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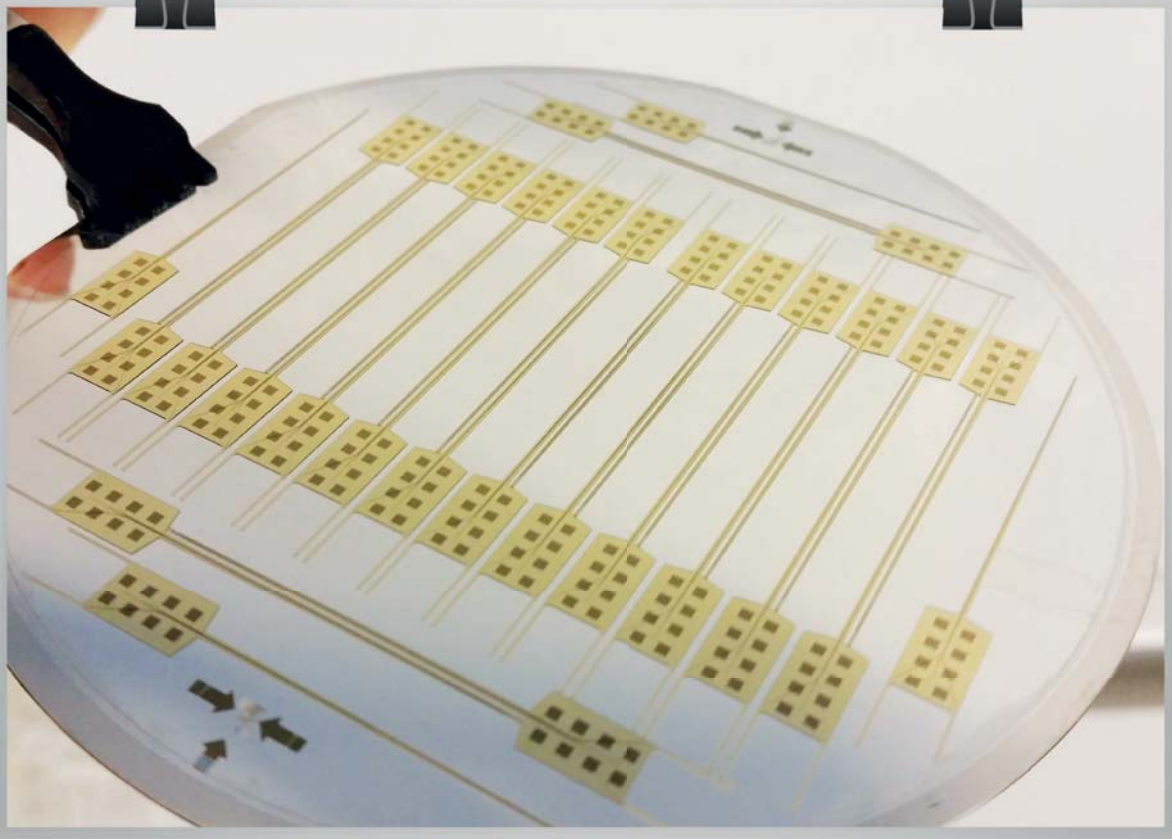

Mass Spec on the Brain

A new device incorporating a neural probe and analysis by laser-ablation inductively coupled mass spectrometry (LA-ICP-MS) allows the direct collection of extracellular fluid from the brain at high temporal resolution, and could open a window into the brain at the chemical level.

Credit: Guillaume Petit-Pierre

Reference: G Petit-Pierre et al., Nat Commun, 8, 1239, (2017).

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

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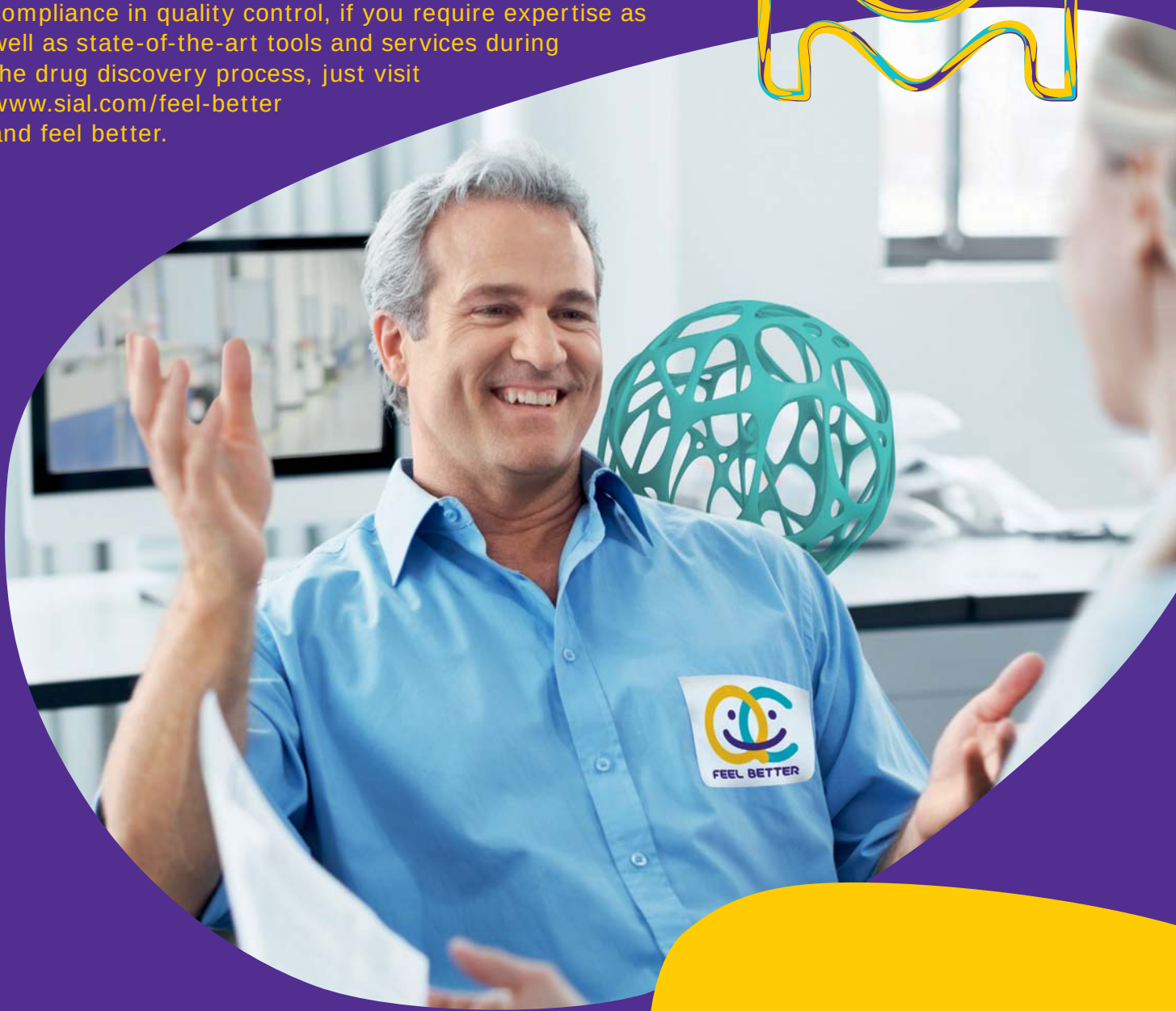

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A Recipe for Innovation

Curiosity, a desire to help others and a hefty dose of teamwork are essential ingredients for creativity.

In our final issue of the year, we reveal the winners of The Analytical Scientist Innovation Awards (TASIAs) 2017. As Content Director Rich Whitworth pointed out in our inaugural TASIAs in 2013, innovation can be a slippery critter (tas.txp.to/Elusive). Sure, it's the lifeblood of science, but what is it? And how can you achieve it? In search of answers, I've journeyed back through our archives to uncover the key ingredients for innovation, according to some of the greatest minds in analytical science…

"I'm easily distracted by shiny objects! I'm motivated by curiosity, and by the prospect of doing something new." – Kevin Schug

"I love a challenge, and if I'm told I can't do something, I'm all the more determined." – Barbara Larsen

"What makes a successful inventor? Unhappiness. Unhappiness with the status quo, including yourself. The same properties that make for successful poets."– R Graham Cooks

"In science, breakthroughs are very few and far between; most progress is incremental. Even a small improvement could be valuable. Look at a gas chromatograph in the 1970s versus one today – it's the same technology, but you wouldn't recognize the instrument." – Hernan Cortes

"A collaborator of ours said to me recently, 'I feel like a kid in a candy store!' And that's exactly the environment that we wanted to create – it encourages people to do great analytical science." – Ron Heeren

"I can follow my own ideas – I'm my own boss, and I can pursue my vision and favorite topics. It's the best job in the world." – Oliver Fiehn

"The thought of all the people who are being left devastated by Alzheimer's disease keeps me focused. It reminds me that we need to aim for more than just incremental improvements in our technology and analytical approach." – Renã Robinson

"What motivates innovation? Curiosity, with eventual utility as the propellant." - Purnendu (Sandy) Dasgupta

"[I want to] apply technology to make this world a better one." – Klaus Witt

It seems the recipe for innovation includes curiosity, intellectual freedom, and a desire to contribute to something bigger than yourself. Of course, having a bright idea is just the start of the process. Bringing a revolutionary concept to market requires a different set of skills, and so it is often industry scientists and instrument manufacturers who nurture ideas sprouting from research, shaping them into fully-grown products. You can see the results on page 20!

I wish you all a happy – and highly innovative – 2018!

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

Detecting Talent

Meet the 11-year-old who was named "America's Top Young Scientist" for her rapid lead detection device

"Imagine living day in, day out, drinking contaminated water with dangerous substances like lead," says Gitanjali Rao, in her video submission for the 'Discovery Education 3M Young Scientist Challenge' (1). Frustrated by the recent Flint water crisis, the 11-year-old spent three months working with mentor Kathleen Shafer and other scientists at 3M to develop a new lead detection system, to provide rapid and accurate water analysis.

Clearly, contamination events extend far beyond Michigan, with millions of people worldwide at risk of exposure to lead and other dangerous compounds. "There are over 5,000 water systems in the US alone with lead contamination issues," Gitanjali says. "Timely detection and preventative action can help mitigate the problem, but today it takes a long time, requiring chemical labs and expensive equipment."

Luckily, Gitanjali had a cheaper, quicker solution to propose based on nanotube sensors. The prototype comprises three parts: a disposable cartridge with a specially treated carbon nanotube chemical sensor, an Arduino-based processor with Bluetooth extension, and a smartphone to display results. She's named it "Tethys", after the Greek sea goddess.

How does the device work? Child's play! "When dipped in non-contaminated water, the arrays have no reaction to the lead, and resistance remains unchanged, showing safe water status," she explains. "When the same cartridge is dipped in contaminated water, the lead in the water reacts (with the arrays) to create additional resistance to the flow of current – which is measured by the Arduino processor and shown on a phone. The change in resistance is proportional to the degree of lead in water."

"I like finding solutions to real problems," Gitanjali says. "I hope this helps in a small way to detect and prevent long-term health defects of lead contamination for many of us." She also hopes that the device could be used to test for other chemical contaminants in potable water with further research.

Gitanjali has some words of wisdom for other kids (and adults) who are interested in a STEM career: "Just have fun with science and keep digging deep for solutions. If you do not succeed the first time, that's OK! There is never a limit to the number of tries it takes to accomplish a goal."

Anyone want to nominate this bright young thing for the next 40 Under 40 Power List?

Reference

1. *2017 National Finalist: Gitanjali Rao (2017). Video available at: http://bit.ly/2i8zxzl. Accessed November 27, 2017.*

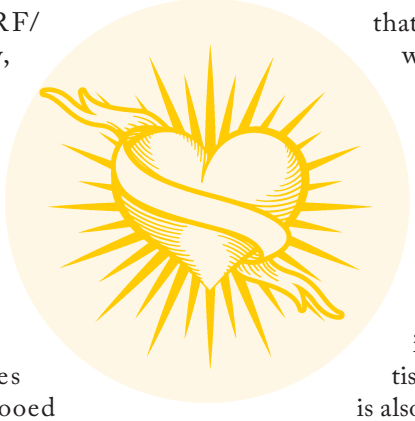
Think Before You Ink

Advanced mass spectrometry finds that tattoo ink can migrate to lymph nodes

With an estimated 30 percent of Americans now sporting at least one tattoo, going under the needle has never been so popular (1). But could the long-term effects of body art be more than skin deep? A study has shown that nanoparticles of tattoo pigments can travel from the skin to the lymph nodes, raising new questions about potential risks (2).

According to scientists from the German Federal Institute for Risk Assessment (BfR), safety concerns have been triggered by the increasing prevalence of tattoos. Earlier chemical analysis of tattooed skin has mostly been in vitro (3), but pigmented and enlarged lymph nodes have been noted previously in people with tattoos (4). The German researchers wanted to examine the phenomenon in more detail.

Using a combination of synchrotron ν-XRF/FTIR microscopy, MALDI-TOF-MS and ICP-MS, the BfR team analyzed skin and lymphatic tissue samples from four tattooed human cadavers down to 50 nm resolution, comparing them with samples from two non-tattooed individuals. They found traces of organic pigments in skin and lymph samples, as well as inorganic elements such as iron oxide and titanium dioxide.



While no impact on health has been shown, some of the compounds found are known toxins or carcinogens, and the authors stated (5), "People should be aware of the unknown risks that might come along with tattooing, rather than presuming that the colors are safe (5)."

In future experiments, the researchers hope to track pigments and heavy metals in other organs and tissues. Further research is also needed to determine whether the nanoparticles cause long-term health effects.

