previously.

Nominator comment: "Andrew has quickly established himself as a leader in developing and applying spectroscopic methods to study atmospheric aerosols – critical for addressing global health and climate change."

Matthew J. Baker

Reader in Chemistry, Department of Pure and Applied Chemistry, University of Strathclyde, UK.

Research
My focus is to impact upon people's lives by understanding the composition and behavior of molecules in complex media. I aim to detect or identify disease, toxic chemicals and pathogenic bacteria via spectroscopy and translate these methods to real-world settings.

Greatest achievement
In January of this year we were able to put a FTIR spectrometer in the Western General Hospital, Edinburgh, that is fitted with the new accessories that we have developed via my spinout (www.clinspecdx.com). We were able to collect serum spectroscopic data from people attending for a CT, finally translating something invented in the lab to the clinic.

Objective
I hope to have fully regulated spectroscopic tests that are FDA/MHRA approved, used in daily practice and cover a wide range of diseases. This will not only benefit patients but also expand our field.

Prediction
The infrared spectroscopy area is very interesting at the moment with the use of new light sources and new techniques coming, such as nanoscale IR and thermal-based analysis.

Zachary S. Breitbach

Senior Scientist, Analytical Research and Development, AbbVie Inc., Chicago, Illinois, USA.

Early inspiration
I was always interested in figuring out how things work and how to make them better. Analytical science is one of the few professions that gives you the advanced tools to really understand complex problems.

Greatest achievement
The launch of AZYP, along with the development and commercialization of superficially porous particle-based chiral stationary phases. It is exciting to be in an industrial setting now, where these columns have transformed chiral separations.

Scientific heroes
I worked with my graduate advisor, Daniel Armstrong, for over 10 years and he is one of the most intelligent researchers in analytical chemistry, as well as an extremely effective teacher.

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

Nominator comment: "Breitbach is the young star of separation science. Among his numerous awards is the 2018 ACS Young Investigator Award in Separation Science."

Ken Broeckhoven

Associate Professor, Department of Chemical Engineering, Vrije Universiteit Brussel, Brussels, Belgium.

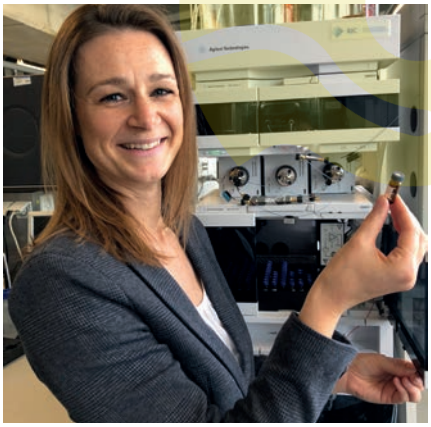
Early inspiration
I can only thank/blame my former promotor, Gert Desmet, for dragging me into the field of liquid chromatography – not a typical choice for a chemical engineer, but one I don't regret.

Greatest achievement
Building and running our very own extremely high-pressure LC system (3000 bar) that can handle the flow rate of typical (2.1mm ID) UHPLC columns, with no serious injuries or accidents in the process (besides some dents in the casing!).

Objective
As part of the Belgian ChIMiC research consortium, we hope to achieve a paradigm shift in the quality of chemical composition measurements of vapors, mixtures, cells and tissues – by developing innovative hardware and software solutions.

Advice
Investigate the unexpected! If your experiments do not give the results you had planned or hoped for, often interesting new things can be learned by figuring out why.

Nominator comment: "Ken is a talented researcher with a deep understanding of the fundamentals of chromatography. He is also a passionate teacher, and an excellent presenter at conferences."



Deirdre Cabooter

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

Research
We are looking into new ways to rationalize and automate liquid chromatographic method optimization for complex samples by developing new software and hardware tools.
Plus, together with Gert Desmet, we continue our work on trying to better understand mass transfer phenomena in liquid chromatography.

Greatest achievement
I'm grateful to have been given a permanent position at the University of Leuven, giving me the space, tranquility and freedom to explore new research ideas. I'm also very proud of my current research group, consisting of smart, enthusiastic people that work together in a very constructive way.

Scientific hero
Gert Desmet, who is my mentor, my friend and my greatest source of inspiration. He is incredibly intelligent, extremely dedicated and one of the most original analytical scientists I know.

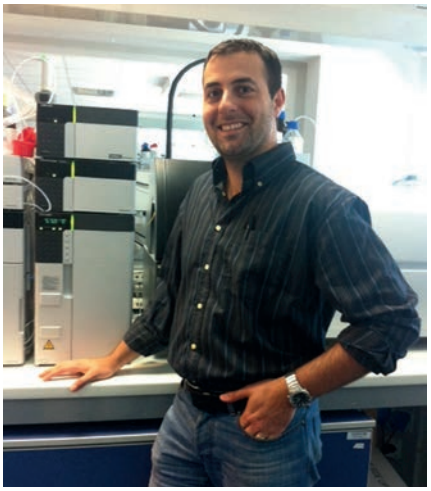
Advice
Work hard, be persistent and don't give up too easily! Take every opportunity you can to learn, and collaborate to expand your horizons.

Francesco Cacciola

Associate Professor of Food Chemistry, Department BIOMORF, University of Messina, Italy.

Research
The application of innovative analytical techniques, in particular comprehensive two-dimensional liquid chromatography, for the characterization of bioactive molecules in food and natural products.

Greatest achievement
The successful development of comprehensive two-dimensional liquid chromatography by using reversed phase in both separation systems for the characterization of food bioactive polyphenolic compounds.



Scientific heroes
Luigi Mondello and Paola Dugo, my mentors and former promoters, who introduced me to the world of chromatography with great enthusiasm. Plus, Pavel Jandera, an extraordinary scientist and my official supervisor when I started my PhD at the University of Pardubice, who pioneered 2D-LC separations of polyphenols in wine and beer.

Objective
To keep pushing forward with the application of 2D-LC separations in the field of food and natural products analysis with the aim of sharing my enthusiasm and passion for research with young researchers.

Nominator comment: "Cacciola is an outstanding researcher in the field of comprehensive two-dimensional liquid chromatography. His findings have enabled significant evolution in the field, especially in food analysis."

Cecilia Cagliero

Assistant Professor, Department of Drug Science and Technology, University of Turin, Italy.

Early inspiration
As soon as I started work in a research laboratory, I saw that an academic career allows you to combine the most challenging elements of the human experience: the possibility of following your natural curiosity through research activity, and transmitting knowledge and passion to younger generations.

Research
Developing new technologies and strategies for the definition of the composition of volatile and nonvolatile biologically active secondary metabolites of plants and plant products of interest in the pharmaceutical, cosmetic and food fields.

Greatest achievement
I was very honored to receive the Leslie Ettre Award during the ISCC meeting in Riva in 2016; however, I think that my best achievement is with regards to the people (colleagues and students) I have worked with.

Advice
The best advice that I can give to a young scientist is to always work with passion: passion helps keep the mind "alive" and active and, even more importantly, a passionate scientist is able to infect everyone in contact with them with their enthusiasm.

Nominator comment: "Despite her young age, Cecilia is a highly creative, motivated, and rigorous scientist."

Tomas Cajka

Associate Professor, Department of Metabolomics, Institute of Physiology CAS, Prague, Czech Republic.

Research
Developing novel strategies using cutting-edge LC–MS technologies to merge untargeted and targeted metabolomics methods, expanding the coverage of spectral libraries and identification of unknowns by using in-silico fragmentation software, and applying these tools in biomedical research to ultimately improve human health.

Objective
In untargeted metabolomics, it is estimated that only 20 percent of features can be identified – a sad balance indeed. Hopefully the field will move toward a higher identification rate of metabolites thanks to open-source MS/MS libraries for more meaningful data interpretation. I would like to contribute a few pieces to this big metabolomic puzzle.

Advice
Make use of every opportunity and challenge! Easy to say, much harder to do, of course. However, solving seemingly intractable problems has always forced me to think outside the box and consequently influenced the direction of my future research.

Nominator comment: "Tomas is the most meticulous, creative and imaginative analytical chemist that I have ever met."

Anna Laura Capriotti

Associate Professor, Department of Chemistry, University La Sapienza, Roma, Italy.

Research
We develop new analytical methods and tools, based on liquid chromatography coupled to high resolution mass spectrometry, for the characterization of proteins and peptides important in life sciences and food analysis.

Greatest achievement
Receiving the EuChemS Lecture Award 2017 really boosted my visibility, which makes this job all the more enjoyable.

Scientific heroes
Aldo Laganà gave me a chance to work in his research group, and taught me to rely on dedication, self-sacrifice and collaboration to reach my goals. No one can become a great scientist without a great research group!

Advice
Never stop believing in your dreams and stay focused on your objective.

Nominator comment: "She is a brilliant young scientist full of energy, enthusiasm and curiosity."

Jennifer Chen

Associate Professor, Department of Chemistry, York University, Toronto, Ontario, Canada.

Early inspiration
I chose academia because of my passion for research, teaching and mentoring. I enjoy the freedom to tackle a problem and to come up with a solution. I find it rewarding to be able to make a difference in students' lives and see them grow into mature scientists.

Research
Developing nanostructures and methodologies for detecting biomolecules down to the single-cell level, thereby enabling rapid and economical interrogation of cellular heterogeneity and microenvironment.

Scientific heroes
I have great respect for Arnold Beckman's contribution in developing analytical technologies that advanced many fields of science, and for his entrepreneurship, involvement in policy, and philanthropy.

Advice
Stay curious, as learning is a life-long journey. Be flexible and open-minded – different career paths may be attractive at different points in one's life.

Nominator comment: "Jen has built an innovative and multifaceted research program in analytical chemistry, which comfortably resides at the interface of materials research, next-generation sensor development and biomedical diagnostics. She and her team are rapidly establishing a center of research excellence in the area of plasmonic sensors."

Lynn Dennany

Senior Lecturer, Department of Pure & Applied Chemistry, University of Strathclyde, UK.

Early inspiration
I wanted to undertake research that makes a difference, and analytical science represented the most challenging and fulfilling way for me to achieve this. That's why I chose this career path; I do the science I love, have an impact on society and share my enthusiasm with younger scientists.

Greatest achievement
My biggest achievement was showing that electrochemical sensors can be successfully utilized in complex matrices such as blood. Prior to this, they had been dismissed for real-world analysis by many. This represented a game-changer and cemented electrochemical research as part

of the mix for portable analysis and real-world applications.

Prediction
Current research is focused on portable sensing for applications in personal medicine, process analysis and forensic science. The biggest challenge for all of this innovative research is translation into active use in these fields. If we can overcome this hurdle, advances in all of these industries will be achievable.

Advice
Collaborate at every opportunity. This can help you direct and shape your area of research while visiting different countries and laboratories. It also gives you a brilliant support network of scientists and friends.

Nominator comment: "Lynn has pioneered the fundamental understanding of electrochemiluminescence to facilitate the translation of electrochemical sensors into the clinical arena and showcase its potential for a variety of other applications. She has written agenda-setting papers, developed new sensor platforms and made advances toward continuous monitoring."

Livia S. Eberlin

Assistant Professor, Department of Chemistry, University of Texas at Austin, Texas, USA.

