

the Analytical Scientist

Upfront

Olfactory puzzle of
world's smelliest fruit

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From 3D printing to 3D-LC,
three is the magic number.

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The Smell of Death

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Clever co-workers

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Nexera Method Scouting system

Image of the Month



The Next Small Thing

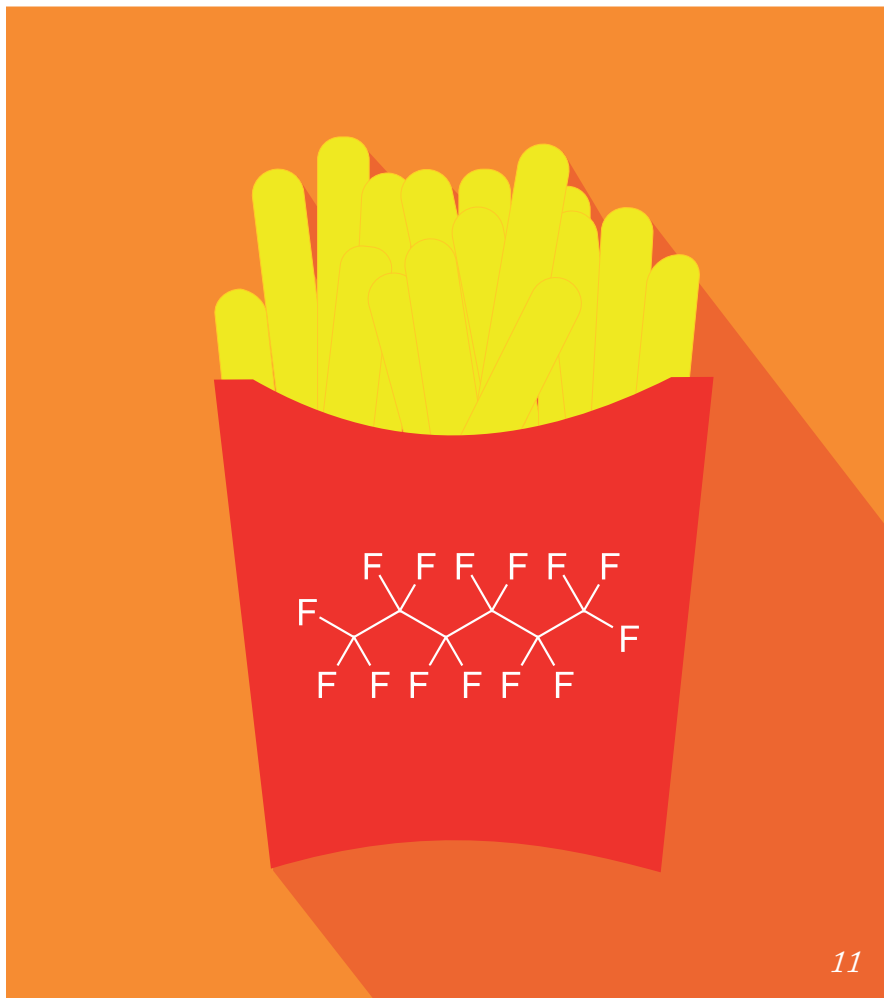
A sample of cocaine is subjected to electrical charges from a triboelectric nanogenerator before being measured in a mass spectrometer. A team at the Georgia Institute of Technology (1) report that by using triboelectric nanogenerators as the power source to ionize molecules, mass spec sensitivity was significantly boosted – in this case, achieving a highly sensitive (~0.6 zeptomole) analysis using minimal sample (18 pl per pulse). If widely adopted, the researchers hope this new technique could allow analytical scientists to measure smaller sample sizes with increased sensitivity. *JC*

Credit: Rob Felt, Georgia Tech Reference: A Li et al., "Triboelectric nanogenerators for sensitive nano-coulomb molecular mass spectrometry", *Nat Nanotechnol*, [epub only] (2017)

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



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By Charlotte Barker

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the Analytical Scientist

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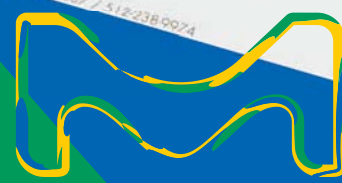
New!

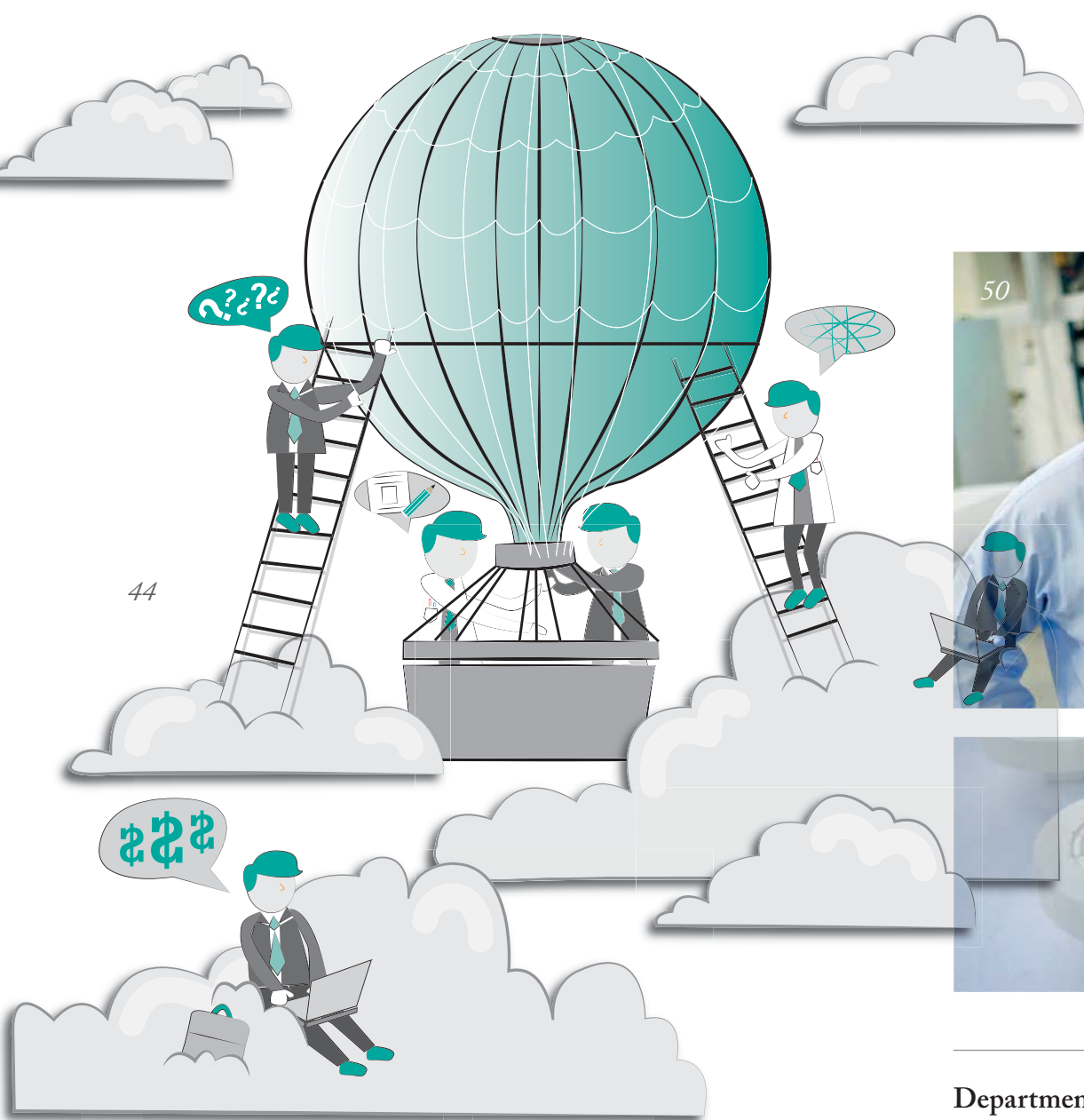
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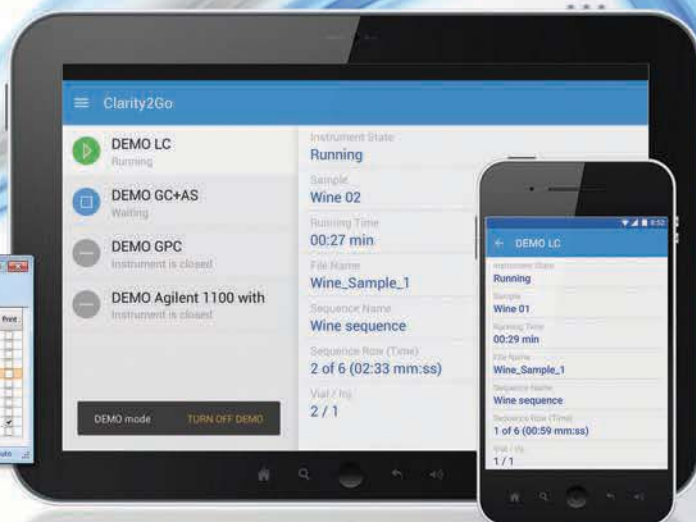
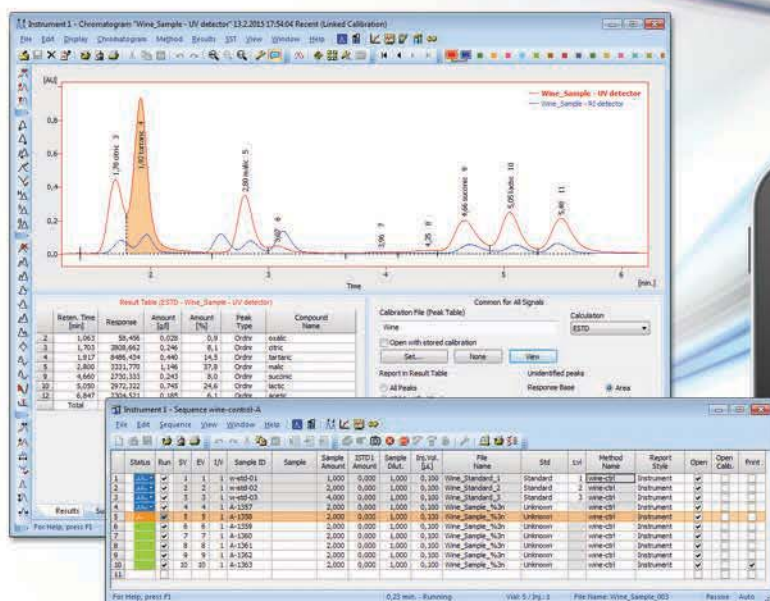
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It's something that those of us who read scientific articles for a living have long suspected; scientific journal articles are becoming more difficult to read. A group of Swedish researchers assessed the readability of 707,452 abstracts published between 1881 and 2015 in top biomedical journals using two standard formulae (Flesch Reading Ease and New Dale-Chall). Both systems calculate readability based on length of sentences, syllables per word, and number of 'difficult' words – and both confirmed that the readability of scientific abstracts has declined over time (1). In fact, the team noted, “more than a quarter of scientific abstracts now have a readability considered beyond college graduate level English.”

But why? Apparently, a sharp increase in the use of scientific jargon – jokingly referred to as ‘science-ese’ – is to blame. Jargon isn't inherently bad – it can convey information to a specialist audience with minimum word count; however, a combination of technical terms and unnecessarily complex language can make even the most scientifically exciting papers a hard slog for the reader. Scientists are only human, after all. Having a PhD doesn't (always) give you superhuman reading comprehension skills – or make you immune to boredom or frustration. In many cases, the concepts being expressed are not hard to grasp – when I talk to scientists about their work, they readily communicate it in a way that I can understand. Shouldn't we strive to do the same in our written work?

As we frequently see in our own pages, some of the most fruitful partnerships are forged by scientists in very different disciplines – and breaking down communication barriers is often an ingredient for success. Writing more readable papers is one way to encourage wider collaborations – and that can only be a good thing. Given the collaborative and diverse nature of the field, do analytical scientists need to be even more aware of the need to communicate clearly? I would say so.

The Analytical Scientist has always aimed for clarity over complexity. By bringing you the stories behind the science, we hope to encourage the free flow of ideas between different disciplines, application areas and techniques. From 3D printing (page 32) to the smell of death (page 22), we want you to be able to explore all of our articles, whether you're a world expert in the topic or simply curious.

How readable do you find The Analytical Scientist? Could we improve? Please let me know: charlotte.barker@texerepublishing.com.

Reference

1. P Plavén-Sigraý et al., “The readability of scientific texts is decreasing over time” (2017). Available at: <http://bit.ly/2nAd3gf>

Charlotte Barker
Editor

Upfront

Reporting on research, personalities, policies and partnerships that are shaping analytical science.

We welcome information on interesting collaborations or research that has really caught your eye, in a good or bad way. Email: charlotte.barker@texerepublishing.com

Stink Fruit

GC-O helps solve the olfactory puzzle of the world's smelliest fruit

If you love the smell of onions in the morning, then allow us to recommend a slice of durian – a tropical fruit that remains very popular in southeast Asia despite its pungent oniony aroma.

Knocked off their feet by the stench, a group of researchers from the German Research Center for Food Chemistry have attempted to quantitate the chemicals that account for the unappetizing aroma and then simulate that aroma (1)...

“My first trip to the tropics took me to Chanthaburi Province, one of the major growing regions for tropical fruits in Thailand, and I was fascinated,” says Martin Steinhaus, Group Leader of Aroma Chemistry. “Among the huge variety of different flavors, that of the durian is exceptional; not only because of its strength, but also because of its extraordinary combination of fruity and oniony odor notes. When I was choosing a topic for a new PhD student, Jia-Xiao Li, I decided it was time to crack the puzzle.”

For the analysis, they used what Steinhaus describes as the “workhorse” of aroma research: gas chromatography-

olfactometry (GC-O). “The volatiles, previously isolated by mild approaches to avoid deterioration of sensitive compounds and artifact formation, are separated by GC, and the column effluent is split into two parts, one directed to a detector such as an FID or an MSD, the other one directed to a heated exit serving as sniffing port,” says Steinhaus. “A panelist places his nose above the sniffing port and identifies the odor-active

compounds among the bulk of odorless volatiles in the chromatogram.”

They detected a total of 44 odor-active compounds in the durian pulp (2), and ranked their odor potency using an approach known as aroma extract dilution analysis (3). After breaking down the chemical composition of the fruit's unique odor, the team attempted to recreate it, and were surprised to find that only two potent compounds were required.

“Typically, 10 to 20 compounds are required to satisfactorily mimic the aroma of a food, but in this case, model experiments showed that a simple binary mixture consisting of ethyl 2-methylbutanoate and 1-(ethylsulphanyl) ethane-1-thiol in their natural concentrations was able to mimic the typical aroma of durian,” says Steinhaus (1).

And how did the team find working with the world's smelliest fruit? “It is not my favorite fruit, but I wouldn't say





it is disgusting either,” Steinhaus says. “And to be honest, if you work in the

field of odor-active food compounds, you get used to strong and unpleasant smells! Moreover, the benchwork was mainly done by Jia-Xiao Li, who is a big fan of the fruit. The problem was much bigger for his lab mates!” *JC*

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1. JX Li et al., “Insights into the key compounds of durian pulp odor by odor quantitation and aroma simulation experiments”, *J Agric Food Chem*, 65, 639–47 (2017)

Chem, 65, 639–47 (2017)

2. JX Li et al., “Characterization of the major odor-active compounds in Thai durian (*Durio zibethinus* L. ‘Monthong’) by aroma extract dilution analysis and headspace gas chromatography-olfactometry”, *J Agric Food Chem*, 60, 11253–11262 (2012).
3. P Schieberle, W Grosch, “Evaluation of the flavour of wheat and rye bread crusts by aroma extract dilution analysis”, *Z Lebensm Unters Forsch*, 185, 111–3 (1987)

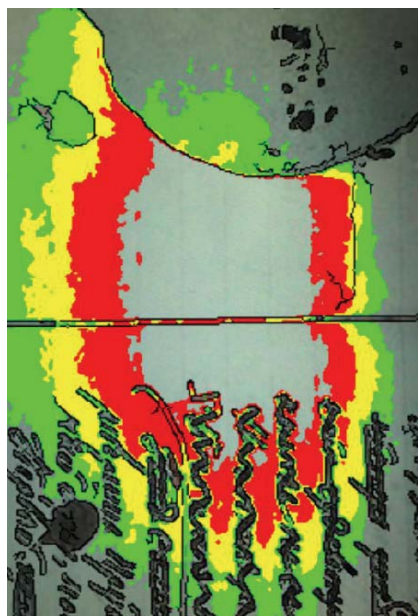
The Master and Macromolecules

LC-MS/MS identifies fingerprints on a 75-year-old manuscript

Mikhail Bulgakov’s allegorical novel, *The Master and Margarita*, tells the story of a visit by the devil to 1930s Moscow, with a naked witch and gun-wielding cat in tow. It’s a satirical portrayal of Stalinist Russia and one of the most celebrated novels of the twentieth century; now, a reanalysis of an original manuscript has helped scientists shed light on Bulgakov’s final years...

The novel was finished four weeks before he died in 1940 but, because of its provocative themes, was not published until 1967. Some experts on Russian literature have speculated that fingerprints found on the margins of one particular foil belonged to the NKVD agents (Stalin’s secret police) who sequestered Bulgakov’s manuscript. However, an Israeli–Italian team has ascertained that the fingerprints belong to the author himself – by identifying the biomarkers of the disease that killed him and the medication he took to ease his pain (2).

“I was introduced to the novel in 1990



Traces of morphine on a page of Bulgakov’s manuscript. Red indicates 10-ng/cm² levels, yellow indicates 5 ng/cm², and green indicates 2 ng/cm². Credit: *J. Prot./Elsevier*

when, upon dissolution of the USSR, a few Russian scientists were housed in my lab in Milan. My co-author on this paper, Gleb Zilberstein, being Russian, knew this novel very well!” says Pier Giorgio Righetti (Politecnico di Milano, Italy). Knowing that Bulgakov suffered from renal disease in the months before his death, the team decided to undertake a two-part analysis. First, they probed the manuscript for traces of drug intake,

using chromatographic beads and GC-MS, and found morphine in all the pages interrogated (1).

To prevent contamination or destruction of the delicate manuscript for the second part of their analysis, lead author Zilberstein (Spectrophon Ltd.) devised a novel film, in which two types of chromatographic beads were embedded on foils of ethylvinyl acetate (EVA). “The film works by capturing any analyte present in the work of art probed – metabolites as well as macromolecules,” Righetti says. Using this method, they were able to harvest and identify 30 different proteins on the manuscript foils – mostly from Bulgakov’s saliva – three of which were biomarkers of his renal pathology.

Righetti believes that the image (left), obtained by tracing the levels of morphine left by his thumbs on the margins of various foils, is as close as they could get to an actual fingerprint of Bulgakov – and notes, “Even Sherlock Holmes would have appreciated these findings!” *JC*

References

1. G Zilberstein et al., “Maestro, Marguerite, morphine: The last years in the life of Mikhail Bulgakov”, *J Proteomics*, 131, 199–204 (2016).
2. G Zilberstein et al., “Unearthing Bulgakov’s trace proteome from the Master I Margarita manuscript”, *J Proteomics*, 152, 102–108 (2017).

Finger Lickin' Fluoroalkyls

PIGE spectroscopy tracks the ecotoxic compounds in our fast food wrappers

Fancy your fried chicken wrap with a side of perfluorinated compounds? When you order fast food, you may be getting a little more than you bargained for – namely, per- and poly-fluoroalkyl substances (PFASs). PFASs are used to render packaging and textiles water and stain resistant. They are also used in a variety of specialty surfactant applications, notably as a primary ingredient in the aqueous film-forming foams (AFFF) used in jet-fuel fire-fighting foams. In food packaging, they are added to prevent water and oil from seeping through paper or cardboard. But how much of them make it into our bodies – and what impact would they have on our health?

Researchers from the University of Notre Dame have analyzed over 400 samples of food packaging for the presence of fluorine and other chemicals, using particle induced gamma-ray emission (PIGE) spectroscopy. “The method is relatively free of matrix effects because gamma rays are very penetrating, and there are no spectral interferences from any other nuclei at these energies,” explains Graham Peaslee, Professor of Physics. They found the chemicals in 56 percent of dessert wrappers, 38 percent of burger and sandwich wrappers and 20 percent of paperboard.

The team had been working on detecting halogenated flame retardants in furniture using particle induced x-ray emission (PIXE), when a fellow researcher asked Peaslee if the technique could be used to measure fluorinated compounds. “I thought about it for a couple of weeks and realized that, though it can’t be done with PIXE, PIGE might be sensitive enough to measure it. The sensitivity of the technique for fluorine

of large numbers of samples, providing a more comprehensive assessment.

Since the paper was published, Peaslee and team have heard from several other companies interested in which wrappers were found to contain high levels of fluorine. “For most fast-food companies, the packaging is subcontracted out to a packaging provider,” Peaslee says. “My guess is that many of these companies have never asked the question of what chemicals are used on their wrappers – until now.”

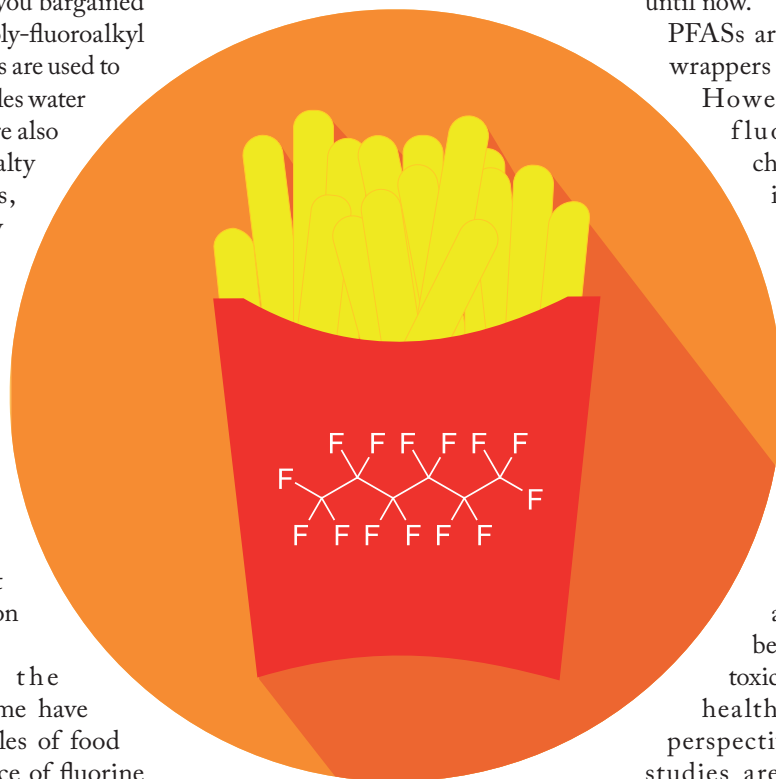
PFASs are perfectly legal to use on wrappers in the US and Europe.

However, Peaslee describes fluorine as a “persistent chemical”, which is absorbed into the bloodstream and accumulates over time, and notes that PFASs have previously been linked to various serious health issues, from cancers to immunotoxicity (2).

The team recently published a separate article demonstrating how a range of PFASs compounds target different organs in mice, a finding that Peaslee believes will be interesting to toxicologists both from a public health and an environmental perspective. “As more toxicology studies are performed on PFASs, we believe it is likely that all these surfactants are likely to demonstrate some ecotoxicity, especially with the extremely long environmental half-lives observed in PFASs,” says Peaslee. The team is now assessing PFAS prevalence in personal care products. *JC*

Reference

1. LA Schaidter et al., “Fluorinated compounds in US fast food packaging”, *Environ Sci Technol Lett*, 4, 105-111 (2017)



is typically in the low part-per-million range, which works well for papers and textiles that have been coated intentionally with PFASs,” Peaslee says. In previous studies on PFAS in food packaging, analysis was carried out with what Peaslee refers to as the “typical gold-standard technique” – LC-MS/MS. But using PIGE in this study allowed the team to undertake rapid screening

Prepping for PREP

Symposium Chair Giorgio Carta tells us what we can expect from PREP 2017 in Philadelphia

Tell us about PREP...

The International Symposium, Exhibit & Workshops on Preparative and Process Chromatography (PREP) was founded by the late Georges Guiochon in 1985. By providing a dynamic forum where scientists, engineers, and suppliers of media, equipment, and technology can come together to comprehensively discuss all aspects of preparative chromatography, PREP helped lay the foundation of the tremendous growth we've seen in this area over the past 30 years. Preparative/process chromatography is now used extensively in the manufacture of fine chemicals, natural products, amino acids, sugars, pharmaceuticals, and a whole host of biotechnology products, including therapeutic proteins, virus for gene delivery, virus-like particles for vaccines, and even whole cells.

Why a dedicated forum for preparative chromatography?

Analytical and preparative/process chromatography both use a stationary phase and a mobile phase, and in both, the separation is driven by the partitioning of components between the two phases. Yet the scope is very different, with analytical applications focusing on sensitivity and speed, while preparative/process applications focus on yield and productivity. The higher load requirements of preparative chromatography mean that predicting and optimizing performance is much more challenging, and process design has to meet more stringent constraints, such as column pressure.

What is your goal as Chair?

When I took over from Georges a few years ago, I wanted to expand the scope of the event to not only serve as a driving

force for scientific progress in preparative and process chromatography, but also as a major technology showcase, and an avenue for advanced education and training in chromatographic process development and design.

What will be the key themes at PREP 2017?

Pharmaceutical and biopharmaceutical applications will play a central role, with increasing emphasis on process understanding and improving manufacturing through more effective designs and continuous processing.

Sessions include:

- Industrial case studies in protein chromatography
- Mechanistic understanding and modeling
- Bioprocesses
- Stationary phases - bioapplications
- Stationary phases - RP HPLC
- Protein A and affinity chromatography
- Preparative chromatography in drug discovery, development, and manufacture
- Continuous and integrated processing
- Supercritical fluid chromatography
- Column and molecule-surface interaction characterization
- Natural products applications and CPC
- Monoliths and alternatives to packed beds
- Virus, VLPs, and cells
- Process modeling and design

Final thoughts?

The event is co-located with the International Symposium on Separations of Proteins, Peptides and Polynucleotides (ISPPP; July 19–21), with a joint day (July 19) and opportunities for networking throughout the week.

PREP 2017 will be held July 16–19, 2017, at Loews Hotel on Market Street, in downtown Philadelphia, Pennsylvania, USA. Visit www.PREPsymposium.org.



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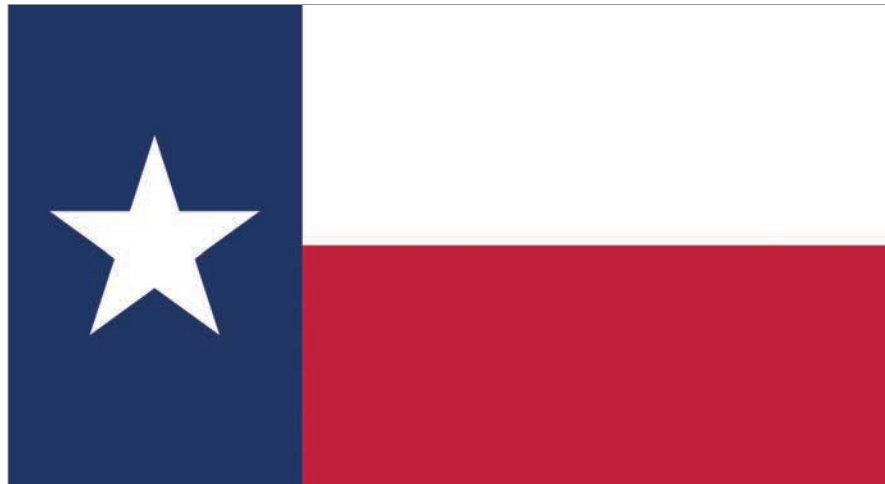
Texas Stars

Saddle up for new adventures and old challenges at ISCC & GC×GC

In May, the International Symposium on Capillary Chromatography (ISCC) and the co-located GC×GC Symposium will be held for a second time in Fort Worth, Texas. We caught up with Sheriff (Chair) Daniel Armstrong for his thoughts on this year's "Riva in Texas."

Armstrong promises a strong and varied program, highlighting hot topics in the field: "I love the way that seemingly established, mature research areas come roaring back with new innovative approaches. GC was such an area: 10–15 years ago, GC×GC and new ionic liquid stationary phases moved it back to the forefront of analytical research. Now, it's GC detectors that are all the rage, with a dedicated session at this year's event." Texas Titan Kevin Schug will give one such presentation on May 18 – and you'll find us "Sitting Down With" him on page 50.

Applications for new multidimensional techniques in health, environmental and metabolomics areas will also feature



heavily, says Armstrong. Indeed, cover feature author Jef Focant (page 22) will chair "Health/Metabolomics II" on May 17. But the program won't just focus on the hot topics of the moment. "Sample preparation is not a sexy topic, but it is tremendously important. Improvements in this area always have a big impact on chemical analysis – so we have devoted a session to it," he says.

Talks to look out for include:

- Monday, May 15 – Carlo Bicchi on better approaches for the analysis of flavors and fragrances

- Tuesday, May 16 – Vince Remcho on novel high-throughput screening consumables
- Wednesday, May 17 – Milton Lee on compact microchip thermal gradient GC
- Thursday, May 18 – Len Sidisky on new ionic liquids in separations
- Friday, May 19 – Richard Smith on interfacing ion mobility spectrometry with mass spectrometry.

ISCC & GC×GC 2017 takes place in Fort Worth, Texas, May 14–19.
www.isccgcxgc.com

SCIEX Safety Notice

Are you the owner of a API 4000, API 4000 QTRAP, or API 5000 model mass spectrometer?

In case you missed the recent announcement – SCIEX is asking owners of these instruments to take them out of service immediately

before visiting <https://sciex.com/tv801safetynotice> to check whether a potentially dangerous fault in the Varian TV 801 turbo pump may apply to their mass spectrometer. To date, no injuries have been reported.

For more information, visit <https://sciex.com/tv801safetynotice>





Beijing and Biotransformation

What's new in business?

Products

- SCIEX announces two new biotransformation solutions powered by MetabolitePilot s/w
- Bruker introduces AVANCE NEO NMR research platform plus new NMR solutions at ENC 2017
- Analytik Jena release novel compEAct for organic elemental analysis
- