NOVEMBER 2019 # 82

the Analytical Scientist™

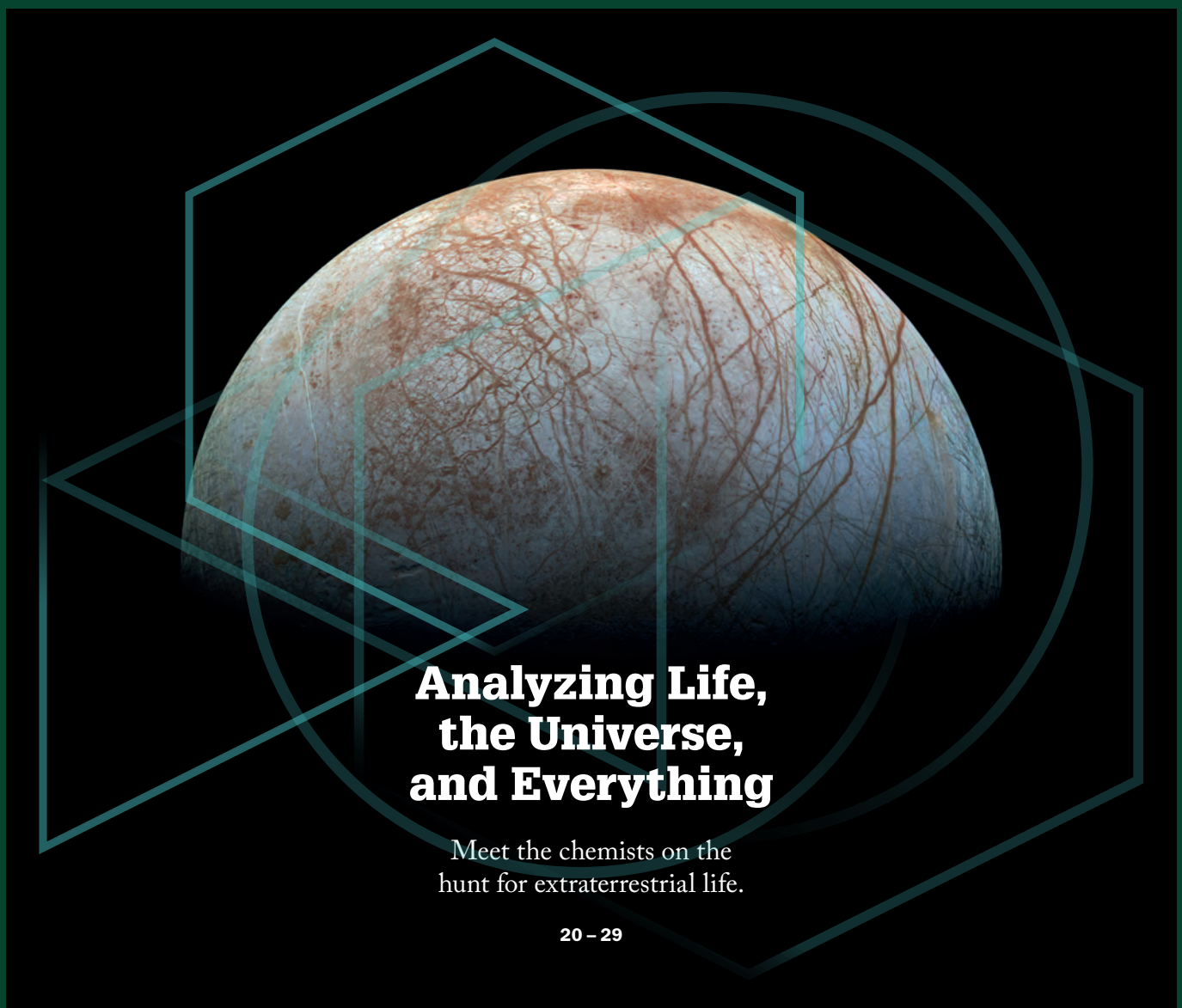

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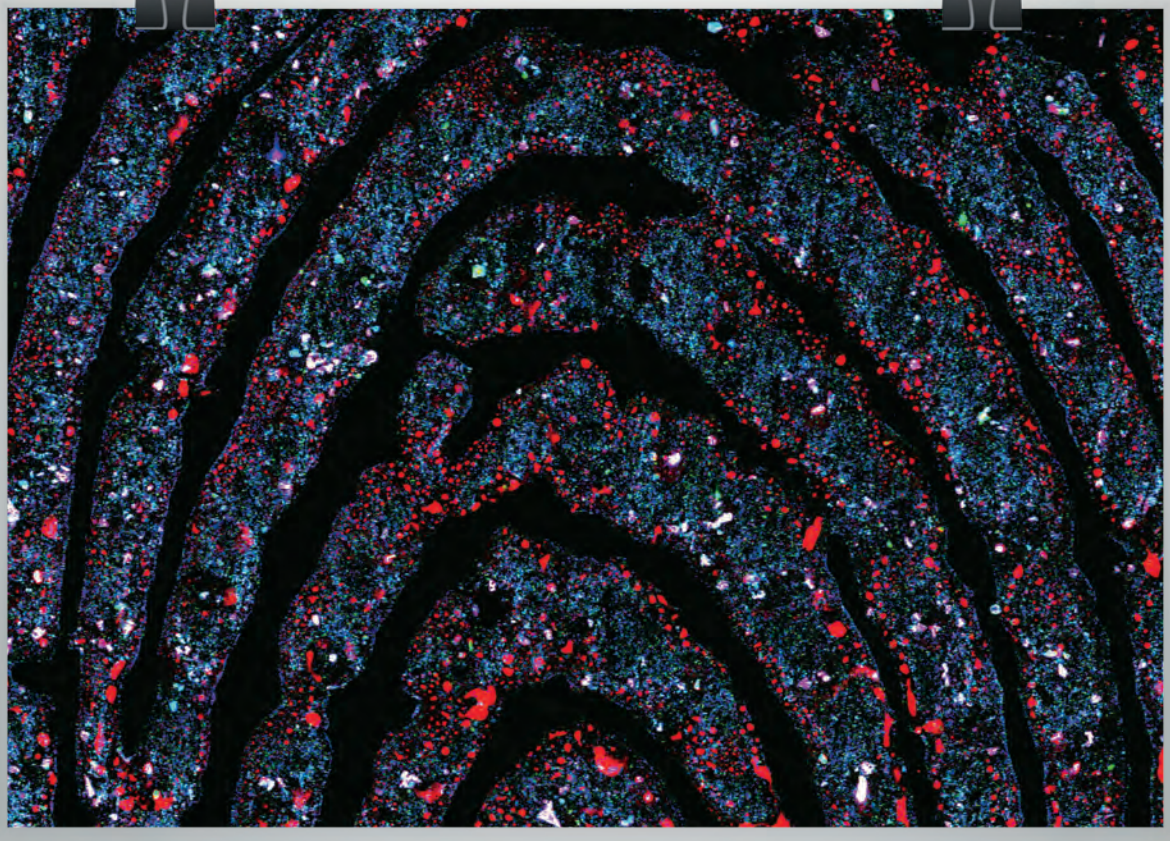
Image of the Month



Elementary. My Dear Watson

Large area synchrotron source X-ray fluorescent microscopy scan of a natural fingermark showing distribution of Zinc (red), Iron (green) and Tin (blue) (Prepared by Rhiannon Boseley). Intrigued? Get the full story on page 12.

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

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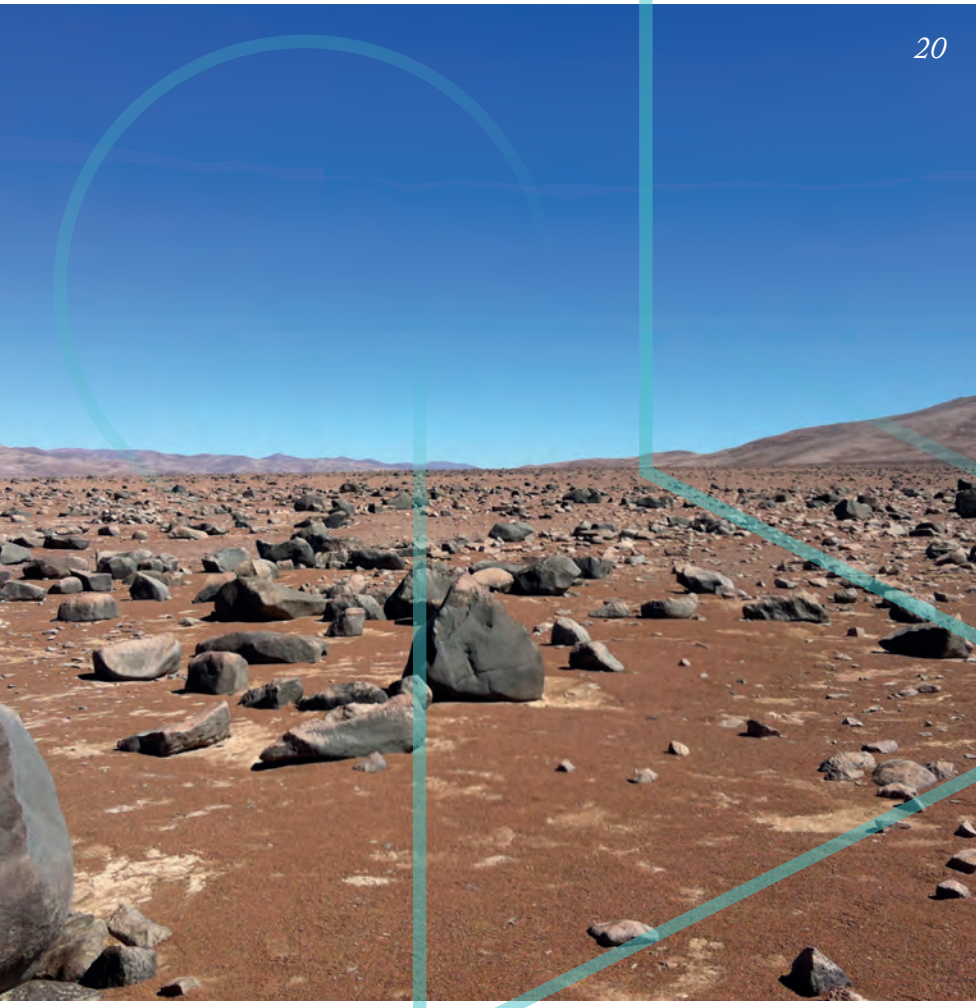

On The Cover

Could the subterranean waters of Europa provide an ideal environment for alien life?

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the **Analytical Scientist**

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Crowdsourcing Toxicology: The Sequel

The current outbreak of vaping-associated lung disease highlights the risks facing consumers when markets move faster than regulation

Back in summer 2018, The Analytical Scientist highlighted the lack of analytical information available to regulators and consumers on the health effects of vaping and e-cigarettes (1); in my editorial, I called it "a global toxicology experiment" (2). The first results of that experiment are now starting to emerge… And it's not good news.

In early 2019, reports started to appear of serious lung injuries in people using vaping products. The situation escalated rapidly; at the time of going to press, America's Centers for Disease Control (CDC) has recorded 37 deaths and 1,888 cases of vaping-associated lung injury.

FDA forensics laboratories are scrambling to analyze hundreds of samples but have been unable to pinpoint the specific chemical(s) causing the condition. So far, the most significant association appears to be with products containing THC, the main psychoactive component of cannabis.

Perhaps it is not surprising that the origin of the outbreak appears to lie at the intersection of vaping and cannabis, two products with a history of minimal safety testing or quality control. The discretion and convenience of vaping e-liquids struck a chord with consumers and it has quickly become one of the most popular ways to consume cannabinoids. Though research on the safety of vaping nicotine products is limited, for cannabis oils it is almost nonexistent.

As legalization spreads, cannabis is cleaning up its act, with tough new regulations for products sold on the legal market. But it's clear that more research is urgently needed into the chemical constituents of e-liquids (whether black market or legal, containing cannabinoids or not). There is no such category as "generally recognized as safe to vape".

In a LinkedIn essay (3), analytical lab CEO Rob O'Brien calls for international standards organizations, analytical laboratories, and government organizations to come together to create standards for a new category: "Products intended for inhalation after high-temperature vaporization."

With the death toll rising every week, analytical scientists everywhere should be asking: "What can we do to help?"

Charlotte Barker
Editor

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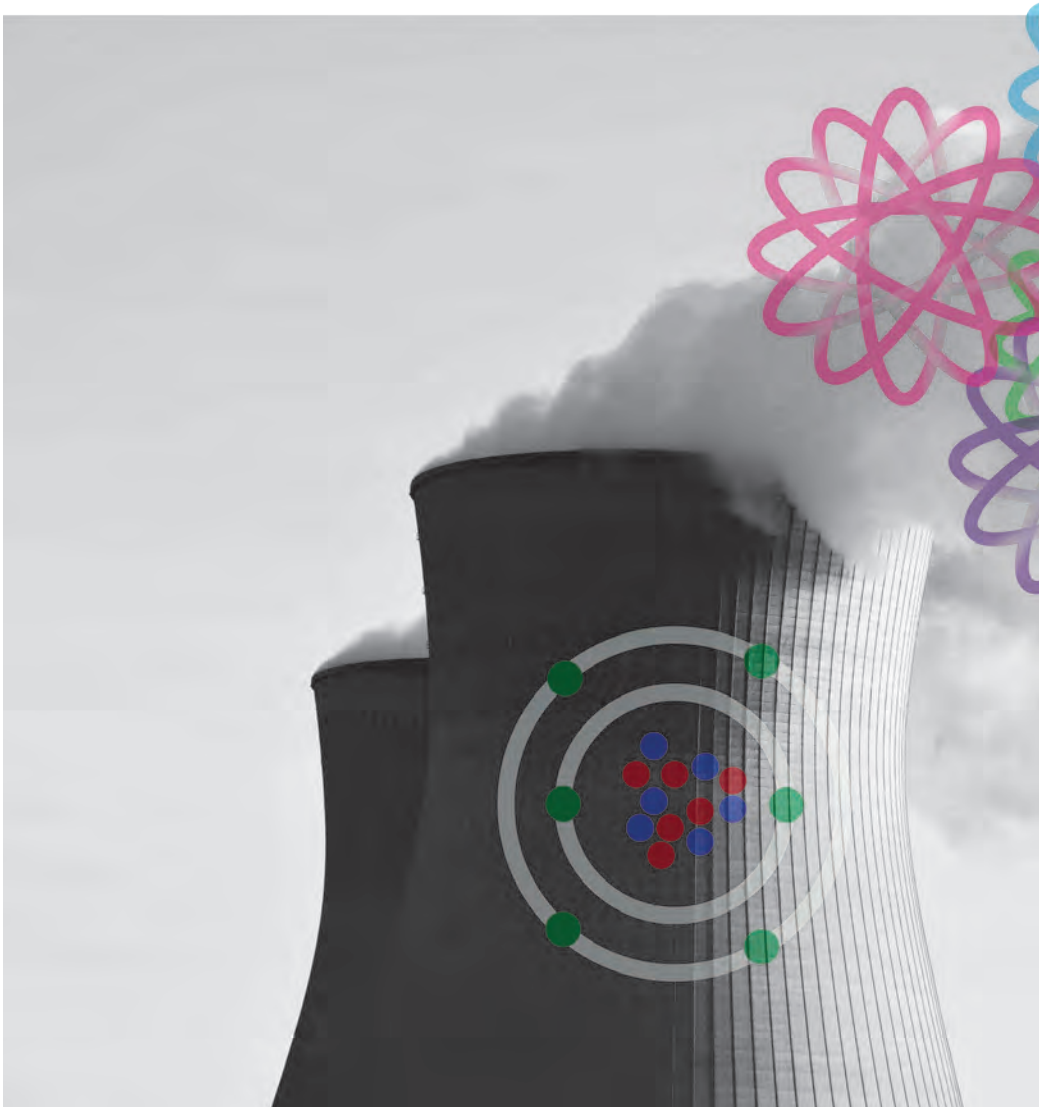
Upfront

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



Emission Impossible?