Nominator comment: "I believe Eberlin is unique among the many talented analytical chemists, specifically mass spectrometrists, under the age of 40. In her short career, she has worked on medically related topics with the aim of improving medical decisions via molecular measurements. Her work (and that of her lab) is exemplified in the development of the MasSpec Pen for intraoperative cancer diagnosis."

Flavio Antonio Franchina

Postdoc researcher, Division of Organic and Biological Analytical Chemistry, University of Liège, Belgium.

Research
As part of a challenging project involving other excellence centers (Bruxelles, Leuven, Ghent), we aim to evolve and establish innovative analytical methods, making them accessible and straightforward for environmental/life science applications.

Greatest achievement
Receiving the Phillips Award for my contribution to the field of comprehensive two-dimensional gas chromatography (GC×GC). It is a tribute to my mentors, who made it possible with their teaching and passion.

Objective
Consolidating advanced analytical methods with robust sample preparation and improving our understanding of the already information-rich data we collect with modern instrumentation.

Advice
Be solid with fundamentals first, then there is no fear in exploring new fields.

Nominator comment: "He is a very promising scientist in the field of comprehensive gas chromatography. Despite his young age, he is a great mentor and teacher for graduates and undergraduates entering the lab."

James Grinias

Assistant Professor, Department of Chemistry & Biochemistry, Rowan University, Glassboro, New Jersey, USA.

Early inspiration
As an undergraduate student, I planned on being a physician. I was lucky enough to be recruited to do research with an analytical faculty member (Heather Holmes) on a fundamental GC project, and I fell in love with the field of chromatography. I haven't looked back since!

Research
My lab has several separations-focused projects that revolve around the theme of "reduction": reducing the size and cost of instrumentation, reducing cycle time and generated waste of analytical methods, and reducing hurdles for new practitioners to learn about analytical chemistry.

Scientific heroes
There are far too many former mentors and colleagues to name just one or two. However, when I look at the authors on my book shelf, I realize how much all of us owe to many giants in the field, such as Giddings, Horváth, Kirkland, Snyder, Dolan and Neue.

Advice
Never stop trying. Research is often difficult when you are trying to make a new observation or discovery, but it makes the eventual success that much more satisfying.

Nominator comment: "Jim trained with two chromatography legends and is now independently successful, securing grants from the NIH and ACS (impressive for a new professor)."

Andrea Gargano

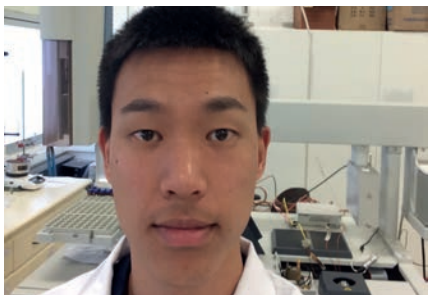
Tenure Track Assistant Professor, Centre for Analytical Science Amsterdam, van't Hoff Institute for Molecular Science, Amsterdam, the Netherlands.

Early inspiration
A lucky set of circumstances got me on a plane to Berkeley at the end of my Master's degree. I haven't quite figured out why Frank Svec accepted a young and quite (scientifically) illiterate Italian as an intern in his group but my experience there was great – it was there I discovered my enthusiasm for science.

Research
My research area is the separation and mass spectrometric analysis of large molecules. Currently, I am working on solutions to analyze proteoforms using LC-MS and I'm starting to look at the characterization of synthetic polymers.

Prediction
In the field of LC-MS, the hyphenation with other detection strategies to allow for more direct quantitative analysis. More generally, in analytical chemistry, maybe something coming from unexpected candidates, like pH meters.

Advice
I benefitted a lot from working in different work environments, so I would suggest everyone try such experiences (and maybe do it multiple times). There are many things that can be learned from seeing different labs, from research vision to lab safety.



Leandro Wang Hantao

Assistant Professor, Institute of Chemistry, University of Campinas, São Paulo, Brazil.

Early inspiration
I had really great advisors that motivated me. Mine has been a dynamic and challenging path that balances teaching, coaching, and research.

Research
Our focus is separation science applied to bioanalysis and the oil and gas industry. To solve such complex problems, we rely on miniaturized techniques for sample preparation and comprehensive two-dimensional gas chromatography coupled to mass spectrometry.

Objective
My group and I hope that our students continue to persevere and find the best opportunities in life. We also intend to expand our research opportunities by diversifying our funding sources to create a solid environment for continuous growth.

Advice
Find balance in your life. Pick a research team that you enjoy working with and that pushes you to be your best self.

Nominator comment: "Leandro has been influential in developing novel, inexpensive modulators for GCxGC and encouraging the adoption of GCxGC as a technique, through a number of high-profile collaborations in Brazil."

Cheng-Chih Richard Hsu

Assistant Professor, Department of Chemistry, National Taiwan University, Taiwan.

Research
We use mass spectrometry platforms to explore the chemistry of complex biological systems. In particular, we focus on technical advances that help develop better understanding of how microorganisms interact with the human body. Plus, we implement ambient ionization mass spectrometry for clinical sciences.

Scientific heroes
Richard Zare, my postdoctoral advisor, for his pioneering work and technical breakthroughs in analytical science – and for his never-ending passion for his research and mentorship of younger scientists.

Prediction
The most game-changing advance we could see in the next five years would be an algorithm that could rapidly and accurately determine the chemical structures of compounds based on their spectroscopic and spectrometric features.

Advice
Stay passionate when you discover nothing, and stay calm when you find something.

Anneli Kruve

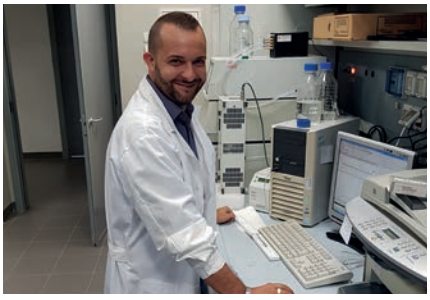
Humboldt Fellow, Institute of Chemistry and Biochemistry, Freie Universität Berlin, Germany.

Early inspiration
I got started in organic synthesis but quickly joined a biomedical lab that needed students to operate a HPLC. From there, moving to LC/MS was a natural step. The ability to incorporate various skills from IT to synthesis with mass spectrometry-based research has kept me motivated to stay on this path.

Research
My field is structural and quantitative characterization of compounds with LC/ESI/IMS/MS. A key focus of mine is developing the possibility of giving a quantitative context to non-target LC/HRMS data without the need for standard substances.

Greatest achievement
I have already seen many students moving from our lab to the workforce and receiving positive feedback from their employers – that definitely makes a former supervisor happy!

Prediction
Mass spectrometry has already changed almost everything; its impact will increase further, as we make non-target screening more efficient with effective algorithms, and make it quantitative. I also have a dream technique: I sometimes wonder what the world would look like with MS-(gas phase) NMR…



Marcello Locatelli

Assistant Professor in Analytical and Bioanalytical Chemistry, Department of Pharmacy, University "G. d'Annunzio" Chieti-Pescara, Chieti, Italy.

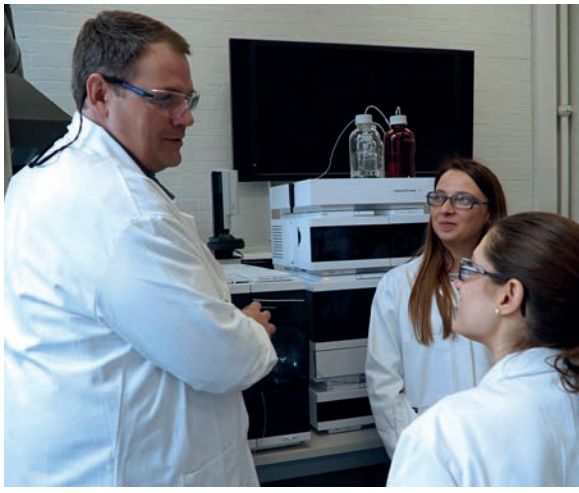
Research
I work on the development and validation of innovative (micro)extraction (FPSE, MEPS, MIPs) procedures and instrumental analysis both in biological matrices (for clinical and pharmaceutical applications) and in natural matrices and foods/food supplements.

Objective
I would like to be able to make a contribution in my field and to transmit this desire to future generations.

Prediction
In the next five years, the most game-changing technology or advance will be represented by increased performance, and online or automatic techniques.

Advice
Have fun and "play" with skills and knowledge. Be open to all areas of science, to develop a complete vision of both the problem and the solution.

Nominator comment: "Marcello is an excellent researcher, with many publications, a vast knowledge in his area of expertise, coupled with great networking skills and insightful ideas for future research projects."



Panagiotis Manesiotis

Senior Lecturer in Analytical Chemistry, School of Chemistry and Chemical Engineering, Queen's University Belfast, UK.

Early inspiration
Growing up, I was always curious to discover the inner workings of everyday items. As a researcher, I worked beside inspirational academics who ignited my passion to convey knowledge and communicate science. An academic career in analytical chemistry means I can do what I love as my day job!

Research
I work on the development of materials and sensors to tackle some of the biggest present and future challenges, such as water quality, nutrient management and sustainable chemical and agri-food production, using my expertise on the interface of analytical, materials and supramolecular chemistry, and collaborating with microbiologists and environmental engineers.

Greatest achievement
The development of a handheld, inexpensive, disposable sensor for phosphate, made predominantly using biodegradable materials. It is able to signal the presence of the nutrient in concentrations under 1mg L-1 in soil, agri-food waste and water streams via a real-time color change and without the requirement of additional chemical reagents or power.

Jean-Francois Masson

Full Professor, Département de Chimie, Université de Montréal, Canada.

Early inspiration
After high school, I was training as a lab technician when an internship hooked me on analytical chemistry research. Plasmonics was emerging in the early 2000s; working on this topic provided an attractive opportunity to contribute to a new analytical field.

Research
I work on surface-enhanced Raman scattering (SERS) optophysiology to monitor metabolite release from cells and neurons. This stimulating project lets me learn more about cell biology, physiology and machine learning data processing. I also work on field-deployable sensors for bioprocess monitoring, energetic materials and, as a true Canadian, maple syrup analysis.

Objective
To make innovations from my lab mature into technologies that will have a long-lasting impact in analytical sciences and in the community.

Advice
Networking is key. The analytical community is very supportive of early career scientists, and senior researchers in the field will gladly help you – so don't be afraid to approach them. You will find new collaborators, generate ideas, create job opportunities and learn a lot.

Nominator comment: "Masson is a very prolific and creative scientist on all levels and a leading authority in portable instrumentation."

Matthew R. Lockett

Assistant Professor, Department of Chemistry, University of North Carolina at Chapel Hill, North Carolina, USA.

Early inspiration
I have always been interested in applying chemical principles to quantify biological systems. Academia has afforded me the chance to work with creative and driven colleagues and students, who continually inspire me to work harder and learn more, as we tackle hard questions at the interface of chemistry and biology.

Research
We are developing a paper-based 3D culture platform, to determine how components of the microenvironment affect cellular behavior (for example, hormone sensitivity or drug resistance). To best quantify the extracellular environment and intracellular responses in these 3D spaces, we are developing new sensors and methods of bioanalysis.

Scientific heroes
I have been very fortunate to interact with a number of very supportive mentors and colleagues, each pushing the field of analytical sciences in new and exciting directions. I am forever indebted to my PhD advisor, Lloyd Smith, who has always encouraged me to pursue hard problems and dream big.

Advice
Love science, even when it does not love you back.

Nominator comment: "Matthew is doing fantastic work developing new tools to analyze cellular behavior in 3D cultures with defined micro environments and gradients."

Christopher C. Mulligan

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

Early inspiration
I have always been interested in science and aspired to a career where I could help others. It wasn't until very late in my education (and after some encouragement from those close to me) that I even considered an academic career. But I'm very glad that I did.

Research
By leveraging portable MS technologies and ambient ionization methods, my group aims to provide the first-response and forensic communities with chemical information on-demand, in a platform that is simple, reliable, and court-admissible.

Prediction
I think advances in miniaturization will eventually yield the consummate, Tricorder-like device that many analytical chemists have sought to create. When this technology joins the "Internet of Things," the data produced could revolutionize fields like medicine and public safety.

Advice
Work hard, but also work smart. Play to your strengths in research, and minimize your weaknesses through effective collaborations. Finally, protect your research and writing time like it's a valuable commodity, because it is.

Nominator comment: "Mulligan has dedicated his professional career to empowering law enforcement agencies with the appropriate analytical instruments and methods to combat crime efficiently."

Sergio C. Nanita

Principal Investigator, DuPont Industrial Biosciences, Wilmington, Delaware, USA.

Early inspiration
I chose industry because its fast-paced R&D delivers products that improve quality of life. It has been gratifying to contribute fit-for-purpose innovations in analytical sciences, while experiencing the entire product commercialization process.

Research
As a mass spectrometrist, my current research focuses on developing state-of-the-art analytical methods and providing chemical structure elucidation expertise for the discovery, development, and support of products from various businesses segments of DuPont Industrial Biosciences, from Biomaterials to Animal Nutrition.

Scientific heroes
My most influential mentor is R. Graham Cooks (Purdue University, USA).

Objective
Develop and apply effective analytical chemistry solutions to advance DuPont R&D programs and deliver renewable bio-based products that benefit society and the environment.

Nominator comment: "Sergio has established himself as a leader in the analytical sciences. He is well-known for his efforts toward demonstrating flow injection MS methods, particularly in quantitative analysis of pesticides. He truly enjoys what he does and makes time to mentor other people within Dupont and outside of the company."

Gary J. Patti

Michael and Tana Powell Associate Professor, Department of Chemistry, Department of Medicine, Washington University in St. Louis, Missouri, USA.

Early inspiration
I think obsessed is a good word. It's the feeling of getting halfway through a jigsaw puzzle and then having to stop. There's an irresistible urge to find that missing piece. That's how I've felt about science for the last 20 years.

Research
Metabolomics and all things related to cellular metabolism. The difference between a good measurement and an excellent measurement could be a missed diagnosis.

Advice
Have the courage to say no. No to collaborations that don't excite you. No to conference invitations that aren't interesting. No to prospective students that aren't a good fit for your lab.

Nominator comment: "Patti has pioneered technologies in the burgeoning field of metabolomics. In particular, he has developed analytical methods for coupling metabolomics with isotope tracing."

Juris Meija

Research Officer, Metrology, National Research Council Canada, Ottawa, Canada.

Research
I explore the reliability of analytical data with a focus on isotope-based methods of quantitation. In a sense, it is all about the attention to detail in chemical measurements.

Greatest achievement
Being elected Chairman of the IUPAC Atomic Weights Commission at age 33 and being part of the team to draft the new definition of the mole.

Prediction
We live in the era of big data, which often favors quantity over quality. This has undesirable effects on the reliability of chemical testing results. I believe that metrology will guide us away from the reproducibility crisis in analytical chemistry.

Advice
Nurture your social skills and be someone others will want to work with.

Katelynn A. Perrault

Assistant Professor of Forensic Sciences and Chemistry, Laboratory of Forensic and Bioanalytical Chemistry, Forensic Sciences Unit, Chaminade University of Honolulu, Hawaii, USA.

Early inspiration
My career as a Professor allows me to balance three things I love: teaching, research, and outreach. Teaching helps me guide others to paths that bring them fulfillment. Research leads me to exciting discoveries that can improve our world. Outreach fosters a personal connection with my community through science.

Research
I develop advanced chromatographic strategies for detecting volatile organic compounds (VOCs) that comprise odors. In forensic science, we can use odor as an investigative tool. Though odor is invisible evidence that has long been overlooked, it has the potential to bring a vast amount of information to forensic casework in the future.

Objective
I hope to become internationally recognized as an expert in my field for the quality of my work and dedication to my discipline. I aspire to advance alongside the cutting-edge developments in separation science so I can continue to advocate for new technology implementation in the forensic science community.

Advice
Learn to wear different hats. Don't be limited by defining yourself as one single type of scientist. We live in a world where multidisciplinary

research, collaboration, and innovation are paramount to forward movement. Imagination does not grow when we constrain ourselves by a single perspective on something.

Nominator comment: "Kate's career thus far has been a tour de force, changing the way we understand odor evidence in forensic science. She leads dynamic programs in teaching, research, and outreach that are more effective than any I have seen before. Kate understands that quality science needs quality communication."

Kerri Pratt

Seyhan N. Ege Assistant Professor, Department of Chemistry, University of Michigan, Ann Arbor, Michigan, USA.

Early inspiration
As soon as I began analytical/physical chemistry research as an undergraduate, I was hooked. Since then, I've wanted to inspire students and use novel instrumentation to pursue complex environmental questions.

Research
My group conducts logistically and analytically challenging measurements of complex mixtures of atmospheric trace gases and aerosols in the rapidly warming Arctic, improving understanding of the interactions between ocean, atmosphere, snowpack and sea ice. Using chemical ionization mass spectrometry, we have measured several atmospheric trace gases for the first time in the Arctic.

Greatest achievement
Using chemical ionization mass spectrometry, we measured atmospheric molecular iodine in the Arctic atmosphere for the first time and showed through lab-in-the-field experiments that it is photochemically produced in the snowpack! This molecule is important for climate impacts associated with ozone (greenhouse gas) and atmospheric aerosols.

Advice
Follow your passions and don't be afraid to be different. I've pursued in-depth training in both mass spectrometry and atmospheric chemistry, and combined it with first-hand knowledge of Arctic science, putting myself in a unique position to advance our understanding of Arctic atmospheric chemistry.

Rawi Ramautar

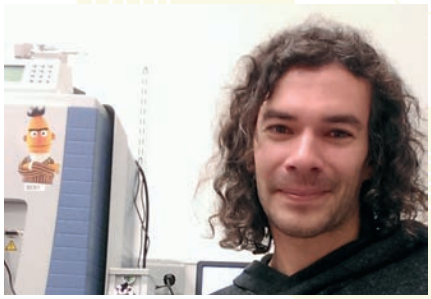
Assistant Professor, Leiden Academic Center for Drug Research, Leiden University, Leiden, The Netherlands.

Early inspiration
Trying to understand the molecular mechanisms of diseases is intriguing, and the use of reliable separation techniques is key for this purpose. Therefore, I decided to follow a career in the development of analytical techniques in metabolomics.

Greatest achievement
Enabling a deeper understanding of biological processes in sample-limited cases will constitute a real breakthrough in metabolomics. Therefore, I am happy that the Netherlands Organization for Scientific Research has recently chosen to fund this ambition of mine with highly competitive personal research grants, allowing me to set up my own research group.

Objective
I hope that the analytical technologies and workflows designed in my group for volume-restricted biomedical questions will be adopted in a clinical setting and used by medical practitioners for the prediction and/or diagnosis of diseases.

Advice
It is important to be a good team player, as research is a multi-disciplinary effort. Moreover, try to work with colleagues who are energetic and passionate about their research, and whose company you enjoy, as they will keep you motivated. Strive for the right work–life balance – family and friends matter!



Mikhail Savitski

Team Leader and Head of Proteomics Core Facility, European Molecular Biology Laboratory (EMBL), Heidelberg, Germany.

Early inspiration
My parents have PhDs in physics and always explained any questions I had in a fun and entertaining way. That drove me to seek out a path where conversations like this are the norm, and where the questions never stop.

Research
We study protein–drug, protein–metabolite, and protein–protein interactions, as well as regulation of disordered proteins, in the context of cellular perturbations and fundamental biological processes such as the cell cycle. To achieve that, we develop and apply novel proteomics technologies for measuring proteome-wide thermal stability and solubility.

Greatest achievement
To have developed a novel proteomics technology – thermal proteome profiling – that enables unbiased assessment of protein–drug interactions inside a living cell. Furthermore, we have shown that this technology uncovers a wealth of new biology in fundamental processes, such as the eukaryotic cell cycle.

Scientific heroes
Alexander Makarov, the inventor of the Orbitrap mass spectrometer. His work has transformed the proteomics field. He is also an incredibly good person and a great inspiration for people in the field.

Nominator comment: "Mikhail has made numerous groundbreaking contributions to the field of proteomics. In particular, thermal proteome profiling has had a significant impact on drug discovery."

Emma Schymanski

Associate Professor and Head of the Environmental Cheminformatics Group, Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg, Belvaux, Luxembourg.

Research
"Big data for small molecules" – non-targeted (mass spectrometry), cheminformatics and data analysis to identify small molecules in complex samples and apply this to tackle key questions in environmental, metabolomics, medical and forensics research.

Greatest achievement
Helping build and shape community thinking by publishing a well-received viewpoint article (DOI: 10.1021/es5002105) that has influenced an entire field, changed the way scientists consider and report identifications, become a de facto standard and, best of all, stimulated countless constructive discussions on future improvements.

Scientific heroes
The work of Antony J. Williams (currently USEPA) has inspired me for almost 20 years and it is a great privilege to collaborate with him to make (environmental) chemistry more open to the public and enable new analytical and cheminformatics approaches.

Prediction
As data science matures, we will see a revolution in the integration of analytical data with model-based predictions. Once non-target data analysis happens at the speed of data acquisition, new worlds of opportunity will open up for big concepts such as real-time monitoring, personalized medicine or predicting ecosystem trajectories.

Danilo Sciarrone

Associate Professor in Analytical Chemistry, CHIBIOFARAM Department, University of Messina, Messina, Italy.

Early inspiration
Since my student days I have been fascinated by mass spectrometry and chromatography, in particular by the multidimensional techniques that went on to become the focus of my career.

Research
The development of multidimensional chromatographic techniques coupled to the most innovative MS analyzers (QqQ, HRToF, IRMS) and the use of hyphenated LC and GC approaches for preparative purposes (LC-MDGC-prep). The aim is to collect highly pure components for structure elucidation and biological tests.

Greatest achievement
At the 2012 International Symposium on Capillary Chromatography (ISCC), I was presented with the Leslie Ettre Award, given to a scientist aged 35 or below for the most interesting original research in capillary gas chromatography in environmental and food safety.

Scientific heroes
I owe much to my mentor Luigi Mondello and key figures in the field like Pat Sandra, who inspired me and showed me how to face the challenges of research.

Hong Heng See

Associate Professor, Department of Chemistry, Faculty of Science, University of Technology Malaysia, Johor, Malaysia.

Early inspiration
I truly care about helping and sharing knowledge with people, and this career allows me to do that.

Research
Electrified sample preparation techniques in combination with chromatographic, electrophoretic, and microfluidic separation approaches.

