FEBRUARY 2019 # 73

the Analytical Scientist™

Química Analítica

Three scientists reveal a vibrant research community in South America.

F-DGSi
Innovative Gas System Company

DON'T BUY YOUR GAS,
MAKE IT !

COSMOS GAS
GENERATORS FOR GC

SECURE YOUR GC WORKFLOW
WITH TECHNOLOGY LIGHT
YEARS AHEAD !

F-DGSi- SMART SOLUTIONS
WITH "GEN SECURE"

SECURE

MODULAR

ADVANCED

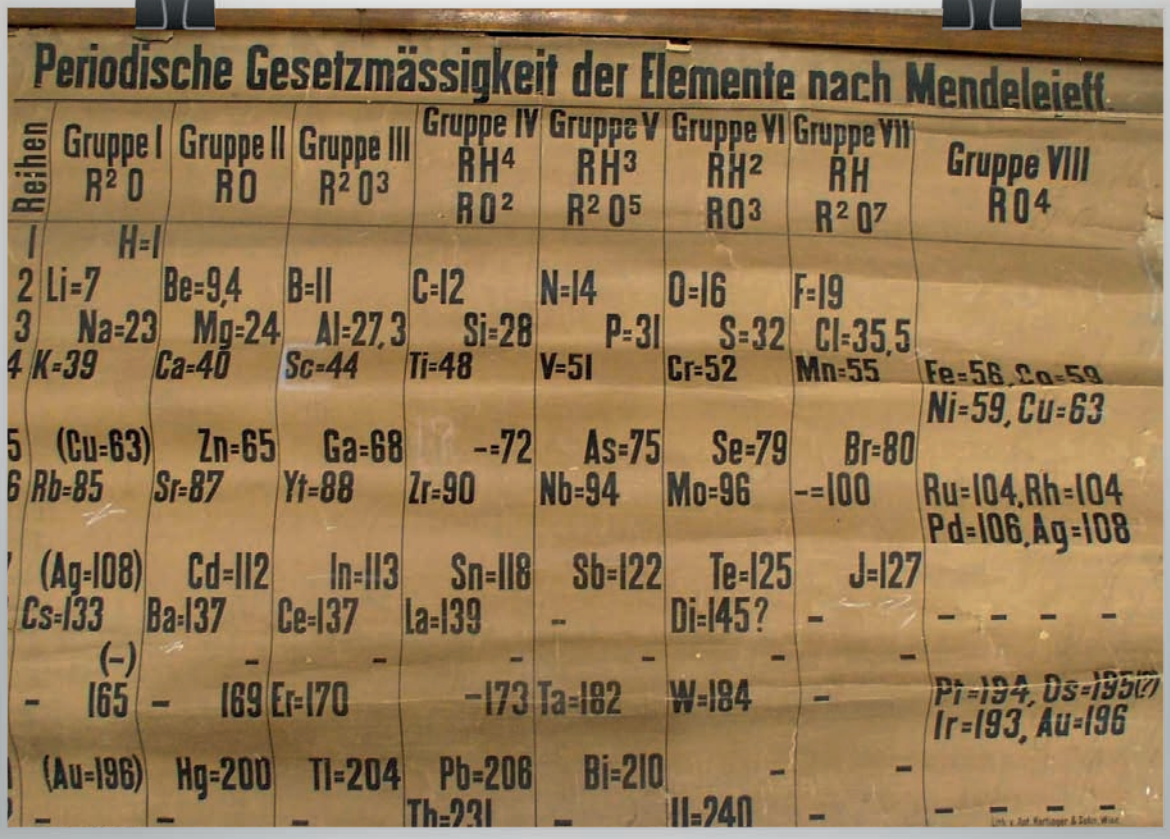
REMOTE CONTROL

TRUSTED

VISIT OUR BOOTH : · PITTCON PHILADELPHIA N° 2811 · ARABLAB DUBAI N° 658

WWW.F-DGS.COM

Image of the Month



From the Archives…

This battered paper and canvas poster is thought to be the oldest surviving periodic table wall chart. Found underneath a lecture theatre at St Andrew's University (UK) in 2014, and featuring just 71 elements, the chart is thought to date from 1885 – just 16 years after Dmitry Mendeleev first published the iconic table. The university shared photos of the restored chart to mark the United Nations-designated "international year of the periodic table."

Credit: University of St Andrews

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

Contents

10

On The Cover

The flags of Argentina, Bolivia, Brazil, Colombia, Chile, Paraguay, Peru and Uruguay celebrating analytical science in South America.

Upfront

In My View

Features

Reports

The Spectroscopist Inside

Sitting Down With

the Analytical Scientist

ISSUE 73 - FEBRUARY 2019

Change of address
info@theanalyticalscientist.com
Hayley Atiz, The Analytical Scientist,
Texere Publishing Limited, Booths Park 1,
Chelford Road, Knutsford, Cheshire, WA16 8GS, UK

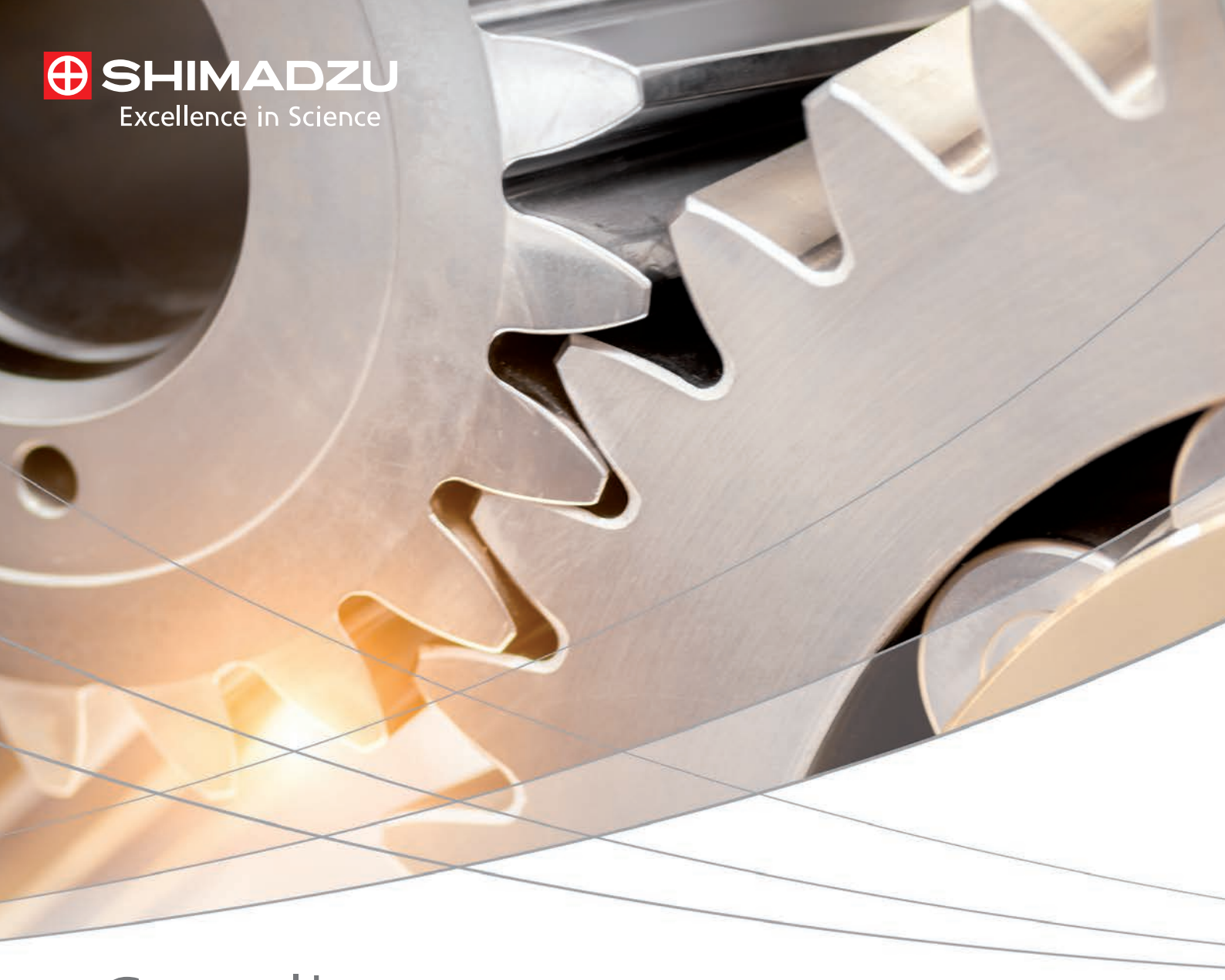
General enquiries
www.texerepublishing.com
info@theanalyticalscientist.com
+44 (0) 1565 745 200
sales@texerepublishing.com

Distribution:
The Analytical Scientist (ISSN 2051-4077), is published monthly by Texere Publishing Limited, Booths Park 1, Chelford Road, Knutsford, Cheshire, WA16 8GS, UK. Single copy sales £15 (plus postage, cost available on request info@theanalyticalsientist.com). Non-qualified annual subscription cost is £110 plus postage

texere publishing ltd

Available on the App Store

SHIMADZU
Excellence in Science



Coupling powers

Pioneering new fields in ultra-trace analysis, the new GCMS-TQ 8050 NX triple quadrupole couples the powers of a world-leading GC and a newly designed detector. Both provide outstanding sensitivity at femtogram and even sub-femtogram levels.

Superior performance of NX technologies
e.g. new flow controller and time management for maintenance

A wide variety of optional products supports trace analysis
such as autosamplers and inlets

Comfortable, easy change of accessories
through the advanced, illuminated GC oven

The GCMS-TQ 8050 NX complements the Shimadzu NX family, coupling the Nexis GC-2030 with the quadrupole series TQ-8050, TQ-8040 or QP-2020. Shimadzu's NX series provides high-end GCMS solutions for every analytical challenge.

www.shimadzu.eu/coupling-powers

Crossing Borders

In science – as in life – it's important to enjoy the journey

"*As you set out for Ithaka*
hope the voyage is a long one,
full of adventure, full of discovery."

I begin with an excerpt from a poem written in around 1900 by Constantine Peter Cavafy. Within its five verses, he tells us to live our life as an adventurous journey, to visit many cultures and countries, to not be afraid, to keep our heads high, and to enjoy that journey fully, while keeping in mind that our destination is – as Ulysses' goal was – Ithaka.

These days, being an analytical scientist can bring a life full of adventure. We work in all kinds of interesting areas of exploration, and our endeavors give many of us the opportunity to see different countries and meet with scientists from many cultures.

Times have changed for the better. When I studied analytical chemistry some 40 years ago, not many of us crossed borders – neither geographical borders, nor the borders of our own specialism. Instead, scientists dug deeper and deeper, like moles searching for the light while, unsurprisingly, it became darker and darker around them.

Since then, analytical scientists have (thankfully) lost their tunnel vision and started to collaborate with a variety of sciences to provide direction, details, facts and figures. The tools we developed made many discoveries possible – in energy, health, biology, medicine, genetics and proteomics.

This issue of The Analytical Scientist is full of adventures and crosses many borders. We take a look into analytical science in South America, go deep into single cell analysis – and in "The Spectroscopist Inside," we ask spectroscopists what's on their ultimate wish list.

So why aim for Ithaka? What if we arrive and find it disappointing? Cavafy gives us an answer:

"Ithaka gave you the marvelous journey.
Without her you would not have set out.
She has nothing left to give you now.

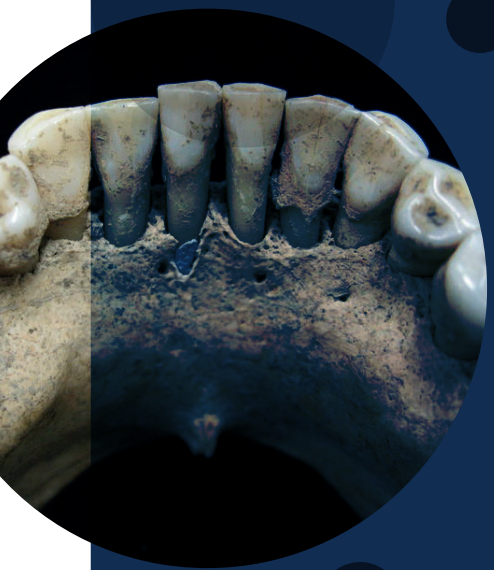
And if you find her poor, Ithaka won't have fooled you.
Wise as you will have become, so full of experience,
you will have understood by then what these Ithakas mean."

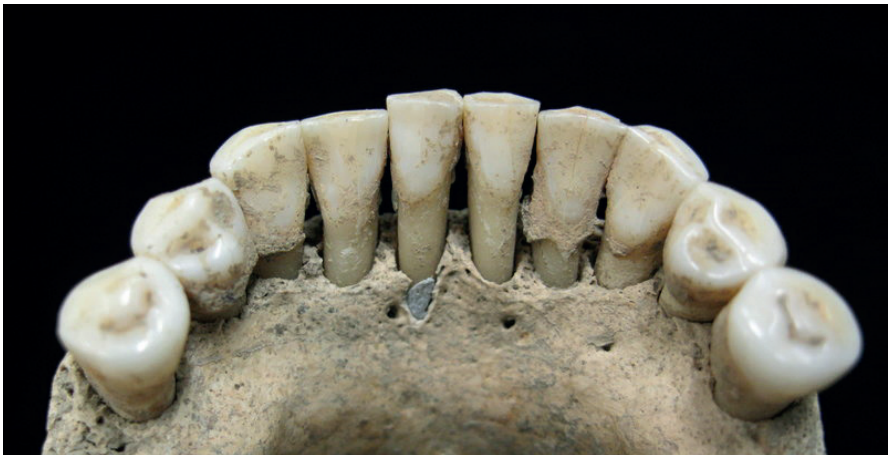
Frank van Geel
Scientific Director

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





Something Old… Something Blue

Lapis lazuli found in dental calculus paints a different picture of medieval gender roles

According to a recent discovery by an international research team, when it came to producing illuminated manuscripts, women in the Middle Ages really got their teeth stuck into the process.

They analyzed the teeth of a female skeleton found in Dalheim, Germany, and discovered a blue pigment in the dental calculus. Micro-Raman spectroscopy confirmed it was lapis lazuli, a mineral used for coloring the manuscripts at the time, and more recently as a semi-precious stone in jewelry.