A novel spectroscopic approach could take radiocarbon emission monitoring out of the lab and into the field

Monitoring radiocarbon emissions (carbon-14, typically in the form of carbon dioxide and methane) from nuclear reactors is no easy task. Laboratory-based methods to detect carbon-14, including accelerator MS and liquid scintillation counting, are effective, but are not easily used onsite – neither are they sufficiently adaptable to monitor atmospheric samples. Guillaume Genoud and colleagues at the VTT Technical Research Center in Finland set out to fill the gap by using an automated laser spectroscopy-based system to detect traces of carbon-14

containing gases in atmospheric-like samples (1). "We employed an optical method to ensure a compact, rapid, and more affordable way of detecting trace gases," says Genoud. "Mid-infrared cavity ring-down spectroscopy (CRDS) was chosen to provide the highest levels of sensitivity."

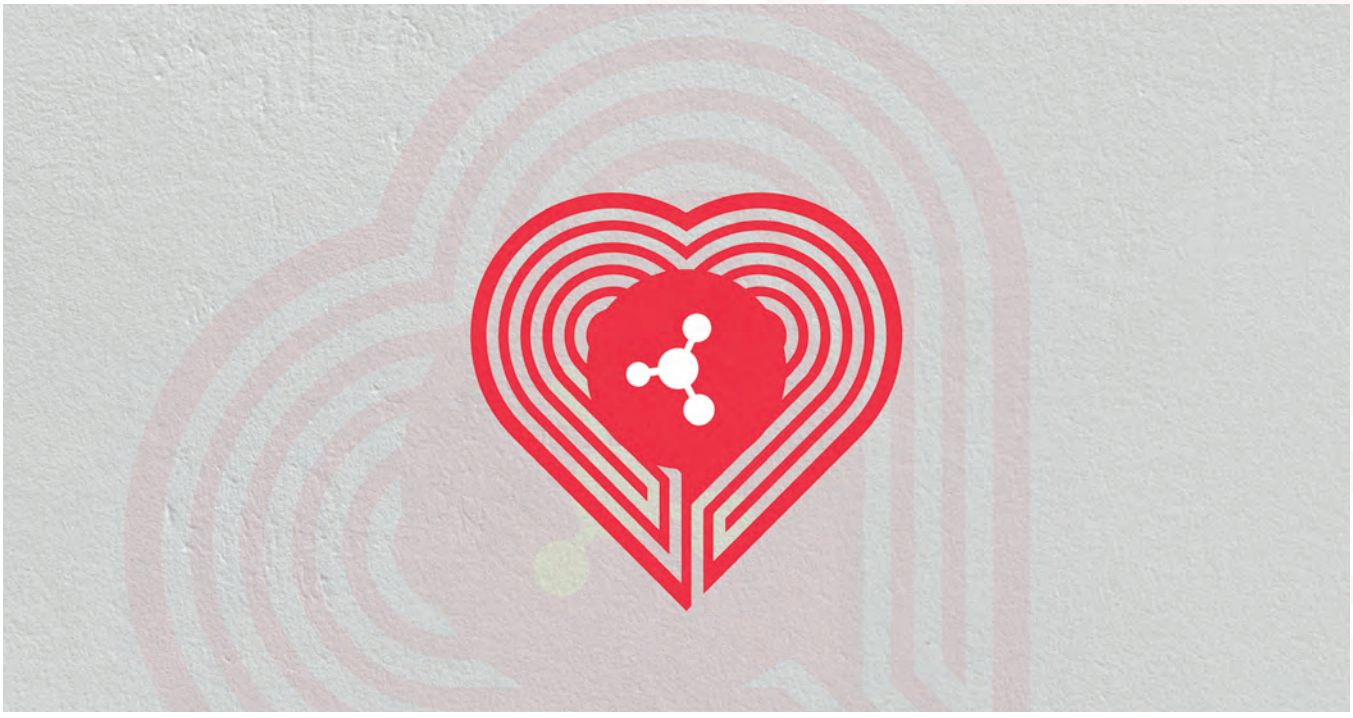
The CRDS instrument was coupled with an advanced, two-part sampling system; a cryogenic trap extracts carbon dioxide from the air sample, while a catalytic unit converts methane into carbon, which allows the approach to discriminate between radiocarbon in organic or inorganic molecular form.

Genoud's research has been conducted in a laboratory so far, but he's confident of its eventual utility: "There isn't anything preventing its use in a real setting for in situ radiocarbon monitoring." In fact, preliminary studies in nuclear facilities are already underway – and the results will be published shortly.

Looking ahead, Genoud would like to enhance the device's sensitivity. "By increasing sensitivity below 1 part-per-trillion, we'll not only be able to monitor emissions from nuclear facilities, but also use this method for other applications where C-14 is diluted in atmospheric samples," he says. And that could take the system even further afield. "One would, for instance, be able to determine the origin of greenhouse emissions as radiocarbon can be used to discriminate between fossil and biogenic emissions– key to developing more accurate climate models and predicting future changes."

Reference

1. *G Genoud et al., "Laser spectroscopy for monitoring of radiocarbon in atmospheric samples" Anal Chem, 91, 12315 (2019). DOI: 10.1021/acs.analchem.9b02496*



Getting to the Heart of Proteoforms

How do we overcome the challenge of characterizing the cardiac proteoforms?

Heart disease is the number one global killer – and recent evidence suggests that proteoform analysis is important to understanding cardiac dysfunction (1). MS can be used to characterize the proteoforms found in cardiac disease states, but the approach suffers a number of problems, such as decreasing signal-to-noise ratio as molecular weight rises. Adapting open-source software, researchers at the University of Wisconsin-Madison have applied MS to identify a novel set of large proteoforms in human heart tissue (2). We asked the team (Lloyd Smith, Ying Ge, Leah Schaffer, Trisha Tucholski, and Michael Shortreed) to tell us more about the work.

What are proteoforms – and how do we identify them?

Different protein forms arise from biochemical processes – RNA processing, post-translational modifications and genetic variability being chief among them. Proteoforms can be identified by their intact mass and fragmentation data. A previous study by the Ge lab introduced a top-down proteomics platform using MS-compatible, serial-size exclusion chromatography to fractionate proteins extracted from human heart tissue – enabling a 15-fold increase in proteoform observations over 60 kDa (3). However, no proteoforms above 60 kDa were identified because of the difficulty in obtaining high-quality MS/MS data on a chromatographic timescale.

What can you tell us about your new workflow?

We previously pioneered an open-source software program – Proteoform Suite – that is capable of identifying proteoforms by intact mass alone, grouping them into distinct families. In this study, we augmented the software to allow us to determine candidate identifications for large proteoforms based on average mass and LC retention time. The large proteoform candidates that we selected informed our interpretation of previously acquired large proteoform fragmentation data, which – until now – had not provided positive identifications.

We've been able to identify a number of important large heart proteoforms – notably, a complex fragmentation spectrum from co-isolation of multiple 72 kDa lamin A and 65 kDa lamin C. We also identified endogenous 140 kDa myosin heavy chain protein C for the first time; proteoforms of this type are associated with various heart diseases.

What main challenges did you face?

We were unable to isotopically resolve the observed proteoforms because of their high molecular weight and the resolving power limitations associated with quadrupole-time-of-flight mass analysis. As a result, we used average mass and a wide search space to determine candidates, but this also generated many false positives and therefore required manual analysis of our data.

Larger proteoforms do not fragment as efficiently as smaller proteoforms, which makes collecting high-quality data challenging. A higher number of fragmentation spectra are required, which is difficult to achieve on an LC timescale. In addition, fragmentation spectra become increasingly complex with larger proteoforms.

What's next?

We hope to use intact mass analysis to construct proteoform families that will facilitate the selection of interesting candidates for more targeted data acquisition. A number of observed masses remain unidentified – likely, at least in part, due to the enormous number of uncharacterized proteoforms. Future work may also see us integrate other types of data, such as bottom-up peptide or RNA sequencing data, to create a more comprehensive database.

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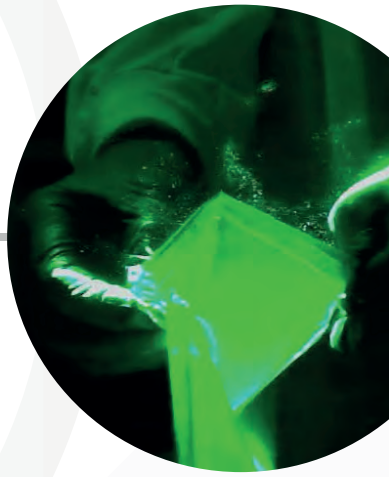

Leaving Your Mark

There's much more to fingerprints than meets the dye

Since their inception in the late 19th century, fingermark detection technologies have played a decisive role in criminal investigations, often providing essential evidence linking suspects to a crime. Yet, many fingermarks go undetected. "We know that we don't detect all latent fingermarks – there's some recent work by Scott Chadwick and co-workers that shows this (1)," says Simon Lewis, a researcher based in Perth, Australia. "If we better understand this chemistry then we could potentially improve these detection rates." While much is known of the organic component of fingermarks, there is a major element that has not been investigated. The missing piece of the puzzle? Inorganic compounds – either originating in the body or transferred by handling everyday items such as coins or cosmetics.

Lewis and colleagues used the ANSTO Synchrotron facility in Melbourne to determine the distribution of the elemental and inorganic components of latent fingermarks using high-powered X-ray fluorescence microscopy (2). "Thanks to this synchrotron's unique detector design and geometry, very large samples can be rapidly imaged at high spatial resolution," says Mark Hackett, who worked with Lewis on the study. The result: highly detailed compositions detailing the distribution of metals and inorganic components of fingermarks. While synchrotron techniques are unlikely ever to become part of the forensic investigators' toolbox, the results contribute to fundamental knowledge in this area. "Gaining a more complete overview of fingermark chemistry will provide an incentive for more robust detection methods in the future," says Lewis.

The immediate applicability of the work is limited by a number of unanswered questions, which are now being studied by Rhiannon Boseley, a PhD student in Lewis's group. For example, how much of these compounds are transferred in a fingermark? And what are the background levels? "We certainly don't have the answers to all the questions yet," says Lewis, "but we're hopeful that work like ours can provide a framework for more detailed understanding of fingermark chemistry – now, and in the future."

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What's in the Bag?

An MS-based approach could let police ID illicit drugs without opening suspect packages

A team of researchers led by Edward Sisco found that their thermal desorption direct analysis in real-time MS (TD-DART-MS) method, coupled with wipe-based sampling, was capable of determining the contents of unopened drug packaging with 92 percent accuracy (1). We sat down with Sisco and co-investigators Elizabeth Robinson and Amber Burns to learn more.

What inspired the work?

Edward Sisco: The study originated from our ongoing work measuring the background levels of drugs in forensic laboratories. Surfaces throughout the laboratory are wiped and the resulting sample is tested for a panel of drugs. This new study using wipes and TD-DART-MS to measure drug levels in packages is a natural extension of this work.

Amber Burns: The goal is to develop a rapid screening test to provide the information necessary to further an investigation or file charges. It's also possible that this approach will detect drugs that are difficult to analyze by other means.

How did you conduct the study?

Elizabeth Robinson: Wipe sampling was performed both on the outer and inner drug packaging prior to opening, and a wipe treated with a single drop of alcohol was used as a control. We then carried out TD-DART-MS and LC-MS/MS; the former was used for non-targeted screening of trace residues, allowing us to compare the substance inside the package with the trace residue on the outside, while LC-MS/MS was used to obtain quantitative measurements of the trace residue from the exterior of the packaging.

What were the major findings?

Sisco: We were able to correctly identify the contents of a package with 92 percent accuracy – much higher than anticipated – simply by wiping the packaging exterior. In most instances, there was more than a microgram of material present on the exterior – a significant amount in trace detection terms. It's feasible that less sensitive techniques could also be employed, which represents an important consideration for field applications. Interestingly, as highlighted in the paper itself, we also detected low levels of illicit substances other than those contained within the sample packaging. Thus, it may be possible to profile the history of drugs present in a particular location – such as a drug dealers' home – by targeting these low-level signatures.

What's next?

Sisco: We're working on a number of new avenues. Firstly, we want to increase the sample size while maintaining the same level of accuracy. We are also keen to expand the study to different types of packaging and are investigating whether it is possible to extract intelligence-level information – such as the source of an illicit substance – from samples.

In addition, we're working on a novel workflow for traditional drug analysis that incorporates presumptive screening from the get-go. Our goal? To complete screening immediately upon receipt of evidence to better inform law enforcement, which should in turn drive more targeted forensic analysis in the field.

Lastly, we're interested in whether the process of handling evidence contributes to trace residues. Given the background contamination in forensic laboratories, we want to ensure that residues on the outer packaging are not being introduced in the lab.

Reference

1. *E Sisco et al., "What's in the bag? Analysis of exterior drug packaging by TD-DART-MS to predict the contents", Forensic Sci Int [Epub ahead of print] (2019). DOI: 10.1016/j.forsciint.2019.109939*

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

Repeat After Me...