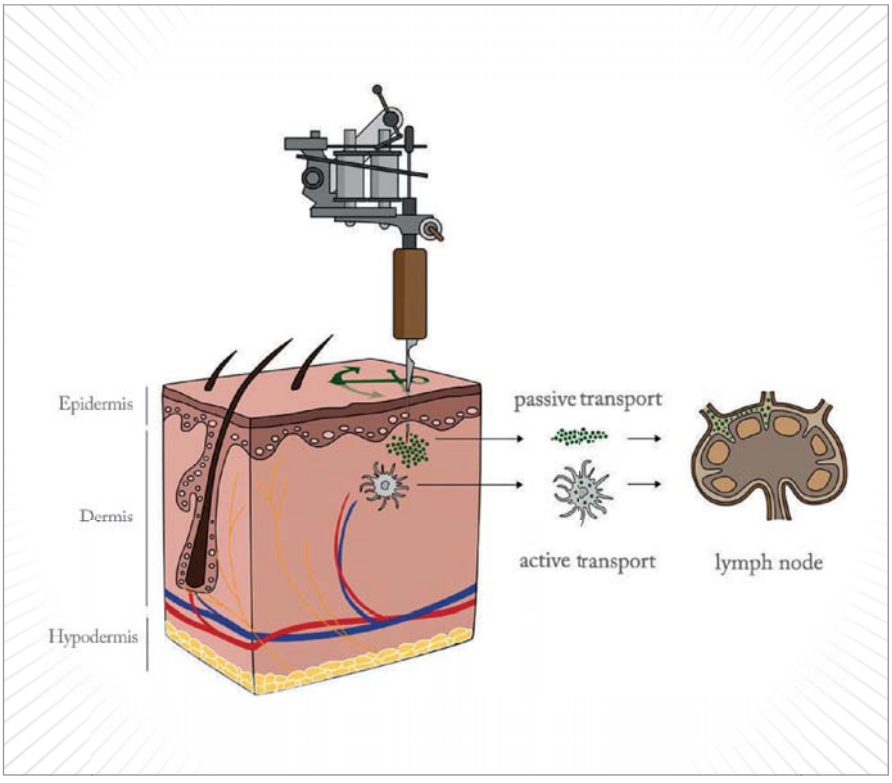


Figure 1. Tattoo ink particles can either be transported passively by blood and lymph or phagocytized and transported actively into regional lymph nodes, and remain present after healing.

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1. *"Tattoo Takeover: Three in Ten Americans Have Tattoos, and Most Don't Stop at Just One", The Harris Poll, (2016). Available at: http://bit.ly/1SQYy0D*
2. *I Schreiver et al., "Synchrotron-based ν-XRF mapping and μ-FTIR microscopy enable to look into the fate and effects of tattoo pigments in human skin", Scientific Reports, 7, 11395 (2017).*
3. *I Schreiver et al., "Identification and hazard prediction of tattoo pigments by means of pyrolysis—gas chromatography/mass spectrometry", Arch Toxicol 90, 1639–1650 (2016).*
4. *LL Anderson et al., "Tattoo pigment mimicking metastatic malignant melanoma", Dermatol Surg 22, 92–94 (1996).*
5. *Bundesinstitut für Risikobewertung, "Questions and answers on the study lead of BfR investigating the distribution of tattoo ink as nano-sized particles in lymph nodes", (2017). Available at: http://bit.ly/2AiiQdC. Accessed November 28, 2017.*

Destination: Hyphenation

Small but perfectly formed, HTC-15 will be held in the Welsh capital Cardiff. Here, we present our top picks for the 2018 symposium

For the second time in its history, the International Symposium on Hyphenated Techniques in Chromatography and Separation Technology (HTC) is coming to the UK.

The 2018 symposium boasts a fantastic array of speakers. Some of the biggest names in the field (including several Power List awardees) will be imparting their wisdom, while dedicated sessions and presentations give early career researchers their chance to shine. We're particularly intrigued by the sessions on Big Data and Green Separations, and keynotes by Caroline West, Luigi Mondello and Hans-Gerd Janssen. Read on for more presentations that caught our eye.

Day 1 (24 January 2018)

UPLC-MS for metabolic phenotyping: Advantages, assays and applications
Elizabeth Want, Imperial College London
Session: Advances in Clinical Analysis

Investigating the potential for improved temperature responsive separations in liquid chromatography
Mathijs Baert, Ghent University
Session: Interfacing and Ionization

The comparison of Unispray and Electrospray for the ionization of neuropeptides
Yannick Van Wanseele, Vrije Universiteit Brussel
Session: Interfacing and Ionization

Day 2 (25 January 2018)

Better living through (flavor) chemistry: Vacuum ultraviolet spectroscopy as a new tool for GC analysis of terpenes in flavors and fragrances
Alex Hodgson, VUV Analytics
Session: Separations by Shape: Instrumentation

Big data – when less is more
Benjamin Woolford-Lim, GlaxoSmithKline
Session: Big Data – What Do We Do With It?

Quantitative proteomics for molecular diagnostics of public health
Jack Rice, University of Bath
Session: Approaches to Maximizing Analytical Data

Day 3 (26 January 2018)

Automated sample preparation: the missing hyphen to hypernation
Camilla Liscio, Anatune
Session: Automating Complex Sample Workflows

Recent advances in the analysis of petroleum-based fuels using GC-VUV spectroscopy
James Diekmann, VUV Analytics
Session: Analysis of Complex Energy Products

Improving untargeted metabolomics with ion chromatography-mass spectrometry
John Walsby-Tickle, University of Oxford
Session: Life Science & Pharma

The HTC-15 conference will be held at Cardiff City Hall, Cardiff, Wales, UK, January 24–26, 2017.
https://www.ilmexhibitions.com/htc

Scent to Try Us

PTR-MS helps explain why some fabrics keep you smelling fresh, while others... don't

If you've ever found your face jammed in a fellow commuter's armpit, you may have noticed that some fabrics seem to make people smellier than others.

So why do some fabrics leave you reaching for the deodorant? Human body odor consists of many known volatiles that can adhere to the textile against the skin; the fibers of different fabrics have been shown to adsorb and release these volatiles differently. So by more fully understanding these interactions, garment manufacturers could develop products to counteract unpleasant odors. At least that's what researcher Raechel Laing of the Centre for Materials Science and Technology, University of Otago, has in mind.

Laing and her co-authors from the Department of Food Science used proton transfer reaction-mass spectrometry (PTR-MS) in multiple ion detection modes to identify the volatiles present. Why not simply use our own offended sense of smell to do the 'dirty' work? "Human noses tend to vary a lot in their sensitivity," explains Laing, "and extensive training is required. There are also practical issues in securing and managing specimens..."

They observed three main patterns, which may confirm long-held suspicions (and act as a guide to those who suffer from misbehaving sweat glands): low relative adsorption and low overall release of the volatiles for cotton, high relative adsorption and continuous release of the volatiles for polyester, and high relative adsorption but low overall release for wool.

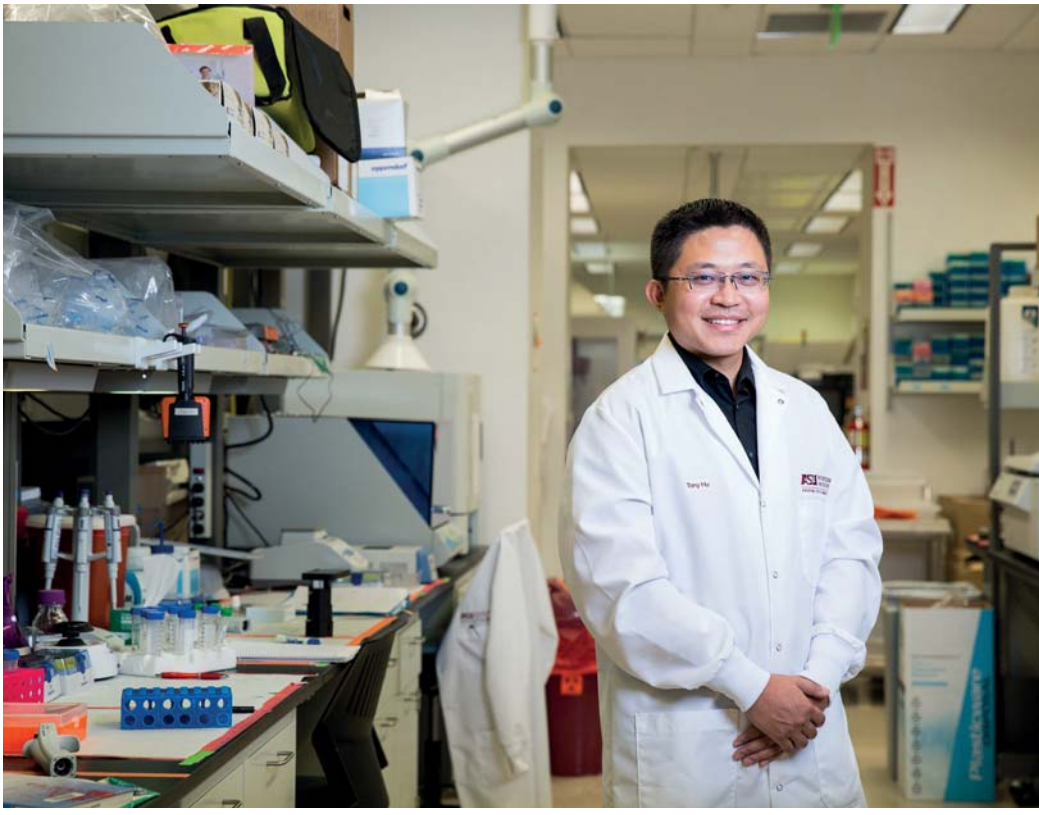
In the future, the team plans to investigate the bacterial breakdown and adsorption of other fiber types, such as polyamide, viscose and silk. In the meantime, it might be an idea to ditch that polyester shirt come summer.

Reference

1. *TM Richter et al, "Textile binding and release of body odor compounds measured by proton transfer reaction – mass spectrometry", Text Res J (2017).*

Dark Fields and Diagnostic Disks

New devices for detecting tuberculosis may speed up diagnosis and improve treatment



Tuberculosis (TB) is the eighth most common cause of death in low- and middle-income countries (1) and a challenging disease on many levels. To begin with, it's difficult to diagnose – symptoms like fever, weight loss and coughing apply to a wide range of illnesses, and many tests are inconclusive or subject to a high percentage of false positive and negative results, especially in patients with additional health problems. To reach a conclusion, doctors require a medical history, a physical examination, and a variety of tests, including skin tests, chest X-rays, sputum smears and microbiological cultures. Even after diagnosis, the battle isn't over; treatment is long, arduous, and side effects are common – and antibiotic resistance compounds these problems. But the longer patients go undiagnosed, the worse the odds of survival become – and it is more likely that they will spread the disease to others.

Tony Hu and his colleagues from the Arizona State University's Biodesign Institute decided to tackle the problem of diagnosis by developing a nanotechnology-based method of detecting and quantifying TB-specific proteins in circulation (2): an antibody-conjugated nanodisk that improves detection by high-throughput MALDI-TOF mass spectrometry. The disk first binds target peptides CFP-10 and ESAT-6, and then enhances the MALDI signal to allow quantification of the peptides at low concentrations. In the group's proof-of-concept study, the disks were highly sensitive and specific, successfully diagnosing culture-positive and extrapulmonary tuberculosis even in HIV-positive patients. The specificity was similarly high in healthy and high-risk patient groups. And during treatment, the nanodisks were able to quantify serum antigen concentrations to assess how well patients were responding.

It seems the new test has everything – speed, sensitivity, specificity, and the ability to offer conclusive results from a single, low-volume blood draw. But it's not the Hu group's only TB diagnostic; they've also developed another proof-of-concept device for use in resource-limited settings (3), which takes the form of a simple dark-field microscopy system with an LED light source, a dark-field condenser, a 20x objective lens, and the user's smartphone. It's small, light, and cheap at under US$2,000 – but the researchers aren't done yet, setting their sights on higher sensitivity, less weight, and a fraction of the cost.

The goal is to make high-quality TB care – and eventually, broad-range infectious disease diagnosis – available to every patient, regardless of location, health status, or resource availability.

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1. *UC Atlas of Global Inequality, "Cause of Death" (2000). Available at: http://bit.ly/2j41zfR. Accessed November 17, 2017.*
2. *C Liu et al., "Quantification of circulating Mycobacterium tuberculosis antigen peptides allows rapid diagnosis of active disease and treatment monitoring", Proc Natl Acad Sci USA, 114, 3969–3974 (2017). PMID: 28348223.*
3. *D Sun, TY Hu, "A low cost mobile phone dark-field microscope for nanoparticle-based quantitative studies", Biosens Bioelectron, 99, 513–518 (2018). PMID: 28823976.*

From Cancer Genomics to Chemical Detectors

What's new in business?

In our regular column, we partner with www.mass-spec-capital.com to let you know what's going on in the business world of analytical science. This month, there are several beneficial collaborations in the clinical and diagnostics fields, and SCIEX develops a new pesticide detection method as a response to Europe's recent "egg scandal" (tas.txp.to/0917/eggs).

Products

- Genedata announces global release of Genedata Selector Version 5
- SCIEX releases new detection method for Fipronil in eggs and poultry
- ACD/Labs announces updates to Spectrus Informatics Platform

Investment and acquisitions

- Eurofins acquires Spectro Analytical Labs Ltd in India
- Eurofins successfully prices €400m new hybrid bond

Collaborations

- Agena Bioscience's liquid biopsy technology used in LIMA Project: EU Horizon 2020 Grant
- Bruker: US Contract for 133 hand-held chemical detectors
- Owlstone Medical breath biopsy platform used in GSK's Phase II respiratory study
- Analytik Jena and German BAM cooperate for elemental analysis
- SCIEX embarks on joint venture with Zhejiang Dian Diagnostics in China
- Agilent Thought Leader Award for Jiandong Jiang at IMM-CAMS
- Bruker: Weizmann Institute installs 15 Tesla UHF MRI system
- Agena Bioscience partners with N-on-One for cancer genomics

People

- PerkinElmer elects Pascale Witz to Board of Directors

Organizations

- Bruker merges its subsidiaries in Sweden

For links to all press releases and more information, please visit the online version of this article: tas.txp.to/1217/BUSINESS

In My View

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

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

Contact the editors at edit@texerepublishing.com

The (Sci)X Factor

The 2017 "Great Scientific Exchange" provided fascinating insights into some of the toughest challenges facing analytical science – and the world.