Illuminated manuscript production in the Middle Ages was previously thought to be the province of men, specifically monks (according to an article in The Atlantic, one expert suggested this woman had come into contact with the pigment because she was the "cleaning lady"). "Microscopic analyses have revealed that dental calculus (calcified tooth tartar) can entrap and preserve a wide range of microdebris related to craft activities," said the authors in the paper (1). One of the researchers' theories for this is that women were involved in the production process, thus painting a different picture of medieval gender roles.

What's more, it gives some insight into trading at the time – the lapis lazuli stone was mined only in Afghanistan, 4,000 miles away. In this case, it was found in "an otherwise unremarkable women's community in northern Germany," which, the authors believe, "powerfully testifies to the expansion of long-distance trading circuits during the 11th-century European commercial revolution."

This isn't the first time a tooth has told the truth; dental plaque has shown that women from ancient societies were partial to smoking (2) and has even helped reconstruct the genome of the bacterium behind the Great Plague (3).

Reference

1. *A Radini et al., "Medieval women's early involvement in manuscript production suggested by lapis lazuli identification in dental calculus", Sci Adv, [Epub before print] (2019). DOI: 10.1126/sciadv.aau7126*
2. *https://theanalyticalscientist.com/techniques-tools/the-tooth-will-out*
3. *https://theanalyticalscientist.com/fields-applications/pestilence-persistence*

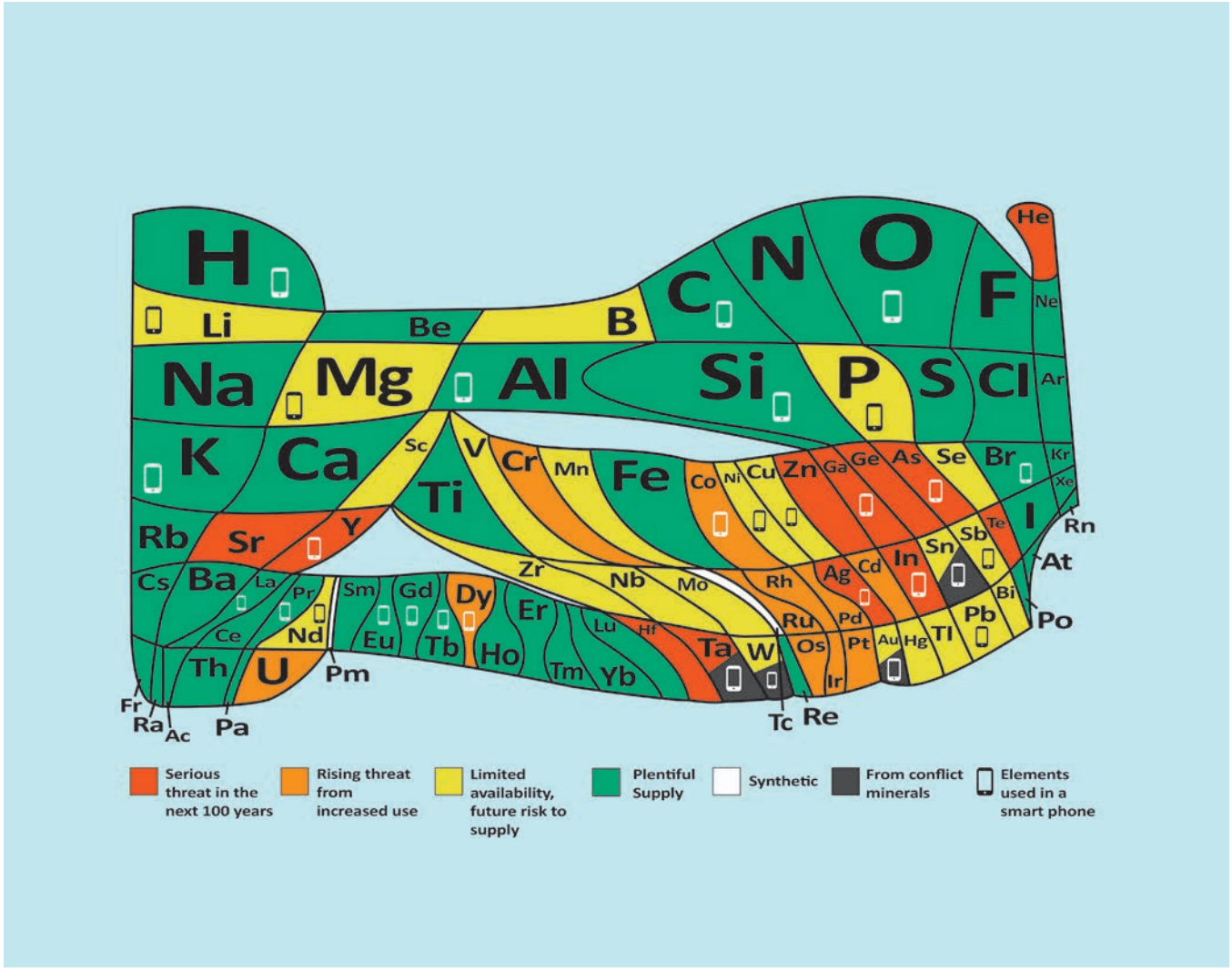


Image credit: European Chemical Society

Red Alert!

A new version of the periodic table shows the elements under threat

Join us in wishing the periodic table a happy 150th anniversary!

It seems that the years have taken their toll, however. On a new version published by the European Chemical Society, each of the 118 elements has been color-coded to show how vulnerable they are to dissipation – in short, the more we use them, the harder they will be to recover.

Elements such as silver (Ag), helium (He) and strontium (Sr) are the most under threat – and many of the elements "in the red" play an important part in our technology, from MRIs to smartphone screens to deep sea diving equipment. The chart also shows (in black) elements that could be more ethically sourced, known as "conflict minerals" because wars are fought and lives lost over their ownership.

This version of the periodic table provides a striking reminder that we need to apply the five Rs – Refuse, Reduce, Reuse, Repurpose, Recycle – at a fundamental level. However, you'll be glad to see that oxygen – for now, at least – is still in plentiful supply.

Reference

1. *A Radini et al., "Medieval women's early involvement in manuscript production suggested by lapis lazuli identification in dental calculus", Sci Adv, [Epub before print] (2019). DOI: 10.1126/sciadv.aau7126*

Sweating the Small Stuff

Tracking the body chemistry of athletes – through perspiration

A new waterproof, flexible sensor could be the latest way for athletes to monitor their health and hydration. Tracking biomarkers through sweat analysis is an increasingly popular technique in diagnostics, but John Rogers and the rest of his US-China team have taken it to the next level, by creating a sweat-collecting sensor that can function underwater and – crucially – stay in place on the body, even during vigorous swimming.

The device combines a waterproof microfluidic, absorbent pad and a near-field communication sensor, all attached using a skin-safe adhesive. Initial trials have been promising; the devices have been able to successfully measure chloride concentration of sweat and skin temperature. The researchers believe it could be used for cystic fibrosis screening in babies (which is also measured by chloride levels in sweat).

Rogers and his colleagues have been working on stretchable sensors for some time (2) and the iterations continue to evolve – next, they plan to try to measure electrolyte losses. Well they do say genius is one percent inspiration and 99 percent perspiration…

Reference

1. *JT Reeder et al., "Waterproof, electronics-enabled, epidermal microfluidic devices for sweat collection, biomarker analysis, and thermography in aquatic settings", Sci Adv, 5 [online only] (2019). DOI: 10.1126/sciadv.aau6356*
2. *2. https://theanalyticalscientist.com/techniques-tools/biomarkers-sweat-and-tears*

Impress in 600 Seconds

Do you have the research focus and the charisma to become… The Separation Science Slam Champion of HPLC 2019?

All young separation scientists (35 years old and under) are invited to submit abstracts for the opportunity to present at a brand-new session at HPLC 2019 in Milan, Italy: the Separation Science Slam.

Successful applicants will have just 10 minutes on the Separation Science Slam stage to inform, engage and thrill the audience – and jury – with the hard-earned results of their liquid chromatography-based research project.

Competition is expected to be fierce, so "slammers" are urged to make use of props, live demonstrations, assistants… anything that will "wow" the crowd.

The reward? Gold = €2000 Silver = €1500 Bronze = €500

Send your short abstract (max 100 words) and brief CV to: rich.whitworth@texerepublishing.com

Abstract deadline: March 29, 2019.

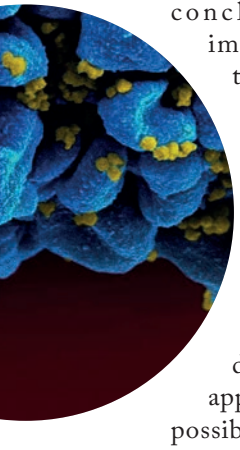
If you have any questions or require further guidance, please contact: rich.whitworth@texerepublishing.com

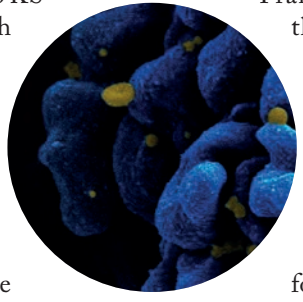
One TINY Step at a Time

How to diagnose Kaposi's sarcoma in areas without reliable infrastructure

First author Ryan Snodgrass uses sunlight to heat TINY at the AIDS Healthcare Foundation-Uganda Cares Clinic, Masaka, Uganda.

Kaposi's sarcoma (KS) presents a diagnostic challenge at the best of times: the disease can form masses in the skin, lymph nodes or elsewhere; lesions can be limited or widespread; they may be flat or raised; and each of the disease's four subtypes may resemble a range of other conditions. Nevertheless, conclusive diagnosis is important, not only for treatment purposes, but also because KS is considered AIDS-defining, meaning that its presence in an HIV-positive patient makes the diagnosis of AIDS official. But histopathologic diagnosis – the standard approach – is not always possible in resource-limited settings, such as sub-Saharan Africa, where KS is endemic, and so KS is often diagnosed through macroscopic observation. Unfortunately, the disease's heterogeneous nature means that clinical diagnosis is error prone.





It's clear that a point-of-care testing device capable of circumventing the need for traditional testing would be invaluable. And so, a team of engineers, pathologists, dermatologists and clinical epidemiologists at Cornell University designed device that can be operated without electricity: the Tiny Isothermal Nucleic acid quantification sYstem – TINY, for short (1).

Jeffrey Martin, Professor of Epidemiology and Biostatistics at the University of California, San Francisco, helped determine the suitability and accuracy of the device. He explains the testing process: "A small biopsy of the affected skin is taken under local anesthetic. DNA is then extracted from the biopsy and tested for the presence of Kaposi's sarcoma-associated herpesvirus (KSHV) DNA via a reaction known as loop-mediated isothermal amplification (LAMP)." Because LAMP needs samples to be heated 154°C, the assay cannot typically be conducted without a power source; what makes TINY unique is its ability to collect and store heat from any source, including the sun and Bunsen burners, allowing it to function without a reliable source of electricity.

Martin is currently working alongside colleagues to test the device's accuracy across a broad range of conditions in Africa. At the same time, the team is establishing demand for TINY and seeking ways to keep its cost low. "Obviously, we need to make this as inexpensive as possible," says Martin. "There is little point on working on such a project if we cannot make it affordable."

References

1. *R Snodgrass et al., "A portable device for nucleic acid quantification powered by sunlight, a flame or electricity", Nat Biomed Eng, 2, 657–665 (2018).*

From mAbs to MALDI

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

Products and launches

- Waters has launched several new products this month, including:
  - The Kairos Amino Acid Analysis Kit, which aims to streamline and speed up LC/MS-MS analysis of human urine and plasma.
  - The BioAccord System, an LC-MS aimed at the biopharma market that should decentralize routine monitoring.
  - Ion-Exchange Columns (BioResolve SCX) to simplify mAb characterization
- Bruker launched the G6 LEONARDO, an inert gas infusion analyser for ONH concentration in organic samples.

Collaborations and company updates

- The San Francisco Office of the Chief Medical Examiner (SFOCME) is partnering with SCIEX to speed up forensic testing in the city.
- Mala Anand (president, Intelligent Enterprise Solutions and Industries) has been appointed to Agilent's Board of Directors. Agilent chairman Koh Boon Hwee said, "[Mala's] depth of experience in technology innovation and cloud-based strategies brings a critical perspective to the board."
- MRM Proteomics has partnered with Biodesix. granting them the rights to use its MALDI technology for the improvement of lung cancer diagnostics.
- The US Department of Defense has selected Smiths Detection (SDI), a threat detection and screening technology company, to design and engineer a new chemical detector. SDI is itself partnered with 908 Devices, which develops the high-pressure mass spec used in their detectors.

For links to original press releases, visit the online version of this article at: tas.txp.to/0219/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 charlotte.barker @texerepublishing.com

Here Be Monsters

Predators lurk in the world of science communication, waiting to trap the unwary – here's how to evade their clutches.

By Peter de Boves Harrington, Ohio University Center for Intelligent Chemical Instrumentation, Department of Chemistry & Biochemistry, Athens, Ohio, USA.

The advancements of the "Information Age" have made it easy to distribute intellectual property such as research reports. Many publishers have moved to an open access (OA) model, in which the authors of the research report pay for publication and retain the copyright. Thereby, the publishers recover the lost revenue of selling reprints, while the research is accessible for all, including scientists in developing nations. These OA journals, many of which are online-only, have reduced production costs, creating the opportunity for many new start-up journals, some based in developing nations.

It's a common scenario. You receive a request to submit a paper to a journal you have never heard of, that has nothing to do with your area of research or publication record. Usually not mentioned in the invite is the publication fee that is involved. In some cases, the editor can be quite forceful, as with the example below, which I received last year:

"As per previous conversation I am eagerly looking for your submission, but yet I have not received that. So I humbly request you to submit your eminent submission at the earliest possibility. In fact I have only few days to reach my goal."

There had been no previous conversation, and the grammar is poor – both giveaway clues that I was being stalked by a predatory publisher.

You may also receive an invite to an editorial board of a journal or be asked to edit a special issue. In one case, a journal recruited an editor for a special issue on chemometrics. The special issue, which was supposed to have no publication charges for the submitted papers, was never published – all the submitted papers were rejected without review, by the Editor-in-Chief.

Before agreeing to submit anything to a journal you haven't worked with previously, check out their website and editorial board thoroughly, and read a few papers from past issues.