How committed are we to reproducibility in science?

By Heather Bean, Assistant Professor, School of Life Sciences, Arizona State University, Tempe, Arizona, USA.

The institutions funding our research and journals publishing our discoveries make, almost without exception, a seemingly simple request: make your science reproducible. Why? Because we owe it to the taxpayers – who often foot the bill – to make the best possible use of their money, and we owe it to our colleagues to ensure that they can trust our conclusions.

To ensure reproducibility, we perform replicate experiments, report standard deviations and conduct significance testing. We also name the sources of chemical standards, reagents and cell lines, document the instrumentation used and software deployed, detail method parameters and cite the studies central to method development.

This information alone, however, is not enough for one to reproduce a given experiment. Consider the following: you ask your most senior researcher to reproduce the results of a paper they're submitting for publication, relying only on the methods section (that is, they can't use the saved method on the instrument software). The result? Disaster! In reality, nobody reports all experimental details, and there are several reasons for this.

Journal articles are restricted regarding their length and formatting. Utilizing supplementary information to provide a more complete overview of methodology has become the workaround of choice; yet, typically this amounts to nothing more than endless lists of parameters in narrative format – hardly easy to interpret, particularly for the non-expert. The ever-growing availability and adoption of black-box methods with hidden default settings that can be difficult to deduce and report is then another issue. Consider a parameter as ubiquitous as a signal-to-noise threshold in a data processing method.

The rise of interdisciplinary science has introduced more diverse and complex technology. The methods outlined in manuscripts for biomarker discovery and validation studies, for example, would include (and may not be limited to): study design, subject recruitment, subject and sample characteristics, sample handling and processing, chromatography, MS, data processing, data post-processing. statistical methods, machine learning, and validation steps The burden of ensuring that every one of these steps is thoroughly reported ultimately falls on the journal's reviewers but, realistically,

"The rise of interdisciplinary science has introduced more diverse and complex methodologies."

it's highly unlikely that the review team will cover all of the necessary expertise.

Bench scientists and reviewers alike suffer from poorly reported methods; I myself have had difficulty in citing a standard data processing parameter due to a lack of previous reports, leaving both myself and the requesting reviewer at a loss. Such issues highlight a central question that we must answer moving forwards: how do we ensure that we, as a community, make our experiments truly reproducible?

As authors, tables and lists are our friends. Not every methodological parameter will fit this style, but many will, and for investigators trying to adapt them to their own software platforms, it is much easier to match against these formats. For greater transparency, why not print the methods, scripts and/or code directly out of the software and provide those printouts as supplementary files? This also reduces the probability of errors.

The responsibility is not, however, that of the authors alone. Reviewers must critically appraise the methods sections of submissions and request more detail where they deem an experiment cannot be reproduced from the manuscript content. To this end, publishers themselves must be more specific in their standards for methods sections and should hire staff with the necessary experience to ensure these standards are fit for purpose in our ever-evolving field.

Software manufacturers can also play their part by streamlining the export of method tables in editable and easily interpreted formats. These tables should also include default parameters not editable by users and should track the provenance of raw, processed and post-processed data to generate reports on how data has been integrated, transformed and filtered.

If we want to provide a firm foundation for the researchers of tomorrow to build on, we need to accept that reproducibility is everyone's responsibility.

Diagnostics Everywhere

Remote self-sampling may improve diagnosis and prognosis while reducing costs, but numerous factors must be considered for appropriate implementation

By Jennifer E. Van Eyk, Erika J. Glazer Chair in Women's Heart Health and Director of the Precision Biomarker Laboratories at Cedars Sinai Medical Center, and Kimia Sobhani, Chief Clinical Chemist and Director of the Core Laboratories at Cedars-Sinai Medical Center, Los Angeles, California, USA.

The precision diagnostic tests that often inform essential treatment decisions can take years to develop and validate – and even then their applicability is often limited to specific indications. Companion diagnostics, for example, are useful for predicting safety- and efficacy-related responses to treatment, but may be considered niche in their window of application. Broader diagnostics that harness the utility of previously validated, well-studied circulating biomarkers can be used to address disease-specific diagnostic and prognostic questions, both in and out of the clinic.

Continuous or semi-continuous biomarker assessment relies on our existing knowledge of changing biomarker concentrations over time and/or in response to disease development. For many clinically established analytes, however, the expected shift in concentration over time is poorly defined, especially in early disease. These days, artificial intelligence can be applied to help pinpoint disease risk and progression from routine lab tests, and – in some cases – routine monitoring can enhance the power of these approaches.

As the quest for novel and clinically relevant biomarkers continues, the most promising discoveries can be combined with existing markers through algorithmic approaches. Such tests that incorporate multiple biomarkers in algorithms have been dubbed "Multianalyte Assays with Algorithmic Analyses (MAAA)," and can receive their own Current Procedural Terminology codes. The untapped potential to develop MAAA tests is vast. But to see the paradigm shift towards enhanced disease prevention by early diagnosis, we will likely need to implement semi-continuous sampling of blood (and other body fluids), thus creating a need for collection devices that are usable by anyone, anywhere, and at any time.

Given the need for intuitive and reliable collection devices, numerous companies have developed methods to enable patients to self-collect blood. In doing so, the following considerations are of the utmost importance:

- the amount of sample to be collected (and how many tests can be performed as a result),
- the reproducibility of the collection method/device,
- the sample matrix (whole blood versus cell-free plasma or serum fractions),
- the location from which the sample is taken (e.g., fingertip vs. other capillary blood draw sites),
- which biomarkers can be measured from the sample type,
- shipping requirements and sample stability, cost, and ease of use.

Serum and plasma represent the critical matrices for measuring most blood-based biomarkers, and are classically obtained by centrifuging blood – a challenge in remote settings. Filtration-based approaches are available, but these often correlate poorly to centrifuged samples. As such, there has been some focus on dried blood samples, because they are simpler to transport and sometimes have greater stability than liquid samples. However, the number of analytes that can be accurately measured from dried blood is limited (because of hemoglobin interference and/or inability to differentiate intracellular from extracellular analytes in whole blood lysates) – and established blood-based diagnostic methods are designed to work on liquid samples. So, if a dried whole blood sample is collected, it must be extracted in an appropriate liquid medium and correlated to liquid results.

As such, we propose that a combination of sampling approaches should be applied to suit the types of analytes being measured and individual patient needs. Of course, this means that additional preanalytical considerations (such as the sample collection method), extended biomarker validation studies, and informatic and statistical support (particularly when establishing MAAA utility) will be needed – but this extra effort is more than worth the benefits for patients.

Healthcare affordability and disease prevention remain at the forefront of the minds of our medical community, government and public in the US. And yet, approaches to improve the situation have not centered on the most obvious tools at our disposal: well validated laboratory diagnostics. The Centers for Medicare and Medicaid have recently cut reimbursements in many areas (including laboratory testing) through the Protecting Access to Medicare Act. Considering the major costs in healthcare, including doctor visits that could have been handled remotely and procedures that could have been avoided with earlier diagnosis, one might consider cuts to laboratory reimbursement counterproductive because of the effects on diagnostic development and patient monitoring.

All things considered, it is imperative that every group developing and validating diagnostics make an effort to refocus major stakeholders (patients, clinicians, payors, and the government) on the utility of diagnostics and democratizing access with appropriate clinical oversight.

Casting Your Net(work) Wide

What's the point of expanding your analytical network? Where do I begin...

By Christina Jayne Vanhinsbergh, PhD student, University of Sheffield, UK.

Networking can be a daunting prospect, and the associated skillset is not always easily developed. And yet it is clearly valuable activity – especially for early-career scientists.

I am a PhD student at the University of Sheffield, UK, with a focus on multidimensional chromatography and its application in oligonucleotide separations. The novel nature of PhD research requires that you widen your sources of expert knowledge beyond that of your academic institution. Integrating into a professional community seemed to be the fastest route, so I went in search of societies that offered events to further increase my network.

I found the Chromatographic Society (ChromSoc.com) and signed up for 'Grass Roots 2', a fundamentals of chromatography training weekend. Alongside an in-depth lecture program, we also participated in hands-on troubleshooting, and attended advice sessions and networking events; the organizers were incredibly welcoming and my confidence improved ten-fold. In fact, the weekend was so useful that I went on to attend many sequential ChromSoc events and ended up joining the organizing committee!

Societies like ChromSoc recognize the importance of providing early-career analytical scientists with opportunities for training and professional development. To this end, ChromSoc organize regular events to communicate cutting-edge technology and research, which also provides the opportunity for scientists to

"The novel nature of PhD research requires that you widen your sources of expert knowledge beyond that of your academic institution."

present their own work. What's more, these events are often conducted in partnership with other established networks, such as the Royal Society of Chemistry or the British Mass Spectrometry Society, which, when coupled with ChromSoc's engagement with industrial sponsors (which builds bridges between equipment manufacturers and users of the technology) significantly boosts the potential network.

If you're low on cash (as many postgrad students are!) there are funding options to support attendance, including student bursaries and the John Dolphin Fellowship. In addition, travel grants are available for early-career analysts in small-to-medium sized pharmaceutical and biopharmaceutical companies, and there are even opportunities for undergraduate students to undertake summer research studentships.

But the benefits for students don't stop there: ChromSoc recognizes contributions to the advancement of chromatography by awarding annual medals to those who make major and significant advances within the field, including an undergraduate student award, which recognizes the importance of early professional development. Nominations for recipients are made by the members of the society network – the same network that drives all society activities. Without networking, the society would not know what events would be of use for the professional development of members. The ChromSoc Twitter and LinkedIn pages are great sources for help and advice.

Through networking with the chromatographers in the society, I have been able to ask for troubleshooting advice, extend my training, seek funding opportunities and – more importantly – build a base of professional contacts. My CV is now thicker, with skills in report writing, project management, networking and presenting due to my work on the organizing committee and at symposia.

Association with a professional society sets me apart from other PhD students and enables me to build my profile within the professional community. I feel I can drive my own development; some opportunities that have allowed me to grow academically and professionally may never have presented themselves, if I had not committed myself to networking.

In my view, all postgraduate students should seek out relevant societies – through them, you can collaborate, engage and grow. It might feel a little scary or intimidating at first but, like all good things, it's worth the extra effort.

Aiming for Peak Uptime

Whether providing clinical diagnostics for busy physicians or pharmacokinetic testing for the pharmaceutical industry, being able to operate 24/7 is mission critical for many analytical labs. We caught up with Ken Lewis, founder and CEO of North Carolina-based analytical laboratory OpAns, to find out how on-site gas generation is helping the company minimize downtime and keep vital testing on track.

Who are OpAns?

We are a contract analytical services laboratory providing support for pharmaceutical discovery, clinical trials, and clinical diagnostics.

How did you come to launch your own laboratory?

I knew from my undergraduate days onwards that analytical chemistry was a great fit for me - it is just the right blend of chemistry, engineering, physics, and mechanics. I earned my PhD in separations and mass spectrometry at the University of Carolina, Chapel Hill, under the direction of Jim Jorgensen. And I was lucky enough to be involved in some ground-breaking work – along with John MacNair, we built the world's first UHPLC system.

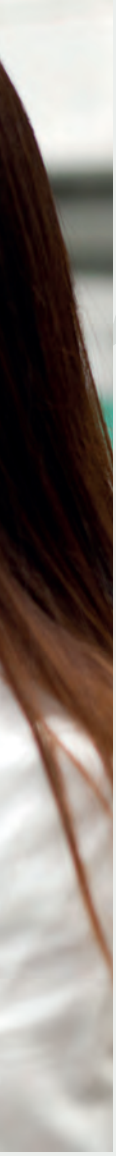
As a postdoc, I worked in the biopharmaceutical sector, first at Affymax and later in the discovery chemistry divisions of Glaxo-Wellcome and Eli Lilly. When the site I worked at was closed in 2004, it prompted me to make a big decision. Rather than move to another site or company, I decided to take control of my fate and use my skills and experience of running labs to start my own company, OpAns. What started as a company of two has now grown into a medium-sized analytical laboratory, employing 30 people.

How does your work in the contract lab world compare with previous roles?

It's satisfying to know that our work is helping people. While important, I was aware that my work in the pharma industry was ultimately driven by stakeholder return; if that return didn't exist then the work could not continue, no matter how noble. OpAns gives me the flexibility to pursue work that I believe in. In particular, a large proportion of our work is in pediatric clinical trials, supporting America's Best Pharmaceuticals for Children Act by studying dosage for children – especially newborn babies.

We also allocate significant resources to research into steroidogenesis; for example, studies of environmental exposure to certain chemicals and how they affect hormone production, screening programs, and work for pharmaceutical companies studying endocrine diseases.

A third area we work in is clinical diagnostics, primarily dry blood spots for toxicology testing and therapeutic drug monitoring. Dry blood spot testing is easier on patients than traditional blood tests and provides better information to physicians compared with saliva- or urine-based toxicology.



The Cost of **Nitrogen Cylinders** vs. **A Gas Generator**

The **cost** of having **nitrogen gas delivered** to your lab is subject to **price increase** and additional, often **hidden, costs**.
A **gas generator** is a more **economical** and **reliable** solution for nitrogen gas supply.

Costs of Buying Nitrogen Cylinders

- Fluctuating nitrogen cylinder costs
- Unused nitrogen gas in cylinders
- Employee safety training & monitoring
- Regular deliveries
- Installation work

Producing your own Nitrogen with a Gas Generator

- One-time delivery for installation
- Annual generator service

What are the workhorse technologies in your labs?

Given that 95 percent of the work we do is quantitative in nature, we primarily perform LC-MS/MS using triple quad MS. To a lesser degree we use time-of-flight and single quad MS, and immunoassays including ELISA.

What are the critical factors when choosing equipment?

It's a balance between performance/robustness and regulatory compliance. The work that we do is regulated by good laboratory practice (GLP) and clinical laboratory improvement amendments (CLIA) regulations. Once you get a compliant solution in place you cannot easily switch vendors, so it's very important that we pick the right partner first time.

Our decision to work with Peak Scientific for gas generation came down to three key factors. First, Peak was recommended and used by a number of instrument providers – it was important to us that they have acceptance from the manufacturer. Second, the support and information from the team at Peak was terrific, and provided exactly the information I needed. Third, pricing was very competitive. Seven years later, I can say it was a good decision!

Why did you originally switch to on-site gas generation?

Previously, we used liquid nitrogen – stored in a 600-gallon tank that had to be re-filled every five days. When we outgrew that tank, we started to look at on-site gas generation and realized there were several advantages.