By Matthieu Baudelet, Assistant Professor, National Center for Forensic Science/ Chemistry Department, University of Central Florida, USA.

It is always a great pleasure to attend SciX – but this year was made all the more special for me, because I was the program chair. And I felt lucky to be able to work with an incredible team that included Becky Dittmar (general chair), Mike Carrabba (exhibit chair), Rob Chimenti and Mark Henson (workshop chairs), Karen Esmonde-White (award chair and program chair 2018).

Our community of analytical chemists is confronted by many challenges. Issues such as gender equality, research in developing countries, and helping young scientists to succeed have never been more important, and events like SciX can act as a central platform to address these challenges.

With this in mind, a new section was created: "Contemporary issues in analytical science" (chaired by Rebecca Airmet). It covered the role of analytical scientists in fighting world poverty, how to increase diversity and equality, and helping students in their education and transition to the job market.

Food safety was a major focus this year in many sessions, with the opening plenary talk given by Janie Dubois, chair of the Laboratory Capacity Working Group at the World Bank's Global Food Safety Partnership. She brought our attention to real problems that the analytical community has helped solve already, but also the new challenges we face as a society.

The critical thinking we rely on as scientists has taken a hit in recent years. The abundance of information, genuine or false, and the speed of access to it, have led to a new generation of students who have not been trained to think as critically as we once were. This shift is being seen in classrooms as well as everyday life, and we were glad to welcome two wonderful speakers for our closing session: Panayiota Kendeou, from the University of Minnesota, and Jevin West, from the University of Washington. They both used their lectures to attack misinformation and misconception, and discussed how we can counter them and clearly communicate our research. Jevin leads an effort with Carl Bergstrom called "Calling Bullshit" (http://callingbullshit.org) that teaches us all how to critically evaluate the information we receive every day in this age of big data.

We are all part of one society, one community – and I believe we should contribute not only with our scientific work but also through direct involvement in charitable initiatives. SciX started a new operation this year to give back to the community with the Wednesday evening gala that included a fundraiser for the Renown Children's Hospital in Reno, allowing us to present a cheque for USD $4,500 to delighted hospital staff.

SciX has shown again this year that it is a conference unlike any other. We are a growing family and, as such, we are looking to strengthen our bonds, invite new members and further extend our knowledge. So I will take this opportunity to invite everyone – students, teachers, professionals and researchers – to join the SciX family and see for yourself what makes this such a special event. SciX 2018 will be in Atlanta, GA (21–26 October), and our first European SciX will be this Spring in Glasgow, UK (17–20 April).

Keeping the Lights On

The threatened closure of Stanford Synchrotron Radiation Lightsource would be a huge loss for the US research community.

By Graham George, Professor, Department of Geological Sciences, University of Saskatchewan, Canada.

The Stanford Synchrotron Radiation Lightsource (SSRL) is known as the birthplace of many of the innovations that have made synchrotron X-ray methods such important analytical tools. It is one of four Department of Energy (DOE)-funded synchrotron radiation facilities that provide X-rays for a wide range of researchers from academia, industry and other national laboratories. The FY 2018 Congressional Budget request (1) contained a substantial reduction for the DOE. DOE's response was to cut the proposed SSRL budget in half, and put the facility in what was called a "warm standby" mode from January 2018. Since most of the cost of running SSRL is salaries for the employees, it seems very likely that SSRL would never have reopened. Fortunately for SSRL, the budget did not pass and the facility will remain open next year. But the FY 2019 budget is being built along the same lines as the FY 2018 budget, and next spring SSRL may be in jeopardy again.

The DOE has an extraordinary legacy of support for research in general and for synchrotron facilities in particular, setting the bar for all such facilities worldwide. SSRL has a vital place in the DOE team of synchrotron radiation laboratories, specializing in X-ray spectroscopy and macromolecular crystallography with access to the hard X-ray regime. Other laboratories specialize in different X-ray energies and in methods that require very small X-ray beams. SSRL is the smallest of the four DOE synchrotron radiation laboratories, but it produces the highest proportion of what DOE calls high-impact papers, which in 2016 was 24 percent of all papers from SSRL. It also provides some unique advanced spectroscopy capabilities. For example: it has the only multicrystal spectrometer array optimized for high-resolution X-ray absorption spectroscopy in the USA; the only tender X-ray emission spectrometer in the USA, which is also the only solution-compatible spectrometer of this type in the world; the only high-solid-angle Raman spectrometer optimized for soft X-ray absorption spectroscopy in the USA; and the only transition edge sensor array detector for soft X-ray spectroscopy in the world. Remote access for protein crystallography experiments had its origins at SSRL, as did many other advanced capabilities. SSRL is streamlined and efficient, and is known for its flexibility and as a can-do facility that enables users' science as a priority. It produces more than 90 percent of the science that comes out of the larger SLAC National Accelerator Laboratory – despite having less than 10 percent of the employees of SLAC overall. SLAC is home to the world's first free-electron X-ray laser source, the linear coherent light source (LCLS), a coherent femtosecond pulsed source of staggering brightness that has potential impacts across many fields of science. Many of the new detector technologies needed for LCLS have been developed in collaboration with SSRL, and should SSRL close, many think that LCLS and SLAC will follow.

The links between SSRL and other DOE-funded laboratories, such as the Los Alamos National Laboratory (LANL) and Lawrence Livermore National Laboratory (LLNL), are especially strong, and very important to the nation from the perspectives of national security, energy and environmental cleanup. SSRL's closure would mean loss of capability for LANL and LLNL, directly undermining core aspects of DOE's mission.

Industrial research, such as petrochemical and new catalyst technology is also a growth area at SSRL. It is important to emphasize that SSRL and the other DOE-funded national laboratories do not engage in corporate welfare; they provide facilities to industrial and academic scientists alike that are well outside the normal scope and capability of industry or university.

SSRL has benefited from years of outstanding leadership, and it is this, combined with talented staff and world-class facilities, that sets SSRL apart, positioning it as a crucial facility for (analytical) science. It is an especially nimble facility, able to respond quickly to new and innovative requests from users, which springs from a pervasive culture of collegiality and less compartmentalization than happens at larger facilities. Its success is confirmed by a consistently high level of satisfaction from its users.

A Heritage Foundation report (2) recommends that the DOE should refocus "on maintaining America's nuclear weapons deterrent and managing the cleanup of the nation's nuclear weapons complex; limiting science spending to government needs and basic research while encouraging more flexibility and responsibility at America's

national laboratories". SSRL's closure would be in direct opposition to these recommendations. DOE's response to the FY 2019 budget should not be to close SSRL; whether for industry, healthcare or national security, the loss of SSRL would have a substantial impact on research in the US and beyond. In short – I believe it would be a disaster.

Graham George is a U.S. Citizen, currently living and working in Canada.

References

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2. *K. Tubb et al., "The Heritage Foundation Backgrounder, DOE Reset: Focus the Department of Energy on Core Missions and Decrease Distractions", (2017). Available at: http://bit.ly/2BGKVeI. Accessed December 4, 2017.*

I Do Not Want Green Eggs and Ham

We've come a long way in food safety – but consumers deserve to know exactly what they are eating.

By Jim Lawrence, Health Canada (Retired), Ottawa, Canada.

Food often contains substances that some of us do not wish to consume. Some substances may be considered undesirable for religious or ethical reasons, while others (for example allergens, lactose or gluten) can cause immediate serious illness or discomfort. Many consumers don't feel comfortable consuming food containing measurable levels of agricultural chemicals (for example, pesticides, hormones or antibiotics) or environmental contaminants (for example, dioxins, PCBs or mercury).

In a perfect world, we consumers would be able to quickly and simply test our food for substances that we do not want to ingest. Although rapid test kits already exist for many allergens, agricultural chemicals and environmental contaminants, none are currently suitable for proper use by the average consumer, so we must rely on the food industry and governments for information through food labeling. Food labeling is not normally required for whole fresh foods such as fruits, vegetables and meat products. And consumers can be confident that the apples or potatoes they are buying do not contain peanuts... But this is not the case with processed foods – a frozen apple pie could very well contain traces of peanut protein. In addition, many non-food chemicals, such as emulsifiers, preservatives, stabilizers, artificial flavors and colors, may be added to processed foods. As a result, processed foods tend to require food labeling that provides the consumer with the information about ingredients with a potential health risk.

Label declarations for allergens and food intolerance substances have improved over the past decade, with suspect ingredients (or constituents) often being specifically highlighted and listed separately. Manufacturers may also include labels such as "gluten free", "dairy free" or "peanut free" on their packages. However, not all statements are so helpful: "May contain peanuts" is of little help if you have a peanut allergy. If you are an allergy sufferer, your only safe option is to avoid anything with such vague information. And what about agricultural chemicals? There are no label requirements for them, which results in many consumers opting for "organic foods". In fact, over the past decade there has been a significant shift in consumer preferences to "organically grown" food and it is a steadily growing segment of the food industry. In the past, the term "organic" was poorly defined and there was no regulation of these types of products. Now, many countries have standards, definitions, certification programs, inspection programs and industry associations. All of this is good news for the consumer.

However, several examples above demonstrate that, despite major improvements in regulation and labeling, we have yet to achieve a point where consumers can be completely confident about what's in their food. So, where do we go from here? Although personalized food testing is still some way off, I believe it will have great value – especially for those who suffer from life-threatening allergies. The challenge for the analytical scientist is to take the current state of rapid testing technology to the next level: into the hands of the consumer. This may not be an easy task, but it is not impossible. Rapid test kits have been in use by consumers for many decades. For example, personalized blood glucose tests and home pregnancy test kits are readily available to consumers. We just haven't yet developed the technology for food testing. In the more immediate future, we must do much more to further enhance the readability of labels, as well as including more substances that may pose a health risk to the consumer. Ultimately, we need to give consumers more power to make informed choices.

HUMANITY IN SCIENCE AWARD

the Analytical Scientist

In partnership with

KNAUER

Richard Jähnke

Meet the Winner

Richard Jähnke

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

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

Could it be you in 2018?

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

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

@Humanityaward Humanity in Science Award

www.humanityinscienceaward.com

Intense Innovation

The TASIAs are back, celebrating the creativity needed to transform colorful concepts into vibrant analytical tools! With a record number of entries, the final 15 reflect the full spectrum of analytical advances, from ingenious software for managing impurity data, to transformative MS imaging technology.

15

CHARON PARTICLE INLET FOR PTR-TOFMS

A single instrument for direct monitoring of gas-phase and particulate organics.

Produced by IONICON

A new inlet enables IONICON PTR-TOFMS series instruments to measure sub-µm particles directly with a versatile, reliable and proven technology for VOC analysis: PTR-MS. One single instrument from IONICON covers VOCs and now additionally allows the molecular-level characterization of sub-µm particulate organic matter at a 1-min time-resolution.

The CHARON particle inlet consists of a honeycomb activated charcoal denuder that efficiently adsorbs organic gases and transmits particles, a high-pressure aerodynamic lens system that collimates and extracts sub-µm particles, and a thermo-desorber that evaporates non-refractory organic particulate matter.

These organics are subsequently analyzed as gas-phase analytes with a high-resolution IONICON PTR-TOFMS instrument. By coupling the CHARON inlet to a PTR-TOFMS, the VOC inlet remains fully operational. An automated valve system allows for scheduled switching between gas- and particle-phase measurements, as well as zeroing of the particle inlet.

Potential impact

CHARON, in combination with the IONICON PTR-MS technology, detects an abundant range of atmospheric organic carbon. Customers can upgrade their real-time analytical instrument to monitor gas-phase organics and particulate intermediate, semi-and low-volatile organic compounds (IVOCs, SVOCs and LVOCs, respectively) in < ng/m^3 concentrations, with a single CHARON-PTR-TOFMS analyzer.

CHARON is a direct inlet system that doesn't sacrifice one of the main benefits of PTR-MS instruments: real-time monitoring capabilities. With its high temporal resolution and the high degree of conserved chemical composition information, CHARON PTR-TOFMS is able to identify and quantitatively follow atmospheric particulate tracer compounds such as levoglucosan and polycyclic aromatic hydrocarbons. One-minute resolved data of hundreds of identified chemical compositions boost the quality of source apportionment significantly.

14

THE TOPAZ SYSTEM

A simplified, fully integrated LC-MS system for clinical diagnostics.

Produced by SCIEX

LC-MS/MS is important for efficient and reliable diagnostic testing, but is not used to its full potential because of its perceived complexity. The result has been an undesirable compromise of costly send-out testing, extended turnaround times, and limiting assay performance. The CE-marked Topaz System, built on SCIEX's most robust technologies to date, incorporates features that enhance usability to help new users build proficiency quickly. The heart of the system lies within the ClearCore MD software, an intuitive platform that simplifies and streamlines workflows and method development, bringing the power of LC-MS technology to the hands of the routine user.

Potential impact

The Topaz System provides accessible LC-MS technology with much-needed gold-standard accuracy to clinical diagnostic labs. Currently, immunoassays are the prevalent technology for routine testing. These tests generally offer a high degree of automation and fast results, but have a number of drawbacks, including issues with accuracy, selectivity and specificity. These drawbacks can have profound diagnostic implications, often requiring use of LC-MS for definitive accuracy. The simple design of the Topaz System lowers the barriers to this powerful technology for the standard clinical lab. Clinical labs will be able to offer improved quality of care for patients without the need for high-level specialists to run the mass spectrometer. In addition, the Topaz System's flexibility enables clinical labs to rapidly expand their testing services and bring previously outsourced tests in-house, saving time and costs.

What the judges say:

"This could be another important step in allowing MS to be used in the clinic."

EPREP SAMPLE PREPARATION WORKSTATION

Simple, low-cost automated sample preparation for every laboratory.

Produced by ePrep

The ePrep Sample Preparation Workstation specifically addresses the need for a simple, flexible, low-cost and reliable automated sample preparation system for analytical laboratories. It targets chromatography laboratories that handle many different sample preparation protocols with varying, often small, batch sizes that are typically analyzed on different instruments.

The design of ePrep makes it easy to program and operate, with most sample preparation workflows created and validated ready for operation in 5–15 minutes. The key to its operation is the predefinition of tasks, syringes, tools, accessories, racks and vials – enabling workflows to be created using "drag-and-drop" processes.

The ePrep solution is more than an automated robotic platform – it also includes a range of novel accessories and consumables such as microSPE, disposable syringes, micro filtering and customizable chemistry that bring enhanced performance to common sample preparation processes.

Potential impact

Sample preparation techniques constitute a high portion of analytical cost, have not kept up with the efficiency of modern analytical equipment, and are the major source of analysis costs and errors. Despite this, most analytical chemistry laboratories are reluctant to automate because of high costs and complexity of sample preparation automation. ePrep has set out to change that paradigm with simple, low-cost and high-flexibility operation for the chromatography laboratory. It can effectively handle 5 to 500 samples and provides laboratories with improved precision, accuracy and operator safety.

What the judges say:

"A new approach to automated sample preparation. Highly flexible and applicable to every laboratory."

13

G908 3-IN-1 CANNABIS ANALYZER

Leverages GC-HPMS to perform three state-required cannabis tests on one device.

12

Produced by 908 Devices

The G908 3-in-1 Cannabis Analyzer combines 908 Devices' patented high-pressure mass spectrometry (HPMS) technology with the separating power of ballistic gas chromatography (GC) to perform three state-required cannabis tests – total potency, terpenes and residual solvents – on one device. Designed for central labs, growers and producers, the device makes it easy for users at all skill levels to accelerate analysis processes for a wide range of cannabis compounds, while reducing analysis time by more than 80 percent.

Unlike legacy lab instruments, G908 is easy to use, offering professional-grade cannabis analysis at the push of a button. Designed for durability and transportability, G908 can rapidly perform testing in the laboratory and at remote field-based settings. Moreover, the device costs less than legacy lab instruments and was designed with field serviceable components, which eases the financial burden placed on growers, producers and labs looking to purchase new instruments.

Potential impact

With state regulations demanding that products pass safety, purity and quality tests before distribution, those involved in the growing, manufacturing and testing of cannabis need a fast, rigorous analysis solution to ensure compliance.

In the lab, G908's small footprint and compound selectivity eliminates the need for multiple, complex analytical instruments. GC-HPMS provides fast compositional analysis, enabling technicians to scale-up operations and successfully manage the hundreds of samples they need to test each day. G908 can perform analysis on residual solvents five times faster than legacy lab instruments.

For growers and producers, G908 will increase their chances of passing state-sanctioned testing. The ability to test products on-site throughout the cultivation, extraction and manufacturing processes provides growers and producers with the ability to determine optimum harvest conditions, and identify potential product quality problems early enough to take corrective action – reducing the risk of having batches quarantined or destroyed.

Q EXACTIVE HF-X HYBRID QUADRUPOLE ORBITRAP MASS SPECTROMETER

An Orbitrap mass spectrometer that accelerates insights, from discovery to verification.

Produced by Thermo Fisher Scientific

The Q Exactive HF-X Hybrid Quadrupole Mass Spectrometer provides sensitive and reproducible analyses of highly complex samples, setting new standards for depth of analysis, quantitative accuracy and reproducibility. The instrument delivers this through fast and accurate mass analysis, two-to-three-fold sensitivity improvements and up to eight-times better signal-to-noise ratio than previous models.

Potential impact

The Q Exactive HF-X Hybrid Quadrupole Mass Spectrometer enables scientists to comprehensively profile and quantify the proteome, discover and verify novel biomarkers, and fully characterize complex biotherapeutics. It allowed Jesper Olsen, Associate Professor and Deputy Director of the Novo Nordisk Foundation and Center for Protein Research at the University of Copenhagen, Denmark – an early tester of the Q Exactive HF-X for protein research – to identify 1,100 unique peptides per minute, setting a new world record. It can provide scientists with the depth of analysis, data quality and analytical precision required, without sacrificing robustness or speed.

11

What the judges say:

"A better Orbitrap! With each generation the Orbitrap gets better and better. This is no exception, pushing the limits of sensitivity and resolution."

LUMINATA

Software for efficient and comprehensive management of impurity data in process development.

Produced by ACD Labs

Luminata is an informatics system that enables organizations to establish effective impurity control strategies based on assembled analytical and chemical information – in a single environment. Built on the multi-technique, vendor-agnostic ACD/Spectrus Platform, Luminata offers comprehensive data standardization – accomplished by aggregating chemical reaction information, and the associated formation and fate of impurities, with chromatographic and spectral data. Luminata facilitates efficient organization of the typically overwhelming quantity of analytical knowledge for processes and associated impurities at every stage.

Luminata's assembly of searchable knowledge provides visualization, decision-support, and reporting capabilities; and facilitates collaboration between process chemistry and analytical research and development groups.

Potential impact

The current processes for managing impurity profile information are cumbersome and overwhelming. The sheer quantity of data generated is almost impossible to effectively organize and manage with currently available systems. Many organizations use Excel in an effort to transcribe scattered information from different sources into a single environment, but this is tedious, error-prone, and time consuming.

Luminata allows the multi-disciplinary teams that undertake process development projects to gather all the relevant chemical and analytical information in a single scientific environment. Furthermore, it supports a Quality-by-Design (QbD) approach to establishing effective process and analytical impurity control strategies. The fear of using old data is eliminated with access to live up-to-date information. This assembled data enables collaboration and information sharing in a manner not previously possible.

10

09

ULTIVO LC/TQ - 1260 INFINITY II PRIME LC

A high-performance LC/TQ, a third of the size of previous generations.

Produced by Agilent

The Ultivo Triple Quadrupole LC/MS delivers the performance of a traditional high-end LC/TQ in a third of the laboratory bench space. It is also designed to be integrated into a stacked LC system to free up additional lab space.

Ultivo's next-generation ion optics are miniaturized without loss of sensitivity. The novel twisted and tapered dodeca-hexapole cyclone ion guide collects ions and transmits them to MS1. Thin DC-only pre-filters provide efficient ion injection into the new reduced-size quadrupoles. The Vortex collision cell confines ions during fragmentation with a twisted and tapered hexapole, with fragmentation patterns comparable to those from traditional collision cells.

A new embedded software computing platform provides smart self-tuning and enhanced diagnostic capabilities. Removable instrument side panels provide easy access for system maintenance, and VacShield allows capillary exchange without breaking vacuum. The 1260 Infinity II Prime LC completes the system, offering the highest sample capacity per bench space for any laboratory.

Potential impact

Ultivo marks the next generation of LC/TQ instruments. It offers performance equivalent to or better than larger LC/TQ systems, with the added benefits of being smaller, easier to use and costing less to operate. Laboratories benefit from its space-saving and stackable design, providing optimal use of lab bench space, plus early maintenance feedback, enhanced serviceability, intuitive operational design, and robust/reliable performance in difficult matrices.

These enhancements along with streamlined data management tools ensure that Ultivo, when coupled with the 1260 Infinity II Prime LC, meets the challenges users face for performance, form factor, robustness, time-to-report, ease-of-use and ROI.

CAPTIVA ENHANCED MATRIX REMOVAL-LIPID

08

Highly selective, efficient and easy lipid removal for complex samples.

Produced by Agilent

Bond Elut Enhanced Matrix Removal-Lipid dSPE sorbent was developed in 2015 and is recognized as an innovative technology in the food industry – it selectively target lipids using a combined mechanism of size exclusion and hydrophobic interaction and integrates into common workflows such as QuEChERS.

Advances in sorbent chemistry now allow EMR-Lipid to function in a pass-through SPE format – Captiva EMR-Lipid. The new format can be integrated into popular protein precipitation workflows and provides bioanalytical scientists with a tool to remove lipids, including phospholipids, without adding additional steps. A non-drip feature in smaller formats facilitates in-cartridge protein crash, while larger sizes support gravity flow elution for food safety labs. The new Captiva EMR-Lipid formats deliver high recovery for a diverse range of analytes and readily accommodate multiclass, multiresidue analysis workflows for complex, fatty samples.

Potential impact

When organic solvent is used in protein precipitation of many plasma and whole blood samples, lipids remain soluble in the sample and cause matrix effects that negatively affect the data, reduce method sensitivity, and lead to poor reproducibility. Lipids can also accumulate over time within the system, affecting column and instrument long-term performance due to contamination and carryover issues within the detection system.

The Captiva EMR-Lipid pass-through SPE format simplifies workflows and reduces sample preparation steps. With cleaner samples (removing >99 percent of phospholipids), the method sensitivity and analyte recovery is improved, which results in faster data analysis, better reproducibility and higher data confidence. By avoiding the introduction of a heavy-laden matrix into the system, unscheduled downtime is reduced.

What the judges say:

"Simplifies sample preparation for complex samples, especially in food analysis."

timsTOF PRO

A new standard for shotgun proteomics.

Produced by Bruker

The front-end TIMS analyzer is optimized for higher-speed shotgun proteomics from smaller sample amounts with high performance single-shot peptide and protein identification. Its dual-TIMS geometry enables the PASEF (parallel accumulation serial fragmentation) method, where ions are accumulated in parallel in the first TIMS section, while ions are released from the second TIMS section for MS/MS fragmentation. PASEF results in a nearly 100 percent duty cycle, giving it excellent performance for reproducible nanoflow LC-MS analysis of enzymatically digested protein mixtures.

07

Potential impact

The PASEF capability delivers higher-sensitivity and higher-speed shotgun proteomics without loss of mass resolution. Higher scan speeds result in lower mass resolution in FT-based MS technology commonly used for shotgun proteomics. These critical limitations are eliminated by PASEF, allowing for a duty cycle near 100 percent and high sensitivity, while maintaining ultra-high mass resolution for both the precursor and the product ions. These benefits give scientists the tools to dig deeper into the complex biology of the cellular machinery and the potential to discover low-level, biologically significant proteins, or validate them in translational and clinical proteomics research on large cohort sizes and in longitudinal studies.

What the judges say:

"Adds an exciting extra separation dimension for complex sample analysis in proteomics."

VASE

06

Vacuum-assisted, solvent-free GC sample preparation for analysis of volatile to semi-volatile compounds.

Produced by ENTECH

VASE (vacuum-assisted sorbent extraction) is a new solvent-free headspace extraction technique, which performs an in-vial extraction for gas, liquid, and solid samples, followed by direct thermal desorption into the GC. The amount of phase is approximately 150 times greater than SPME, with adsorbents increasing the surface area by thousands of times relative to the low surface area of a PDMS coating. The top of the adsorbent tube contains a seal that allows the vial to be evacuated through the adsorbent immediately after insertion. Under vacuum, the sample collects faster than at atmospheric pressure, enhancing the recovery of low-volatility compounds and often achieving exhaustive extractions. VASE allows analytes to diffuse onto and collect at the front of the adsorbent bed, achieving a better recovery of heavier compounds than dynamic headspace, while eliminating common carryover issues.

Potential impact

VASE has the potential to provide a more sensitive solution than purge and trap for volatiles in water and other matrices, while also replacing solvent extraction for analysis of pesticides, PAHs out to six rings, and other SVOCs in water.

VASE increases the number of applications compatible with headspace extraction by:

- enabling reproducible headspace extractions of low volatility compounds with minimal matrix effects
- combining the strengths of SPME and dynamic headspace to achieve excellent precision and sensitivity over a boiling point range as wide as -50°C to +500°C
- performing complete extraction to equilibrium, which has been shown to eliminate the need to perform isotope dilutions
- enabling exhaustive extraction of samples at 25°C, making VASE suitable for analysis of flavor compounds and contaminants in consumer products.

PORTABILITY

05

A portable mass spectrometer with TDESI direct ambient ionization source.

Produced by BaySpec

BaySpec Portability is specifically designed for field applications, with a lightweight and compact size. It is the only compact mass spectrometer using miniaturized linear ion trap technology to achieve ppb-level detection. The instrument is also equipped with two inlets for low pressure and atmospheric sampling. It is compatible with in situ and real-time detection methods, including electrospray, thermal-desorption electrospray, atmospheric pressure chemical ionization and most of the ambient ionization techniques, such as DART and DESI. This extremely compact instrument is easy to operate and maintain, and is suitable for a variety of bulk or trace on-site detection in real time.

Potential impact

Performing chemical analysis in situ, without the need to deliver samples to the off-site analytical laboratory, is an advantage in many areas of chemical analysis, from environmental monitoring and food control to chemical process monitoring. In-situ monitoring is also crucial for early warning of a chemical or biological release. Many field-deployed instruments are based on optical spectroscopy or electrochemical sensors, because miniaturization of these technologies was relatively straightforward. Using cutting-edge technology in miniaturization of vacuum, ion optics and mass analyzers, BaySpec has developed its new portable mass spectrometer for onsite analyses. Portability combined with TD-ESI makes it possible to perform fast pesticide screening to discover elevated levels of residual pesticides, to monitor exposure of chemical warfare, drugs, explosives, and any other harmful toxins.

What the judges say:

"A portable ion trap with ppb sensitivity – a breakthrough."

NEOSPECTRA MICRO

The world's smallest FT-IR spectrometer enables ubiquitous spectral sensing.