The activities of predatory publishers now extend to conferences too. If conference invites, flyers, and descriptions are poorly written, or you haven't heard of the event, proceed with caution. I was once invited to be a plenary lecturer at "the 9th Edition of International Conference on Analytical Chemistry" (although, strangely, no evidence of the previous eight editions could be found online…). The conference, from EuroSciCon Ltd, could not process my credit card because of previous reports of fraud by the company (another warning sign). When I authorized my credit card company to override the fraud alerts, the conference overcharged me for registration, but I was assured that they would reimburse me later – of course, this never happened. The night before the conference was to begin, I was informed that the conference organizer would not be present and that I would be the conference chair with the responsibility of giving the opening address, moderating all the sessions, and dealing with any problems, of which there were many. After the conference, my emails went unanswered, and I never received my refund. I have heard of other three- or

four-day conferences ending after day one, because so few authors of the submitted abstracts attended the meeting.

Apart from poor grammar and a lack of online history, you may find other discrepancies in the claims made by these conference organizers. Two recent conference invites claimed that the number of attendees in the previous years had topped 400, but inspection of the website and the conference photograph showed no more than 20 people. Another tip is to check the technical programs from previous years – all too often, it is a hodge-podge of talks unrelated to the theme of the conference. Bear in mind that these conferences may list organizing board members, sponsors, and exhibitors without their consent, so if you have any doubts do not hesitate to contact a member of the board by email.

More information on what to look for is available at http://thinkchecksubmit.org/check and a list of known or suspected predatory publishers is available at https://beallslist.weebly.com/

No Longer the Tool of Last Resort

It's a versatile method with widespread applications – isn't it time people overcame their fear of Raman spectroscopy?

By Ian R. Lewis, Director of Marketing, Kaiser Optical Systems, Inc. – An Endress+Hauser Company, Ann Arbor, Michigan, USA.

I think there is still a certain negative viewpoint of Raman amongst many in the wider analytical science community. Perhaps older scientists used Raman during their studies and found it unwieldy and complex – but that's simply not true for modern Raman.

Raman has changed considerably in the last 35 years. The Raman instruments that started to become commercially available in the late 1980s were the first to overcome this hurdle. There had been Raman microscopes before that, of course. The predecessor of HORIBA, Jobin-Yvon, produced a Raman microscope in the 1970s, but it was not very sensitive and lost a lot of photons through the multiple monochromators. The polychromator-based systems with notch filters were an order of magnitude – or maybe several orders of magnitude – more efficient than some of these older designs.

Over time, smaller, more compact lasers were developed and combined with high-quality detection elements. The fact that these instruments were compact enough to stand on a small optical breadboard that could fit on benchtops – or that they didn't need a breadboard at all – allowed Raman to come into labs that would never have used it before. Some of the many applications that had been written about since the 1960s became more of a practical reality. For example, Raman (coupled with fiber-optic probes) proved very useful for polymer characterization or pharmaceutical characterization of formulations. At that stage, Raman became more mainstream – or perhaps it's better to say that it wasn't being dictated by any single type of application; people were trying it in a variety of areas, whether it be explosives, forensic samples, environmental samples, or biological samples. It was changing from a complicated optics tool to a more usable device. And, as the equipment stabilized and became more user-friendly, the number of spectrometers installed increased – as did the number of people exposed to Raman spectroscopy.

Today, we see a great deal of interest in the pharmaceutical and chemical industries, in the polymer and material science space, and in art and archeology – where its non-destructive nature means you can take the spectrometer to the sample using a fiber optic probe. Another hot area is in the biomedical sector – where the coupling of spectrometers to probes can be used on patients to assess diseased tissue, for example.

All that said, I believe that it remains underutilized. In my view, there is serious scope for it to have an impact on many other fields.

Despite the many positive application stories noted above – where Raman has evidently evolved into a far more accessible technique – many scientists still appear to be "afraid" of the technology. Those "missing out" on Raman likely see it as a technology that requires a PhD spectroscopist and a laser lab – and comes at a cost of hundreds of thousands of dollars in equipment. With such a misperception, it's no wonder that people are not giving Raman the chance that I believe it deserves. As scientists (and vendors) in this space, it's our job to convince people of the virtues of Raman; to ensure that the naysayers know that the technology has moved on significantly; to gently persuade the fearful that modern instrumentation is far more user-friendly.

We are now at a point where the application is no longer limited by the lack of the right equipment, no longer limited by the necessity to take the sample to the Raman system, no longer limited to the academic lab, but rather by (misinformed) misgivings or the inability to look at a problem with fresh eyes. In my view, on the one hand that is a real loss to the world of analytical science and on the other a real opportunity for the future.

Supelco®

Analytical Products

IMAGINE THE NEXT 350 YEARS

Supelco® analytical products from Merck. Accurate. Precise. Consistent.

We know only the most accurate analytical products will do. That's why Merck offers the Supelco® portfolio of analytical products. Whatever your needs, our portfolio is always fit for purpose, ensuring your results are accurate, precise and reproducible, and your systems fully certified. Our comprehensive portfolio, developed by analytical chemists for analytical chemists, covers a broad range of analytical solutions, and every product is meticulously quality-controlled to maintain the integrity of your testing protocols. And with Supelco® scientists dedicated to your analytical applications, the expertise you need is always on hand.

1668
Merck beginning with a pharmacy in Darmstadt, Germany

1827
Merck transformation into a research-based company

1850
Establishment of partnership E. Merck

1935
Sigma Chemical Company Founded

SIGMA

1951
Aldrich Chemical Company Founded

ALDRICH

1966
Supelco Founded

SUPELCO, INC.

1975
Merger to form Sigma-Aldrich Corporation

SIGMA-ALDRICH

1993
Supelco Acquired by Sigma-Aldrich

SUPELCO®

1995
Establishment of Merck KGaA and public listing

SigmaAldrich.com/Supelco

The life science business of Merck operates as MilliporeSigma in the U.S. and Canada.

Lit. No. MK_AD2917EN 10/2018

Founders of Supelco

Dr. Walter Supina
Born in Hartford, Connecticut, Walt obtained his doctorate in chemical engineering in 1960

Mr. Nicholas Pelick
Born in Scranton, Pennsylvania, Nick obtained his master's degree in biochemistry in 1964

Footprint of Supelco

1966: Enters GC business with adsorbents and packed GC columns
1971: Enters carbon adsorbent business with Carbosieve®
1979: Enters HPLC with SUPELCOSIL™ line of stable 5 µm spherical particles with true monolayer bonding
1983: Enters the air sampling market by introducing a line of solvent desorption tubes for industrial hygienists to help protect workers from being exposed to toxic chemicals
1985: Enters sample preparation business with Supelclean™ SPE tubes
1993: Launches SPME fibers
1994: ISO 9001 – Quality Management System
2006: Sigma-Aldrich acquires Astec®: leader in chiral chromatography
2007: First to market globally Fused-Core® particles jointly with Advanced Materials Technology, introduced Ascentis® Express
2018: Supelco® expanded to include all analytical products from Merck KGaA for a comprehensive range of analytical techniques

TODAY

2015
Acquisition of Sigma-Aldrich®

2010
Acquisition of Millipore

MILLIPORE

Analysis with mobility and ease-of-use

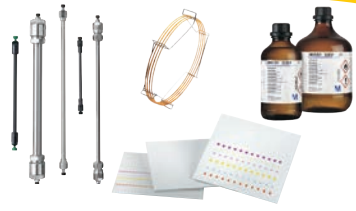
Mobile Analysis

Reference materials for accurate results

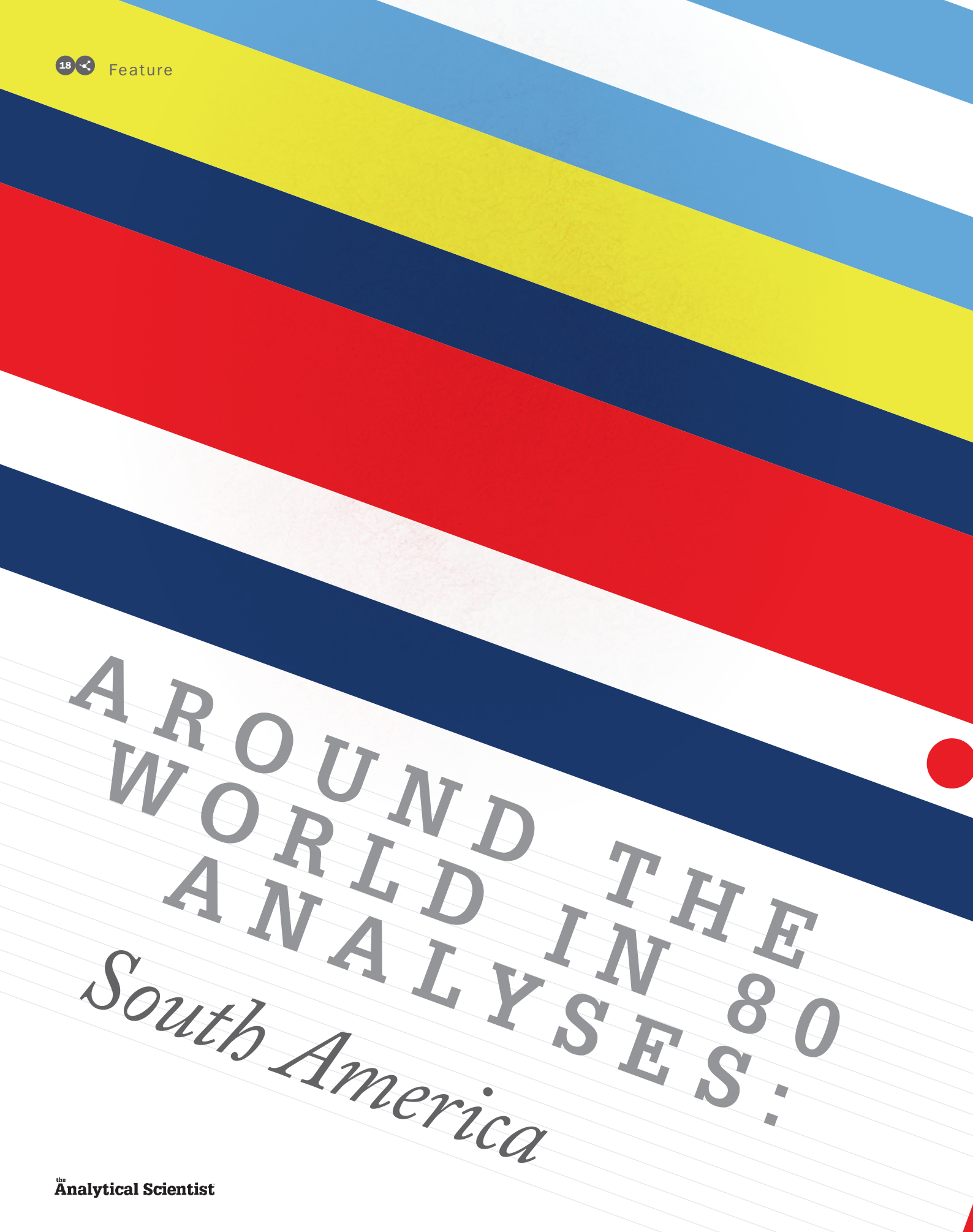
- Cerilliant®, Certipur®, TraceCERT®

Chemical Standards and Certified Reference Materials

Comprehensive analytical portfolio



Chromatography, Titration, Spectroscopy, Photometry



AROUND THE WORLD IN 80 ANALYSES: South America

Look back at our previous Power Lists; you'll notice the USA or Europe dominating in terms of numbers, but good science is not constrained by geography. Here, we take a look at a region that has seen rapid development in the analytical sciences in recent years through the eyes of three analytical chemists working at the cutting-edge in Brazil, Chile, and Colombia.

BRAZIL

Analytical science is booming in Brazil, but more effective collaboration with industry could accelerate the field.

By Fernando Mauro Lanças

My research

My work at São Paulo State University (UNESP) encompasses all aspects of separation science, with an emphasis on chromatographic techniques – from the synthesis of stationary phases to new coating and packing procedures to the development of instrumentation, accessories, and coupled systems, such as supercritical fluid extraction-capillary electrophoresis (SFE-CE).

Over the years, my research interests have evolved. I started working on the production and characterization of alternative fuels (from coal, shale and biomass) and shortly moved almost exclusively to separation sciences and related techniques (such as mass spectrometry). Having obtained the required background on this subject, I developed an online fully automated system consisting of sample preparation, chromatographic separation, and mass spectrometric detection. I am now working on the miniaturization of this system by developing more universal, robust and economical miniaturized extractions columns; capillary (both filled and open tubular) nano-LC separation columns; and the coupling of these with tandem mass spectrometry. By selecting the proper micro-extraction column, a simple switching valve is able to selectively transfer analytes to a nano-LC separation column for a final separation before MS/MS analysis.

> *My own area, separation science, is evolving more rapidly than anyone would have expected 10 years ago.*

For the next 5–10 years, the main goal is to finalize this ambitious project by developing the best possible extraction column (we have been investigating the proper tubing material, dimensions, novel sorbents, and so on) and the ideal nano-LC columns (packed, monolithic, WCOT and PLOT– from novel materials to improved column packing and coating systems). In addition, the coupling of these nano extraction-nano separation columns to mass spectrometry is under investigation by evaluating alternative approaches to electrospray ionization, including electron ionization (also termed electron impact, EI), which has been the standard GC-MS ionization technique for decades.

Ultimately, I intend to work on the "chromatographer's dream" – unified chromatography. We have published some work on this concept, but I always felt that the existing technology was not ready for such an ambitious project. However, if we can miniaturize all forms of chromatography and achieve efficient coupling with MS, we will be ready to develop the proper instrumentation, columns and accessories to perform gas, liquid, and supercritical fluid chromatography (and various combinations thereof) in a single experiment.

Analytical science in Brazil

Excellent research in analytical chemistry is performed at public and private universities, governments agencies and research centers. The number of PhD students defending analytical chemistry theses in Brazil over the last three years (2016–2018) is estimated to be over 3,000 – and the number is growing.

By its nature, analytical chemistry is an applied science, and analytical tools are widely used across the country. Many laboratories are very well equipped with state-of-the-art analytical chemistry equipment, including WCOT GC columns, UHPLC and superficially porous technologies, as well as high resolution and tandem MS systems.