Since swapping, we have increased our gas consumption threefold, so there are significant savings compared to liquid nitrogen. It's not just the cost of the nitrogen itself that adds up either – there is the cost of tank rental, delivery and various other surcharges, all of which increase year on year. By contrast, the cost for maintenance of our on-site gas generator has proved to be quite consistent. Overall, we've cut our nitrogen costs by more than half.

Maintenance is not just a cost issue – it's also an important source of downtime for labs, and on-site generation has proved advantageous in this respect too. We have never experienced failure of the generation system itself, but the associated air compressors do require some maintenance. Our unit contains four air compressors, but will run with three so, if a compressor goes down or needs maintenance, we have redundancy and can continue to operate.

How do you maximize uptime in your lab?

The most important thing is to take a systematic approach and keep up with preventative maintenance. After all, a small amount of scheduled downtime is much better than the unscheduled downtime that results if something breaks – and when you need to have samples running 24/7, unscheduled downtime must be minimized at all costs.

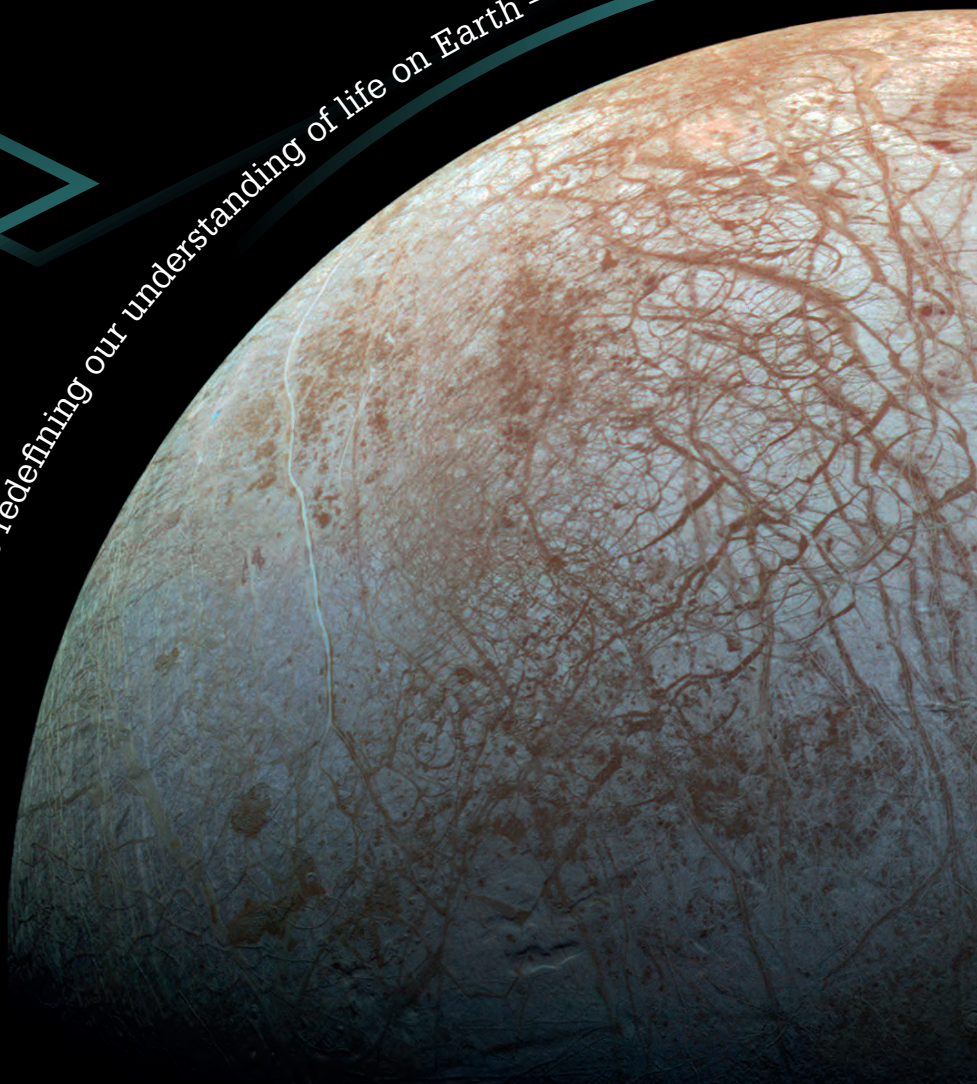
You have to get to know your equipment, and learn when maintenance is needed. Making sure staff understand how the equipment works can also help minimize downtime - when something goes wrong, they can do basic troubleshooting and give service engineers enough information about the problem to select the right parts for the job and resolve the issue quickly.

Why is uptime so important for you?

We work in clinical diagnostics, so physicians and their patients are waiting on results that matter – results that will inform important decisions. I can think of no more crucial analytical need than that.

ANALYZING LIFE, THE UNIVERSE, AND EVERYTHING

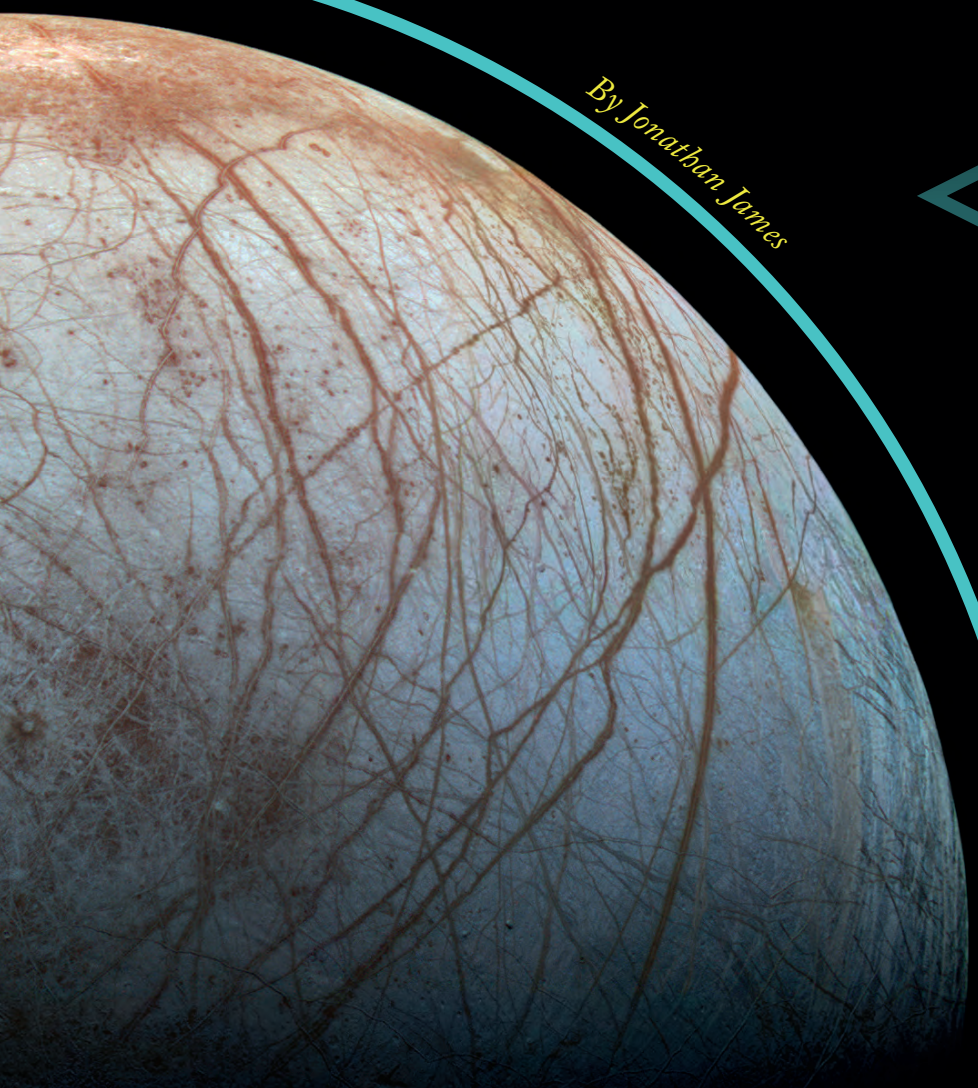
Planetary science is redefining our understanding of life on Earth – and beyond



Long have we sought to understand our place in the Universe. It's easy to imagine even the first *Homo sapiens* looking up at the stars and wondering: are we alone? But only in the past 50 years have scientists been able to even begin formulating an answer to this short but profound question. By studying extreme environments on Earth, planetary scientists piecing together the conditions necessary for life – painting a picture of the ideal alien habitat. Such discoveries are informing the future of exploratory space missions by determining both the destination and the analytical instrumentation needed onboard to confirm the likelihood of life.

Here, two extreme analytical scientists discuss their work on Earth – and further afield.

By Jonathan James



SEARCHING FOR SIGNS OF LIFE

By Dirk Schulze-Makuch,
Professor of Planetary Habitability and Astrobiology at the Technical University of Berlin, Germany, and Adjunct Professor at Washington State University and Arizona State University, USA.

My goal is to characterize the environmental conditions of other planets and moons. I'm particularly enamored with one of our nearest neighbors: Mars. Of course, obtaining samples from the Red Planet is an enormous undertaking, so the overwhelming majority of our research is carried out far closer to home. Analog environments – regions of the earth with conditions resembling extra-terrestrial landscapes – provide the perfect foil. The Atacama Desert in Chile mirrors the surface of Mars superbly, while Pitch Lake, a liquid asphalt lake in Trinidad is an excellent stand-in for the lakes on Saturn's largest moon, Titan. Each location has its own challenges, and we must be willing to adapt – repurposing existing technologies in new ways. The first step in any investigation is the most important: defining precisely what it is you're looking for. In the context of Martian studies, the question becomes: are you looking for ancient fossils - indicative of prehistoric life - or evidence of recent (or even ongoing) metabolic activity?

The Atacama Desert is a very dry environment, which lends itself well to traditional measurements; geologists, organic chemists, and soil scientists can work together to obtain a wealth of information. The multidisciplinary nature of our work is vital to our success: each discipline provides critical information, which when brought together allows us to paint a clearer picture of a habitat – and its inhabitants.

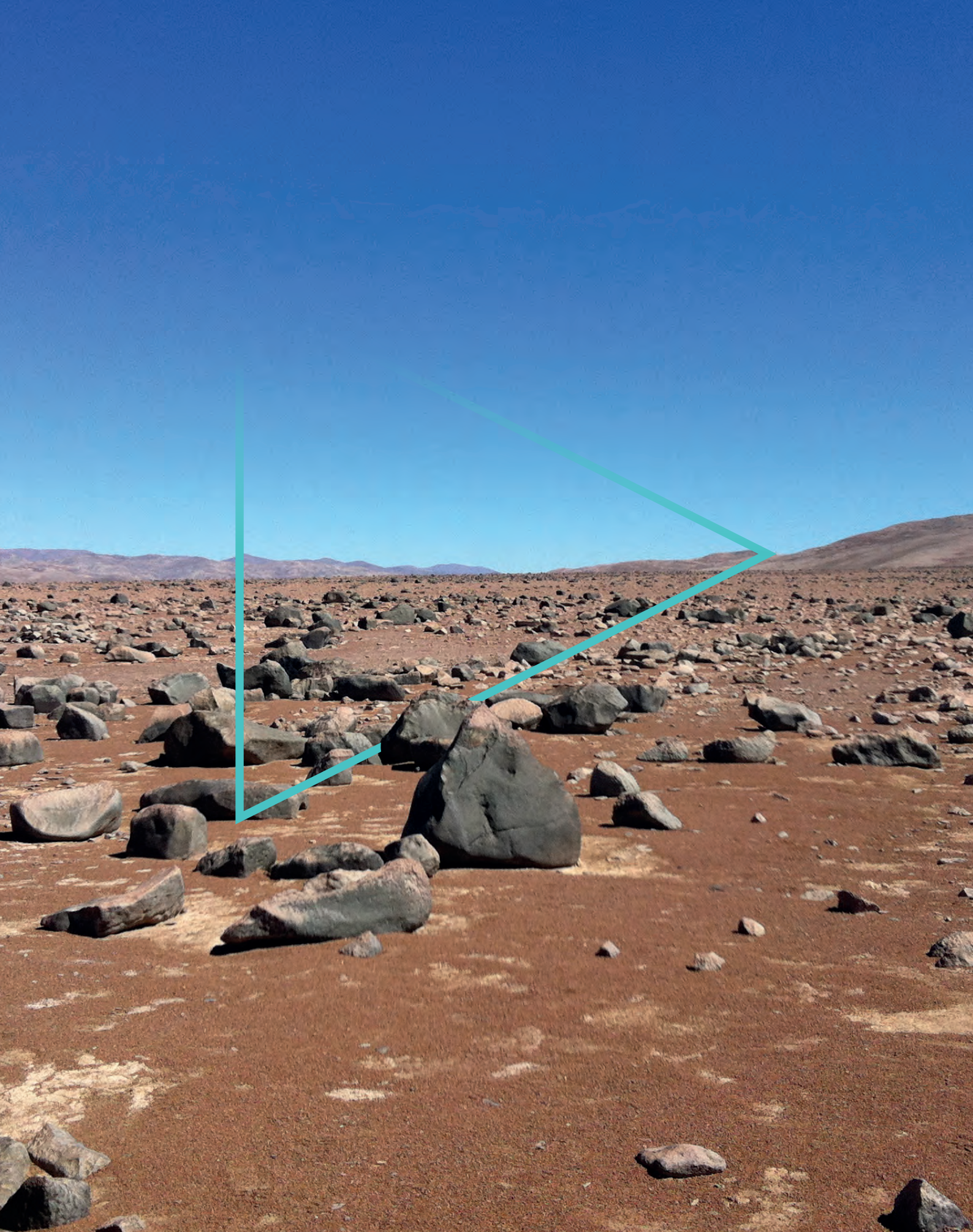
Discovering signs of microbial life in the driest regions of the Atacama Desert – previously considered uninhabitable – was a major scientific discovery, but it was important to remain skeptical. Had these microbes been swept in on desert winds only to die? Or had we discovered a new habitat in which microbes are able to grow and reproduce (1)? Analysis and study design proved challenging: we knew that, even at the limits of today's best technologies, we would struggle to detect many biological markers and organic compounds. Our first round of analysis – comprising DNA sequencing, metabolomics, phospholipid fatty acid analysis, and ATP analysis – provided us with data, but not enough evidence to draw any concrete conclusions. And so, we relied on metagenomic tools to identify replication forks within the DNA of detected microbes to make the necessary breakthrough and confirmed that these microbes called the desert home.

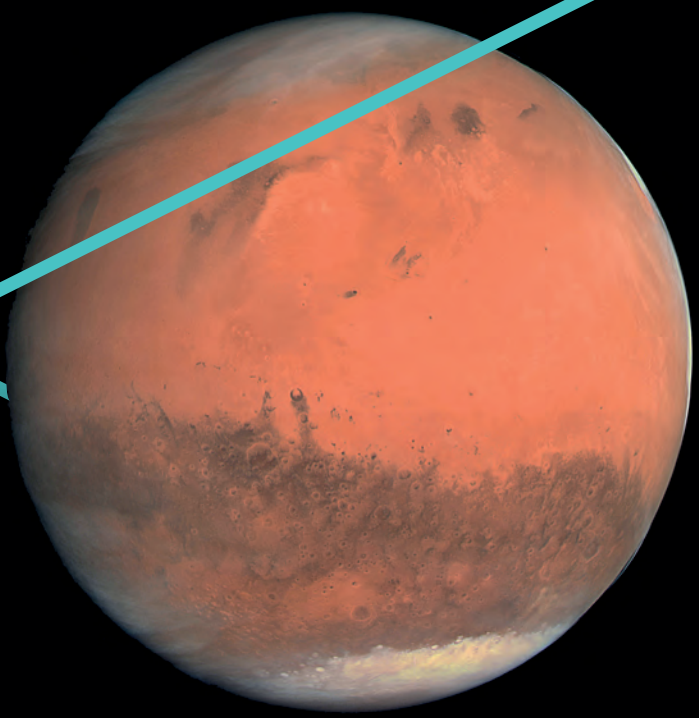
MARTIAN MUD

No matter how robust or complex your study, there's no substitute for primary samples. As every scientist would agree, in-field analysis is far more preferable than working in a laboratory. Sample transportation inevitably alters conditions, irrespective of the number or extent of precautions in place. Add in the challenges associated with transit – magnified enormously by the vast distances of space – and it should come as no surprise how stringent NASA and the European Space Agency's (ESA) standards are for any new piece of equipment. Each new device must undergo extensive testing to ensure functionality under non-terrestrial conditions. Marrying the desire to perform analysis in the field with smaller and more portable instrumentation is an ongoing technical challenge.

"NO MATTER HOW ROBUST OR COMPLEX YOUR STUDY, THERE'S NO SUBSTITUTE FOR PRIMARY SAMPLES"

There have been several missions to Mars, each of which has been prescribed a particular objective; as a result, each set of instruments is unique. X-ray diffraction technology proved an early pacesetter and was used throughout the 1990s to study the mineralogy of compounds – determining whether particular compounds had been exposed to water, and if certain minerals had formed as a consequence.





The dawn of the new millennia saw a shift in priorities, and with new objectives came new technologies. The Curiosity Rover, which landed on Mars in 2012, was tasked with identifying habitable environments. In contrast, the ExoMars mission, set to land in 2021, has an altogether different objective: detecting organic molecules that could be associated with life. The ExoMars Rover will be fitted with Raman spectroscopy instrumentation and the latest GC-MS technology to corroborate results and provide a broader range of applications.

TITANIC TRINIDAD

The solar system's outer moons – particularly those orbiting Jupiter and Saturn – have attracted significant attention in recent years. As planetary exploration expands in scale and scope, the challenges have grown accordingly. Fortunately, there are numerous analogous environments on earth, providing the perfect location for terrestrial study. The asphalt lake of Trinidad represents a prime example, providing the perfect stand-in for the liquid hydrocarbon lakes found on the surface of Titan – regarded by many as a likely location of life in our solar system (2). Any organisms residing here would be beyond exotic by Earth's standards.

"AS PLANETARY EXPLORATION EXPANDS IN SCALE AND SCOPE, THE CHALLENGES HAVE GROWN ACCORDINGLY."

We've had to be inventive. Parameters used to characterize aqueous environments, such as pH, cannot be applied to liquid asphalt. To compensate, we extracted microdroplets of water – some as small as a few µl in size – entrapped in the oil. What we uncovered was breathtaking: an entire ecosystem comprised of complex methanogenic bacteria actively degrading the oil into a range of interesting metabolites (3). Do similar communities thrive at the bottom of Titan's lakes?

SPACE SAFARI

I'm a firm believer that life is flourishing throughout the Universe. In fact, I co-authored a book – The Cosmic Zoo: Complex Life on Many Worlds – with William Baines at The University of Cambridge. Its intention, in part, was to provide a counter argument to an older book, Rare Earth, penned by Peter Ward and Donald Brownlee. Their hypothesis is that complex life is extremely rare in the Universe. In contrast, we argue that once life is established on an extra-terrestrial body, the steps to complexity are not prohibitive. With enough time, life is highly likely to develop.

From that belief came the idea that the Cosmos is teeming with intelligent life. There are several paths to intelligence, but what we can't know for sure is whether technologically advanced species on the level of *Homo sapiens* exist elsewhere. After all, over a period spanning 4.5 billion years, it has only emerged once on Earth.

The origins of life on Earth are vague. What we do know is that this process must have happened in a relatively short time frame. We can reasonably assume that if you have other celestial bodies that meet habitability criteria, life will emerge there too. The rise of bacteria would provide organisms capable of exchanging genes. Give them enough time and they will begin to interact; food chains will develop, and complexity evolves. As a jump is made from simple bacteria to eukaryote, colonies begin to form and multicellularity emerges. I don't believe any part of that progression to be particularly challenging. Rather, the process is simply dependent on favorable environmental conditions and the passage of sufficient time.

There's much work to do – we've only begun to scratch the surface. I've been extremely privileged to be able to turn what began as a hobby into a standalone career. What keeps me striving is simple: an endless fascination and desire to find the answers to some of life's biggest questions.

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CHEMISTRY AMONG THE STARS

What role does analytical science play in the search for life?

Planetary science is a young and rapidly growing field – and as analytical technologies continue to evolve, their application within it continues to grow. We spoke with Sam Kounaves, Professor of Chemistry at Tufts University in Massachusetts, USA, and a visiting Professor in Earth Science and Engineering at Imperial College London, UK, to learn more about his career in this somewhat… alien field.

What inspired your passion for analytical science and planetary exploration?

It's pretty simple really – I grew up in the Star Trek era! Since a young age, I've always wanted to explore alien worlds, particularly Mars. I'm driven by a desire to search for life on other worlds. Determining if we are alone in the Universe is an enormously important question – not just for me personally, not even for the scientific community more broadly, but for the whole of society. Just one other source of life in the solar system or the wider cosmos would be an enormous discovery. It would give credence to the theory that life thrives in the Universe. Equally striking would be the opposite realization – that we are truly alone. Either option has profound consequences.

"JUST ONE OTHER SOURCE OF LIFE IN THE SOLAR SYSTEM OR THE WIDER COSMOS WOULD BE AN ENORMOUS DISCOVERY."

What have you focused on during your career?

My career in planetary science began about 25 years ago when I first got involved in a proposal to NASA to send a robot containing analytical instrumentation to Mars. The end result – the Phoenix mission – launched in 2007 and landed in 2008 (1). I've spent many years involved in chemical analysis of the Martian surface; most recently, investigating process that generate intermediary oxychlorines and highly oxidizing radicals that have implications for the production of perchlorate (ClO_4^-) and the alteration of organics on Mars and perhaps throughout the solar system and beyond (2,3). In parallel, I've also been involved in studying Antarctic soils – great analogs for extra-terrestrial worlds.

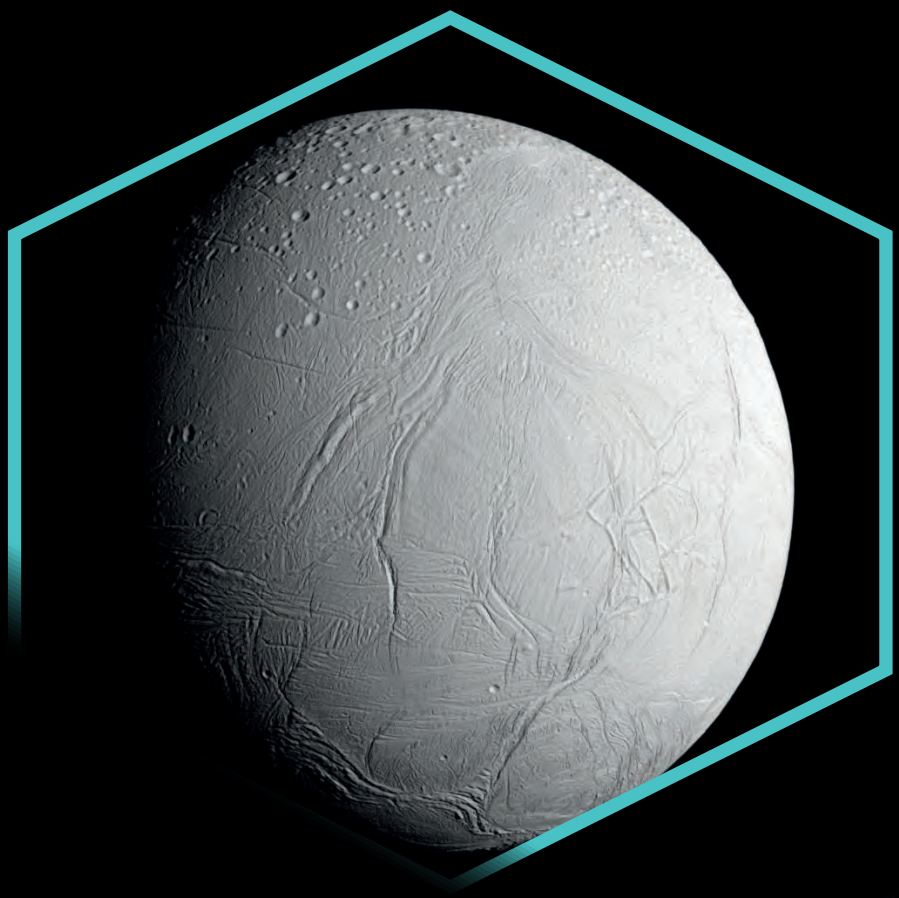
What have you learnt from studying Antarctica?

Antarctica is the closest we can get on earth to a truly alien world. The McMurdo Dry Valleys – vast hyperarid areas gouged out by enormous glaciers over 20 million years ago, are some of the best analogs for Mars. These high-elevation valleys are the perfect place to test the limits of habitability; for many years we assumed nothing lived there. Now we know that some organisms, particularly cyanobacteria, call them home. Understanding how to go about remotely detecting such organisms has provided clues as to how we might go about a similar process on Mars. It also provides the ideal location to test instruments destined for future missions to the Red Planet.

We confirmed the presence of perchlorate in Antarctica (4), which proved a major breakthrough. Until that point the consensus was that most perchlorate on Earth was the result of human contamination – e.g., generated as a byproduct during explosives manufacturing. In fact, it's now clear that perchlorate forms in the upper atmosphere and falls to Earth as perchloric acid. Perchlorate is ubiquitous, but it doesn't usually show up in the soil because it is so easily washed away or used by bacteria as an energy source. In contrast, it collects in the McMurdo Dry Valleys due to a lack of water to wash it away. The discovery that perchlorate is also found on Mars is reason for excitement: perhaps ancient (or indeed, still living) lifeforms adopted similar biochemical processes?

What challenges face the field?

To really reach our goals, new instrumentation will be essential. In addition to developing instruments focused on habitability, we also need new tools that will allow researchers to analyze for different kinds of organic compounds. In new proposals



to NASA, we've outlined a setup comprising of capillary electrophoresis (to analyze amino acid patterns and chirality) and GC-MS (to analyze lipids.) In short, we need complementary instrumentation. In parallel, we need other instrumentation capable of analyzing biomolecules, such as DNA and proteins, to ensure that we don't have contamination in samples.

Selecting which compounds we should try to identify is a crucial step; simplistic biomarkers must be the focus. These components would be easier to detect than DNA; at a more profound level, we have to consider whether DNA would even exist on other worlds. We can't be sure that life would rely on the same forms of coding molecules to store genetic information. An entirely different system – one not conceived by even the most open-minded of scientists – could be used.

How do you adapt technology to study Enceladus and Europa?

"ANTARCTICA IS THE CLOSEST WE CAN GET ON EARTH TO A TRULY ALIEN WORLD."

Distance is the obvious challenge. Enceladus and Europa are so far away that instrumentation must be very low mass – around 1/10th that used for Mars. Why? Because it takes an enormous amount of energy to launch spacecraft; even more to travel the vast distances and successfully land on another planetary body. Instrumentation must also be especially rugged, capable of surviving several years at temperatures down to -70 °C or lower within the vacuum of space, in addition to extremely high levels of solar and galactic radiation. Upon reaching their destination, such devices are then expected to function correctly over an extended period of time, with no hope of repair.

We're now working with NASA to develop this instrumentation, tying our work into the recent discovery of perchlorate deposits on Mars and the importance of organic compounds. One example is the microfluidic flow through cells we're developing for Enceladus; these are an array of selective electrodes built into a manifold. Though the device appears easy enough to construct, it actually presents a significant challenge; each component must be customized to withstand the aforementioned extreme changes in temperature and radiation while remaining small and compact.

Enceladus and Europa have oceans beneath their ice shells and they are among the few places in the solar system where collection of potentially life-containing samples is viable. Both moons are home to geysers that shoot plumes of water from the ocean underneath their icy shells directly into space. These oceans, home to potential hydrothermal vents, are perhaps some of the most life-friendly in the solar system outside of Earth.

What would proof of life look like?

Right now, we're working with the European Research Commission (ERC) on a proposal to answer that exact question. We're outlining precisely what scientists should be looking for. These include specific patterns of organic compounds not produced by any known abiotic process. Chiral amino acids, or non-racemic mixtures, are also a good sign. When you look at the composition of amino acids in chondritic meteorites they are dominated by glycine and alanine, with very small amounts of the others thrown in. On Earth we find a variety of amino acids, the sort of pattern one would expect when surveying for life elsewhere.

Another indicator is complex lipid profiles. Abiotic processes produce very simple lipid molecule patterns expected via chemical reactions; in contrast, life creates unique patterns and lengths of lipid chains. Finding all of these patterns would allow you to conclude, quite definitively, that you've uncovered organic compounds produced by biology. We hope that fellow scientists – and the ERC – will consider these points in the context of future missions to Enceladus, and Europa... and beyond!