Produced by Si-Ware Systems

NeoSpectra Micro is the world's smallest FT-IR spectrometer. Thanks to innovative solutions, it is integrated in a chip-sized 18 × 18 mm package. It offers the widest spectral range at the higher end of the NIR range among all micro-spectrometers, which enables identification of more materials and more accurate quantitative analysis. NeoSpectra Micro can be produced with scalability that enables massive volumes (more than hundreds of thousands) with a price that is affordable to the average consumer. The whole system is alignment-free, calibration-free, shock-resistant, and reliable. The combination of these features and benefits removes the barriers that used to hinder the adoption of NIR spectroscopy in mainstream markets and enables the creation of new usage models, including handheld gadgets, smart phone cases, and IoT sensors. There is a lot of innovation behind the NeoSpectra Micro and it is protected by more than 30 patents, 20 of which have already been granted.

04

Potential impact

By transforming what used to be a lab instrument into a chip-sized module, NeoSpectra Micro could have a real impact on society. For instance, in the food sector, it could enable regulators to monitor the quality of food from farm to fork and make it possible for consumers to detect the authenticity, freshness, presence of allergens, and nutrition facts of their food. In the agriculture sector, it enables huge numbers of in-field smart-farming sensors that can analyze soil, crops, seeds, fertilizers, feed, and many other materials to enhance yield and productivity. In the biomedical sector, patients could monitor health conditions with minimum intervention from physicians.

03

i-RAMAN PRO ST

Raman for seeing through opaque packaging and coatings.

Produced by B&W Tek

The i-Raman Pro ST uses a patent-pending probe that illuminates and collects Raman signal from a large area and depth of the sample. Many visually opaque packaging materials, such as pigment-filled plastic bottles, paper or fabric products can partially transmit laser and Raman light. The depth of sampling over the large sampling area offered by i-Raman Pro ST enhances the relative contribution of the content material in the collected spectrum over that of the packaging material. The intelligent software (patent pending) is able to separate the spectral features of the content material from that of the packaging, and compare with a large spectral library to achieve reliable identification of samples inside the container.

Potential impact

With its high-throughput design, the i-Raman Pro ST analyzer can non-destructively identify common chemicals through thick packaging material in seconds. The system design has the versatility to be adapted for conventional surface Raman measurements with a variety of sampling accessories from a microscope to zoom lenses for standoff measurements. Normal confocal Raman measurements can be made with an adaptor attached to the ST Raman probe, converting it to the confocal configuration. The ability of the i-Raman Pro ST to see through opaque layers expands Raman spectroscopy to more applications. It can be used for identification of materials non-invasively and for improved analysis of heterogeneous samples thanks to its larger sampling area. These capabilities plus its portability make the i-Raman Pro ST a useful tool for a variety of applications, from QC to research.

What the judges say:

"High sensitivity and great flexibility, allowing high performance non-destructive analysis. A big improvement in portable Raman."

MICRO PILLAR ARRAY COLUMN: µPAC

For high-resolution chromatography of complex biological samples.

Produced by PharmaFluidics

µPAC is the first micro-chip chromatography device that is manufactured using lithographic micromachining techniques. The layout of the stationary phase support structure is carefully designed, and the perfectly ordered backbone of the separation bed is formed by etching interstitial volumes out of a silicon wafer.

The low "on-column" dispersion, obtained thanks to the perfect order, virtually eliminates axial peak dispersion, resulting in higher column plate numbers with sharper peaks and higher concentration of compounds. The freestanding nature of the pillars also leads to much lower backpressure, allowing the use of very long columns. These properties result in chromatographic performance with high resolution and high sensitivity. This new approach, compatible with all commercial nano-LC equipment, improves LC analysis in complex mixtures of biological samples.

Potential impact

The past few years have seen the introduction of advanced bioanalytical technologies such as next generation sequencing (NGS) and LC-MS, which together provide more power for integrated and systematic investigation of cellular genomes, transcriptomes, and their proteomes and metabolomes. The holy grail of proteomics and metabolomics is the ability to decode the proteome and metabolome at the single-cell level, which imposes enormous challenges to sensitivity, as there are no amplification methods for proteins and metabolites comparable to those of nucleic acids. The µPAC column is a promising tool for limited sample proteomics. The combination of ultra-high resolution µPAC HPLC columns and high accuracy mass spectrometers allowed the identification of more than 3,000 proteins from the equivalent of 50 HeLa cells. Recently, the device has also been used to characterize monoclonal antibodies.

02

01

HYPERION IMAGING SYSTEM

An imaging solution for comprehensive analysis of cellular phenotypes and their interrelationships.

Produced by Fluidigm

The Hyperion Imaging System brings together high-parameter CyTOF technology with imaging capability, enabling the simultaneous detection of 4–37 metal-tagged protein markers in the spatial context of the tissue microenvironment. Offering a new solution to current challenges in tissue imaging, Hyperion surpasses the capabilities of standard immunohistochemistry (IHC) and fluorescent imaging.

This new approach allows a comprehensive view of complex cellular phenotypes and their relationships in context – from a single scan. Researchers can profile precious FFPE or frozen tissues at subcellular resolution, and identify new biomarkers, visualize cellular social networks, or see how the immune system attacks tumors, identifying which immune subtypes are participating in activation or suppression of the immune system.

The system is accompanied by a pathologist-verified Maxpar imaging antibody portfolio, a software suite for image acquisition and data analysis, plus service and support.

Potential impact

Translating discoveries into better clinical outcomes takes dedication and a desire to use new approaches to ask the most difficult questions. Current solutions restrict our view and thus limit our understanding. Changing the course of how diseases are treated and ultimately cured requires a comprehensive understanding of cellular phenotypes and their relationships in the context of the tissue microenvironment.

The Hyperion Imaging System has the potential to revolutionize disease research by providing unprecedented visualization of complex cellular phenotypes and their relationships in the context of cancer, immuno-oncology, and a wide range of diseases.

What the judges say:

"Combines tissue imaging with cytometry, allowing correlation between biomarkers and cell interactions. This technology has the potential to be truly transformative."

THE INNOVATORS 2017

Whether ensuring consumer safety, speeding up biomedical research, or just making life in the lab a little bit easier – meet the companies advancing analytical science.

SAMPLE PREPARATION WITH TOUCH-OPTIMIZED CONTROL SOFTWARE

Sample preparation with gel permeation chromatography as basic technique can be controlled via the portable and touch-optimized software Mobile Control®.

Time and labor should not be wasted on manual work that can be done by automated processes. Very often, manual sample preparation can be handled by automated Gel Permeation Chromatography (GPC cleanup). Further, reproducibility and quality of your sample is improved. The dedicated system processes up to 15 samples while requiring minimal bench space. The cleanup process can be performed by the AZURA® GPC cleanup system which is operated by touch-optimized Mobile Control®.

GPC Cleanup (Gel Permeation Chromatography) is primarily employed for performing general cleanup tasks on a wide range of sample matrices such as foodstuffs, tissues, plants and environmental samples. The separation of components takes place according to their molecular weight due to the heterogeneous pore size of the stationary phase. High-molecular substances such as lipids, proteins, natural resins, cellular components and steroids interfering with subsequent analysis (for example, of pesticides) are efficiently removed.

The AZURA® system features 15 sample loops controlled by two 16-port multiposition valves. The GPC tubing guide sorts outlet tubings of fraction collection. The wound-up sample loops are stored in a tray with drainage system and are easily accessible for inspection and replacement. An additional multiposition valve supports collecting up to 15 fractions. All multiposition valves and the manual injection valve are integrated in an AZURA® Assistant ASM 2.1L. Elution of separated compounds is monitored by a variable single wavelength UV detector. A second assistant harbors a small detector, the system pump with a pressure sensor and a valve to bypass the GPC column or select between two columns.

The GPC Cleanup system is operated with Mobile Control®. This clearly arranged user interface is run on a tablet directly mounted at the system. It automatically recognizes devices and facilitates system configuration. Due to block programming, methods are created fast, with a minimal number of clicks. Mobile Control® makes sample loop loading easily manageable by synchronously switching both valves at the push of a button. The software Mobile Control® provides an intuitive and cost-effective user interface for device control directly at the system.

Learn more at www.knauer.com

A SMALL POWERHOUSE OF BIG BENEFITS TRIPLES LAB CAPACITY AND MAXIMIZES PERFORMANCE

Agilent's Ultivo Triple Quadrupole LC/MS delivers the performance of a traditional high-end LC/TQ in 1/3 of the laboratory bench space

Welcome to a new era of mass spectrometry

Decades of innovation have brought us into a new era of mass spectrometry with the design of Agilent's revolutionary Triple Quadrupole LC/MS. Ultivo is packed full of the same power and accuracy you'll find in the big guys, but at a fraction of the size. It's on a transformative mission to reshape expectations, reinvent capabilities, and redefine what's possible when small meets powerful.

Innovations for enhanced results

Ultivo is specifically designed to maximize quantitative performance, enhance instrument reliability and robustness, provide the quickest sample analysis to report time – not to mention it also promotes more uptime and fastest return on investment.

Ultivo's innovations empower you to:

- Optimize lab technician productivity with VacShield that allows seamless MS maintenance without the cumbersome necessity of venting the instrument
- Maximize performance in a smaller footprint via the Cyclone Ion Guide which tightly focuses more ions into the detector, thereby delivering greater signal for low-level quantitative and qualitative analyses
- Increase sample throughput and enhance MS/MS performance with the Vortex Collision Cell for more efficient collimation of the ion beam and faster transmission of targeted analytes
- Increase ion transmission with the virtual pre/post filters promoting faster switching and allow more MRMs to be performed in less time
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Enhancing productivity to improve your experience

Ultivo is powered with Agilent MassHunter, so you'll experience new features like an updated user interface and data collection modes that make your method and worklist interactions easier. Experience 50 percent faster autotune–optimizing instrument performance and producing more uptime–along with intelligent diagnostic feedback. After acquiring data, Quant-My-Way empowers lab managers to provide users with just the features they need to convert their data into results, simplifying the user workflow. All this combined makes your MS analyses faster and more productive.

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The PURA water bath series comes in five models ranging from 4 to 30 L. All models cover a working temperature range from +25 °C to +99.9 °C with a temperature stability of ±0.2 °C via digital PID control. Heating capacity ranges from 800 W in the PURA 4; 1.1 kW in the PURA 10 through PURA 30 at 115V; 1.3 kW in the PURA 10 and PURA 14 at 230V and 2 kW in the PURA 22 and PURA 30 at 230V.

JULABO offers an extensive range of accessories for added flexibility in everyday laboratory operations. All bath sizes have a clear plastic lift-up cover accessory available. The cover installs without tools and enables sample viewing while minimizing water evaporation. The range of accessories also includes flat stainless-steel bath covers with sets of rings for tempering Erlenmeyer flasks or other tall vessels. The diameters of the ring openings vary from 92 to 190 mm. Three plastic test tube racks are also offered. They are designed for 60 or 90 test tubes or 21 tubes up to 30 mm diameter. A stents lifter and a stainless-steel hygiene insert are available as dentistry accessories for the small PURA 4 water bath.

For more information please visit https://julabo.us/new-pura-water-baths/

MICRO-CHAMBER/ THERMAL EXTRACTOR

Fast and flexible sampling of chemicals and odors

Markes International's Micro-Chamber/Thermal Extractor™ (µ-CTE™) is a compact unit for the sampling of volatile chemicals emitted from products or materials. Its impressive versatility and ease-of-use mean that it is used in a wide range of industries:

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- Automotive testing
- Consumer goods
- Foods and fragranced products

Operation of the µ-CTE is simple. The sample is placed in one of the sampling pots, the lid is closed, the sample warmed, and a flow of air or nitrogen is used to release the volatile organic compounds (VOCs) onto sorbent-packed tubes. This typically only takes 30 minutes, and the dynamic nature of the sampling ensures excellent sensitivity. The sorbent tubes are then analysed by thermal desorption GC–MS (alternatively, formaldehyde can be monitored by sampling onto DNPH cartridges, followed by HPLC).

Application range

The speed of sampling mentioned above is actually the main reason for the instrument's popularity, and underpins one of its key applications – screening the profiles of regulated materials used indoors and in vehicles. Although final certification testing in these fields is often performed using environmental chambers, the multi-day tests stipulated are very time-consuming.

As Wolfgang Horn at Netherlands-based engineering group BAM points out: "The Micro-Chamber helps us to look at many material samples in parallel and quickly identify what chemicals are being emitted. This can be a real help before we start emission tests in large environmental chambers."

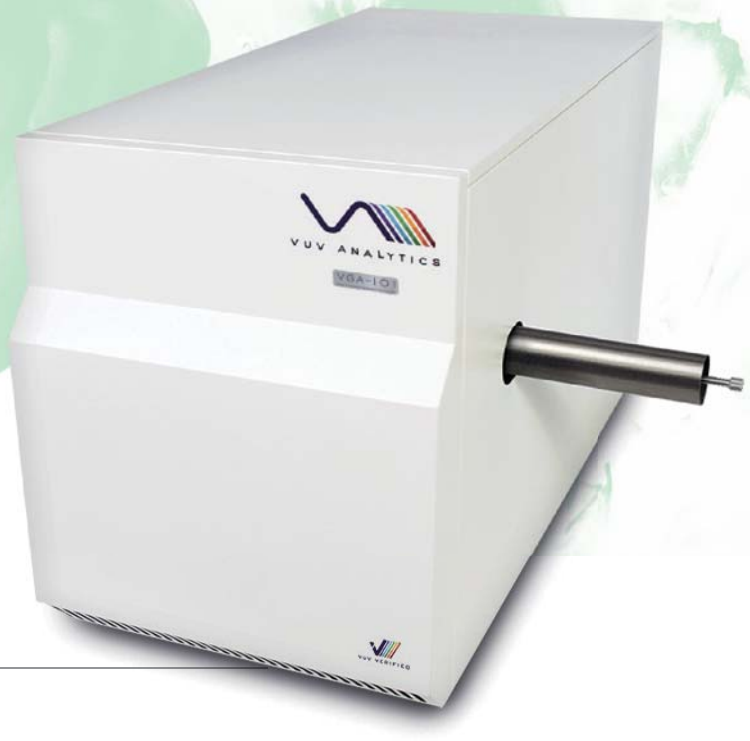
However, the µ-CTE isn't just used to assist regulatory compliance. It is also widely used for:

- Quality-control of final products and raw materials
- Comparing products to those of competitors
- Product troubleshooting and R&D
- Aroma profiling and shelf-life tests
- Time-profiling

Versatile accessories

The µ-CTE continues to evolve, with citations in an increasing number of standard methods, and the release of accessories for profiling flat samples, determining chemical permeation through membranes, and humidifying purge air. All this is testament to the growing popularity of this product and its expanding application versatility – making it a valuable tool in any GC laboratory.

To see the µ-CTE in action and hear from customers, watch the video at http://chem.markes.com/micro



GAS CHROMATOGRAPHY: PROBLEMS SOLVED

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Joining Forces: Breaking the Mold

In our ongoing series profiling collaborations between industry and academia, we look at a partnership finding better ways to detect dangerous fungal toxins in our food.

With Franz Berthiller, Associate Professor, University of Natural Resources and Life Sciences, Vienna (BOKU), in Tulln, Austria, and John Lee, Global Food Market Manager – Agilent Technologies.

Tell us about your project...

Franz Berthiller: Mycotoxins are poisonous metabolites produced by fungi, which can pose a serious food safety threat. A famous fungal metabolite is aflatoxin B1 – it's one of the most carcinogenic compounds known to mankind, and we're still finding it in food. John approached us because BOKU is a leading center focused on researching mycotoxins, with expertise from analytical scientists, toxicologists, and plant biologists. Mycotoxins are highly diverse and so we used to have separate methods for each mycotoxin, with different extraction, clean-up, and measuring modes. In 2005, I published the first method that could analyze nine mycotoxins at once. John wanted to work with us to come up with easier methods for mycotoxin testing, allowing Agilent to offer labs a "mycotoxin testing kit" including the instrument, method, standards and set-up. So Agilent offered to provide us with a high-end tandem quadrupole LC-MS instrument and technical support to help us in that goal.

John Lee: It's academics like Franz who truly understand not just how to make methods more efficient, but also to increase their scope – they're the people we want to work with so we can offer truly cutting-edge workflows.

"Our first goal was to develop accurate methods for measuring regulated mycotoxins."

How did the two teams work together?

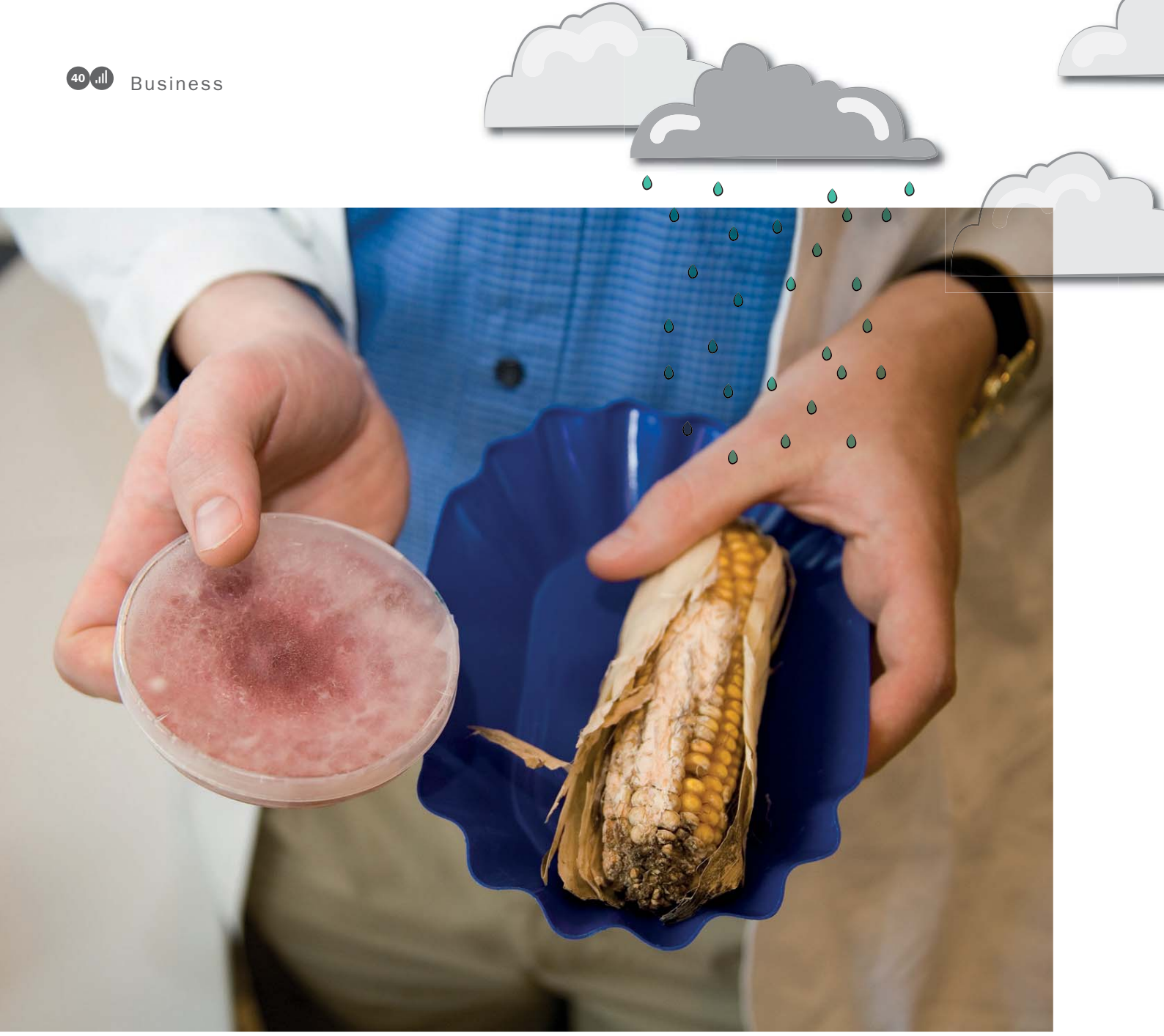
JL: Thomas Glauner is an LC-MS expert in Agilent and it was he who started working closely with Franz's group.

FB: Thomas was our major collaborator during that project; whenever we had questions about the software or struggled with settings, Thomas was just a call or email away. And we had several productive meetings at our lab and Agilent's facility in Germany. Sometimes in projects like these, only one partner publishes – but this is truly a joint work and, as such, our publications include authors from both groups.

What are the aims of the collaboration?

FB: Our first goal was to develop accurate methods for measuring regulated mycotoxins. The regulation of mycotoxins is a complicated issue, and Europe has the strictest regulations in the world. We developed a method to measure all of the regulated mycotoxins found in solid foodstuffs, using stable isotopes. It was published in 2012 (two years after the collaboration began) and looks set to remain the gold standard for quantification for years to come (1). Using sensitive modern instruments, this method allows us to measure mycotoxins at the regulated level even in baby food – for which the acceptable limit is lowest of all.

JL: What was really neat about Franz's idea of using stable isotopes is that the resulting workflow is so simple – it's easy for any lab to replicate at minimal cost. Usually, when you're analyzing



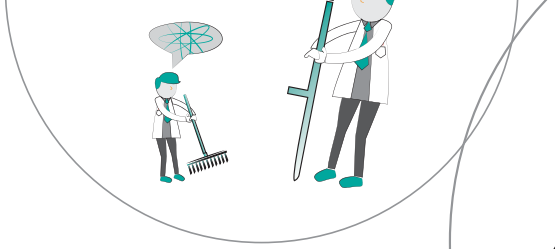
compounds at the very low levels necessary for mycotoxins, you have to do extensive sample clean-up to compensate for matrix issues. With stable isotopes, you can correct for matrix issues, and simplify the sample prep. The sample preparation workflow that Franz and his team developed is very straightforward, and therefore productive.

Earlier this year, a lab in China published an application note with Agilent describing how they had extended Franz's method from 11 to 16 mycotoxins in cereals (2). This shows how Franz's work is not just of academic interest, but of real interest to people doing food testing around the world.

FB: In academia it's easy to feel that once you publish a paper, that's the end of the story. It's great to hear that people as far away as China are adopting our approach.

What was the next phase of the project?

FB: Besides the increasing sensitivity of instruments, a key trend in analytical chemistry is multiplexing. There are tens of thousands of fungal metabolites; we don't know the toxicity of the vast majority of those compounds, but we do know that several hundred have some degree of toxicity. So the second phase of our collaboration was to develop a multi-mycotoxin method that can screen for hundreds of metabolites (3) – preferably without the need for standards. This second phase started with tandem



"As well as access to powerful technology and next-level technical support, we appreciated the opportunities we were given to disseminate our work."

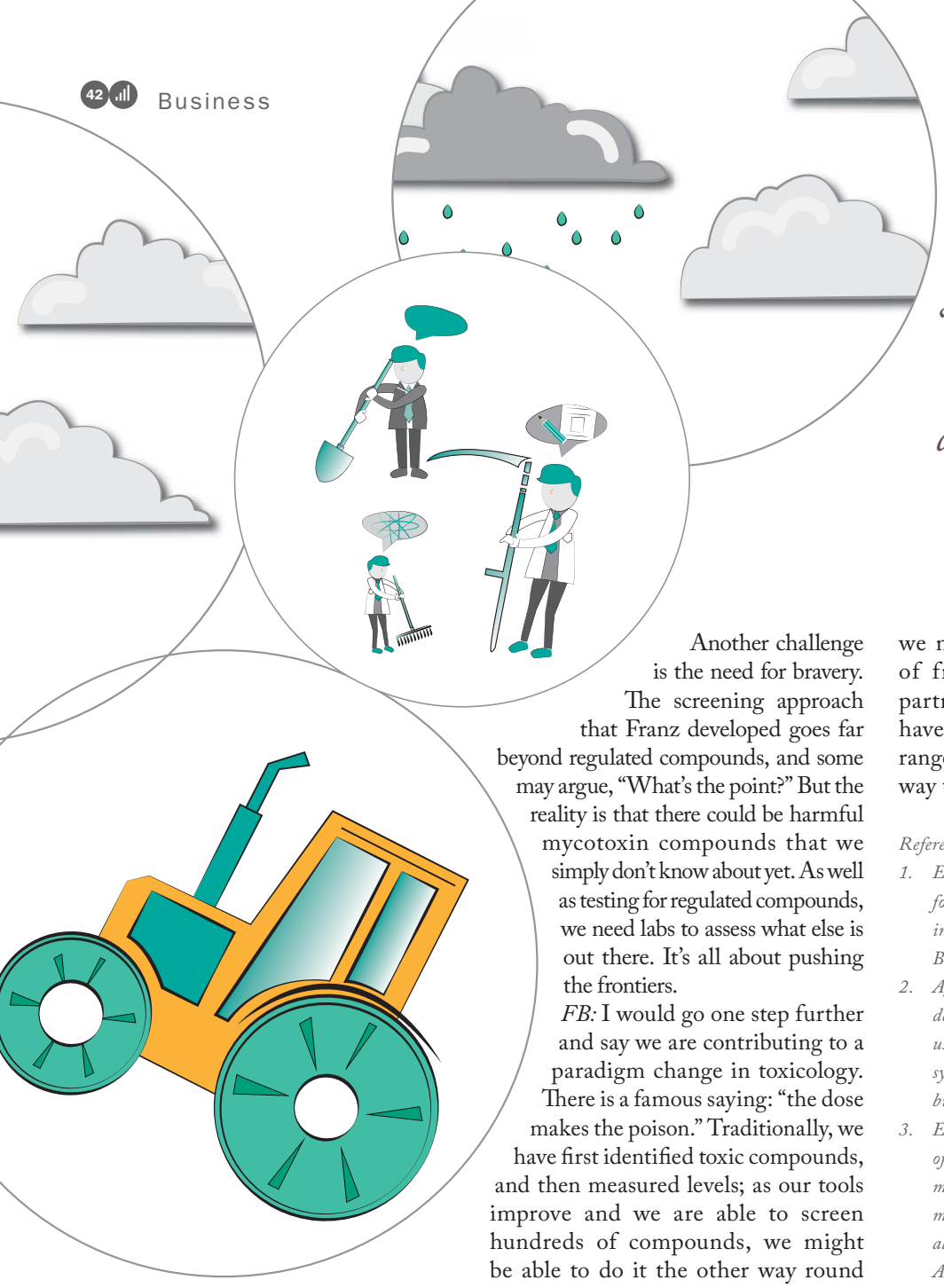
quadrupole LC-MS but ultimately led to the use of high-resolution mass spectrometry, which allows you to scan for anything that ionizes. We used an Agilent QTOF instrument and set up a workflow to screen for over 400 mycotoxins (4), which was challenging for a couple of reasons; first, we had a new instrument to get used to; second, we needed new types of workflows. The idea was to make a library for most of our targets using our specialized collection of standards and isolates. That would then allow any user of that instrument model to screen for the same compounds, even though they wouldn't have access to the standards (5).

What were the greatest benefits of collaboration?

FB: As well as access to powerful technology and next-level technical support, we appreciated the opportunities we were given to disseminate our work. We have had the chance to talk at several scientific conferences, and share our experiences in a WebEx organized by Agilent.

JL: I agree that dissemination is key – making sure that new methods are communicated in public conferences, but also through Agilent-organized events, like the meeting we run every spring for the food and environmental testing community (6). We want to communicate a whole workflow to our customers – and we can only do that through collaboration with experts l ike Franz.

Franz's work also informs our own efforts, allowing us to go back and develop the technology further.



What kind of challenges are typically encountered in such collaborations, and how do you deal with them?

JL: One of the challenges of any collaboration is simply that it takes time. Especially when you're trying to create something for the first time – like a library and databases for hundreds of mycotoxin compounds! Great work doesn't happen overnight, and it can be a challenge to keep focused, stay motivated, and keep driving things forward.

Another challenge is the need for bravery. The screening approach that Franz developed goes far beyond regulated compounds, and some may argue, "What's the point?" But the reality is that there could be harmful mycotoxin compounds that we simply don't know about yet. As well as testing for regulated compounds, we need labs to assess what else is out there. It's all about pushing the frontiers.

FB: I would go one step further and say we are contributing to a paradigm change in toxicology. There is a famous saying: "the dose makes the poison." Traditionally, we have first identified toxic compounds, and then measured levels; as our tools improve and we are able to screen hundreds of compounds, we might be able to do it the other way round – it might not be feasible to assess the toxicity of every compound, but we can start by assessing compounds that occur at high levels.

"I would go one step further and say we are contributing to a paradigm change in toxicology."

What's next?

JL: Franz is now working on yet more innovative workflows looking at "masked" mycotoxins – metabolites made in the plant that don't show up in testing but may still be toxic once ingested by an animal or human.

FB: This new line of work is something we never anticipated, but the degree of freedom that we enjoy in this partnership has made it possible. We have the flexibility to look at a wide range of issues, and that's a really nice way to work.

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Entering the Fifth Dimension

The analysis of complex food and petrochemical samples often demands multiple sample preparation and separation steps – time consuming and prone to error. Could we streamline the analytical method by combining five chromatography and mass spectrometry dimensions into a single automated instrument?

By Mariosimone Zoccali

The problem

I spent most of my PhD and postdoc years analyzing foods and petrochemical derivatives using various chromatographic techniques, starting with gas and liquid mobile phases, and graduating to CO_2 supercritical fluid. The samples I work with are very complex, encompassing not only multiple components but also a huge variety of chemical classes and concentrations. Moreover, most require a sample preparation step before the chromatography separation. Consequently, a number of different analytical techniques and sample preparation steps are usually needed to obtain reliable results. The challenging nature of such analytical methods led me to ask, "Is it possible to combine sample prep and complex analysis in a single fully-automated system?"

Background

Working in the laboratory of Luigi Mondello at the University of Messina, I have spent a great deal of time coupling different analytical techniques (liquid, gas, and supercritical fluid chromatography) to generate more powerful instruments. Under the supervision of Mondello and Peter Tranchida at the Separation Science Center in Messina, I later widened my focus to include both spectroscopy- and spectrometry-based detection methods.

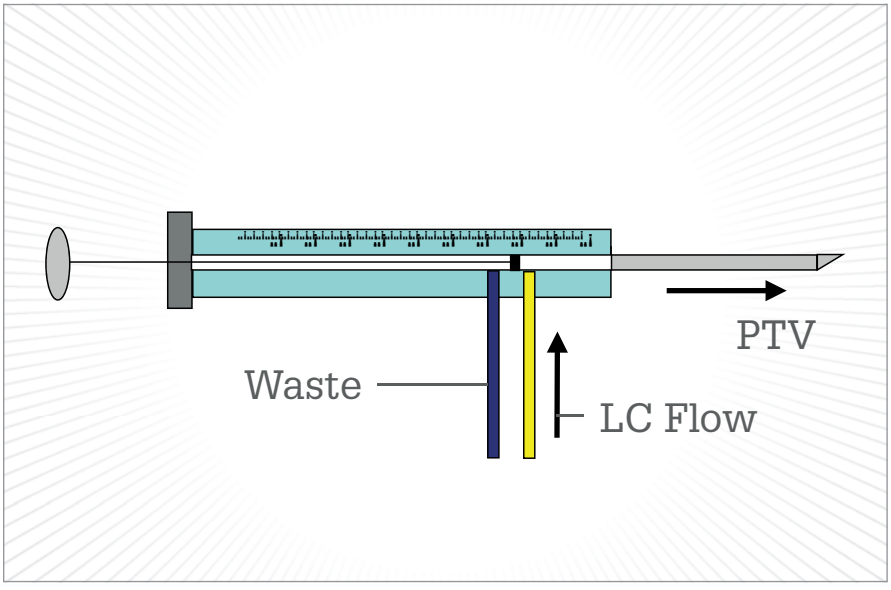
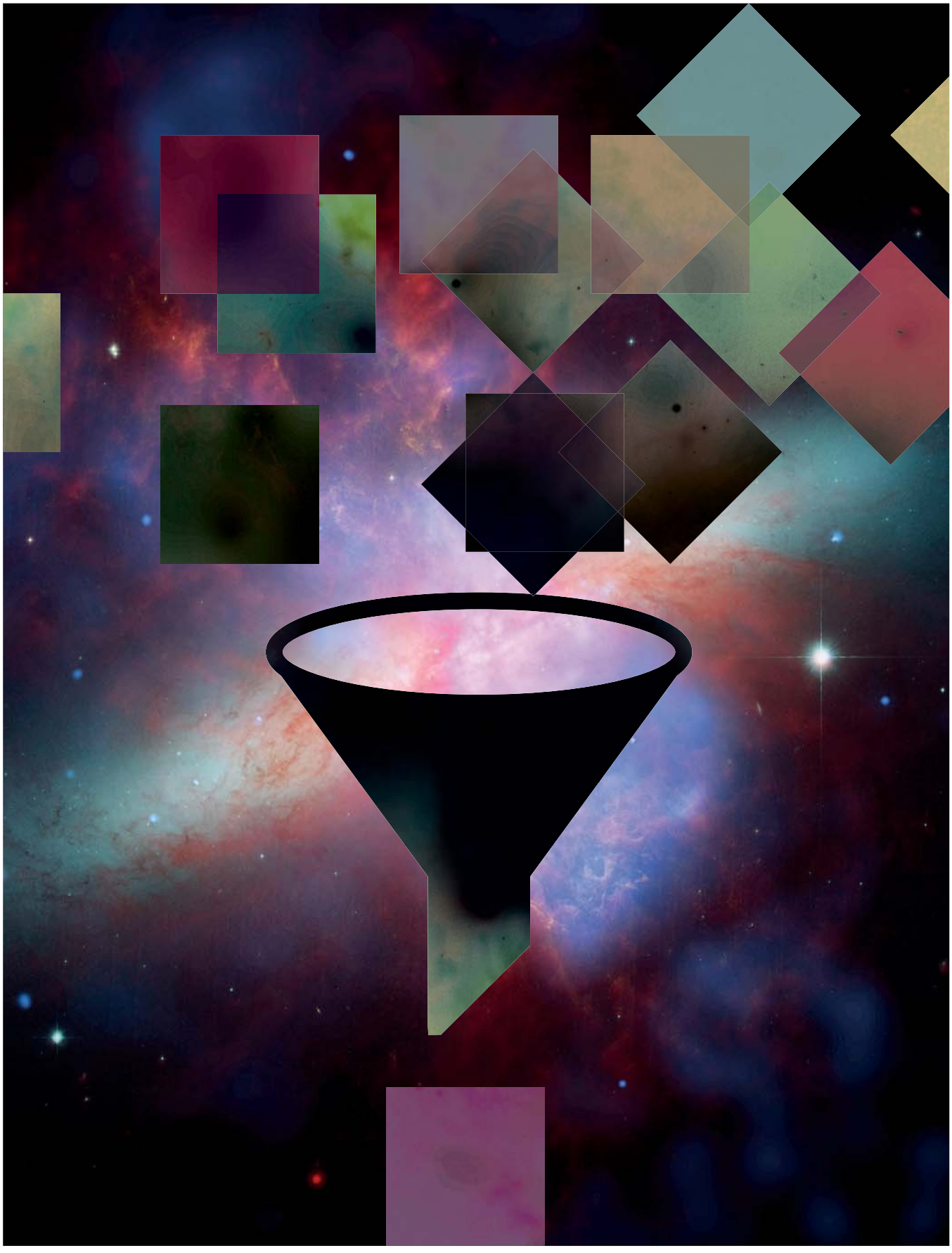


Figure 1. The syringe transfer device used for multidimensional LC-GC analysis.

My introduction to the world of separation science was via standard gas chromatography, and later comprehensive two-dimensional gas chromatography (GC×GC), which showed me the incredible resolving power of hyphenated techniques.

Later, my research focused on the analysis of volatile contaminants in foodstuffs that contained a large number of non-volatile components, such as vegetable oils, which are mainly composed of triglycerides. Here, a sample preparation step is mandatory for a reliable qualitative and quantitative analysis but is time consuming and carries a risk of sample



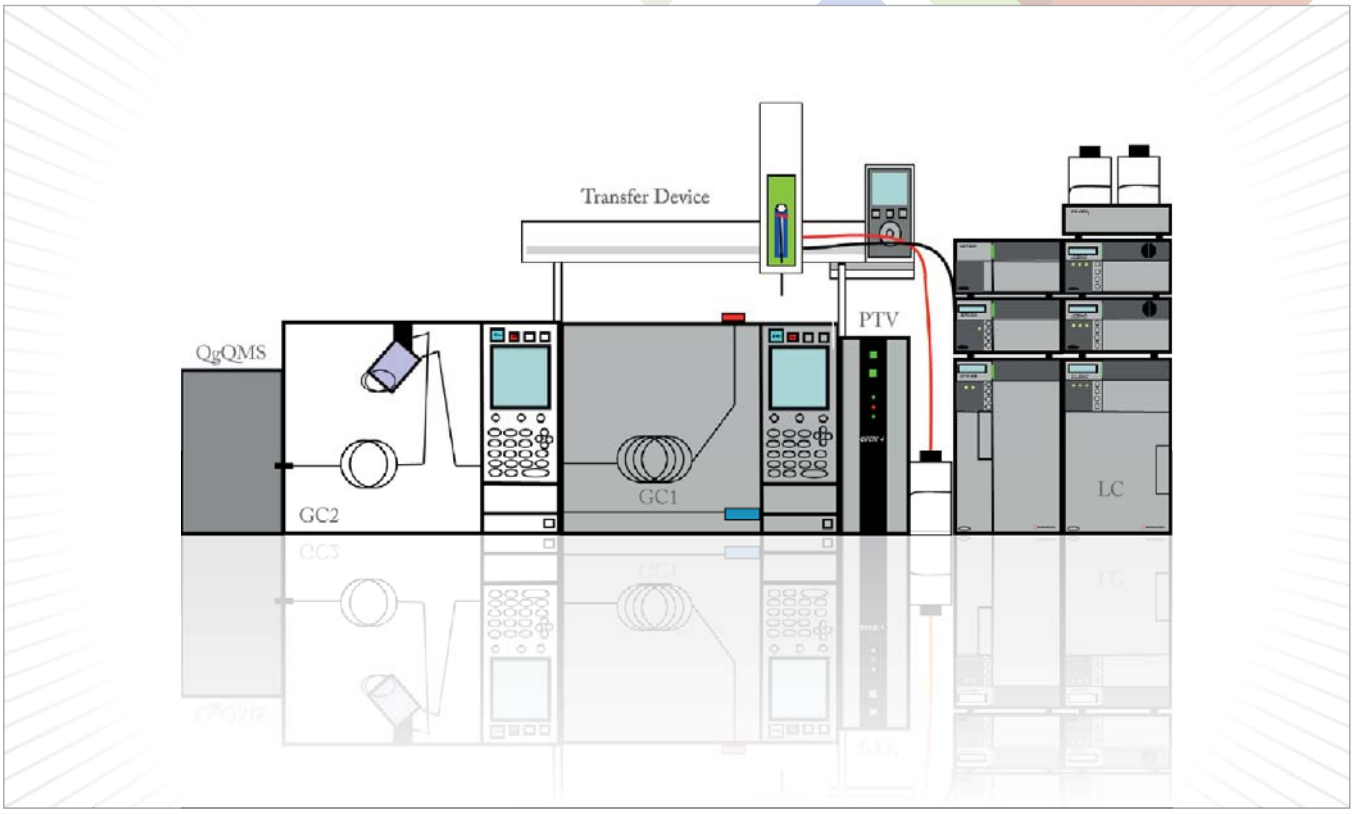


Figure 2. The LC-GC×GC-QqQ MS system.

loss or contamination. An on-line system coupling sample preparation and separation seemed an obvious solution. Normal-phase liquid chromatography can be used to retain the triglycerides, while non-polar solvents are well suited to gas chromatography, allowing the transfer of a purified fraction containing the volatile contaminants. Coupling the two techniques (LC-GC) creates a very powerful separation tool with enhanced selectivity and sensitivity.

However, in the Mondello lab we always want to push things further. So we designed a prototype of an on-line tool coupling LC with GC×GC, hyphenated with a very fast triple quadrupole mass spectrometer. LC is useful for sample preparation/pre-separation, GC×GC brings a very high separation power and sensitivity, and the detector offers both targeted and untargeted applications. Such a system represents the first five-dimensional analytical tool; three chromatographic and two mass spectrometry dimensions are combined.

The solution

After a weekend spent connecting parts of instruments from the lab (with help from service engineer Alessandro Visco), we were able to perform the first run.

The first part of the instrument is a conventional LC system with two dual-plunger parallel-flow pumps, making it possible to perform gradient analysis for the most challenging samples. The PDA detector was connected via PEEK tubing to a dedicated dual side-port syringe, installed in an auto injector, and was employed as transfer device (see Figure 1). Chromatography fraction transfer was achieved, in the stop-flow mode, through a modified 25 µL syringe. Briefly, the lower part of the syringe has two transfer lines – one to the LC detector exit and one to waste. A Teflon plug is located at the end of the syringe plunger; the latter is characterized by a lower outer diameter with respect to the barrel ID, enabling mobile-phase flow inside the syringe. In waste mode, the syringe plug is located below both lines and the effluent is directed to waste. In the transfer position, the syringe plug is located between the lines and the effluent flows to the GC. It is worth noting that potential band broadening during the stop-flow mode could be observed through continuous PDA monitoring. To handle very large amounts of solvent from the LC system,

a programmed temperature vaporizing injector (PTV) was used.

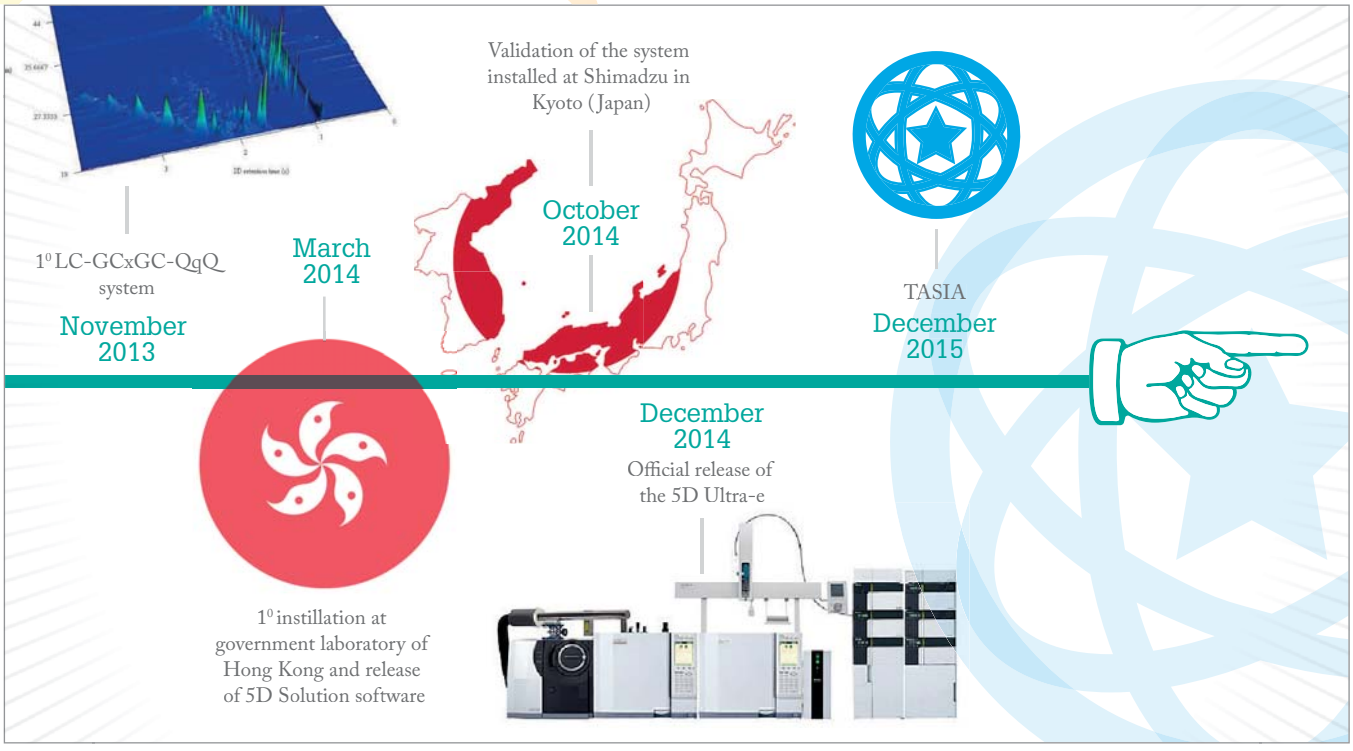
The GC×GC side consists of two gas chromatographs and a cryogenic modulator. The presence of two independent gas chromatographs allows a very high analytical flexibility, with the opportunity to perform two different GC oven temperature programs.

Finally, we decided to use a very high acquisition rate triple quadrupole MS detector, allowing both targeted and untargeted analysis. The mass spectrometric system generated a more-than-sufficient number of data points/peaks for both identification and quantification purposes (Figure 2 shows the configuration of the final instrument).

Having finalized the hardware configuration, we then focused our attention on software development. I spent a lot of time with Shimadzu engineers Tomohiro Kawase and Jun Nagata, and visited the beautiful city of Kyoto, Japan, to help develop intuitive software to control each part of the instrument. The resulting software allows the user to perform single or multiple LC cuts – sequential or not – with repetitive or different transfer times, and use different PTV and GC methods, optimized according to the transferred fraction. Moreover, to make GC×GC analysis easier, we developed software to calculate the average linear velocity inside the first and second dimension and the delay loop.

The LC-GC×GC/QqQ_MS system represents a unified and flexible instrument that can perform one-dimensional, heart-cutting and comprehensive two-dimensional chromatography analyses:

"Such a system represents the first five-dimensional analytical tool; three chromatographic and two mass spectrometry dimensions are combined."



"It's been amazing to see the technology progress from idea to prototype to commercial instrument."

LC/PDA, LC-GC/QqQ MS, LC×GC/QqQ MS, LC-GC×GC/QqQ MS, LC×GC×GC/QqQ MS, GC×GC/QqQ MS, and GC/QqQ MS. The system can be used in any of the seven configurations, depending on the sample complexity, simply through selection of the appropriate software settings.

I've condensed the story here but of course in reality there were many more twists and turns (one reason that the project was so fun!), with both hardware and software presenting significant challenges. Communication between modules had to be carefully considered – a single start signal for seven different devices (LC, transfer device, PTV injector, two GCs, modulator, and MS) means a lot of cables! Similarly, the main software challenge was compatibility between the modules. A single OS is not enough for their coexistence, so we had to install a virtual machine to overcome the various incompatibilities.

Beyond the solution

Today the technology, now known as 5D Ultra-e, is mainly used for the analysis of food and environmental contaminants, such as mineral oil, saturated and aromatic hydrocarbons, polychlorinated biphenyls, and polycyclic aromatic hydrocarbons. Another application is the analysis of highly complex petrochemicals.

The on-line nature of the system, compared to off-line approaches, reduces the risks of sample contamination, improves run-to-run precision, and enables the setting of batch-type applications. The system can be used in a variety of configurations, depending on the specific analytical requirements. Practically all GC-based applications can be covered using one of the seven operational modes.

Combining five dimensions into one system wasn't easy, but it's been amazing to see the technology progress from idea to prototype to commercial instrument (and be recognized in the 2015 Innovation Awards); it has certainly given me a great deal of a personal satisfaction, and I look forward to the new analytical challenges ahead.

Mariosimone Zoccali is a Postdoctoral Research Fellow at the University of Messina, Italy.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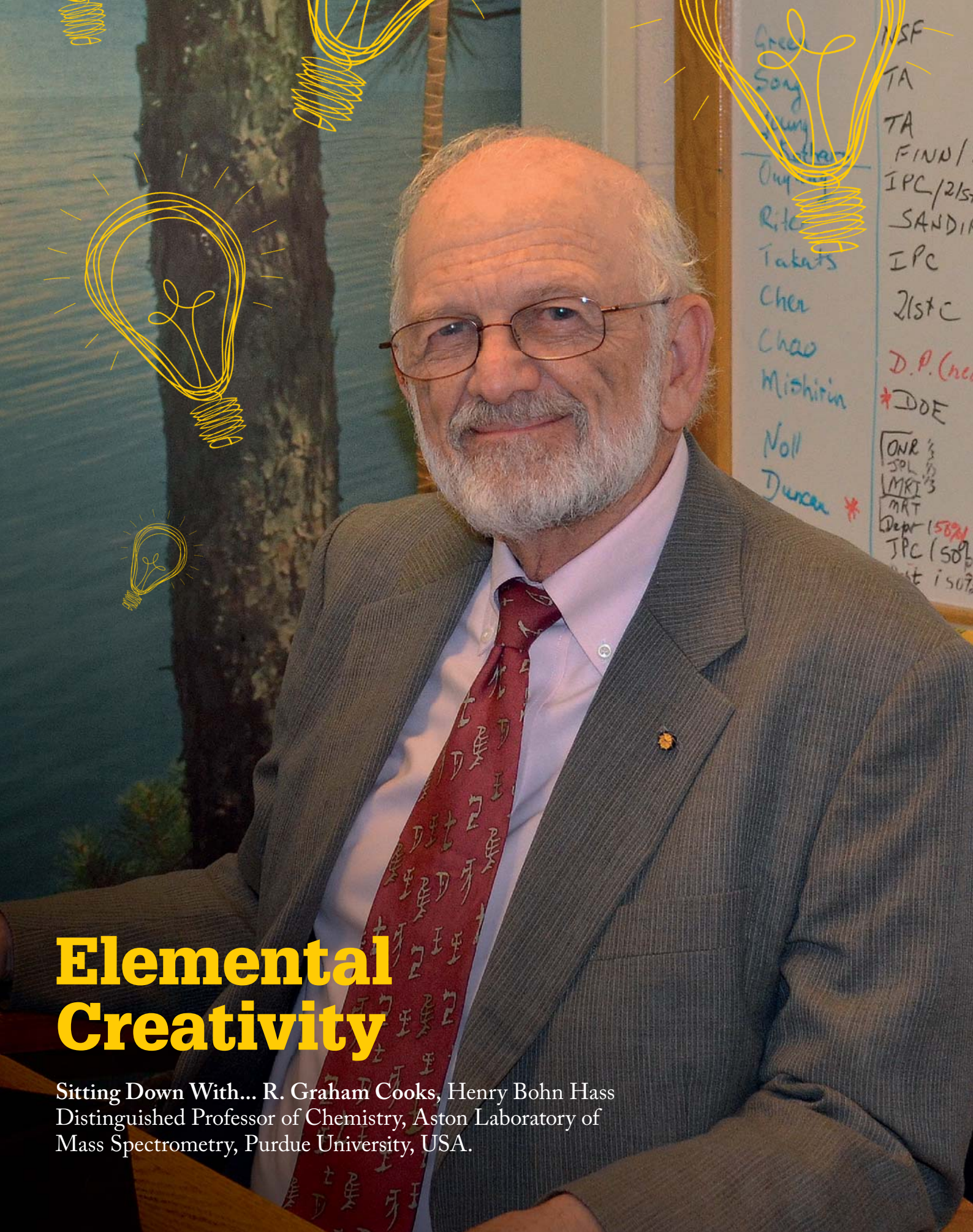

Elemental Creativity

Sitting Down With... R. Graham Cooks, Henry Bohn Hass Distinguished Professor of Chemistry, Aston Laboratory of Mass Spectrometry, Purdue University, USA.

Why did you go into mass spectrometry?
During my PhD at Natal University in South Africa, we were visited by Carl Djerassi. I was doing natural products research at the time, and told him I wasn't making much progress in finding the structure of a certain alkaloid using chemical methods. He asked me for a sample, took it back to Stanford, and recorded a mass spectrum. Ten days later my professor received an air letter with the structure. It was obvious that I had to work with mass spectrometry after that!

What was mass spectrometry like back then?
Well, when I went to the University of Cambridge in 1965 to continue my PhD studies, there weren't any commercial mass spectrometers – just home-built systems. A commercial instrument came soon after I started – and so I got to use one of the first – it wasn't until the instruments of this time that organic chemistry and MS first properly "met," and measurement of exact masses was accepted as a substitute for CHN elemental analysis.

What does your research group focus on?
We work on instrumental development, but that's really a means to an end. One of the merits of analytical chemistry is that it's at the center of all chemistry – almost anything is fair game. You could say we mostly do measurements – but it wouldn't be true. We don't simply record mass spectra (that's just the tip of the iceberg), and we seldom do classical chemical analysis. We work much more on reactions, and on disease diagnostics with MS, to infer in vivo properties of biological systems. We also study the chemical reactions of charged with uncharged species in and on the surface of microdroplets.

What do you most enjoy about your work?
I love that my research group is essentially a band of hunter-gatherers, seeking out information and monetary resources. Internally, we're seeking to understand, or waiting for inspiration... But maybe the biggest surprise to me in my career is the amount of external hunting required; we cross the globe to exchange information about research. It's a strange way to hunt, but it strengthens a shared enterprise.

How has research changed throughout your career?
Being an academic used to mean being semi-cloistered – to give you the time and leisure to think. As research became a larger component of society and a major part of the economy, it could no longer be ignored or left "uncontrolled." People came to depend on the state for funding, and so research became woven into the control mechanisms that run the rest of society. It's a very different enterprise now, and not without benefit – the successful implementation of ideas for societal good is definitely something to be welcomed.

What's the main contribution of mass spec?
It has evolved into the major methodology in analytical – and pretty much all of biomedical – science. The reasons are simple. If you've got charges on molecules, you can handle them, move them around and measure them much more easily; that fact, plus the sensitivity, broad applicability and high specificity with which you can identify particular species means that MS has huge potential, only some of which has been realized. For example, we are just starting to see the emerging capabilities of MS in making medical diagnoses in the clinic.

In my lab we are focused on intrasurgical tissue analysis using desorption electrospray ionization mass spectrometry. It's the easiest type of MS imaginable; low resolution, low performance, simple single-stage instrumentation, and yet you get a huge amount of information from the distributions of lipids and other small molecules. Diagnosing the disease state of brain tissue during brain surgery in a couple of minutes is actually "state of the art" – but it's done with instrumentation several generations behind.

How do you envisage the next few years?
I would say one big change is that MS will transition from being a predominantly analytical technique to a synthetic technique. Unlike other forms of spectrometry or spectroscopy, MS is based on matter, which happens to have charge. It can be individual atoms and collections of molecules, or it can be organized collections of proteins. It's only natural that MS should be an important component of bond-forming chemistry. People may dislike the term "mass spec synthesis," but it emphasizes its versatility. I think that this is one of the major directions in which MS will go – it will begin to shed its purely analytical cloak and take on others.

You have said before that unhappiness makes for a successful inventor…
I've always found research to be extremely emotional – a world apart from the cold and rational stereotype of the scientist. Grappling with problems, as well as concepts and ideas you'd like to make a reality, sometimes takes a long time; for example, we first tried ion soft landing in 1976, but it wasn't till the 1990s that we were successful. We also worked on surface-induced dissociation, which was laughed at for decades, but has now been found to have really important applications. There is an emotional drive that comes from getting difficult experiments to work – and an equally strong emotional reaction when you fail. Musicians or poets occasionally succeed in saying something – but most of the time they don't. The same could be said for scientists. I have always been agnostic as to discipline. I'm happy for any measure of creativity – whether it's in poetry or mass spectrometry.

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