Greatest achievement
Hooding my doctoral students upon the completion of their doctoral degree.

Scientific heroes
It has to be Michael Breadmore, an inspiring analytical scientist who transforms great ideas into reality, and an excellent mentor who always goes above and beyond to provide guidance to the scientists he mentors.

Jacob Shelley

Alan Paul Schulz Career Development Professor of Chemistry, Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, New York, USA.

Early inspiration
My excellent research mentors during my undergraduate degree, Diane Stearns and Jani Ingram, gave me the freedom to fix and tinker with instrumentation.

Research
We are developing new tools and approaches for mass spectrometry to simplify analyses and/or expand the range of detectable species. This includes everything from portable/fieldable atomic mass spectrometry to ubiquitous ionization sources for elemental, small molecule, and biopolymer detection to multimodal chemical imaging.

Prediction
The development of robust, easy-to-use, and inexpensive portable mass spectrometry will have a profound impact on analytical science, and society in general.

Advice
Work hard and stay focused, but more importantly, enjoy what you do.

Nominator comment: "Shelley has become world-renowned for his work in developing, testing, and application of novel plasma-based ion sources for mass spectrometry. One such source, the solution-cathode glow discharge (SCGD) has been found to be useful for a range of samples and to produce information ranging from elemental and isotopic composition, to molecular fragmentation, to peptide sequencing."

Hiroshi Tsugawa

Researcher, RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa, Japan.

Research
Computational mass spectrometry and computational metabolomics.

Greatest achievement
The development of MS-DIAL and MS FINDER packages.

Scientific heroes
Oliver Fiehn, UC Davis.

Objective
I want to better understand the mass fragmentation of small molecules to deepen our understanding of metabolism.

Prediction
The complete prediction of mass fragmentations, at least in some metabolite classes.

Advice
If you want to work in mass spectrometry-based omics science, learn programming.

Nominator comment: "In my laboratory, Hiroshi is referred to as 'genius'. He single-handedly upended the way untargeted LC-MS and GC-MS data processing is handled by programming MS-DIAL, software that is now used across the globe. He also programmed MS-FINDER, the first software that predicts mass spectra from rules and that integrates H-rearrangement in the algorithm."

Muhammad Farooq Wahab

Research Engineering Scientist-V, Department of Chemistry & Biochemistry, University of Texas at Arlington, USA.

Early inspiration
The question of how to determine the elemental composition of materials fascinated me as a young student. I collected hundreds of classic texts, including Hillebrand's "Inorganic Analysis" and Feigl's "Spot Tests" – books that got me addicted to analytical chemistry. At home, I did spectroscopy experiments in my mother's shoeboxes, and eventually published them.

Greatest achievement
Achieved world's fastest separations in 0.5-1 cm homemade columns, and developed "peak processing" mathematics. This allows chromatographers to operate columns above their peak-capacity, reducing long separations to a few seconds with intact quantitative information even when peaks partially overlap.

Prediction
3D printing of high-efficiency columns with custom chemistry and low-cost, high-resolution MS are in the foreseeable future. Coupling this with multidimensional chromatography would facilitate biological analyses, where millions of elusive molecules are to be discovered.

Advice
Don't be afraid to make mistakes –this allows you to think outside the box, and science has an excellent self-correction mechanism.

Nominator comment: "He is a brilliant young research scientist – few have his ability to formulate experiments to better understand chromatography and separation science."

Caroline West

Associate Professor, Institut de Chimie Organique et Analytique, University of Orleans, ICOA, France.

Research
I have not yet finished exploring supercritical fluid chromatography (SFC). This is an exciting era for SFC, with many people getting involved coming from different application fields, which is raising new questions and challenges.

Scientific heroes
The innovators, those who dare to think differently. Science is not a religion – every bit of knowledge lasts only until someone finds a new truth.

Objective
To do something that matters. I hope that I can propose something that will be useful to people.

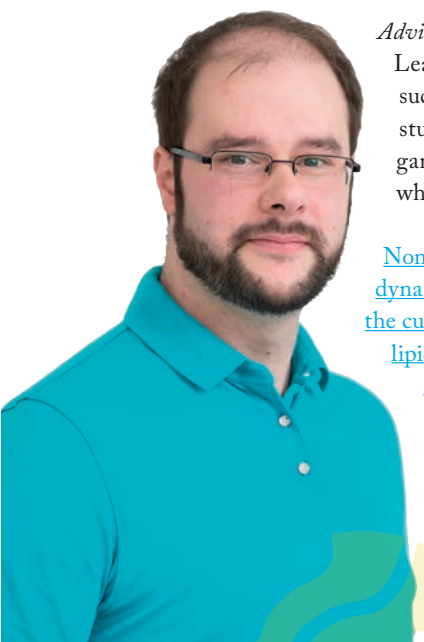
Advice
Be modest in your achievements, and learn about the work of others before pretending to novelty.

Nominator comment: "Caroline has developed many tools for the understanding of supercritical chromatography and is a member of the University Institute of France, which is a high distinction."

Michael Witting

Research Scientist, Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, Neuherberg, Germany.

Research
Developing analytical methods for the analysis of metabolites and lipids from single Caenorhabditis elegans (959 somatic cells). Such methods will enable me and other scientists to study the metabolic heterogeneity of an otherwise isogenic animal to learn more about metabolism and its regulation.



Advice
Learn from both your failure and your success. All great scientists started as students and had to learn how to play the game. Do it your way and be authentic in what you are doing.

Nominator comment: "Michael is a dynamic young scientist working at the cutting edge of metabolomics and lipidomics. He is developing new methods for the analysis of the C. elegans metabolome and lipidome, as well as working on new approaches to data analysis."

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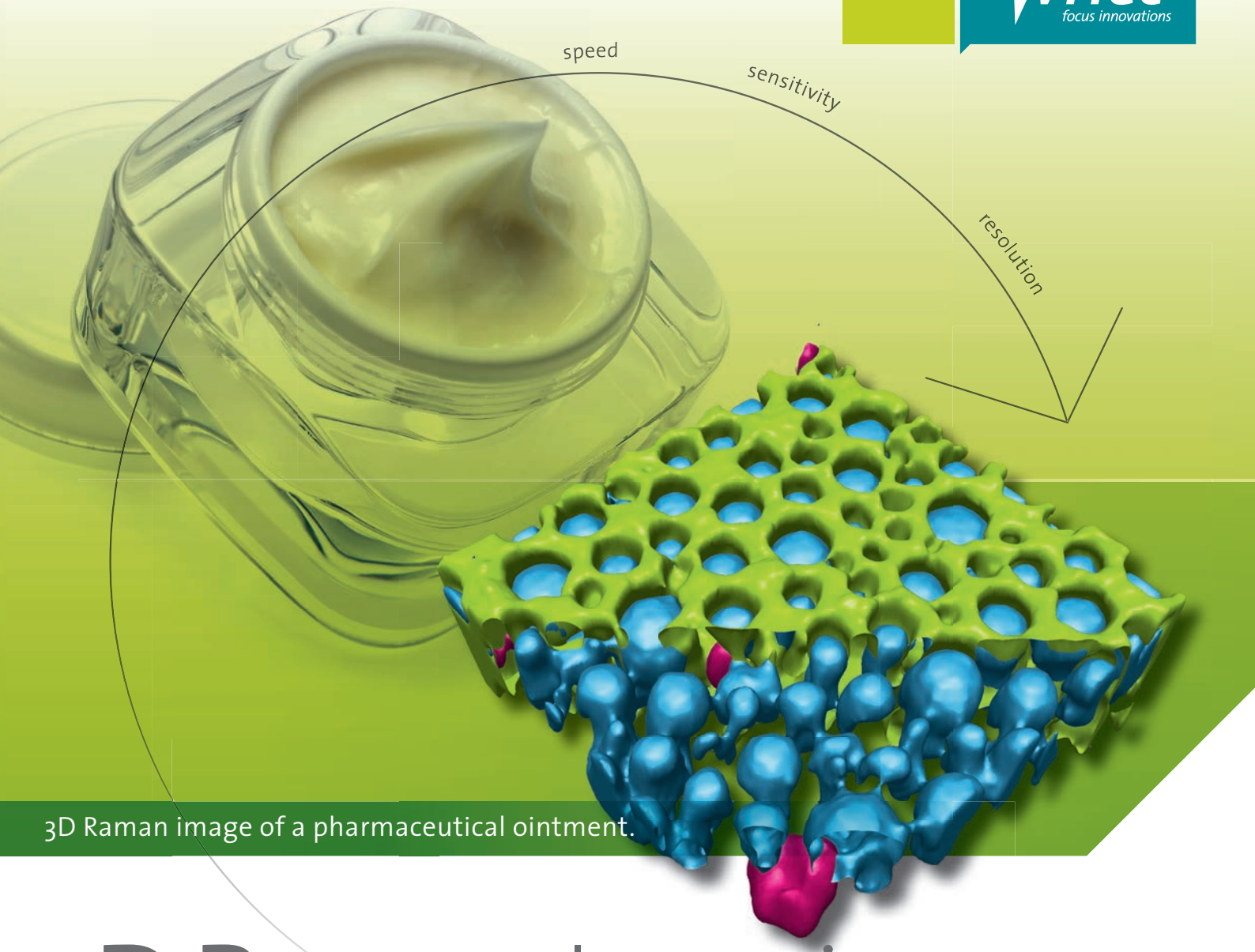

3D Raman image of a pharmaceutical ointment.