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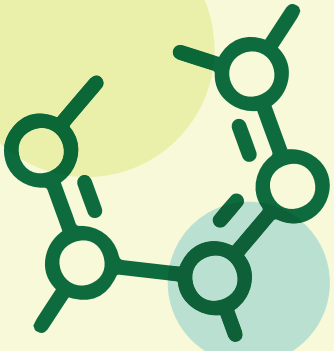


Cleaning UP OUR ACT!

How analytical science is contributing to a greener planet

With continuing pressure from dedicated groups and scathing headlines fueling wider frustration, pollution is never far from government agendas or the public consciousness. The Greenpeace Research Laboratories – established more than a quarter of a century ago – have played a significant role in raising the profile of microplastic and heavy metal pollution. We spoke with David Santillo, one of eight scientists employed at the Laboratories at the University of Exeter, UK, to find out more.

What motivated you to work at Greenpeace?

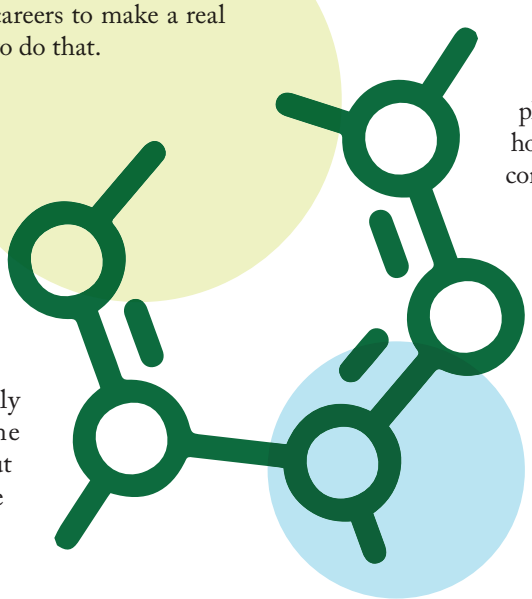
Central to Greenpeace's mission is the idea of "bearing witness" – reporting on environmental pollution using advanced analytical techniques. My greatest hope is to shed light on the monumental problems that we face, and that's a real motivator. Whether dealing with chemical or plastic pollution, the goal is always to address the issue at its source.

Analytical science plays a vital role: if you don't have high-quality evidence to back up your case, then all you can speak about are generalities, which don't provide solid foundations for good policy. You can only understand the complexity of chemicals in the environment by applying analytical techniques.

More generally, I'm invested in the use of the methods, skills and experience gained throughout our careers to make a real difference – and Greenpeace allows me to do that.

What major areas do you focus on?

There are a number of key themes we explore. The major ones are complex waste analysis, analysis of environmental matrices (soil and sediments), and water analysis. We try to go beyond simply identifying common contaminants by forensically screening our samples to determine what other chemicals are present (but not necessarily being recorded). These molecules can be anything, from organic compounds to non-organic pollutants and heavy metals; we're looking to uncover the real story by identifying these components in industrial and environmental waste, consumer products, and food samples. We're driven broadly by Greenpeace's overarching campaign goals, but within that we are afforded some flexibility, which allows us to develop novel research programs that drive the understanding of the wider scientific community.



We've found that there are a lot of more chemical pollutants in the environment than those typically screened for. Part of the problem is that these chemicals are never found on their own – they're always a component of more complex mixtures. Documenting this has revealed just how important it is to deal with these chemicals at their source, before they have the chance to enter the environment.

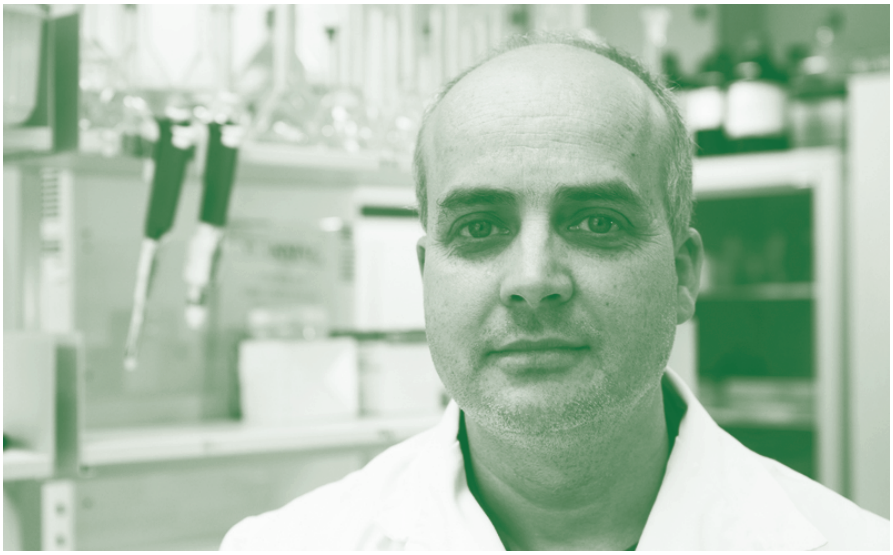
A recent example of our application of environmental forensic analyses is our study documenting soil pollution at a landfill site in Poland that was thought to be receiving hazardous waste (1). The waste was building up but then periodically catching fire, making it potentially very difficult to trace the problem. However, through a combination of our own analyses and working with another external laboratory, we were able to characterize the contaminants in soils impacted by those fires, revealing that complex chlorinated products and dioxins were leaching into the soil and damaging the local environment.

Among the biggest concerns at the moment – and certainly the one that's gaining the most media attention – is microplastics. There are two sources of chemical contamination when it comes to microplastic (besides the plastic itself): i) plastic additives, which provide color, structural stability, or texture, ii) additional chemical contaminants gathered from the broader environment or a wastewater treatment process. Last year, we studied this particular problem in the coastal waters of Scotland, and were able to characterize not just the types of plastics involved, but also the pesticides, household chemicals, metals, and other contaminants attached to them.

How do you ensure the quality of your science?

We publish everything we do in some form – either in peer-reviewed papers (our preferred route), results papers or technical reports. We make all of those available to the public for free on our website so that, even if some of our work doesn't undergo formal peer review, it is still open to public scrutiny – anyone can download it, anyone can read it, and anyone can criticize it. Clearly, people may have different views on the policy implications of our work, but the science itself is very rarely challenged.

Many of the methods we've developed have been adopted by the wider community. The more we can publish and the more attention we can garner, the greater the benefit for society. Of course, for our science to have that effect, we need to have absolute confidence in the research that we do. And that's why we apply state-of-the-art methodologies and work to the same standards as any other analytical laboratory. We can never compromise on the quality of our work.



What are the main contaminants of interest right now?

We're currently reviewing chemical contamination generated by ineffectual plastic recycling processes in Malaysia. We've identified a wide range of contaminants that we're now bringing to the attention of the local authorities. And that's really our main objective – to point out when pollution is being generated "under the radar"; often even the producers themselves are unaware. At the same time, we aim to equip the authorities with the evidence they need to hold to account those responsible.

In general, decision makers around the world are willing to look at our results and see them for what they are – whether that's in East Asia, Europe, or South America. There is a degree of acceptance that the work we're doing is valid and valuable. Our role is not simply to represent scientific issues to the public, but rather to capitalize on the serious opportunities provided through our capabilities in environmental forensic analyses to carry out primary research, thereby bringing awareness to these problems, and encouraging those with the power to effect change to do so.

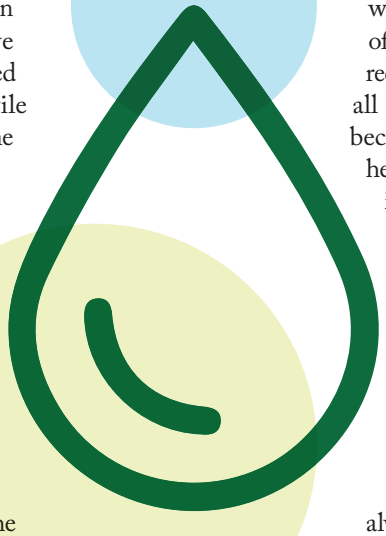
You spoke about microplastics at LabAnalyse 2019...

I gave an overview of the work that Greenpeace scientists have conducted over the past 12 months, with a particular focus on pollutants. We participate in collaborative projects examining how chemical contamination has been affecting wildlife, including

turtles, whales and dolphins, with researchers at the University of Exeter and across the UK. Microplastics and plastics are a major pollution problem; they're found not only in just about every sample of river or seawater, but are also evident in the wider environment. They can be found in the guts of stranded whales, dolphins, and seals, as well as inside turtles killed by fishing trawlers.

We also discussed the forever-changing nature of the contaminants' chemical composition – a major problem. With microplastics, every sample we take from surface seawater or a river – even when it's from the same location one hour later – is unique. It makes analysis extremely challenging, and means that averaging exposure and risk for assessment of potential impacts is almost impossible.

There are also more technical challenges to consider: degradation of the samples, degradation of plastics, recovery, cleanup, quantitative detection, and so on. Fourier-transform infrared spectroscopy is a powerful and very versatile technique, but ideally, we would also examine samples for the presence of much smaller fragments and fibers. Other techniques are available for microplastics analysis, but each of those methods has its own limitations. Looking forward, there's a need for method development that would allow for more rapid sample screening and, in particular, to have some form of quantitative indicator to reveal microplastic levels in sediment. If – as is the case currently – that remains a time-consuming process, then I believe most regulators will be unwilling to devote the necessary time to conduct these analyses.



A new system capable of more rapid sediment sample screening represents a niche yet to be filled. An efficient and reproducible way to retrieve all contaminants through further analysis is needed if we are to look for microplastics in sediments in a quantitative way; that can be a lengthy and complicated process, with lots of potential for contamination. The only thing that's crystal-clear right now is that there is no easy answer!

What are the highlights of your career?

Every time we publish a report that has any kind of impact is a moment of personal delight – even more so when it's picked up by the press and drives changes in policy. Some of our work examining electronic waste has been particularly impactful, helping to tighten regulations, both on the chemicals used in the production of electronics, and the management of the resulting waste. More broadly, we've carried out a lot of work around textile production, ensuring that the chemicals used both in production and the finished product are held to the highest standards.

However, one example that I would highlight more than any other is actually the product of foresight. About 20 years ago, we began using MS instruments in "scan mode", which allowed us to examine a broader range of pollutants. At the time, some viewed such approaches as unconventional and of little value; the convention being that you ought to focus only on particular contaminant groups in detail – there was simply no time or justification for spreading the net wider with broad-spectrum analysis. But gradually, the fact that we were able to identify complex mixtures of pollutants that, though previously undetectable, were nonetheless of enormous relevance in terms of environmental protection, began to lead to a recognition that we may have been on to something all along. It took a long time for our approach to become common practice, but increasingly we hear from other laboratories that MS screening in "scan mode", rather than merely for a finite list of chemicals, is one of the fastest growing requests from clients today. A change we instigated 20 years ago is becoming part of the gold-standard today!

What does the future hold?

To some extent, more of the same. There's always value in investigative research, particularly if that involves regions or contaminants to which nobody else is paying much attention. There is a huge amount left to uncover. I think there's a certain danger in assuming that we know everything there is to know about a certain type of contaminant or its movement through the environment.

More broadly, we're witnessing the start of a major cultural shift – one in which our work is beginning to seriously impact public policy and corporate development. At the same time, with the development of smarter materials, smarter products, and smarter processes, we will see a shift away from environmental investigation towards pollution prevention – from the river into the factory at long last!

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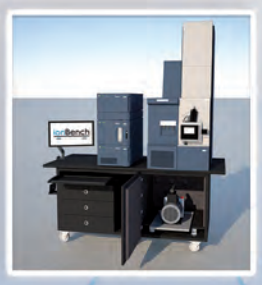

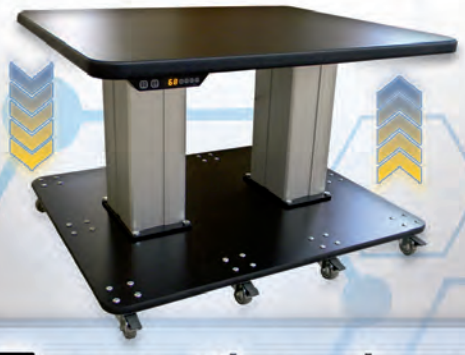

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Separation Science – Slammed!

We celebrate the success of three up-and-coming analytical chemists who excel at an all-important "soft" skill: communication

HPLC 2019 in Milan bore witness to something special. Six young scientists took to the stage in the main auditorium to share their research – but these were no ordinary conference talks. Inspired by poetry slams, "science slams" are slowly taking over the world. The obvious next step? The Separation Science Slam. "The most fun I've ever had at HPLC," said one unnamed but esteemed figure of the field. "Well – at least outside of the social calendar…" they admitted.

Assessed by a panel of judges for both "science and style," the quality was high across the board. But three presentations stood out in particular: a gripping tale of two brother molecules, a compelling love story, and a story about insulation foam… Our three winners were awarded spectacular trophies and cash prizes – courtesy of KNAUER and Merck. And the final part of the prize comes from the third sponsor…

Here, we introduce two bold orators and one even bolder rapper to find out what went down at the HPLC 2019 Separation Science Slam.

Can you offer a few more details about your research project?

Breuer: My work is part of the Separation Technology for A Million Peaks (STAMP) project at the University of Amsterdam, under the supervision of Peter Schoenmakers. A lot of fields – and particularly omics – are struggling with the increasing complexity of samples. Our aim is to improve separation power by giving a peak capacity of one million via three orthogonal separation mechanisms. Our next step? Further development of the substrate, on which the effluent from the microfluidic device is stamped; I would like to increase the sensitivity and reproducibility to better deal with low volumes and concentrations.

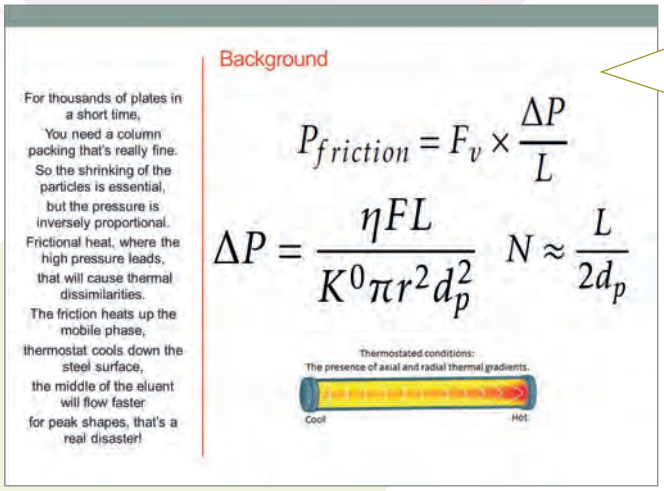
Lambert: The thermal conductivity of the insulation material is crucial to minimize the size, and reach the adiabatic conditions in chromatographic columns. Gritti and colleagues showed that the utility of vacuum-based columns can be effective, but fabrication of this hardware is difficult and expensive. Our (super cheap) polyurethane column insulation demonstrated similar efficiency, and we hope that this can be commercialized in the future.