My own area, separation science, is evolving more rapidly than anyone would have expected 10 years ago. Traditional applications include petrochemical (from field exploitation to final product quality control), ethanol and sugar, pharmaceutical and veterinary drugs, food and beverage safety, food-derived products (such as fruit essential oils), sports doping, and many others. As one of the world's largest botanical reserves, Brazil has always been a center for research into active ingredients from natural products – extraction, purification and analysis of these materials requires skilled separation scientists. In addition, Brazil has the largest reserve of fresh water worldwide, so water quality research is a priority for Brazilian officials and scientists. Notably, more rigorous regulation of food, pharmaceuticals, and veterinary drug production is also driving advances in separation science. As one of the largest food producers in the region, the country has to maintain a

strict control on food safety for both exportation and the internal market.

To meet the country's growing need for analytical chemistry expertise, I would like to see an ongoing analyst training program to help scientists adapt to more efficient and environmentally friendly technologies.

In contrast to the USA or Europe, research funding in Brazil (and Latin America as a whole) comes almost entirely from the government, with little money coming from industry. As a consequence, the public universities are better equipped with modern instrumentation for teaching analytical chemistry in general, and separation sciences in particular. I'd like to see more investment from private companies in research and educational projects in separation sciences. Although the industry–academia interaction is maturing in Latin America, the rate of progress is currently too slow to allow full benefit on both sides. My university, São Paulo State University, awards special funding for industry–academia research. It is a relatively new program, but the results have been positive so far.

> *In contrast to the USA or Europe, research funding in Brazil comes almost entirely from the government*

Looking ahead

Analytical chemistry in general, and separation science in particular, are key tools to improve quality of life everywhere. The growth of analytical chemistry in Brazil can be seen in the ever-increasing volume of scientific presentations and publications coming from the country. According to a recent publication by the Brazilian Chemical Society (1) the proportion of research originating from Brazil across 12 analytical science journals is rising year-on-year – demonstrating the growing visibility of Brazilian scientists in the global community. Brazilian scientists were particularly active in chemometrics, microextractions, and green chemistry.

The Brazilian National Symposium on Analytical Chemistry (ENQA) in September 2018 was the largest yet, with more than 1,200 participants. COLACRO (Latin American Symposium on Chromatography and Related Techniques) and SIMCRO (Brazilian Symposium on Chromatography and related techniques) also seeing increasing attendance. The next COLACRO will be in July 2019 (www.colacro2019.com); more than 1,000 participants are expected.

In many countries, the analytical sciences are not considered an independent discipline but rather a toolbox to be used by other disciplines – but in Brazil we have a clear and growing space for fundamental research in this area. As the nation demands more efficient and selective drugs, higher quality drinking water, improved air quality, safer food, and solutions to many other challenges that affect our daily lives, we can look forward to the increasing involvement of analytical chemistry – and separation sciences.

Fernando Mauro Lanças is a Professor at São Paulo State University, Brazil.

Reference

1. *CC Nascentes et al., "Current status, trends and challenges on analytical chemistry in Brazil", Quim Nova, 40, 643–649 (2017) http://dx.doi.org/10.21577/0100-4042.20170080*

CHILE

Analytical science has a key role to play in developing the economy of the future.

By Pablo Richter

My research

Currently, I am focused on the development of microextraction technologies to improve sample preparation (environmental, food and biological) and its coupling with chromatography and mass spectrometry. In the last few years, we have paid special attention to emerging organic pollutants (including endocrine disrupting chemicals, EDCs), developing not only quantitative analytical methodologies, but also biomimetic strategies to determine the bioavailable fraction of a pollutant.

Our group developed rotating disk sorptive extraction (RDSE) in 2009, which has been applied to various sample types for the extraction of analytes of interest, both in liquid samples and bioavailable fractions of solid samples. RDSE is a very simple, rapid and inexpensive approach with several additional key advantages:

1. The high surface-area-to-volume ratio of the device;
2. Extractions are performed from a low volume of liquid samples;
3. The recirculating regime prevents the collapse of the filter in complex samples, allowing continuous contact between solid and liquid phases;
4. The geometry of the device permits a high rotation velocity;
5. The adsorptive phase is easily replaceable, allowing the use of either commercial, natural or laboratory-synthesized sorbents.

Now, we are continuing to work on microextraction techniques, but we are migrating towards bioanalytical applications. As I am not a biochemist, we have established a collaborative relationship with my colleague, Alfonso Paredes, to study the effect produced by some EDCs on the endocrine system, using microextraction and mass spectrometry to identify biomarkers in biological fluids. We are supervising the PhD thesis of a Venezuelan student, Daniel Arismendi, who has accepted the challenge of addressing new bioanalytical problems.

I hope in the coming years to achieve a consolidated research line in the interdisciplinary field of bioanalytics – a fascinating challenge for an analytical chemist who has mainly covered applications in more classical fields (inorganic and organic chemistry).

> *Analytical chemistry has a clear role to play in solving important challenges facing Chilean science and society.*

Analytical science in Chile

The area of analytical chemistry did not start to develop in Chile until the 1980s, with the first PhDs formed in Chile in analytical chemistry in the 1990s. As recently as 20 years ago, the position of analytical chemistry in Chile was troubling. The discipline was seen as subordinate to other areas of chemistry, with no more than four active groups dedicated to the field. There were no analytical chemists in the evaluation panels or study groups of the main scientific and technological agency (CONICYT), making it hard for analytical chemists to access research funds. Thankfully, the tide has gradually turned. Today, analytical chemistry is recognized alongside other branches of chemistry, and is an increasingly popular choice for PhD projects.

The Chilean food industry is a substantial contributor to our economy (in particular, fresh fruit, forestry, wine and fishery products). Before export, food products must be certified safe – a process conducted by accredited public and private laboratories, using modern equipment. The laboratories must be accredited by the ISO 17025 standard and undergo regular audits by government regulators. One of my PhD students worked with such a laboratory to introduce analytical methodologies based on RDSE technology and LC-MS, to validate new veterinary pharmaceuticals for approval by the Agricultural and Livestock Service of Chile.

Looking ahead

Analytical chemistry has a clear role to play in solving important challenges facing Chilean science and society. For example, we need to find responses to environmental emergencies, such as the recent air pollution event from the Ventanas Industrial Park, at the border of the Puchuncaví and Quintero communes. Typically, government agencies are only detecting pollution after it has caused a negative effect on the population. There

is a lack of coordination among the analytical scientists in the country, particularly those belonging to the academic sector. By coordinating a collective opinion, we would be better able develop solutions to pressing problems.

The biggest challenge for researchers in Chile is funding. The budget for science, technology and innovation in Chile represents only 0.38 percent of GDP (compared with 1.17 percent in Brazil and 2.74 percent in the USA) – a figure that has remained relatively static since 2011.

Funding must increase, if Chile is to achieve its goal of moving the economy away from the export of natural resources to one that develops competitive advantages through innovation. In 2018, the main science-funding program (FONDECYT) approved 38 projects out of a total of 138 submissions in chemistry, with about 8 projects related to separation sciences.

Industry funding is similarly scarce. Though the government has instituted some policies to encourage industry collaborations with academics, they have been largely weighted in favor of short-term projects that benefit companies, rather than longer-term partnerships with more scientific value. Of the 18 PhD theses supervised in my lab, only three have been developed in collaboration with the commercial sector. Clearly, we need to strengthen these relationships.

Thankfully, the President appointed the first Minister of Science, Technology, Knowledge and Innovation in December 2018, and we hope that the newly created ministry will be given the resources to fulfil the expectations of the scientific community.

Pablo Richter is a Professor of Chemistry at the Faculty of Chemical and Pharmaceutical Sciences of the University of Chile, Santiago, Chile.

COLOMBIA

Lack of funding remains a challenge, but green shoots are emerging.

By Elena Stashenko

My research

Our group uses separation science to investigate essential oils and extracts of aromatic plants. We have gradually extended the scope of our work from laboratory experiments to field work with farmers' associations to examine all the steps of the essential oils value chain. Basic work included the detailed chemical characterization of complex mixtures of secondary metabolites and the determination of various biological activities, mainly antioxidant capacity.

High chromatographic resolution and high mass spectrometric resolution are our key areas of interest, because of their applications in natural products research, environmental, food, forensic and other analyses. Comprehensive chromatography, in particular, is challenging and rewarding.

Notably, some of our projects look likely to result in the development of commercial bioproducts, which will demand a shift in gear towards fractionation and separation at a larger scale. In fact, we plan to create a spin-off company to manage such commercial applications. However, I do not see myself ever becoming a businessperson – I intend to remain a scientist!

> *"Newly minted chemists return to the country from studies abroad and are frustrated by the lack of funding for their projects."*

Analytical science in Colombia

Analytical chemistry is a core requirement for undergraduate chemistry students in Colombia, but there are also optional higher-level courses on NMR, X-ray diffraction, chromatography, mass spectrometry, electrochemistry and other specialized topics based on analytical methods, such as forensic chemistry. In addition, industry uses universities for their technical and scientific personnel training. For example, at our university, we organize the National School of Chromatography – hands-on training courses for small groups (fewer than 15 people) on topics, such as sample preparation, gas chromatography, GC-MS, experimental design, and applications in food, natural products, environmental and forensic analysis.

Not all universities have sufficient equipment. Most instrumentation is used for research purposes, but there is a growing use in analytical services for industry or other laboratories. The installed infrastructure is not high-end in terms of sensitivity or resolution – there are few high-resolution mass spectrometers, for example. However, although instrumentation is important, I think that the main obstacle is sample preparation. There are many manual steps, subject to variations and errors from the analyst. More automation and higher throughput are needed – and that will represent an increasing focus of our work going forward.

Like several other Latin American countries, Colombia spends an extremely low percentage of its GDP on science and technology – 0.24 percent. A large proportion of these funds was used in the last decade for scholarships to increase the number of PhDs formed both abroad and in Colombia. Very little is left for research projects. Newly minted chemists return to the country from studies abroad and are frustrated by the lack of funding for their projects. The dearth of funding for public universities was the cause of many protests from students and educators during 2018. Unfortunately, science and education are not an ongoing Government priority – they are mentioned during campaigning but are forgotten once elections are over.

Moreover, there are limited cases of investment from industry into academia – and most requests are for assistance on a very narrow, urgent problem. This situation is not helped by the increasing bureaucratization of academia, which is not compatible with the quick answers demanded by industry. However, there are successful partnerships in the area of pesticide residues in coffee and other exported agricultural and meat products.

Looking ahead

To date, the main role for analytical science is in quality control of products for the final consumer. For example, there is illegal gold mining, which causes mercury contamination in streams and rivers. The sophisticated techniques and qualified personnel that allow us to detect these disturbances are not well understood by the public or politicians, however.

I would like to see more focus on herbal medicines and

natural products for human consumption, both generated in Colombia and imported. There are cases of counterfeit products, false claims about composition, contamination, and many more problems that require the participation of analytical chemistry. As a stark and worrying example, we know of a company that produces a medicine purporting to be based solely on marigold (*Calendula officinalis*) extract, but in fact it is based on the prescription drug diclofenac. Other areas that need more attention include the control of pesticide use, air or water contamination and oil spills.

When I arrived in Colombia, close to 40 years ago, there were one or two GC-MS systems in the whole country. Today, we have over 1,500 gas and liquid chromatographs in universities and industry. There are several world-class laboratories, equipped with high-resolution GC-MS, LC-MS, NMR and X-ray diffraction, and the work being done at these centers demonstrates the great value of analytical science in the future development of the country.

Elena Stashenko, Director, Research Center for Biomolecules - CIBIMOL Research Center of Excellence, CENIVAM Universidad Industrial de Santander Bucaramanga, Colombia.

Where Next?

We hope this article will be the start of an ongoing series highlighting the achievements of analytical scientists in different regions, particularly areas that are under-represented at conferences, in journals and in our own Power List. We'd love to hear where you think we should turn our spotlight next – email charlotte.barker@texerepublishing.com or leave a comment online.

RESTEK | ADVANTAGE

See What It Can Do for You and Your Lab

- Technical Articles & Applications
- Videos & ChromaBLOGraphy
- FAQs & Troubleshooting
- Education & Instruction
- Online Tools & Calculators
- Product Selection Assistance

Sign up today to access Restek's years of chromatography knowledge at

www.restek.com/advantage

RESTEK Pure Chromatography

Your Efficiency Challenge – Part V

In the final part of our series, three laboratory efficiency experts offer their must-read advice for ambitious (or complacent) laboratory managers. Drawing on our in-depth reader survey and distilling just some of the key points in our video webinar (http://tas.txp.to/0918/YEC), we start you on your path to improved laboratory efficiency. To continue the journey, look out for our forthcoming eBook.

How will you survive in an increasingly competitive world?

Our survey discovered:

- 1 in 3 labs is under competitive pressure
- 1 in 5 labs is viewed as dispensable
- 1 in 5 labs is already in direct competition

Oliver Rodewyk has been in the chromatography business for 32 years and is now a strategic account manager in the service sales division at Agilent.

Here, Oliver offers advice on boosting efficiency in labs – old and new…

When considering laboratory efficiency, you should always start with a critical reflection of where you are today. Also, keep in mind that equipment is not the only important factor in efficiency – your team members are the ones who will drive improvement. Are they trained in the best approach to the task? Are they open to change? It's crucial you have the right people, with the right training, at the right time.

An "old" lab

- When inheriting an existing lab where much of the equipment is outdated, the priority for laboratory managers should be to identify critical systems and target investment to those areas.
- Don't do all your upgrades at the same time, but stagger them to spread the cost and avoid having multiple parts due for replacement at the same time in years to come.

A new lab

- When setting up a new lab, the most common mistake I see is to take a "copy and paste" approach – assuming that if it worked perfectly in the past, it will work in the future.
- Instead, use a "copy and adapt" approach that builds on a foundation of past facilities, but invest at least 10-15 percent of your time and capital on adapting to new challenges and looking for ways to evolve or develop the lab.

Our survey revealed that respondents are often challenged to improve throughput and do more with less.

- 64 percent said they would benefit from shorter LC run times.
- 44 percent said that sample numbers are increasing – but staffing levels are not.

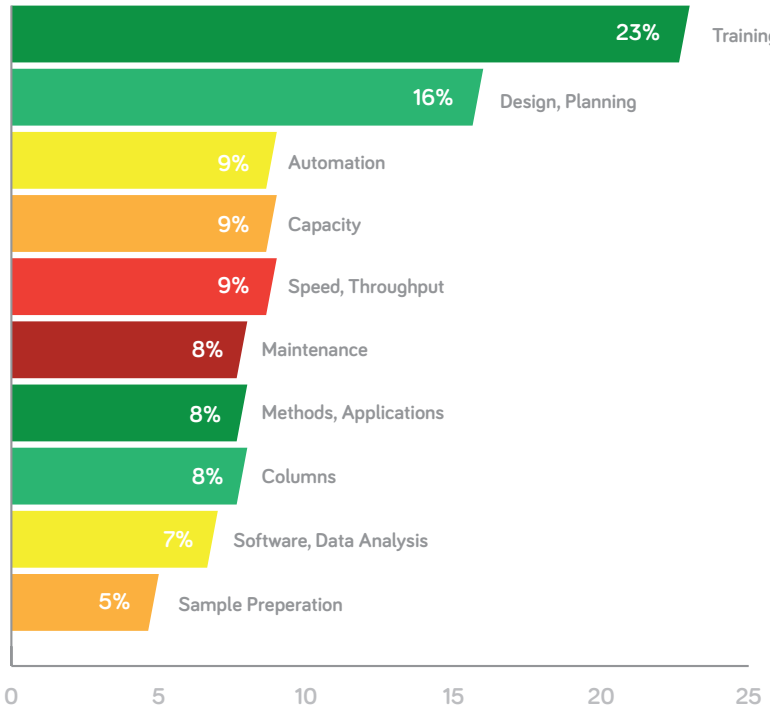
We asked survey respondents where they had made successful gains in laboratory efficiency and got a wide range of answers, with the most successful being training and planning or design.

Wolfgang Kreiss is an independent consultant in laboratory management, working on strategic and operational projects for analytical laboratories in industry and government agencies.

Here, Wolfgang helps you take the first step towards efficiency gains…

- To improve efficiency, you must first quantify it – and that means considering how best to assign numerical values to various efficiency parameters.
- You could think of efficiency as a simple ratio between input (amount of work, operating costs) and output (number of analytical results, timeframe or monetary value); this gives a firm basis for comparing efficiency with different setups.
- The laboratory is a very complex unit – it's not enough to simply collect numbers for the various efficiency parameters, you also have to look at all the possible influences that might affect the numbers.
- It's not easy to measure efficiency – do not be afraid to seek external support!

Martin Hermsen is a senior R&D analyst in the organics department in the Eurofins environmental lab based in The Netherlands, where he is in



charge of technical aspects of data automation and robotics

Here, Martin shares his approach to making efficiency gains…

- To improve efficiency in any lab, one of the first things that I do is go to the work floor and look at the process.
- Talk to the staff. You may think that you have the 'right way' of doing something, but remember to consider the people who must do a particular task day in, day out. It's best to adapt to their experience and preferences wherever possible.
- I sometimes get insight from someone that has no lab experience; I ask them to look at the process with a fresh pair of eyes. Often, it brings up things I have never thought of.
- Look at the bottlenecks in your workflow – seek ways to remove them
- Where is the most downtime occurring? Think about where replacement systems would be most impact.
- Consider introducing automation – it can be a very powerful tool. Robots can take over the time consuming, low-skilled aspects, leaving staff free to focus on more complex issues.
- Above all, don't stand still.

The Road to Improved Efficiency

Are you a scientist, laboratory analyst or lab manager – or all of the above? Are you willing to challenge your perception of efficiency or do you already know you need to make efficiency gains?

Join our experts – Kelly Zhang, Udo Huber, Stéphane Dubant, Adrian Dunn, Wolfgang Kreiss, Martin Hermsen and Oliver Rodewyk – for an exclusive series of video webinar masterclasses:

Webinar 1 – Analytical efficiency: How to push your results to the next level by selecting suitable technology

Webinar 2 – Instrument efficiency: How to survive the sample onslaught and even create a little breathing room

Webinar 3 – Laboratory efficiency: How to plan for success and secure your future

For more details, visit: http://tas.txp.to/0918/YEC

What Does Laboratory Efficiency Mean to You?

A simple question, but ask a room of laboratory managers and you'll get a surprising variety of answers. We'd like to know your definition of efficiency – get in touch at charlotte.barker@texerepublishing.com.

SMALL WONDER

Imagine the vast chemical complexity that exists within each of our cells. Concentrations of DNA, RNA, proteins, lipids, and metabolites range from a single molecule to billions – and molecular weights cross more than six orders of magnitude. A molecule may disappear almost as soon as it appears, or may long outlast the cell in which it originated. How can we capture a snapshot of just one cell's intricate inner workings?

By Marina C. Philip and Jonathan V. Sweedler

Chemical interactions can drive cell function. Because of the striking chemical heterogeneity found within cell populations, analyzing cells individually can uncover mechanisms not observable when studying the chemistry from homogenized cellular populations. However, the intricacies of single cell investigation become more overwhelming the more we consider them; from sample preparation to analysis, smaller scales increase our risk of failure.

For decades, the hyphenation of approaches, often incorporating volume-matched separations, has aided chemical measurements (1). So it's not surprising that methods to analyze individual cells using multiple combined measurement techniques have expanded our capabilities. Here, we highlight several serial approaches that boost the information obtained from single cell analyses.

SEPARATING CELLULAR COMPLEXITIES

Our lab has spent many years creating measurement technologies using capillary electrophoresis (CE) to explore the chemistry of volume-limited samples – in some cases, even smaller than single cells (2). We have characterized single neurons and subcellular features, and uncovered chemical complexity in animal models ranging from mollusks to mammals. CE requires nanoliter volumes and thus reduces sample dilutions from single cell separations (3). By hyphenating CE to mass spectrometry (MS) (4), we have expanded our ability to explore complex single cell chemistry and characterize both familiar and new compounds from selected cells.

The traditional and easiest methods for CE sample preparation involve placing the sample into an extraction buffer or, in some cases, injecting the entire cell into the capillary. The limited sample remaining after a measurement often precludes follow-up analysis, especially once technical replicates are performed. Accordingly, we and other scientists have gotten creative in our efforts to develop sampling techniques that reduce analyte losses and enable multiple distinct measurements. For example, we used patch-clamp electrophysiology to identify and characterize neurons, and then used the same patch-clamp pipette to extract a few picoliters of cell cytoplasm for follow-up CE-electrospray ionization (ESI)-MS metabolite profiling (5). Other labs have used similar micropipette sampling techniques, leaving much of the cell intact and alive (6).

More recently, we developed a liquid microjunction (LMJ) sampling probe that enables the extraction of cellular content from cells located on a microscope slide (7). The probe consists of two concentric capillaries; solution is pumped through the outer capillary and aspirated through the inner capillary. Cellular material is collected as fluid migrates from the outer to inner capillary. Analysis can be carried out before or after metabolite extraction, depending on our needs and the measurement technique being used. Not only can we perform CE-ESI-MS metabolite profiling, we can add other minimally destructive slide-based chemical measurements of the same cell. We validated the approach by hyphenating matrix-assisted laser desorption/ionization (MALDI) MS to CE-ESI-MS to analyze single cells from rat pancreatic islets of Langerhans, micro-organs that perform the canonical glucose-regulating functions of the pancreas. Pancreatic cell types are defined by the presence of a peptide hormone; beta cells contain insulin and alpha cells contain glucagon. We screened cells for peptides (revealing cell type) using MALDI MS, selected the cells of interest, and extracted the small molecule metabolite content with the probe. We then performed follow-up metabolite profiling with CE-ESI-MS, reporting one of the first direct detections of canonical neurotransmitters in single pancreatic alpha and beta cells. Our ability to perform these combined measurements has opened the door to studying pancreatic chemistry from human islets used in islet transplantations.

SAMPLE SAVIOR

The crux of serial analyses for single cell studies lies in the preservation of cellular material from the first analysis for use in the next measurement. An early study in our lab established that at least 60 percent of cellular material remains on the surface following MALDI MS analysis (8). Although the laser shots do consume cellular contents, the extent is less than most think, and MALDI MS measurements do not preclude the cell from being re-assayed.

To achieve a more robust reanalysis, we created microMS (9), open-source cell-finding software that enables single cell targeting on a microscope slide. Multiple research groups have developed strategies to target single cells beyond simply imaging the entire slide. In our approach, we use optical imaging to register the spatial locations of cell nuclei on a slide and then direct the laser, electron beam, or LMJ probe to the desired cell locations. During development of the software we also determined that, in addition to leaving chemical material behind, such analyses do not displace the cell.

The microMS software enables single cell analysis on a high-throughput scale; we can analyze thousands of cells in several hours. We have performed sequential profiling using several different mass spectrometers: MALDI time-of-flight (TOF), MALDI Fourier transform-ion cyclotron resonance (FT-ICR), and C60+-secondary ion mass spectrometry (SIMS). We can leverage the advantages of each instrument to collect complementary information for single cell samples; for example, lipid and peptides via MALDI-TOF MS, high-resolution spectra and elemental composition confirmation with MALDI-FT-ICR MS, and small molecule content from SIMS (Figure 1).

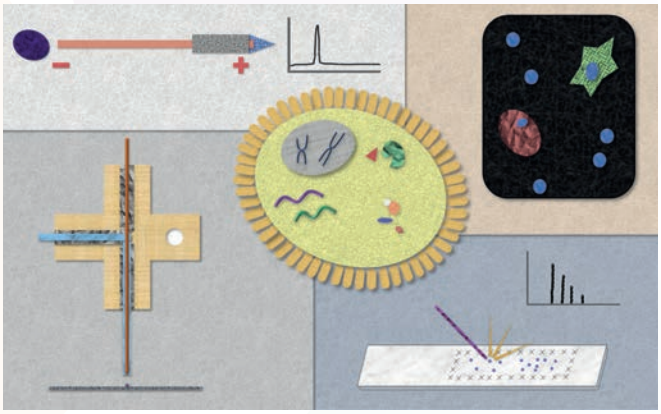
NARROW (BORE) FOCUS, WIDE APPEAL

Join us at ISCC & GC×GC to hear more about the next big (or small) thing in separation science!

By Kevin Schug, Conference Chair

This exciting work by Philip and Sweedler is a perfect example of the cutting-edge research and technical advancements on display at the 43rd International Symposium on Capillary Chromatography and the 16th GCxGC Symposia held in Fort Worth, Texas, in May. Professor Sweedler will be one of several high-profile plenary speakers amongst a vibrant and well-attended scientific program. Analytical science is moving to smaller scales, and to multidimensional and automated platforms, trends that will be front and center at the event. Here, you can both learn the fundamentals from the world's leading experts and view the newest advances in technology and applications. Not too big and not too small, ISCC & GCxGC 2019 provides ample opportunity to rub shoulders with key opinion leaders in a relaxed and welcoming atmosphere, underscored by a Texas-style social program. Register now to attend the key event of 2019 for advances in capillary and comprehensive separation technologies.
Plus, abstract submission for both oral and poster sessions is currently open – apply now to join the conversation!

The 43rd International Symposium on Capillary Chromatography (ISCC) and the 16th GCxGC will be held in Fort Worth, Texas USA on May 13, 2019. Register at www.isccgcxgc.com



A WIDER WORLD OF MEASUREMENTS

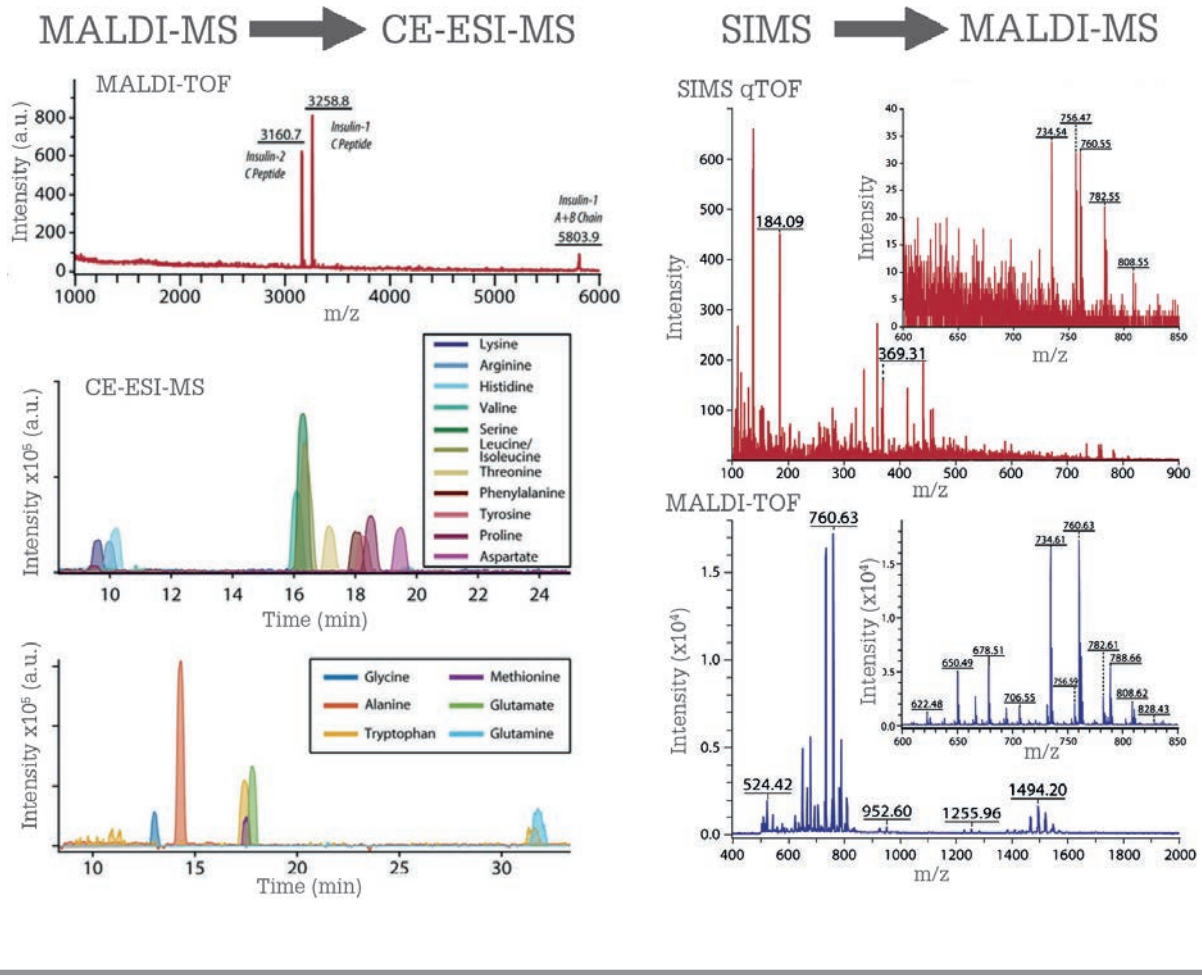
Our lab has employed various strategies to hyphenate MALDI MS to a number of analytical approaches, including immunocytochemistry, spectroscopy, and transcriptomics. Despite the potential for sample destruction, by carefully sequencing our experiments, we can add the advantages inherent to each individual technique.