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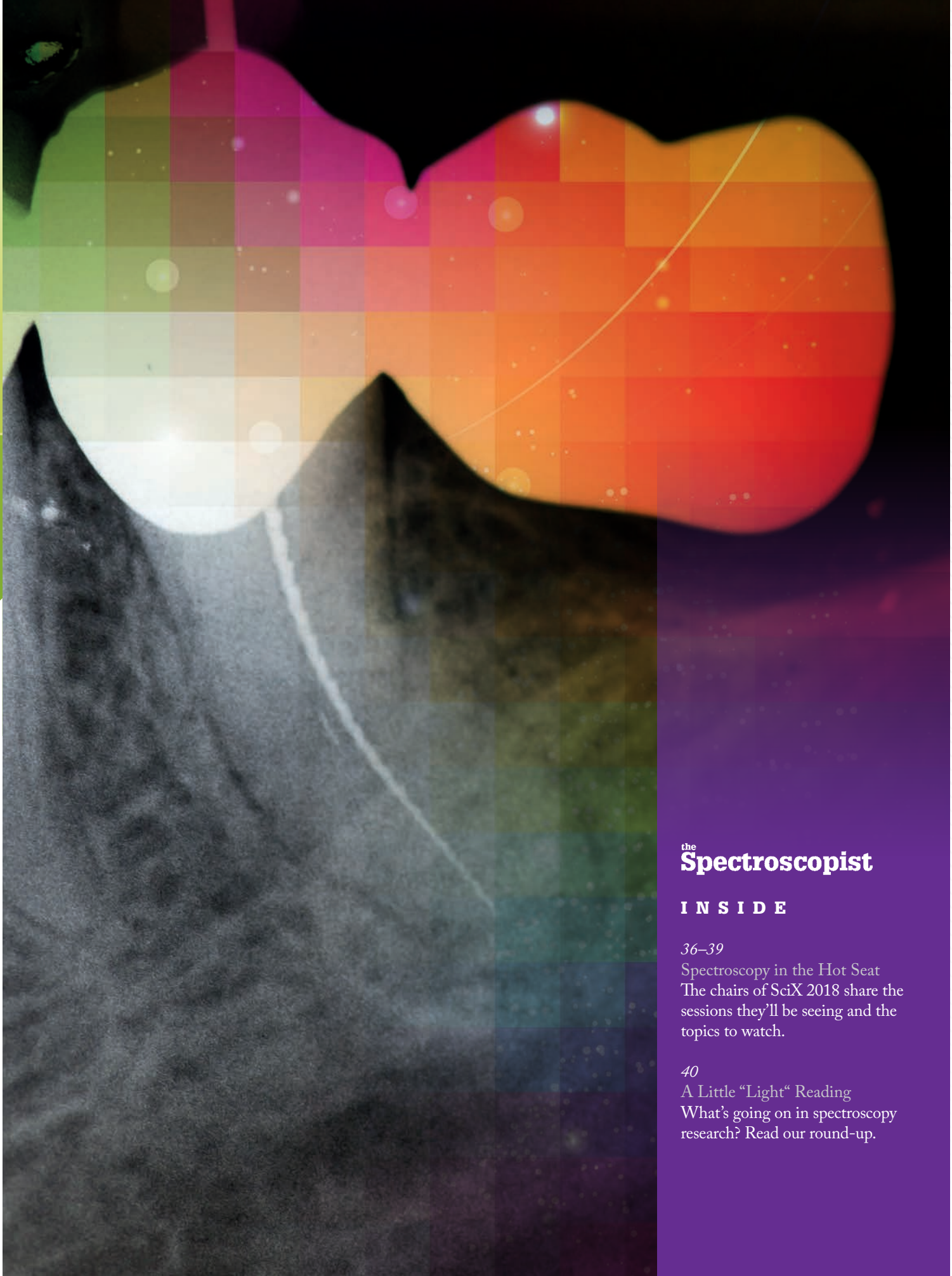


the Spectroscopist

INSIDE

Spectroscopy in the Hot Seat

SciX 2018 – held in Atlanta – showcases cutting-edge research in the spectroscopic arena and demonstrates the impact of the technology on diverse fields. Here, several SciX chairs "pull up a pew" and share their tips for getting the most out of the conference – and their insights into the future of spectroscopy.

Process Analytical Technology

Chair: Jim Rydzak, Founder, Specere Consulting, New York, USA.

Must-see sessions

I anticipate that "Enabled Flow Chemistry and Continuous Manufacturing," and "Modeling for Continuous Manufacturing" will be highlights of the PAT sessions. These offer the cutting-edge application of in-process on-line spectroscopy to continuous manufacturing practices, which is beginning to gain traction in the pharmaceutical area.

I am also really looking forward to the Speed Mentoring session (Monday 22, 12:15-1:30, Room A602) – a fun, fast-paced session that allows young scientists to talk to over a dozen spectroscopists from various industry, academia, and government labs to get an understanding of what it's like to work in those areas. These interactions will be a wonderful networking opportunity for job hunting or just getting a better understanding of life as a spectroscopist, and could even be the basis of an ongoing mentoring relationship. Register at members.coblentz.org to take part and receive a free boxed lunch.

I'll also be attending:

- Workshop on PAT: Out of the Lab and into the Line.
- Charles Mann Award session on the Driving Forces Behind the Growth of Raman Spectroscopy
- Celebrating 60 years of Spectroscopy by the Society of Applied Spectroscopy

After hours

Be sure to bring your favorite sci-fi costume to wear to the Wednesday night Gala – who said spectroscopists were boring?

Chair: Xiaoyun (Shawn) Chen, Research Scientist, The Dow Medical Company, Midland, Michigan, USA.

Topics to watch

This is the fourth year we have organized a session on Industrial Applications of Vibrational Spectroscopy. Our original motivation was very simple. There were many SciX talks from academic groups, but the limited number of talks from the industry tended to be heavily focused on (bio)pharmaceutical companies. Despite their important role, you could count the number of talks from the chemical industry on the fingers of one hand. Organizing these sessions allows industrial speakers to showcase their research work to the outside world and learn from each other and the wider community.

These sessions are tough to organize as those industrial speakers who do breakthrough research often cannot get approval for external release, but over the years we have been lucky enough to feature spectroscopists from industry-leading companies including Eastman, Stepan, DuPont, Infineum, and Dow Corning.

Must-see sessions

On Thursday, October 25, we will have speakers from Dow, 3M and Chevron to present on topics ranging from machine learning, to quantification of hydrocarbon in soil, to real-time reaction monitoring.

Raman Spectroscopy

Chair: Duncan Graham, Head of Department, Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow, UK.

Topics to watch

Stimulated Raman scattering (SRS) – there's a real opportunity for SRS to take over where fluorescence has been used.

Must-see sessions

The Analyst Emerging Lectureship Award lecture by Wei Min is something I'm looking forward to a great deal. Min has been producing excellent data for many years now, pioneering the use of small, inert tags for use in cell imaging with stimulated Raman scattering (SRS), which is quite stunning to see. The accompanying award session dedicated to him will also be of interest.

Chair: Ian R. Lewis, Director, Marketing, Kaiser Optical Systems, Inc, Ann Arbor, Michigan, USA.

Must-see sessions

This will be the 22nd year I have organized/co-organized a session or symposium at FACSS/SciX. With such a vibrant and

established symposium, it's difficult to pick out individual presentations, although the sessions on Emerging Raman and SERS are consistently cutting-edge. Outside the Raman field and as someone who works in the application of spectroscopy to industry, the industrial sessions, including the SAS-sponsored PAT sessions, are of interest.

From a wider impact perspective, the ocean plastics and clinic sessions (as well as the plenary on ocean plastics) are topical and should be educational.

Networking

I am looking forward to the networking opportunities that I have as a member of the Coblentz Society, SAS, IRDG, ANACHEM, and RSC. In some cases, it has been a year since I have seen some of my international friends. The oral sessions, the poster sessions, and the exhibit give me a venue to start discussions and the evening networking opportunities allow time for these discussions to be concluded.

Contemporary Issues in Analytical Science

Chair: Rebecca Airmet, Airmet Editing.

Must-see sessions

One of the core missions of SciX is to foster unexpected connections between attendees, and the Contemporary Issues in Analytical Science section is always a great opportunity to move the science out of the lab and into the real world. The section represents the human counterpoint to the technical, measurement-driven topics of the overall conference.

This year's section embraces social topics, science advocacy and education, and development for early-career professionals. I'm most looking forward to this year's session on "Scientists Easing World Poverty", which focuses

this year on low-cost healthcare, especially for point-of-care diagnostics. This session always sparks new ideas and connections. If you're a student or in the early stages of your career, don't miss the "mini-workshop" and panel on speaking and presentation skills. Sessions devoted to the development of open source equipment, the impacts of 3D printing, and the role of citizen scientists also promise to be relevant across industry, academia, and even government. Every year, these narrative-driven sessions bring surprising information, passionate speakers, and opportunities to connect and collaborate across the boundaries of disciplinary silos, and this year will be no exception.

After hours

I always look forward to the Wednesday night Gala. It's a great opportunity to connect with old friends and meet new ones. Networking is one of the elements that sets SciX apart. Take advantage of these great opportunities!

Biomedical & Bioanalytical

Chair: Juergen Popp, Leibniz Institute of Photonic Technology, Jena, Germany.

Topics to watch

In my opinion, SciX is the best conference in analytical science. The organizers have put together a wonderful program and it is very difficult to choose a particular symposium or presentation – but since my own research focus is on biomedical Raman spectroscopy, I am particularly looking forward to the numerous Raman symposia, which showcase an immense range of applications of Raman, ranging from biology to ancient artifacts. A particularly exciting field of application is the diagnosis and therapy of infectious diseases. We recently founded the InfectoGnostics research campus in Jena, Germany, a public–private partnership for the development of new methods in infectious disease diagnostics (https://www.infectognostics.de/en.html), and the research campus will chair two very exciting symposia on this subject.

Another exciting topic will be Raman labeling. Raman spectroscopy, in particular fast coherent Raman imaging (CARS, SRS), allows the targeted observation of specific molecules (such as metabolites, lipids and amino acids) in combination with specific Raman tags. These Raman tags differ in size and multiplexing ability from fluorescent labels. Though fluorescence probes can often be larger than the labeled molecules, Raman tags are small modifications of the target molecules that do not change their functionality and do not affect the cells. The modifications can involve stable isotope labeling or the addition of a single molecular group with a large Raman scattering cross section (such as nitrile or alkyne groups). The combination of coherent Raman microscopy with multiplex Raman tags makes it possible to study a variety of small biomolecules with high specificity and sensitivity in living cells, at tissue level or even in vivo.

Must-see sessions

"Infectious Diseases. The Unmet Medical Need" and "Analytical Technologies for Infectious Diseases I: Molecular Methods." These will address the unmet needs in infectiology and modern analytical/diagnostic approaches. Alex van Belkum, R&D Director of bioMérieux, and one of the world's leading experts on infectious diseases, will give a lecture on tests for antibiotic resistance – one of today's most urgent public health threats.

Surface Plasmon Resonance

Chair: Jean-François Masson, Professor, Département de chimie, Université de Montréal, Quebec, Canada.

Topics to watch

This year's plasmonic program at SciX will feature an outstanding group of established leaders and rising stars in the field. Attendees will have the chance to discover the latest in the synthesis of new plasmonic materials and their use in a series of important biomedical, clinical, environmental and industrial applications. These applications are rapidly reaching a maturity level, which means technology transfer is on the horizon. Plasmonics are poised to have a much broader reach outside the realms of academia in the near future.

Mass Spectrometry

Chair: Glen Jackson, Co-Editor-in-Chief, Forensic Chemistry and Ming Hsieh Distinguished Professor, Forensic and Investigative Science, West Virginia University, Morgantown, West Virginia, USA.

Must-see sessions

SciX 2018 provides an amazing opportunity to see some of the highest-impact mass spectrometrists in the USA. The mass spectrometry section comprises sessions organized by leaders in mass spectrometry who are based in Georgia or its neighboring states. The theme of the mass spectrometry (MS) section is "Top-Down and Intact MS Analysis". Facundo Fernandez from Georgia Tech is organizing a session

on "Advances in MS Ionization." Ronghu Wu, also from Georgia Tech, is organizing a session on "MS-Based Protein Analysis." Leslie Hicks from UNC, Chapel Hill, is chairing a session on "Activity-Based MS", and Lissa Anderson from the National High Magnetic Field Lab in Tallahassee, Florida is chairing a session on "Intact Protein Analysis." Finally, Jonathan Amster from Georgia University will be chairing a session on "Native Mass Spectrometry". This latter session, on Wednesday morning, features presentations by Joseph Loo from UCLA, Brandon Ruotolo from U. Michigan, Jon Amster, Francisco Fernandez-Lima from FIU and Henry Shion from Waters Corp. In addition to the other MS sessions, this session will be a great opportunity to see cutting-edge research by some of the world leaders in top-down and intact protein analysis.

Atomic Spectroscopy

Chair: Jorge Pisonero Castro, Department of Physics, Faculty of Science, University of Oviedo, Oviedo, Spain.

Must-see sessions

This year, I am looking forward to attending the sessions on Atomic Spectroscopy, as well as some related to LIBS. In particular, I am interested in new developments related to solution cathode glow discharge, FAPA sources, and microwave plasma sources. I am also very keen on new methodologies for fast elemental imaging using LIBS and LA-ICP-MS.

Topics to watch

- Fast high resolved elemental imaging using LIBS and LA-ICP-MS with probable new applications in biochemistry, geology and material science.
- Robust microwave plasma sources for multiple applications, including elemental analysis, CO_2 conversion, etc.
- Portable devices for fast liquid analysis based on solution cathode glow discharge.
- New software and hardware development for multi-elemental analysis of nanoparticles, including ICP-TOFMS.

Pharmaceutical Analysis

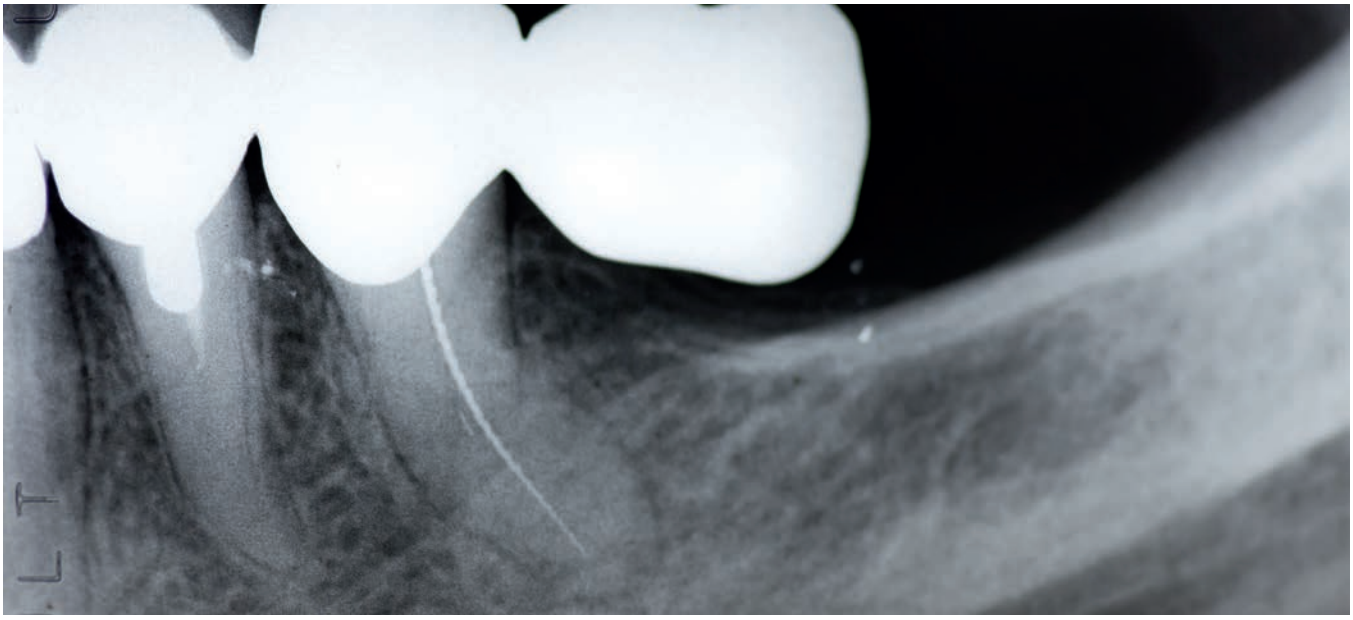
Chairs: Anna Luczak and John Wasylyk, Scientists, Bristol Myers Squibb, New Brunswick, New Jersey, USA.

Must-see sessions

SciX 2018 promises to meet – and exceed – expectations yet again! This year we have increased the number of sessions in the Pharmaceutical Analysis section from 9 to 11, with a heavy emphasis on biopharmaceuticals. There are presentations by top speakers from industry and academia, covering topics from pharma/biopharma counterfeits and real-time fermentation monitoring, to advances in aggregation tracking and chiral analyses. On a personal level, we are looking forward to sessions on some of our favorite topics, such as Raman, PAT, and Chemistry in Art and Archeology – the challenge at SciX is trying to squeeze them all in! The only "rest" we get is during the many networking opportunities, which always seem to energize us and provide an excellent platform to catch up on recent advances.

Top tip

Make sure you plan your day using the SciX app. Bring your most comfortable footwear... and perhaps download another app to count your steps!



A Little "Light" Reading

Presenting the latest spectroscopic research in bite-sized chunks

Root of the Matter

A recent proof-of-concept study analyzed the impact of sodium hypochlorite – the medication of choice for root canal therapy – on dental collagen. FTIR spectroscopy confirmed that the compound causes degradation in the collagen structure. Another reason to take good care of your teeth…

Read the paper: http://bit.ly/2NfM3e4

Bad Blood

Raman continues to make its mark in forensic science; Igor Lednev and Kyle Doty (University of Albany, New York, USA) successfully distinguished between chronological ages of blood donors in a new preliminary study. Unlike sex or race, age is something that clearly cannot be determined through DNA profiling.

Read the paper: http://bit.ly/2NhW8H9

Lucky in Lava

Spectroscopy took a dive lately, when researchers used LIBS to discriminate between samples of rock taken from various volcanoes. Able to identify different regions and sources, handheld LIBS could be a viable option in the field when analyzing and dating geological samples.

Read the paper: http://bit.ly/2NhuF8L

To the Bone

Vanderbilt University Medical Center researchers have successfully used Raman spectroscopy to analyze collagen integrity in bones – meeting the need for a non-destructive means to diagnose brittle bone disease.

Read the paper: http://bit.ly/2NfHMXV

Free-from Fries

When the chips are down… it looks like spatially resolved spectroscopy can detect it. Lien Smeesters and his colleagues from the Vrije Universiteit Brussel have developed a new laser scanning technique to find out which potatoes have the lowest amounts of acrylamide – making them most suitable for the production of fries. The technology can scan tons of potatoes per hour.

Read the paper: http://bit.ly/2P4skj1

Baby Brains

MRI scans can check for brain damage in newborn babies, but doctors often have to wait several days to perform them. However, a team at University College London have discovered a possible alternative that allows earlier screening and treatment – broadband near-infrared spectroscopy. A clinical trial will soon be underway.

Read more: http://bit.ly/2P822wo

Find it in Your Heart

Could NIR spectroscopy identify patients at risk from angina and acute coronary syndrome? When combined with intravascular ultrasound (IVUS), a team headed by Ron Waksman (MedStar Heart Institute) discovered NIRS was capable of identifying lipid-rich plaque, which is associated with increased risk of certain cardiovascular diseases.

Read more: http://bit.ly/2P5PuWh

Heroin – rapid identification for immediate action!

ID Kit and Mira DS handheld identification system

1. Apply sample onto paper strip
2. Insert into Smart SERS attachment
3. Unambiguous result at the touch of the screen – that's it!

ID Kit was developed with the help of Criminal Forensic Laboratories in the US and enables instant identification of heroin and other opioids, even in complex samples.

Watch a demo on **metrohm.com/ID-Kit**

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Industrial Revelations: Theo Jelink, AkzoNobel Chemicals

In our ongoing series championing scientists in industry, we look at one chromatographer's experience of innovation and knowledge transfer in the field of specialty chemicals.

Theo Jelink has worked at AkzoNobel Chemicals for almost 40 years. After a stint in the army, a series of speculative letters to chemical companies saw him gain a position in the Research, Development and Innovation (RD&I) Department of AzkoNobel, where the chance to experiment with multiple analytical tools soon had him hooked. Here, he tells us more about working with cutting-edge tech and the collaborative culture at the company.

What are the advantages of working in industry?

It is very challenging, but highly enjoyable. The scope of my company is broad and we have sites located all over the world, with colleagues from America to Japan, from Sweden to Africa. There are no borders these days with modern communication. Within our RD&I group, I come into contact with all kind of analytical techniques – challenging projects can often only be solved by multidisciplinary teams. Having close contact with our

"For me, the most interesting projects these days are those that implement 'green' technology in our processes."

customers all over the world gives me the chance to meet people from other cultures, so I've ended up with a large, international network. I am also directly involved in the practical implementation of the solution within each project, which is a real highlight for me.

How would you characterize the culture in your area of work?

It is very open – a result of working in a real team-oriented environment. We have plenty of opportunities to keep up-to-date with developments in other fields, or with other techniques, via workshops, lectures, knowledge cafes, and so on. The chance to continually improve on your knowledge and develop your skills is positive and very important.

Tell us about your day-to-day…

It involves providing chromatographic solutions for incoming projects companywide, but also advising different customers about implementing chromatography systems in their laboratory or processes. I also try to implement chromatography as an on-line or at-line tool for many processes, and try to take the analytics to the customer – instead of bringing the customer to our lab.

Another responsibility for me is data management; I implemented the current data system in our laboratories and am now system administrator, responsible for maintaining and updating our system. I am currently rolling out the system in different locations across the site.

It is also my role to keep up-to-date with developments in my scientific field through regular and intensive contact with instrument suppliers – and this can lead to collaboration for the development of new instruments and testing prototypes. When it comes to potential investment opportunities for new technologies and instruments, I am often called on to advise about the best fit – based on testing and experience.

Can you give us an example of a collaborative project you've worked on?

Several years ago, I got a request from a specific business unit of our company to develop an instrument, one which would control a particular process, and perform analysis both at percentage level and at ppb level, simultaneously and at high speed. But the most challenging

factor was it had to be controlled by someone without any knowledge of chromatography; the system needed to run unattended so it had to be fully automated. It took me several years to develop a special capillary analytical column and an automated setup, and it even involved a collaboration with glassblowing technicians and electronics departments. Ultimately, we were able to produce an instrument that fit every one of the stringent requirements.

"I get enjoyment from this job every day – I'd happily continue until the day I retire!"

What has been your biggest success so far?

One of my most successful projects was related to environmental analysis in one of our plants. I developed a method for personal air sampling to monitor the exposure of people in a plant to potentially toxic chemicals. The work resulted in a much better working environment for the operators, and great job satisfaction for me.

Are you working on any interesting projects at the moment?

For me, the most interesting projects these days are those that implement "green" technology in our processes. Our code of conduct means that I am not allowed to share more about these developments right now, but the fact they are both necessary and challenging makes them exciting to work on.

Do you often get a chance to explore new initiatives?