Felletti: My research uses experimental overloaded measurements and theoretical computer simulations to identify a suitable adsorption isotherm model, capable of describing the adsorption behavior of enantiomers. This approach may shed some light on important unanswered questions concerning enantio-separations, such as the effect of experimental variables on the chemical composition of the surface around the

Gold: Nándor Lambert, *University of Pécs, Hungary*

Silver: Simona Felletti, University of Ferrara, Italy

Bronze: Pascal Breuer, University of Amsterdam, the Netherlands

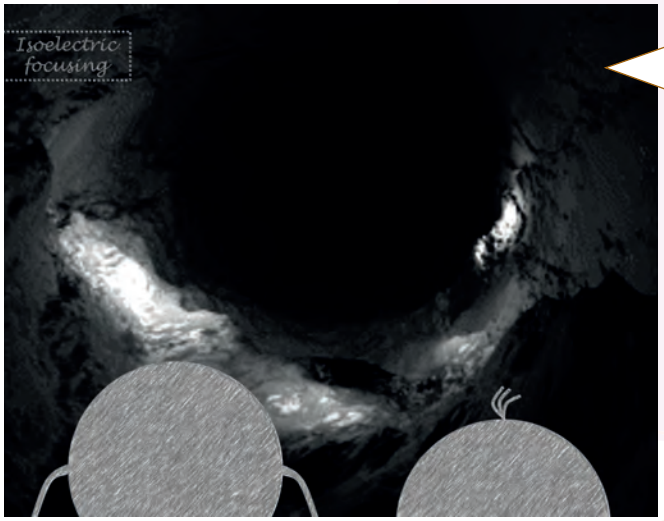


Nándor Lambert

I've been working on chromatographic column insulation to minimize the well-documented band-broadening caused by evolving radial thermal gradients during frictional heating. I created a polyurethane insulation to maximize column performance in isocratic separations, and presented my work by rewriting the lyrics of a rap song (Jon Lajoie; Everyday Normal Guy 2), with an accompanying video...

Simona Felletti

My research focuses on the adsorption and enantio-recognition mechanisms in chiral LC. I presented my research with the help of LEGO characters by comparing the (complicated) relationship between enantiomers and chiral selectors to a love affair – and presented a guide on how to become "the enantiomer's Cupid" regarding selection of the best chiral selector for a given enantiomer.



Pascal Breuer

I develop detection methods for a microfluidic device capable of performing multidimensional spatial LC separations. I took the audience on a journey through such a device, including current detection approaches and challenges, through the eyes of a molecule undergoing separation.

chiral selector, or how loading the loaded amount of chiral selector affects enantio-recognition.

What inspired your creative approach to the Separation Science Slam?

Felletti: I've always been creative, open-minded... and a little bit crazy. I'm also very interested in art, which may explain (in part, at least) my bizarre fantasy.

Lambert: The motif of the song "I'm just a regular everyday normal guy" is frequently used online to ironically highlight peoples' skillsets. Given the uncommon approach that my group takes to chromatography, I found some parallels between the song and my presentation topic.

Breuer: I was focused on the issue of peak splitting when I heard about the Separation Science Slam, and had been noting my ideas with simple illustrations. That's when the idea was born; all I had to do then was to switch the perspective to that of the molecule, which came naturally to me!

What were the challenges in creating your masterpiece?

Lambert: Everything. I used to write poems in my mother tongue, but that was just for my own fun. And rapping, especially in English, was not particularly easy for me.

Breuer: The challenges are best summed up in my lack of artistic skills. I used hand-drawn slides to present my story, but in developing them it soon became clear why I chased a scientific career, not an artistic one. Suffice to say I'm grateful for technological developments, among them the options in PowerPoint that alter reality to a point it's hard to discern what is hand drawn from what is not.

Felletti: I used graphics programs to modify photos I took and had to think of interesting things to convey in a comedic way. Modifying the lyrics to Gloria Gaynor's "I Will Survive" and recording the final song was also a challenge.

Were you nervous ahead of the Separation Science Slam? And what did your colleagues make of it?

Felletti: The Separation Science Slam was more stressful than a usual oral presentation, but I had a great time both during and after the presentation. Overall, it was very exciting, and the feedback I received was great too – my peers said they died with laughter. To would-be separation science slammers of the future, I say: go for it, and be as creative as you like!

Breuer: All was (relatively) fine until an hour before the actual Slam – that's when the nerves kicked in. I think I saw the ground floor of the building from every possible view in that hour while walking around to get my mind at ease, but I became totally at ease as my talk began. The audience were great, and the applause I received still gives me chills. As for my colleagues, they gave comments ranging from "crazy boy" to awesome. In retrospect, maybe I did sway too far towards the more fun side of the assignment; some scientific results may have boosted me up a place or two!

Lambert: I have honestly never practiced so much for a presentation in my life. I was really excited and nervous before the presentation, but could hardly believe the incredible response I got from the audience! The whole experience was really enjoyable. My supervisor only saw my presentation when it was half prepared, but he's a fun guy – and I think he liked it.

What are your views on the importance of science communication?

Breuer: Science is generally not understood by those outside the field. A lot of what we do sounds like science fiction to a layman – and our community is partly to blame. Once the public hear of scientific endeavors, they become interested and ask questions, opening the door for us to provide them with even more information. Science communication today has the power to change the views of many, and we should capitalize on this opportunity. Good communication is one of the many reasons I admire my supervisor Peter Schoenmakers – his confidence and use of humor is inspiring.

Lambert: To say that we are living in an accelerating world is a cliché, but it's also true. It's hard to capture the attention of some – particularly young people – when we are surrounded by so many stimuli on a daily basis. Communicating science is important – whether it be a short chat during a coffee break or wider discussion of key topic, and can result in long-lasting collaborations and change.

Felletti: Science communication is very important to spread and share our ideas and our studies. Moreover, presenting our research in a simple and attractive way can be useful to make science accessible and open to everyone, since it is the link between the science world and non-scientists. It's for these reasons that I admire all those who had the courage to present their work – we can all learn something from one another when we share in this way.

Finally, where do you want to be in 10 years?

Lambert: That's hard to visualize. Though I would like to try my luck in an industrial environment, I feel that I will always find my way back to academia. In ten years I also hope that I am close to Pécs again.

Felletti: I hope to conduct research as part of a large, international group to continue contributing to science.

Breuer: On a personal level, the common story of a nice house, wife and kids. On a professional level, I would like to be in a position focused on problem solving. Finding a solution and (over)seeing the development is what thrills me, and what I would love to do in the future… As long as it is science related that is.

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INSIDE

The Infrared Invasion in Our Hospitals

With Matt Baker, Reader of Pure and Applied Chemistry at the University of Strathclyde, Investor and Chief Technology Officer at ClinSpec Dx, UK

I've always been interested in analysis and applied science, so a PhD using MS to study "dirty samples" felt like a natural progression. I subsequently worked at the Robert Koch Institute in Berlin and Harvard Med in Boston, where I studied combined spectroscopy and imaging MS, and later moved into the Ministry of Defense, conducting real-world analyses of bacterial samples and toxic chemicals. In my current research, I'm looking into the expression of disease markers in blood, and developing methods to detect them simply, quickly and efficiently, particularly for brain tumors.

For many, the idea of translating spectroscopy into the clinic remains a pipedream, but the potential is enormous. And though that may sound like a sweeping generalization, we're clearly moving away from single biomarker approaches, which I don't believe can accurately characterize heterogeneous diseases. The more we understand a given disease, the more we understand that a single biomarker or single genetic mutation often cannot accurately describe it; for example, breast cancer is associated with huge variation between subsets and cases.

The field of clinical spectroscopy has already come a long way. Ten years ago, we were only beginning to regularly apply particular algorithms and techniques for such applications, but we're now discussing these processes in practical terms. Many start-up companies have also flourished – ClinSpec Dx and Biotech Resources (Monash) are just two examples.

Of course, the field remains young. We are more than capable of conducting spectroscopic analysis; what we need now is for users to perform the work, and to run clinical trials when the opportunity arises. (On a legal note, more intellectual property and patents supported by new technologies are also needed.) Once such steps are fulfilled, translation can begin in earnest, and more people will become interested in the benefits of this field.

"For many, the idea of translating spectroscopy into the clinic remains a pipedream, but the potential is enormous."

My group is paying particular attention to brain tumors because they remain an area of unmet need. They're also difficult to diagnose. Did you know that 38 percent of patients visit their primary care provider at least five times before receiving a diagnosis? (1) And that could mean a year and a half before a patient reaches the clinic – and the disease may have progressed significantly.

There are hundreds of different central nervous system tumors, and the ability to characterize these growths with a single biomarker in spite of their distinct biological origins represents a major challenge.

Brain tumors shed "messengers" into the blood and humans shed "messengers" to feed the tumors, which leads to the rise of multiple potential markers through biochemical changes. Spectroscopy can be used to detect multiple markers for diagnostic purposes with a single measurement. Of course, there are downsides, namely the fact that IR can't identify the exact molecules under analysis that are causing the variation. As a result, it will be important to instill confidence in the technology before it can be used; clinicians of course require evidence, and the requirement for direct evidence is yet to be fully satisfied.

We have recently been awarded a Cancer Research UK grant, and we are working to identify the changing signatures of different brain tumors with improved precision. We are also planning to use electrochemistry and mass spectral analysis to investigate genetic markers in serum.

But the question is, what threshold for these measurements is good enough? Reports suggest that anything above 80 percent would be a game changer for a triage test (2); for a diagnostic test, I imagine it will have to be much higher. Regardless, we will continue working to achieve our goal to produce a rapid, easy-to-use and reliable blood test that will ultimately improve the lives of patients.

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Double or Nothing

A dual-system approach could deliver more detailed spectroscopic imaging of chemical and biological samples

Infrared (IR) absorption and Raman scattering spectroscopy (RSS) are two well-known and widely used imaging techniques, yet neither can deduce the entire spectrum of vibrational activity within a sample. Recognizing the unmet need, Takuro Ideguchi and colleagues at the University of Tokyo have developed a complementary vibrational spectroscopy (CVS) instrument that combines aspects of IR and RSS, returning spectral information over a wider bandwidth than either approach alone (1).

Underpinned by an ultra-short, near-infrared pulsed laser and a Michelson interferometer, the CVS system is inspired – at least in part – by dual-model Fourier transform infrared spectroscopy, a staple of the modern-day analytical laboratory. "In truth, our CVS instrument could have been assembled more than a decade ago from existing technologies," says Ideguchi. "This study was simply the result of following our interest from concept to implementation."

Preliminary proof-of-concept

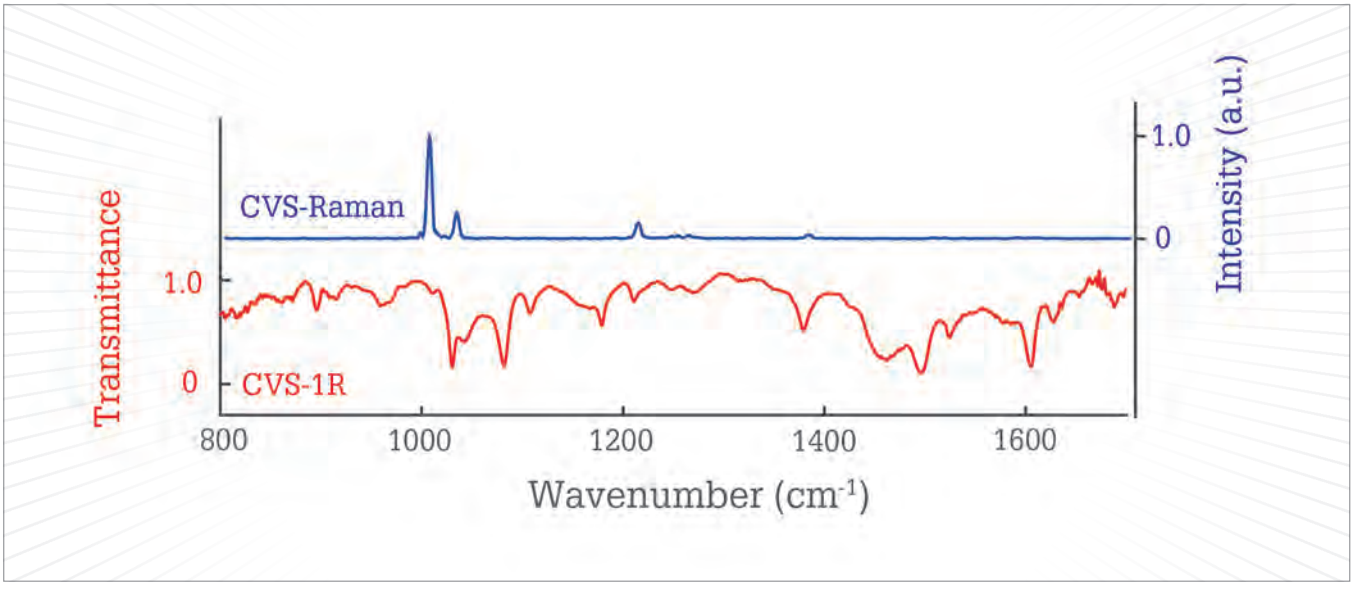

Figure 1. Dual-system vibrational spectra (790-1800cm-1) of toluene.

"At least one other major challenge remains: improving measurement speed – an essential goal to ensure applicability"

work has focused on simple organic compounds – toluene (Figure 1), benzene, chloroform, and dimethyl sulfoxide – and the generation of vibrational spectra covering a wavelength range of 790 to 1800 cm^{-1}. But this is only the first step on a long journey towards real-world application; the dream, according to Ideguchi, has always been to cover a spectrum that goes out beyond 3000 cm^{-1}. "We're exploring a number of different options, including deploying a variety of different lasers or adopting a non-linear approach to analysis," says Ideguchi. "Such approaches would allow us to increase the breadth of our analysis, opening up new avenues for investigation."