For instance, immunostaining for proteins is the gold standard method for cell classification, including defined cell types such as neurons, astrocytes, and other brain cells. However, immunostaining requires fixation of the cells, which renders much of the cellular chemistry difficult to characterize because of the crosslinking of proteins, peptides, and even lipids and sugars. This presents a challenge in validating our single cell separations and MS data.

We address this issue by performing single cell MALDI MS prior to fixation and immunostaining. In addition, in collaboration with the Bhargava laboratory, we have combined vibrational spectroscopy with both mass spectrometry imaging (10) and single cell measurements to provide enhanced information on lipids, nucleotides, and proteins.

In summary, we have enhanced our ability to investigate a population of cells using more than one omics measurement. We can sequentially measure an individual cell using multiple distinct approaches. By analyzing a single cell multiple times using techniques suited for distinct classes of molecules, we further our ability to probe biological systems on the cellular scale. Combining these measurements dramatically increases the potential for advancement while creating an analytical toolkit that is as diverse as the chemistry within a single cell itself.

Marina C. Philip is a graduate student pursuing a PhD in chemistry and Jonathan V. Sweedler is the James R. Eiszner Family Endowed Chair in Chemistry and Director of the School of Chemical Sciences, both at the University of Illinois at Urbana–Champaign, Urbana



Acknowledgements

The authors gratefully acknowledge support under award No. P30 DA018310 from the National Institute on Drug Abuse. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.

References

1. *T Hirschfeld, "The hy-phen-ated methods", Anal Chem, 52, 297A–312A (1980). https://doi.org/10.1021/ac50052a870.*
2. *SS Rubakhin et al., "Measuring the peptides in individual organelles with mass spectrometry", Nat Biotechnol, 18, 172–175 (2000). https://doi.org/10.1038/72622.*
3. *JA Jankowski et al., "Assaying single cells with capillary electrophoresis", Trends Anal Chem, 14, 170–176 (1995). https://doi.org/10.1016/0165-9936(95)98315-Y.*
4. *T Lapainis et al., "Capillary electrophoresis with electrospray ionization mass spectrometric detection for single-cell metabolomics", Anal Chem, 81, 5858–5864 (2009). https://doi.org/10.1021/ac900936g.*
5. *JT Aerts et al., "Patch clamp electrophysiology and capillary electrophoresis–mass spectrometry metabolomics for single cell characterization", Anal Chem, 86, 3203–3208 (2014). https://doi.org/10.1021/ac500168d.*
6. *RM Onjiko et al., "In situ microprobe single-cell capillary electrophoresis mass spectrometry: metabolic reorganization in single differentiating cells in the live vertebrate (Xenopus Laevis) embryo", Anal Chem, 89, 7069–7076 (2017). https://doi.org/10.1021/acs.analchem.7b00880.*
7. *TJ Comi et al., "MALDI MS guided liquid microjunction extraction for capillary electrophoresis–electrospray ionization MS analysis of single pancreatic islet cells", Anal Chem, 89, 7765–7772 (2017). https://doi.org/10.1021/acs.analchem.7b01782.*
8. *JS Page, JV Sweedler, "Sample depletion of the matrix-assisted laser desorption process monitored using radionuclide detection", Anal Chem, 74, 6200–6204 (2002). https://doi.org/10.1021/ac025898k.*
9. *TJ Comi et al., "MicroMS: a Python platform for image-guided mass spectrometry profiling", J Am Soc Mass Spectrom, 28, 1919–1928 (2017). https://doi.org/10.1007/s13361-017-1704-1.*
10. *EK Neumann et al., "Multimodal chemical analysis of the brain by high mass resolution mass spectrometry and infrared spectroscopic imaging", Anal Chem, 90, 11572–11580 (2018). https://doi.org/10.1021/acs.analchem.8b02913.*

Better, Smarter GC

How the Agilent Intuvo 9000 GC is boosting productivity in two very different application areas.

The Scent of Innovation

Alessandro Casilli, a senior scientist at Firmenich, tells us how the Intuvo helps sniff out efficiency gains.

What is Firmenich? And what is your role?

Firmenich is the largest privately-owned company in the flavor and fragrance business – we create fragrances and flavors for the world's most desirable brands. Our clients operate in the food & beverage industry, as well as in the cosmetics, perfumery and home care products industries. Firmenich has nearly 125 years of existence and, with more than 7,300 employees in around 100 countries and with various dedicated research centers worldwide, we are among the top companies in the world in this market. Innovation is crucial to our success.

As a senior scientist in the Analytical Innovation team in the U.S., I work with my team to identify and implement state-of-the-art instruments in routine or R&D applications across the company – we are always striving to improve our analytical capabilities. Sometimes that might be a small innovation; sometimes we'll integrate a completely new instrument – or even a completely new concept in order to provide the best products in terms of performance, guarantying the safest standard levels. And so the work is never boring! We have to understand the needs of internal stakeholders and work with suppliers to help make that a reality.

As you'll imagine, much of our research is focused on volatiles, so gas chromatography is a critical tool.

Why did this industry appeal to you?

Flavor and fragrance are such an important presence in our lives – just think of the flood of memories released by the scent of a familiar perfume, or the taste of a favorite childhood food. It's also a tough field for analytical chemists, who must routinely carry out analyses ranging from separating thousands of components to extracting a single ingredient. I enjoy the challenge of developing methods accessible to all users.

How do you maximize productivity in the lab?

Productivity and high throughput are not only buzzwords – they are also important goals. But I've learned that you must proceed with caution; otherwise, the time taken to develop or adjust a method can outweigh the advantages. You can invest a great deal of time trying to improve throughput, and end up with a method that is too complicated to apply on a daily basis.

We aim to boost productivity by identifying instruments that simplify day-to-day procedures. The Agilent Intuvo 9000 GC system is a game changer in this regard. A more efficient oven and easier column installation reduces time spent on maintenance and makes the instrument more accessible to non-expert users. And yet, its conventional column and inlet means that it can slot easily into existing procedures.

How have you applied the Intuvo?

We have found the innovative chip technology to be the most unique and valuable feature of the Intuvo – it is absolutely unprecedented. The Guard Chip provides an independent, programmable heating zone between the inlet and the column, which we are using as a trap. We inject samples in the inlet, and they are transferred into the Guard Chip, which is initially kept at a low temperature before heating up to allow the transfer of the fraction of interest; for example, going from 40 to 120 degrees. This process reduces the need for sample distillation/extraction and protects the column from heavy fractions that might cause contamination.

We have found the Guard Chip to be particularly powerful when used in a mid-column backflush configuration. Once the fraction is transferred into the second part of the column, we can backflush the first portion of the column and Guard Chip, meanwhile the second part of the column is finalizing the analysis. Before the end of the analysis we are ready to start the next injection, with a clean Guard Chip and first part of the column. It has proved impossible to perform this procedure with any other instrument but, even in this relatively complex configuration, we found that the Intuvo was robust and reliable.

Though the Intuvo will not replace all conventional GC systems, we see it playing a key role in applications where high throughput, ease of use and reliability are paramount.

"Put simply, the Intuvo is one of the best, most robust and most sensitive devices we have in our lab."

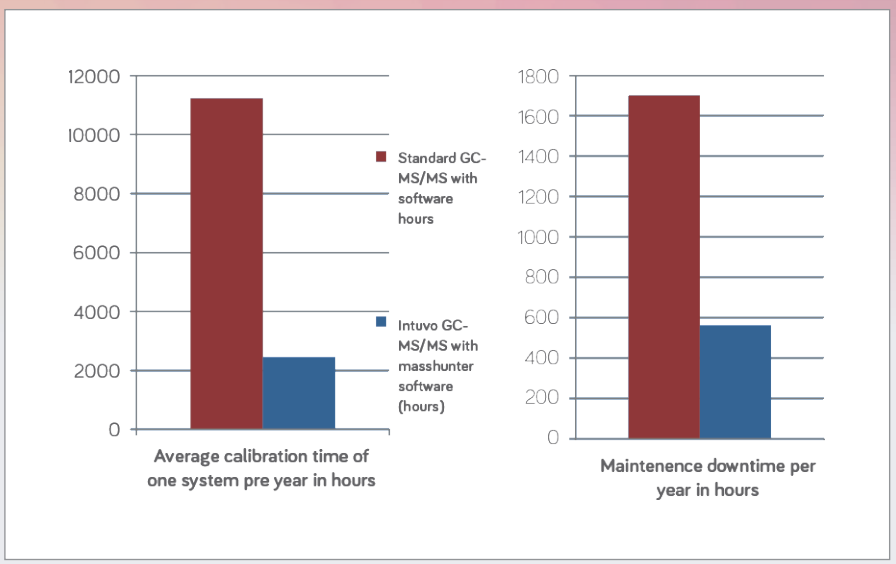


Figure 1. Calibration time and downtime over a year with standard GC-MS/MS and Intuvo GC-MS/MS.

The Taste of Success

Eurofins is a world leader in food, environment and pharmaceutical products testing. Marvin Overbeeke, Khalid Bensbaho and Elisa Platjouw tell us how the Intuvo is speeding up pesticide testing at Eurofins Lab Zeeuws-Vlaanderen.

How do you use GC-MS in your work?

Both the pesticide and the dioxin departments at Eurofins have GC-MS instrumentation, and our challenge is always to achieve more with less. One method that is currently under development aims to quantify 400 pesticides in a single run.

What are the most important factors for you when it comes to choosing a GC-MS instrument?

In short, sensitivity, selectivity and robustness. We also consider how easy it is to work with; our analysts should be able to use and maintain the machine – and add new methods – as quickly and as easily as possible. The ease of use of the Intuvo was one of the main attractions for us.

What difference has the Intuvo made in your lab?

One big difference is that, thanks to the Guard Chip system, we can now analyze dirty matrices (for example, oily or spicy foods) with significantly less maintenance of the system. And when we do perform maintenance, it is quicker and easier, so there is less downtime. At the 2018 European Pesticide Residue Workshop (EPRW) we presented a poster demonstrating a 67 percent drop in downtime (Figure 1). Put simply, the Intuvo is one of the best, most robust and most sensitive devices we have in our lab.

Your poster also mentions the MassHunter Workstation software…

The new software is more intuitive and user friendly than previous software, with more options to automate processes. It is very visual – you can look at your sample and your control simultaneously to see immediately if you have found the right compound. Another feature is that we can tailor what the analysts see, making sure each analyst only sees the options they need for their analysis.

We found that the MassHunter software reduces calibration time by 78 percent (Figure 2).

Find out more about Intuvo in our eBook: tas.txp.to/intuvo-ebook-2019

Making the Leap

A new GC system is a major investment – why choose Intuvo?

By Eric Denoyer, Marketing Director, Agilent Technologies.

The Agilent Intuvo 9000 GC System compares with a typical GC system the way a smartphone compares with a traditional telephone. It has a fast direct-heating design, uses half the power, and takes up half the bench space of a conventional air-bath oven GC instrument. New ferrule-free direct connections with plug-and-play flow path components eliminate a major source of maintenance and complexity, while built-in automatic leak checking ensures connections are made correctly. A unique disposable Guard Chip protects the column from undesirable high molecular weight contaminants and eliminates the need for cumbersome column trimming.

Spending less time on maintenance and reducing potential errors that can lead to unplanned downtime leaves more time for running samples, which is a real time and cost saving for lab managers. In addition, as the Intuvo's direct heating system can heat a capillary column as fast as 250 °C/min, while also having the capability to rapidly cool the column, inject-to-inject cycle times are faster.

Although the Intuvo system improves efficiency in several ways, it was designed to use previously developed, capillary GC applications, which means it can be adopted in an existing lab with little or no disruption. For example, the Intuvo continues to use the familiar time-proven fused silica capillary column, although it is wound in a more efficient and convenient planar format. It also leverages proven inlet and detector technologies. Therefore, the chromatographic behavior of, and analytical results from, an Intuvo system will look and feel very familiar to individuals comfortable with conventional GC systems.

«Our Ion Chromatographs are very robust and reliable»

Lledó Altava is a senior laboratory technician at IPROMA, a leading provider of laboratory testing, monitoring, and consulting services in Spain. Working at IPROMA's large environmental laboratory near Valencia, **Lledó relies on the robust performance of her fully automated Metrohm ion chromatography systems.** They are on duty 24/7 almost 364 days a year – helping IPROMA to keep its competitive edge in a highly competitive market.

www.metrohm.com

Metrohm 75 YEARS PEOPLE YOU CAN TRUST

the Spectroscopist

INSIDE

The Wish List: Spectroscopy

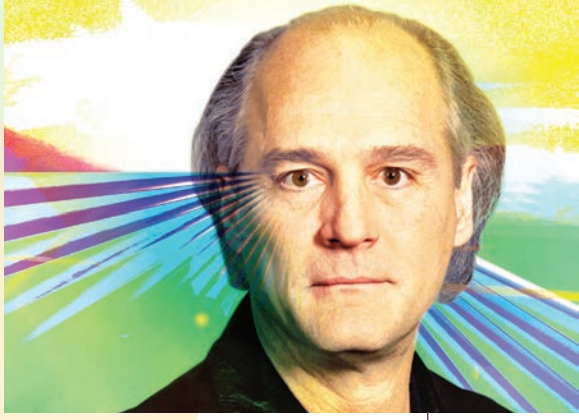
What are the biggest research priorities in spectroscopy today? We asked leading spectroscopists what advances they would most like to see and why. Here's what they told us...

"Top of my wish list would be turnkey ultrafast laser systems. Studying dynamics in systems ranging from molecular movement in macromolecular systems to electron dynamics within molecules (and even photo-ionization) requires the ability to detect phenomena over shorter and shorter time scales. Thirty to forty years ago picosecond measurements were just becoming routine. Today, there are numerous turnkey femtosecond systems used by scientists who are not hardcore 'laser spectroscopists.' My wish is for a turnkey attosecond laser system that would allow a wide array of researchers to study complex system electron dynamics. Next year, I'll wish for the zeptosecond version!"

Frank Bright, Frank Bright, Henry M. Woodburn Chair and SUNY Distinguished Professor, Department of Chemistry, University at Buffalo, USA.

Recent advances in mass spectrometry allow for rapid and efficient fragmentation of naturally-occurring cyclic peptides in the gas phase (UVPD fragmentation); however, our ability to determine the sequence of these mass species is hampered by the difficulty of interpreting the MS/MS spectra. On my wish list, I would like to see advanced algorithms that can help us to sequence these highly complex MS/MS spectra, by reducing the redundancy of sequence coverage normally generated via fragmentation of cyclic species with multiple points of cleavage. To the same end, selective cleavage of specific bonds/residues in the gas phase could alleviate MS/MS complexity and enable the rapid sequence determination needed to characterize these interesting cyclic peptides.

Leslie Hicks, Assistant Professor, University of North Carolina, Chapel Hill, USA.



"After devoting almost 40 years to laser ablation (LA) for chemical analysis, I'd like to see a true direct solid sample analysis instrument – not laser ablation hooked up to an ICP, but an instrument that is specific to solid sample analysis. LA with ICP (OES, MS) and LIBS has advanced considerably over the decades and there are many early adopters at universities and research laboratories who are using the technology successfully. However, for industry use we need a turnkey instrument that can be operated by technicians and is amenable to easy methods development, access to appropriate standards, database libraries, and machine learning tools to complement rapid direct solid sample chemical imaging and analysis."

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

"I would like to see a new generation of detectors for mass spectrometry (for example, arrays) able to simultaneously detect ions from a large mass to charge interval, with high sensitivity, high mass resolution and with a large dynamic range. In this way, technology such as distance of flight (DoF)-MS or multi-collector(MC)-MS could have a big impact in multiple applications – specifically, analysis of multi-elemental nanoparticles/quantum dots, multi-elemental imaging, and determination of multi-elemental isotopic ratios."

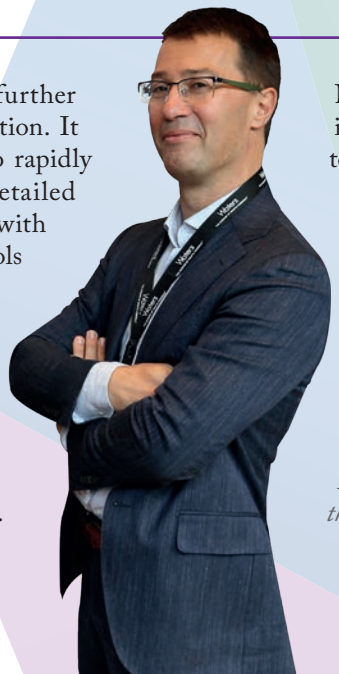
Jorge Pisonero Castro, Associate Professor, Department of Physics, University of Oviedo, Spain.

"My greatest wish is not for technological advances, but rather that scientists get more freedom in research – and less nannying by the state, administration, and interest groups. I believe the scope to follow our own ideas would do much to open new fields of research and accelerate progress in science.

Focusing on analytical spectroscopy, I would like to see more work using laser spectroscopy. Tunable lasers showed their tremendous capabilities in basic atomic and molecular physics more than 30 years ago, but remain underused in analytical spectroscopy. Extremely high detection powers have been demonstrated in absorption as well as fluorescence measurements; moreover, laser spectroscopy offers the possibility to apply sub-Doppler high-resolution spectroscopy. The use of different Doppler-free detection techniques would not only be of interest for high-precision isotope ratio measurements of atoms and molecules, but also for the application of isotope dilution for matrix-independent accurate concentration measurements."

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

"I would like to see further and easier data integration. It has become possible to rapidly generate large and detailed sets of molecular data with a variety of 'spectro' tools on identical samples. Yet, most analytical scientists seem to struggle with data fusion and lack the ability to turn data into reliable answers to their analytical problems.



New innovative and integrative software tools are badly needed."

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

On a lighter note...

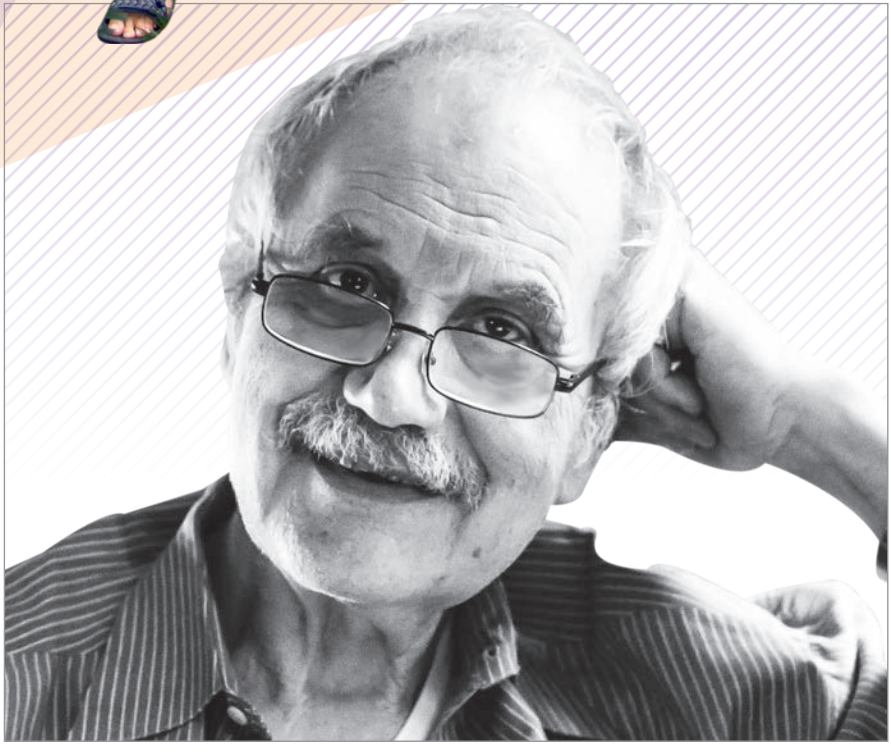
"A wearable ion mobility spectrometer – so that when going shopping one can detect the artificial scents to which businesses increasingly expose their customers and know when to don protective gear!"

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

"There are a number of developments I would like to see in the field, including:

- A broadly tunable narrow-band UV-Vis laser. This would provide greater selectivity in fundamental molecular spectroscopy and make multi-element analysis by atomic absorption, atomic fluorescence, and laser-enhanced ionization spectroscopies possible.
- A micro or nano optical spectrometer based on molecular filters. This would simplify remote, unattended analysis, new generations of high-selectivity optical sensors, and possibly implantable optical spectrometers.
- An ICP replacement with little or no argon consumption, low power requirement (less than 100W), and no matrix interferences to allow ICP-AES and possibly ICP-MS in unattended, remote operations.
- A low-cost multichannel ion or electron detector (analogous to a charge coupled device, CCD), which would provide 'all the signal, all the time.'
- A field-compatible mass spectrometer. Once widely available, such devices could transfer many laboratory mass-spectrometric measurements to the plant, physician's office, or field.
- A glow-discharge emission or mass spectrometer that offers both depth-resolved and surface-resolved elemental concentrations, offering many of the advantages of secondary-ion mass spectrometry (SIMS) but at lower cost and greater speed.
- A source for ambient desorption/ionization mass spectrometry (ADI-MS) that is free from matrix interferences and offers accurate quantification information."

Gary Hieftje, Distinguished Professor Emeritus, Mann Chair in Chemistry, Indiana University, Indiana, USA



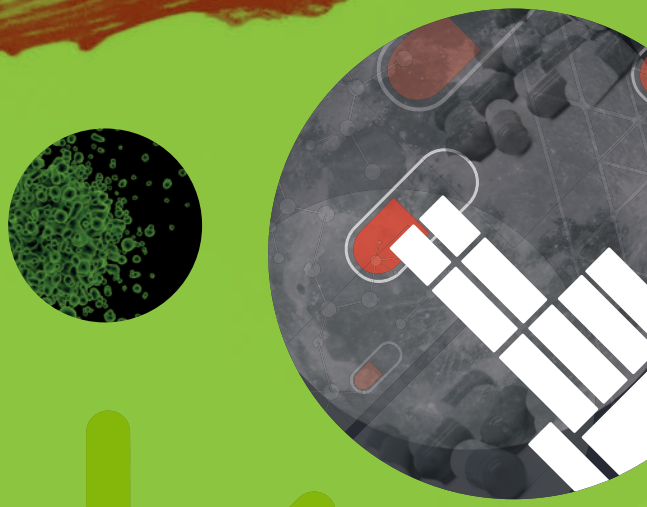
"On the instrument side, I would like to see more hybrid developments of LIBS with other instrumental approaches (Raman–Fluorescence–Absorption, TOF–MS). Such instruments take advantage of the differing information capabilities of each technique, allowing the near-complete characterization of the sample.

In data treatment, I would welcome a universally accepted, pitfall-free, chemometric protocol, responding to the different analytical problems encountered with different types of samples.

On the fundamental side, I would like to see increased attention and effort devoted to the absolute calibration of the instrument, from sample to signal (ions or photons). It's a huge challenge, but even small steps forward will be beneficial."

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

the Translational Scientist™



Meet…

… the researchers overcoming the obstacles of bench-to-bedside research

Explore…

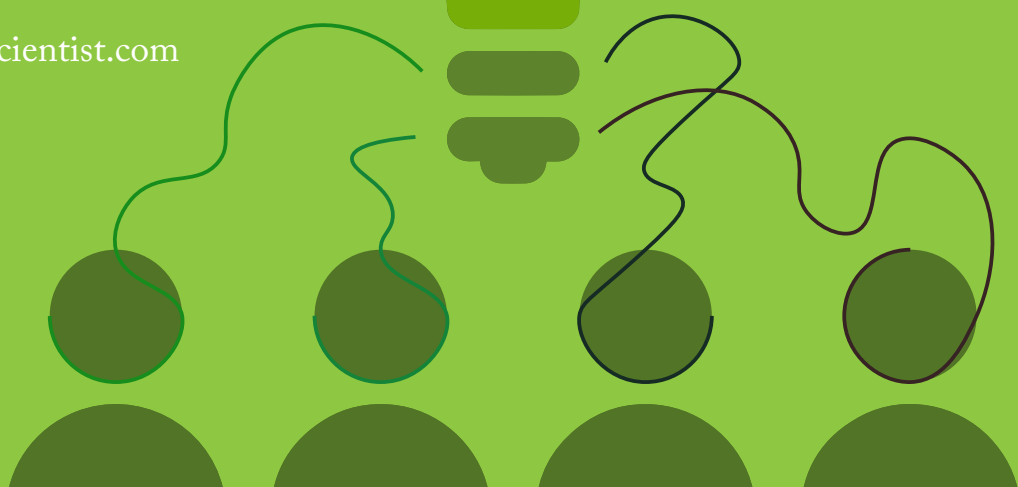
… the technologies and techniques driving robust, cutting-edge life science

Connect…

… with the scientists, engineers and clinicians, who work together to improve global health

Visit…

… www.thetranslationalscientist.com



Thermal Extraction of Phthalates in Polymers based on IEC Method 62321-8 using a Pyroprobe

Phthalate calibration, reproducibility and MDL studies using an IEC standard method

By Karen Sam

Certain phthalate additives are known to be harmful to humans, resulting in regulations regarding their use. With growing environmental awareness and perceptions, the use of phthalates has been restricted in many countries, including the European Union and the United States of America. As a result, a few international standards and conformity assessment bodies such as the International Electrotechnical Commission (IEC) and the American Society for Testing and Materials (ASTM), have published standards for determining certain phthalates in polymeric materials. The recent IEC Method 62321-8 defines approaches to determine di-isobutyl phthalate (DIBP), di-n-butyl phthalate (DBP), benzyl butyl phthalate (BBP), bis-2-ethyl hexyl phthalate (DEHP), di-n-octyl phthalate (DNOP), di-isononyl phthalate (DINP) and di-iso-decyl phthalate (DIDP) in electronics using GC-MS and TD-GC-MS.

Thermal extraction of additives is a straightforward approach involving only a few steps and therefore the possibility of greater recovery when compared to solvent extraction techniques. Sample is simply placed in a sample tube and dropped into the Drop-In-Sample-Chamber (DISC) of a 6150 Pyroprobe. The Pyroprobe thermally extracts the sample using two sequential temperature ramps as defined in the Experimental Parameters, straight to a single quad GC-MS. Resulting chromatograms closely match the chromatograms in Annex C.2 of the IEC Method (Figure 1). Calibration curves based on a one-point calibration (as indicated in the method) are also shown in Figure 1.

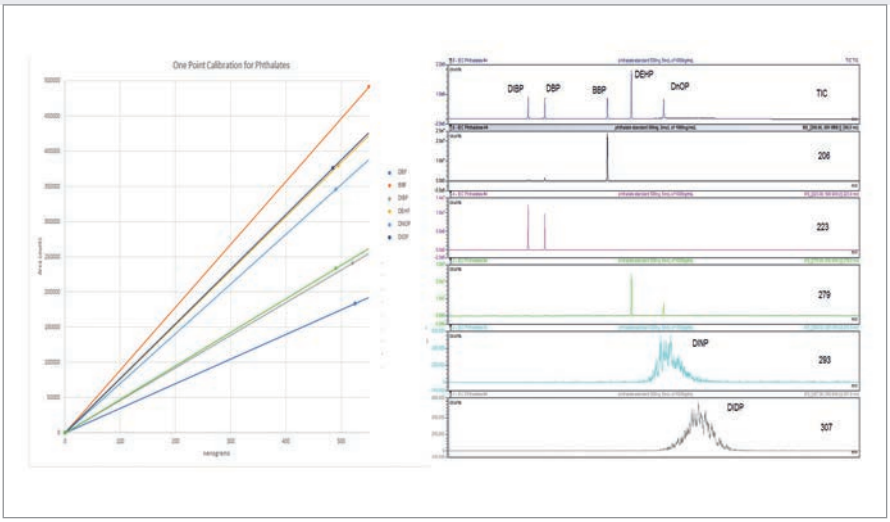


Figure 1: Calibration curve and chromatograms (TIC and EIC) of phthalates.

Phthalate	Quant Ion	RSD (%)	MDL (mg/kg)
DIBP	223	3.2	21.7
DBP	223	2.3	21.0
BBP	206	4.3	21.0
DEHP	279	2.9	14.7
DNOP	279	3.2	9.4
DINP	293	3.0	17.9
DIDP	307	3.2	13.6

Table 1: Area RSDs and calculated MDLs of phthalates

The statistical measures related to reproducibility depend on temperature precision, along with sample related issues like homogeneity and sample preparation. Eight replicates a 500ng phthalate standard provided area RSDs of around 3% for most of the phthalates, which gives a very small statistical variation. Furthermore, when method detection limits were studied in accordance with the IEC method, seven replicates produced calculated MDLs ranging from 9.4 to 21.7 mg/kg, 78-91 percent lower than the 100mg/kg requirement (Table 1).

The latest version of the Pyroprobe from CDS Analytical ensures repeatable, reliable results for thermal extraction of phthalates in accordance with standard methods, like IEC Method 6321-8 for determination of phthalates in electrotechnical products.

Experimental Parameters

The samples were thermally extracted in a CDS Pyroprobe 6150 with an Autosampler, equipped with Drop-In-Sample-Chamber (DISC) technology. A DISC tube was used as the sample vessel.

Pyro Chamber:
Ramp 1: *200°C to 300°C at 20°C/minute*
Ramp 2: *300°C to 340°C at 5°C/minute*
IsoZones: 300°C

GC-MS:
Column: *5% phenyl (30m x 0.25mm)*
Carrier: *Helium, 50:1 split*
Injector: *320°C*
Oven: *80°C for 13 minutes*
20°C/min to 300°C
Mass Range: *50–1000amu*

How to Ensure Analytical Accuracy and Reliability with an Inert Flow Path

Regulations and smaller sample sizes have placed utmost importance on getting accurate results quickly without instrument downtime.

An inert sample pathway is critical for accurately quantifying low levels of active sample that are common in today's analytical applications. Regulations and smaller sample sizes have placed utmost importance on getting accurate results quickly without instrument downtime.

An inert flow path in HPLC is becoming more and more important as the industry standards and government regulations require lower and lower detection levels. Without an inert flow path, analytes can be lost, peaks can be broad, and testing can be unreliable. Dursan® is capable of coating everything in the flow path from injection to detector, including parts that other coatings cannot handle, like frits.

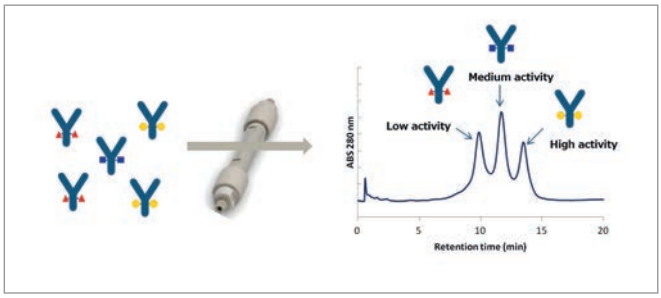
If you're testing sensitive molecules that might bind or have issues with stainless steel, Dursan® coated components can only make your chromatography better. Until now, PEEK has been the industry standard for inertness in HPLC. Dursan® has the inertness of PEEK with the robustness of stainless steel. This gives you the ability to confidently measure compounds such as proteins, chelating agents, and biologics with ease. Because Dursan® coating is applied via chemical vapor deposition, there are negligible effects on pressure and packability. A Dursan® column is not only inert, but it's also versatile, as it can be used anywhere that stainless steel, titanium, or PEEK is used.

For more information visit https://hubs.ly/H0gpQsy0

Evaluation of mAb ADCC Activity through Fc Receptor Affinity Chromatography

Antibody-dependent cell-mediated cytotoxicity (ADCC) is a mechanism of action of anti-tumor antibodies in which the Fcγ receptor (FcR) plays a key role. Hence, affinity chromatography using recombinant FcR can deliver valuable information about ADCC activity. Data on the analysis of therapeutic mAbs with the new TSKgel FcR-IIIA-NPR HPLC column are provided.

The N-glycans of antibody Fc domains are known to play an important role in Fc-mediated effector functions. Accordingly, separation patterns of therapeutic antibodies on TSKgel FcR-IIIA-NPR can be correlated to mAb glycoforms. Early eluting peaks (low affinity to Fc receptor) represent mAb glycoforms with low ADCC activity while late eluting peaks represent glycoforms with high ADCC activity.



FcR-IIIA affinity chromatography separates mAb glycoforms according to their ADCC activity

Chromatographic conditions:
Column: TSKgel FcR-IIIA-NPR (5 µm 4.6 x 75 mm); Mobile Phase: A: 50 mM Citrate, pH 6.5; B: 50mM Citrate, pH 4.5; Flow rate: 1 mL/min; Detection: UV@280 nm; Sample: Rituximab

Read the full application note at http://bit.ly/FcR-2p

Touch Express OPSI coupled to the Advion expression CMS provides a simple, fast, direct sampling method for fentanyl screening in urine

Solvent is delivered to the open port sampling area through the outer pair of concentric tubes at ~250 µL/ min. Paired with the electrospray ion source of the expression Compact Mass Spectrometer, the solvent forms a meniscus at the open port before being drawn down the inner path into the ion source of the mass spectrometer under the Venturi effect of the nebulization gas. The control and fentanyl-spiked urine samples, contained in a pipette tip, are simply touched in sequence to the OPSI sampling port and results are obtained in < 30 sec.

The mass spectra of fentanyl and fentanyl-D5 (Figure 1) show protonated molecules at m/z 337.2 for fentanyl and 342.2 for fentanyl-D5. These ions are used in a Selected Ion Monitoring (SIM) method for the quantification of fentanyl in urine. The OPSI sample technique provides an effective, high-throughput assay for fentanyl screening applications.

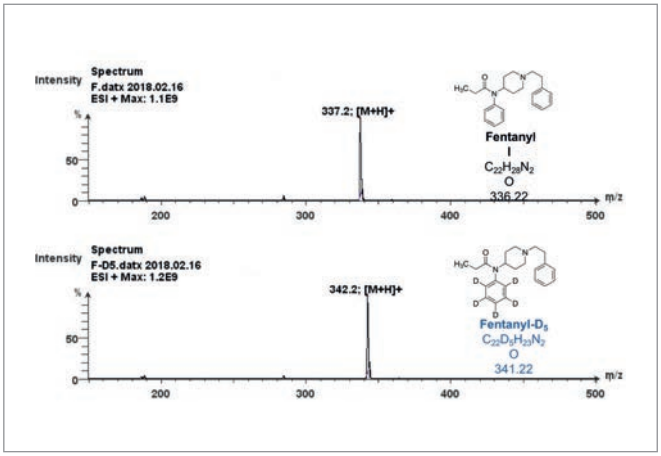


Figure 1: Mass spectra of Fentanyl & Fentanyl-D5 in control urine.

For more information visit www.advion.com

Spotlight on... Technology

CDS 7550S Thermal Desorption Autosampler

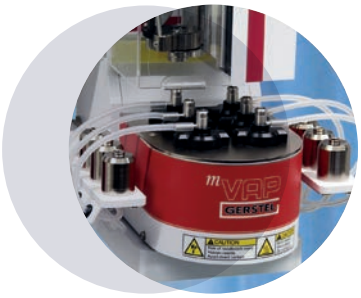
The CDS 7550S is a stand-alone 72-position thermal desorption autosampler. Equipped with the 2nd generation autosampler platform, the CDS7550S offers a worry-free 24/7 automation. With the high-temperature 350 °C oven, and the optional Peltier electric cooling module, the system is capable of handling C2-C44 level VVOC.

https://www.cdsanalytical.com/thermal-desorption-7550s

The Original Immobilized Chiral Stationary Phase

Whelk-O 1 gives broad selectivity toward a wide range of product classes and alternate selectivity to polyssacharide chiral stationary phases, making it perfect for chiral screening. Benefit from high loading capacity and broad range of particle sizes and dimensions for ease of scalability to preparative applications.

For more information visti: www.registech.com



Evaporative Analyte Concentration System

mVAP is a six-position evaporation station for the GERSTEL MultiPurpose Sampler (MPS). Following automated SPE or liquid/liquid extraction, solvent evaporation is performed at user defined temperature and vacuum combined with injection to GC/MS or LC/MS. Solvent change for optimized chromatography and MS ionization can be included in the workflow.

For more information contact: gerstel@gerstel.com or visit: www.gerstel.com

IonSense DART-QDa

Near instantaneous identification of contaminants or drugs of abuse. The IonSense DART source is coupled to the Water ACQUITY QDa mass detector for reliable analysis in seconds per sample. Little or no sample prep is required to obtain direct analysis of powders, surfaces, or solutions – in a compact configuration.

Contact info@ionsense.com for more information

Touch Express™ Open Port Sampling Interface

The Advion Touch Express OPSI is a one-touch solution for mass analysis, offering a unique, prep-free technique that provides direct analysis of solids, liquids, surfaces and fibers. Paired with the electrospray ion source of the expression Compact Mass Spectrometer, any soluble sample touching the port is analyzed in seconds.

Learn more about Touch Express at www.advion.com

Vocus PTR-TOF

The TOFWERK Vocus PTR-TOF mass spectrometer measures trace volatile organic compounds (VOCs) in real-time. TOFWERK's novel Vocus proton transfer reaction cell and high-performance time-of-flight technology combine to offer market-leading sensitivity and separation power for online analysis of industrial, laboratory, and environmental VOC samples.

https://www.tofwerk.com/products/vocus-ptr-tof/

Ocean HDX Spectrometer

Ocean HDX is anchored by High Definition Optics for high throughput, low stray light and great thermal stability. Its X-Platform Electronics include powerful onboard processing and communications including USB, Gigabit Ethernet, Wi-Fi, AP Wi-Fi and RS-232. The Ocean HDX is compact, robust and ideal for integrated, industrial, biomedical and research applications.

More information available at https://oceanoptics.com/product/ocean-hdx/

Confronting Challenges – Big and Small

Sitting Down With… Christy Haynes, Elmore H. Northey Professor, Associate Department Head, Department of Chemistry, University of Minnesota, Minneapolis, USA.

We hear you're currently in Valencia – what are you working on?

I received a Guggenheim Fellowship to support a research collaboration between the Polytechnic University of Valencia (the MPV) and the Instituto Tecnológico. The lab here is focused on biomedical applications of nanoparticles, and the team has developed some really nice mass spectrometry methods for characterization of protein absorption. It felt like a good time for a sabbatical…

How so?

I've been on faculty for 13 years, and I wanted to take a step back and re-evaluate. Sometimes in academia, people have a very singular focus – and become famous by working on their own. But I don't fit into the traditional chemist box – I'm interested in the messy spaces between fields and in truly collaborative work. This sabbatical allowed me to come in with a "beginner's mind."

How did you find yourself in analytical science?

I don't have a very traditional trajectory. There are no scientists in my family, and mine was the first generation to go to college. All I knew was that I wanted to have an impact on the planet. For me, chemistry is really pragmatic; I had to get through college faster than most – I couldn't afford a fourth year of college and so I did it in three – so part of me wanted to stick with what I knew. My PhD focused on physical chemistry but I was orientated towards the analytical, not least because it helped me cross disciplines. As a grad student I did single-cell chemistry, which was a great gift; ultimately, I ended up with unique skillset that really helped when applying for jobs. I tell my grad students that it's important to have many strings to your bow, so that you can set yourself apart.

What are the pressing issues in nanoscience?

Nanoparticle toxicology as a field emerged about 15 years ago and, for a decade or more, it has been largely focused on the exposure of organisms to high concentrations of nanoparticles for short periods of time. That is important, of course – but even more important is to understand the impact of long-term low-dose exposures. A great example are lithium-ion batteries, which contain nanoparticles such as nanoscale nickel manganese cobalt oxide (NMC). Electric vehicles are using these batteries, which is great, but there's something like 40 kg of this NMC in each one – how will that impact on the environment in the long term? I think we have a responsibility to be proactive and consider issues of safety and sustainability in the lifespan of those batteries. My focus is on bacterial interactions with nanoparticles – the bottom of the food web.

What challenges do you encounter in nanoparticle analysis?

Our biggest problem is that we need to find methods that can track nanoparticles in real time in complex matrices and, at the same time, help us to understand how the particle is transforming chemical signatures for dissolution or adsorption. Right now, that is impossible, so we pull together complementary methods to try to paint the whole picture – such as electron microscopy, dark field scattering, hyperspectral imaging and EDF. Unfortunately, most of those methods can't be employed in situ in real time. One of the really complicated aspects of this work is identifying thoughtful and appropriate controls, so that you don't misinterpret data.

In a more general sense, when you're straddling fields, it's sometimes hard to reach the audience that needs to hear about your results. With nanoparticle sustainability, for example, we would like to be able to talk directly to policymakers, to help create smart regulations.

"There are no scientists in my family, and mine was the first generation to go to college. All I knew was that I wanted to have an impact on the planet."

You're a champion for diversity in science – why tackle these thorny issues?

It's still important to acknowledge the challenges that women – and other minorities – face in science. However, I must admit that it's sometimes hard always being the person who points out gender discrepancies or discrimination. In a way, I'd just like to get my science done without bothering about social politics – but I recognize that comes from my own privilege. Plus, I believe that if you have any sort of power, influence or visibility you have a responsibility to talk about these issues. Being an underrepresented person has definitely influenced me – and it has driven me to try to improve things for those who follow. It's also important to remember that diversity contributes to the vibrancy of any field.

Not seeing the forest for the ...?

Get a clear view of the big picture and relevant details: Use intelligently automated GERSTEL solutions with PrepAhead productivity to get your work done in a transparent, efficient and precise manner.

Sample preparation for GC/MS and LC/MS analysis:

- Liquid/liquid extraction
- Clean-up and matrix removal
- Analyte concentration
- Derivatization and liquid addition
- Generation and addition of standards

Our solvent-free, solvent reduced and µL-scale sample prep techniques improve LOQs and provide a clearer view while reducing cost and environmental impact.

What can we do for you?

Derivatization, Adding Standards, Mixing

SPE, Filtration, Clean Up, Solvent Evaporation

Automated Liner Exchange ALEX (QuEChERS)

SPME, SBSE, Thermal desorption

Headspace & Dynamic Headspace (DHS)

Agilent Technologies
Premier Solution Partner

GERSTEL

www.gerstel.com