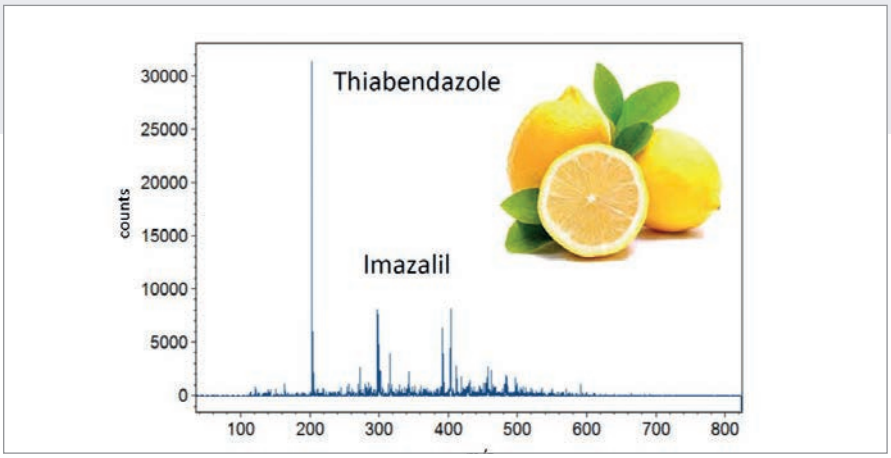
In our department, we have a budget for development, which allows us to investigate trends in our scientific area. We also generate ideas through collaboration with instrument manufacturers and "brainstorming" sessions with other users worldwide. An example of this is the "Voice of the Customer" event organized by Thermo Fisher Scientific; customers from all over the world met in Milan to discuss the function of the autosamplers of the future. Another example is a collaboration with C2V (now Thermo), which makes micro-GCs using MEMS-based technology. We worked with them to test a prototype and made suggestions to improve the instrument. It feels good to be at the cutting edge!

How easy is knowledge transfer between industry and academic research environments?

It is sometimes difficult to organize because of the differences in culture and attitudes to "knowledge-sharing" in different countries and organizations. For example, within our company we have a "code of conduct" that each person has to sign, a way of preventing people sharing confidential details with people outside the organization. Most of the time, on-site cooperation is the best way to get things done.

What does the future hold for you?

My job continues to provide many challenges and a broad scope of projects. I have contact with a large network all over the world, and a great team to work with on-site. I get enjoyment from this job every day – so all I know is that I'd happily continue until the day I retire!



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

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

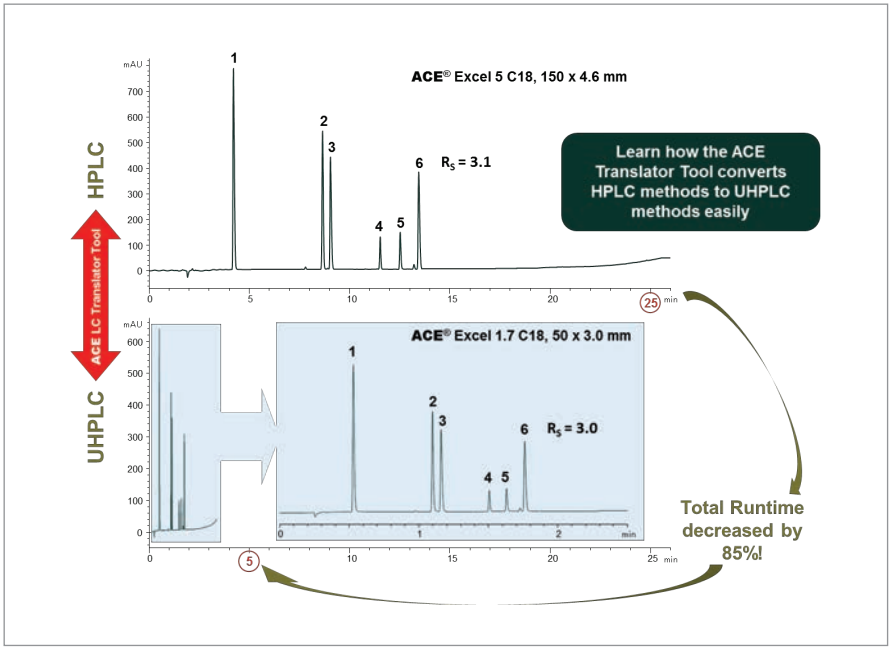
A case study for residual pesticide screening on fruits and vegetables is reported. All produce was purchased from a local market in San Jose, California and immediately analyzed by TD-ESI coupled to the Portability™ mass spectrometer without any sample preparation. The portable analyzer was able to detect ppm levels of pesticides such as thiabendazole, imazalil, flutolanil, and permethrin. Featuring light weight and compact size, BaySpec's novel mass analyzers based on linear ion trap technology are the most sensitive portable devices available on the market with parts-per-trillion detection sensitivity. These extremely compact instruments are simple to operate and maintain, and they are ideal for a variety of bulk or trace on-site detection in real time. Learn how you can bring the lab to the sample with portable analytical tools from BaySpec by reading our educational application note for pesticide screening of produce.

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

Practical Ultra-High Performance Liquid Chromatography (UHPLC)

The potential to increase chromatographic efficiency and resolution along with significant savings in solvent cost and analysis time have driven the uptake of UHPLC to many application areas. This discussion outlines how instrument and column technologies continually evolve to meet the requirements of UHPLC, providing new options for chromatographers. Example data are provided to show the high speed and high resolution options of UHPLC. Advanced topics such as HPLC to UHPLC translations using free downloadable tools are also covered.

Read the full app note at
http://tas.txp.to/1018/app102



Top: separation of six peptides on an ACE Excel 5 C18 HPLC column installed on an HPLC instrument. Bottom: the same separation translated to an ACE Excel 1.7 C18 UHPLC column installed on a VWR Hitachi ChromasterUltra Rs UHPLC system.
The method translation was achieved using the ACE LC Translator Tool. Mobile phase: A = 0.05% TFA in H2O, B = 0.05% TFA in MeCN. Temperature: 60 °C. Detection: UV, 220 nm. Sample: 1. Gly-Tyr, 2. Tyr-Tyr-Tyr, 3. Val-Tyr-Val, 4. Oxytocin, 5. Angiotensin II, 6. Leu-enkephalin.

Comprehensive Drug Metabolism Using Electrochemistry-MS (EC-MS)

Fast mimicking and prediction of oxidative metabolism "in electro" as a comprehensive technique to analyze in vivo and in vitro drug metabolism

By J-P. Chervet[1], N. Reinhoud[1], M. Eysberg[2] and N. Santiago[2]
[1]Antec Scientific, Zoeterwoude, Netherlands
[2]Antec Scientific (USA), Boston, MA, USA

So far, most drug metabolism studies have been based on traditional in vitro techniques initially using liver microsomes, and at later stages in vivo techniques using rodents and finally human.

Both techniques are time-consuming and can be very costly. In addition, they require isolation from the biological matrix (i.e., microsomes, urine, plasma) with the risk of sample loss due to adsorption and/or binding to the cell membrane or constituents. Furthermore, conjugation reactions (Phase II reactions), such as adduct formation with glutathione, are difficult to perform in a controlled manner.

Recently, it has been shown that drug metabolites are formed instantaneously in an electrochemical cell, thereby mimicking the enzymatic Cytochrome P450 reactions that usually take place in the liver (Phase I reactions). By on-line coupling of an electrochemical reactor cell with MS (EC-MS) a drug compound can be easily oxidized in a precise and controlled manner within a few minutes, mimicking/predicting the oxidative drug metabolism to become a true biomimetic tool for enzymatic REDOX reactions.

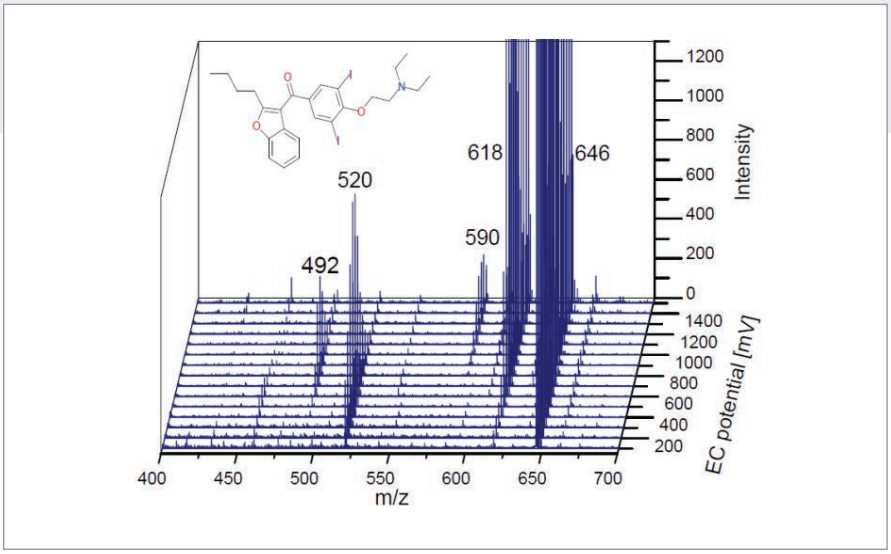


Figure 1. MS voltammogram of amiodarone m/z 646 and its major oxidative metabolites m/z 618, 590, 520 and 492 generated by on-line electrochemistry-MS using the ROXY™ EC system (Antec Scientific) equipped with µ-PrepCell2.0 and connected to an MS. Total experimental time < 15 min.

Why EC-MS in drug/xenobiotic metabolism?

Beside substantial cost and time savings, other advantages of an in-electro approach to metabolism studies result from the absence of any biological matrices. Only clean solvents such as MeOH, ACN or water with formic acid or volatile buffers are used, making the isolation steps obsolete and direct coupling with MS for identification possible.

In addition, the on-line coupling offers the possibility for the measurement of reactive and/or short-lived metabolites – sometimes very difficult, if not impossible, to perform with in vitro or in vivo techniques.

In Figure 1 a typical oxidative "fingerprint" of the drug compound amiodarone (antiarrhythmic agent) is shown. In this MS voltammogram, the signal intensity is plotted versus the m/z and the applied voltage of the electrochemical cell. Simply by increasing the voltage from 200 to 1600 mV all major metabolites could be generated in less than 15 minutes.

Conclusions

Both Phase I (i.e., oxidative metabolism), and Phase II (i.e., conjugation/adduct formation with GSH or proteins) can be performed easily using the Antec Scientific ROXY™ EC system.

Figure 2. ROXY EC system. From left to right: dual syringe pump with ROXY Potentiostat equipped with electrochemical cell (µ-PrepCell™2.0 or ReactorCell™).

With over 100 peer publications from academia and industry available, "in electro" using the ROXY EC system is a truly comprehensive EC-MS technique to in vivo and in vitro drug metabolism.

For more information see www.AntecScientific.com or scan

Molecular Weight Determination for Dextran 40/60/70 According to USP/ EP Monograph

A specific e-workflow in PSS WinGPC MCDS allows for calibration and molar mass determination for Dextran 40, 60 and 70 as stated by USP and EP.

By Wolfgang Radke, Daniela Held, Huub Bock and Peter Kilz

Dextran is used as a blood plasma volume expander or blood flow improver. The dextran molar mass is crucial for the success of the therapy.

PSS WinGPC UniChrom is a macromolecular chromatography data system (MCDS) that offers comprehensive solutions for the characterization of macromolecules with GPC/SEC/GFC, interaction polymer chromatography (IPC) and 2-dimensional chromatography (2D) supporting all multi-detection techniques. Specific e-workflows in WinGPC guide scientists through special tasks such as United States Pharmacopeia (USP) and European Pharmacopoeia (EP) recommended low-molecular-weight (LMW) heparin calibration and analysis, sieve curve and MW cut-off determination or gelatin-specific calibration and multi-area analysis.

The latest addition to the e-workflows in WinGPC is the molecular weight determination of dextrans. A specific routine allows for calibration and molar mass determination for dextran 40, 60 and 70 as stated by USP and EP. USP/ EP recommend aqueous size exclusion chromatography (SEC), with a specific dextran calibration to determine the molar mass information. Specific results for dextran samples include the weight average molar mass (M_w) for the whole dextran as well as for the fractions at 10 percent and 90 percent. USP additionally requires M^n and the polydispersity index (DI).

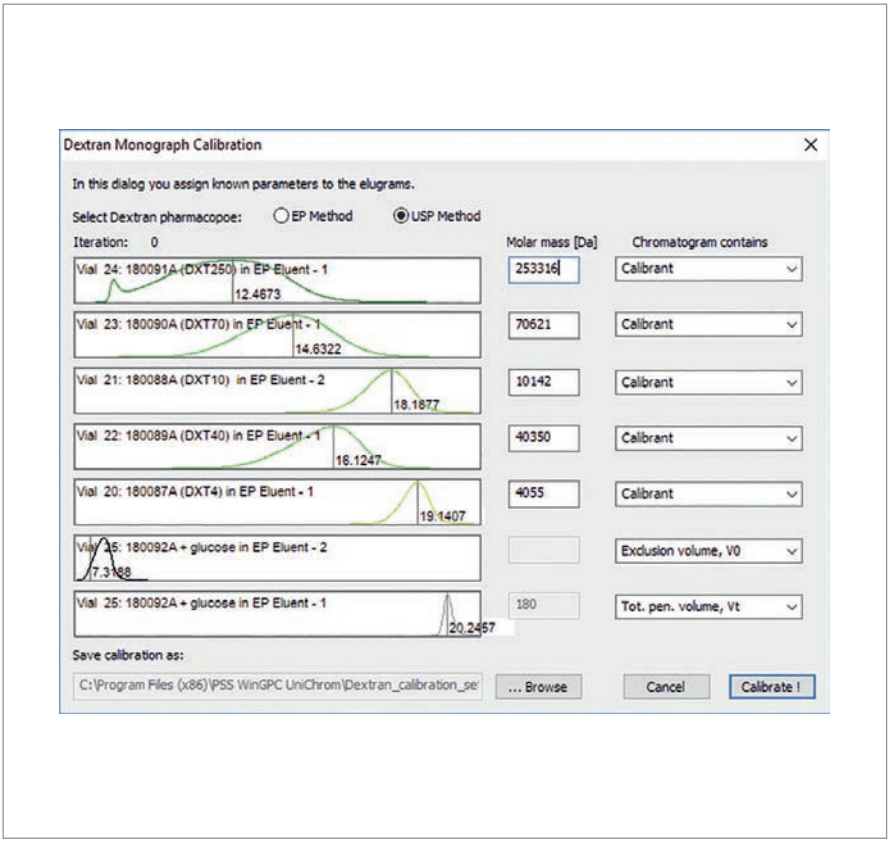


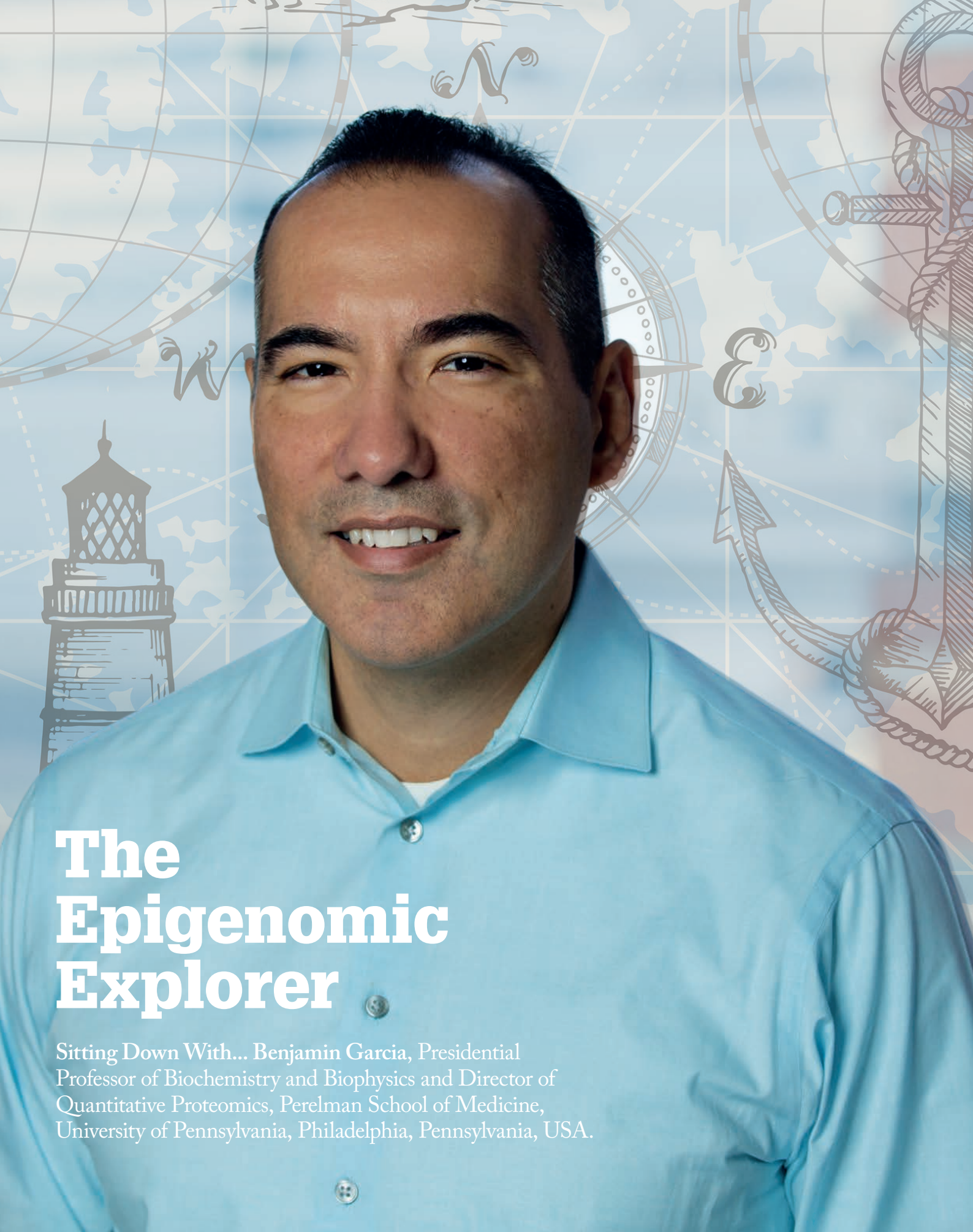
Figure 1. "Dextran Monograph Calibration" dialogue in WinGPC.

PSS WinGPC Software has a specific e-workflow implemented comprising data capture, specific dextran calibration, data analysis and compliant reporting. Regulated laboratories should opt for the WinGPC UniChrom Compliance Pack for FDA 21CFR11 support, including audit trails and electronic signatures.

The "Dextran Monograph Calibration" dialogue (Figure 1) uses five dextran standards of known molecular weights ranging from 4,000 to 250,000 Da, Glucose (180 Da, total column volume [V_t]) and a value for the V_0 (column void volume) to start the iterative non-linear regression fit based on the concept by Nilsson and Nilsson. As the monographs differ slightly in their requirements, scientists have to choose between the EP method and the USP method. If the data can be successfully fitted, a WinGPC calibration file is saved and a report is printed.

Recorded data of the verification samples (System Suitability, Performance) and unknown dextrans can then be evaluated using the calibration curve created above and a specific menu item. WinGPC will automatically determine three different areas for the full dextran, 10 percent eluted mass and 90 percent eluted mass.

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



The Epigenomic Explorer

Sitting Down With... Benjamin Garcia, Presidential Professor of Biochemistry and Biophysics and Director of Quantitative Proteomics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, USA.

Congratulations on receiving the 2018 Biemann Medal at ASMS! What does the award mean to you?

It's an amazing honor. Every person who has received this award has been an incredible pioneer in the field and has made significant contributions. I am overwhelmed to have my name on the same list as them, and to continue deserving my place on that list, I feel that I must still achieve more!

When you said, "It takes a society to raise a scientist," in your acceptance speech – what did you mean?

In any field – and especially in science – we achieve very little alone. To become independent and rigorous scientists with the vision to ask and answer important questions, we must be trained and mentored, supported and encouraged. I definitely couldn't have become the scientist I am without that support. Even now, I'm not doing it alone; I have a fantastic research group with scientists at all levels and from all backgrounds.

Many minority groups are underrepresented in science – how can we change that?

As a young scientist, not seeing people like you at faculty level can be discouraging. It's a "catch-22". We don't have enough senior scientists from underrepresented groups and so the next generation may not think it's an achievable goal. I cannot change the whole field, but I can work hard to bring diversity to my own lab. Diversity isn't just a worthy goal in its own right but hugely beneficial to our work – the most creative and productive times in my group have been when the lab has been at its most diverse.

Who have been your most influential mentors?

During my undergraduate studies at UC Davis, I met Carlito Lebrilla, who has been an amazing mentor – from that first day we met, right up to the present. I came into his lab as part of a summer undergraduate research program, knowing nothing about analytical chemistry – he engaged with me, and held me accountable. I really felt that I was part of the group. He also introduced me to several well-known scientists who went on to become mentors to me, such as Jack Beauchamp, who I worked for at Caltech. In graduate school, I worked with Donald Hunt, studying tandem mass spectrometry of complex biological mixtures. It was amazing to be around a scientist of that caliber – very few people have the vision he has. He is a great mentor and knows exactly how much flexibility and freedom to give you. By that stage, more was becoming known about histone modifications, but it was all bottom-up mass spectrometry, looking at a few modifications at a time. I knew we needed to take broader approach, so I applied for a postdoc in Neil Kelleher's group. Neil is an incredible, infectiously enthusiastic scientist, and it was the perfect training with him – both in top-down proteomics and in running a group. Lastly, David Allis (Rockefeller University), who just won the Lasker Award for his chromatin research, has been a collaborator, mentor and friend for a long time as well.

Why did you choose to focus on histones?

Quite simply, because they are such amazing proteins. I'm fortunate that the fields of proteomics and epigenetics have taken off and I'm in the crossroads of both. But I didn't have a master plan; I just kept studying what I was interested in, without thinking too hard about what would be "fundable" in future or whether I'd be able to build a career.

What upcoming projects are you excited about?

"The most creative and productive times in my group have been when the lab has been at its most diverse."

Fifteen years or more since the role of histone modifications in controlling gene expression was first suspected, we have certainly made progress, but there are still so many unanswered questions. I'm excited about taking our fundamental knowledge and applying it to health and disease by reprogramming a diseased epigenome with small molecule inhibitors or histone-modifying enzymes. I truly believe that is a feasible long-term goal. I use the analogy of a computer: the computer hardware is your genome, but no computer works without the software to control it, and the epigenome is that software. If a virus infects your computer, you can often combat it by resetting the computer to its original state. I think we're going to be able to do that in human disease states.

What do you hope to achieve in your career?

I won't judge my ultimate success on the scientific breakthroughs I make or the awards I receive – gratifying as it is to be recognized by my peers. Instead, when I look back on my career, I will judge myself on the impact I have on others. Seeing those I have trained and mentored take their place as leaders across multiple fields would be more satisfying than any award I could ever receive.

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