At least one other major challenge remains: improving measurement speed – an essential goal to ensure applicability (and the likelihood of any commercial success). "There are numerous avenues ripe for exploration," says Ideguchi. "That might include implementing dual-comb spectroscopy into our setup; alternatively, further enhancing our use of rapid-scan Fourier-transform spectroscopy holds plenty of promise."

And how might a refined version of the tool be applied in the future? "Our approach could see application in biological imaging and chemical analysis," he says. "Using CVS in this way could provide higher specificity of molecular species, allowing the community to conduct much more precise analysis of biomolecules in cells or tissues."

Reference

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Raman in the Clinic

Ananya Barui discusses the potential – and pitfalls – of Raman spectroscopy in the clinic

What's the focus of your work?

The goal of my group at the Indian Institute of Engineering Science and Technology in Shibpur is to develop effective diagnostic tools for early cancer detection. Despite histopathological methods being the clinical gold standard, their invasive nature prevents real-time disease monitoring – a clear objective for pathologists worldwide.

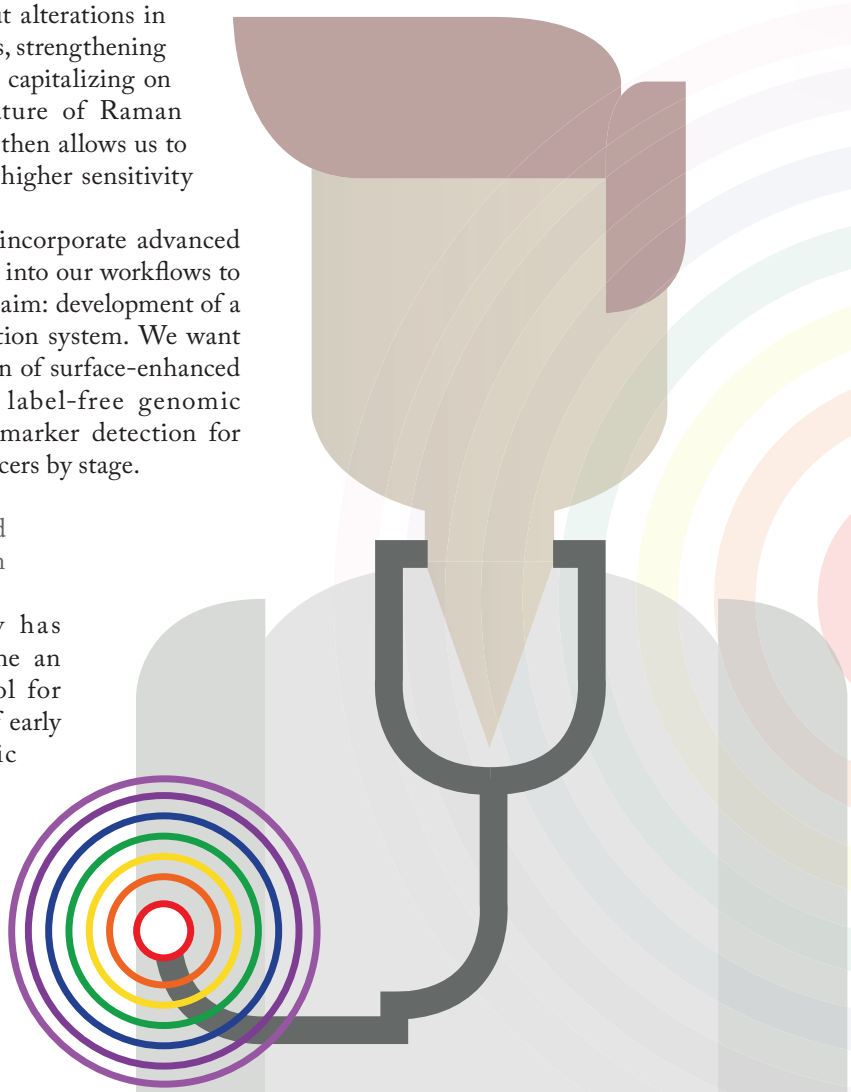
We've started collecting exfoliated cells from susceptible regions of oral and cervical tissues, and are analyzing these using different modes of quantitative microscopy. The evaluation of collected samples using Fourier-transform infrared (FTIR) spectroscopy provides useful information about alterations in cellular functional groups, strengthening our screening processes; capitalizing on the complementary nature of Raman and FTIR spectroscopy then allows us to give our measurements higher sensitivity and specificity.

We're now trying to incorporate advanced chemometric techniques into our workflows to aid in data analysis. The aim: development of a label-free cancer prediction system. We want to explore the application of surface-enhanced Raman scattering in label-free genomic and transcriptomic biomarker detection for stratifying epithelial cancers by stage.

Why should we be excited by Raman spectroscopy in the clinic?

Raman spectroscopy has the potential to become an important clinical tool for the real-time analysis of early disease. The inelastic interaction of light with biological tissues can highlight abnormal characteristics, by monitoring molecular level changes with high sensitivity and specificity. By reducing the chance of false negative results, we have the opportunity to develop "optical biopsies."

Each Raman subspecialty has something to offer. For example, Wei and colleagues developed a Raman-based volumetric chemical imaging method capable of elucidating the complex 3D architecture, chemical composition, and metabolic dynamics of a variety of different tissues (2). Elsewhere, Raman scattering microscopy has been used to image chemical bonds with high sensitivity, resolution, speed, and specificity (3). Other groups have used Raman to characterize the microheterogeneity of oral cancer tissues, which would otherwise have remained undetected (4). All in all, there's clearly enormous scope for Raman spectroscopy to transform a number of research fields.



"We're now trying to incorporate advanced chemometric techniques into our workflows to aid in data analysis."

Despite great promise, translation has proven difficult. Why?

The clinical acceptability and utility of any new technology is dependent on performance, cost, and sustainability. Compared with clinical biopsies, so called "optical biopsies" may not conduct measurement in the same location; moreover, the small sampling volume of Raman-based approaches may not necessarily reflect tissue heterogeneity. As a result, a more detailed histopathological assessment is required to compensate.

The nature of biological tissue, which auto-fluoresces when studied, also enhances the undesired noise in Raman spectra; thus, appropriate signal processing is required to obtain a useful signal. One must also select an appropriate laser source and power setup. The repeatability, cost, and duration of analysis – particularly to withstand competition from other technologies – are also important considerations.

How will the field move forwards?

The development of clinical technologies is influenced either by "technology push" or "clinical pull." In the early years of development, these technologies were developed for non-clinical purposes, but found a clinical utility. Now, the technology is being developed specifically to address clinical needs; in the next few decades, we can expect a proliferation of biomedical optics – providing information for screening, diagnosis, interventional guidance, treatment response, monitoring, and, ultimately, disease treatment.

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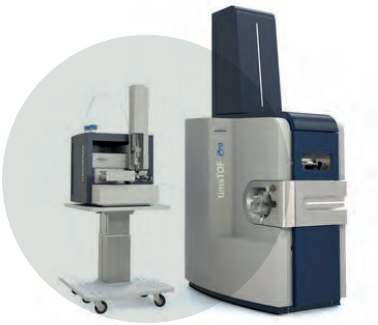

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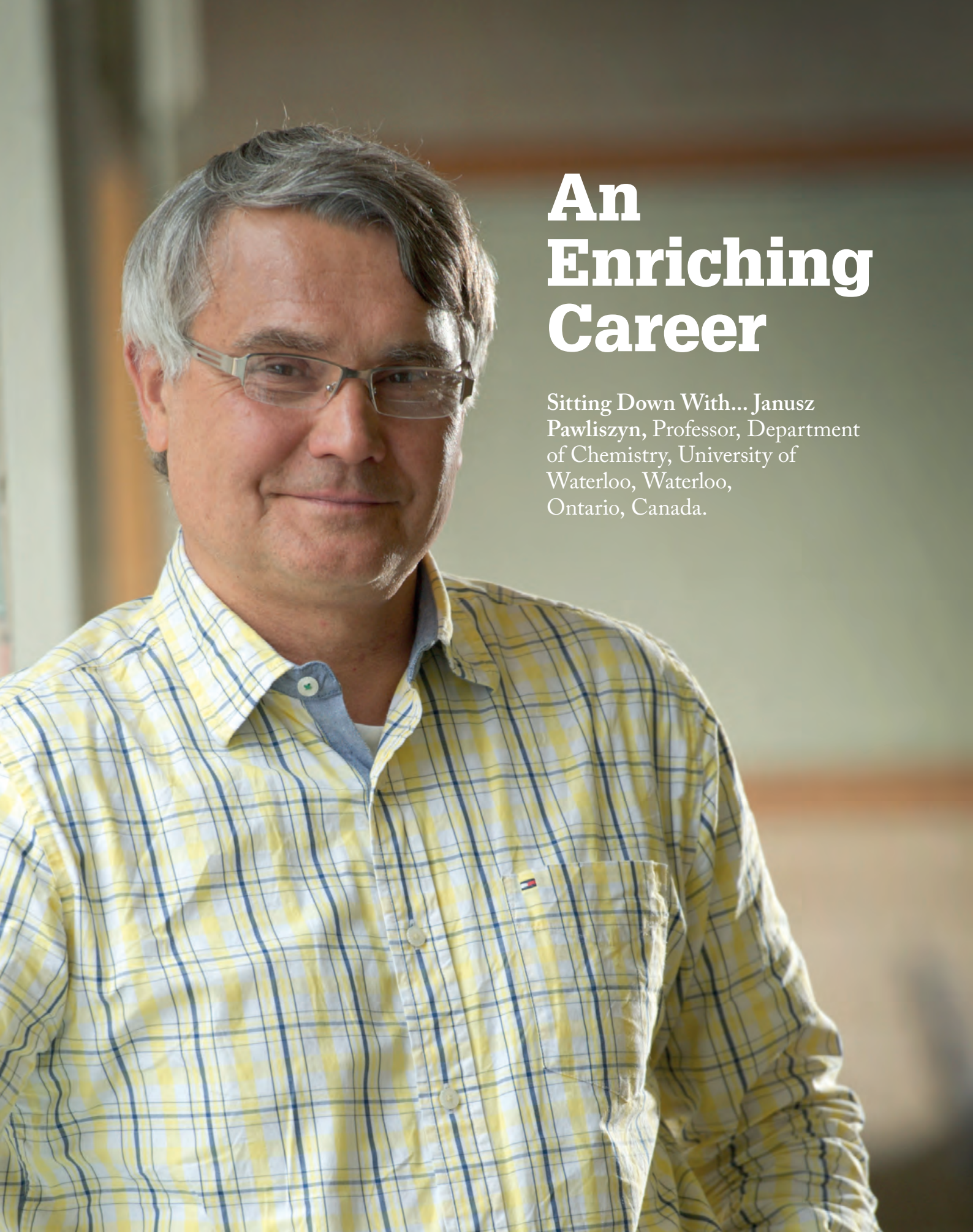

An Enriching Career

Sitting Down With... Janusz Pawliszyn, Professor, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada.

What motivates you?

I'm driven to have a positive impact. Doing science is an ongoing process of discovery, and just as Copernicus was inspired by the need to discover the truth about the cosmos, we're inspired to elucidate the principles underlying analytical technologies, new instrumentation and methods, simpler measurements, and more environmentally friendly approaches. Being able to build strong collaborative partnerships also keeps me excited and motivated to continue driving new discoveries.

You invented solid-phase microextraction (SPME) over three decades ago – what are you working on today?

We're developing optimum devices and conditions for novel integrated sampling and sample preparation strategies that will have a positive impact on all manner of fields, from the clinic to food and environmental determinations. The challenge lies in ensuring the mass transfer is controlled by diffusion through the boundary layer, rather than the thickness of the sorbent coating. Recently, we have developed sampling and extraction devices in the form of thin films, such as a carbon fabric or metal blade, that has proven to be significantly more efficient than previous structures. We're also working with magnetic particles to enhance the efficiency of sample enrichment by taking advantage of radial diffusion effects followed by MS or ion mobility spectrometry-MS with appropriate ion sources, including direct introduction approaches combined with extraction and the use of drones to facilitate on-site analysis.

What's your most satisfying career milestone?

The translation of SPME into the operating theater for the evaluation of human organs. We've developed SPME devices the size of an acupuncture needle that surgeons are not afraid to put into the human body, and which provide a chemical signature indicative of organ function and quality. This success implies that the approach could be translated into other settings too, because looking at food or the environment also requires chemical signatures. This application has been around 30 years in the making, so it's very satisfying to see that finally fulfilled. We're now using it to sample the human lungs and brains for cancer treatment applications.

Would you say analytical scientists are responsible for more than just data?

When analytical chemists get involved in a project, they typically work to provide the necessary feedback rapidly. As such, familiar approaches are preferred, and newer, more powerful techniques may be ignored unless standard approaches do not fully address the challenge at hand. In an ideal world, analytical scientists would consider the utility of all approaches when tackling a problem; of course, the analyst is responsible for demonstrating the usefulness of technologies to contribute to specific issues.

Global warming and pollution are issues with which we are all familiar, and as the challenges associated with them continue to grow, momentum is building – particularly amongst younger people – to address the problems. Analytical scientists will play a key role in providing and presenting data to government and citizens as efforts to combat the issues continue. Greener, cheaper and faster screening methods will prove central to these challenges.

Is that why you're such a prominent proponent of green chemistry?

It's simple: green chemistry is the future. We're facing an enormous challenge, and you can argue that analytical chemistry contributes little to the broader picture. But we too should play our part. One way to address the problem is to incorporate green technologies into our work, and to find ways to reduce the pollution originating from analytical laboratories.

What are the barriers to adopting green technologies?

Speaking to analytical scientists feels like preaching to the converted. The discrepancy, however, comes in practice, where there seems to be a mental barrier preventing the field from adopting new green technologies. Do people worry that it will be inconvenient or do they believe they don't have the expertise? That's difficult to determine. What's clear is that the technology has been around for a long time and it's not difficult to implement; it's not something out of this world. If we want to look more seriously at adopting alternatives, we must employ a form of leadership; we cannot always pass the responsibility onto others. Swift action is needed.

What is your message to analytical scientists – young and old alike?

Life is like a series of laboratory experiments – complex and ever changing. If you want to be successful, don't just start doing something out of the blue. Instead, you need to look at current trends and identify areas that need technological improvements. When I first started my career, the effect of pollution on the ozone layer was already known, and I realized then that this was just the beginning of a long-term shift towards greener technologies. If you can identify an area in need, and find a way to solve the problem, then you're never going to lose. Of course, your approach has to be unique, because you will face competition. If you're a young scientist working on the same problem as your senior peers, it's going to be very difficult to gain recognition – but that's not to say you can't with a little ingenuity!

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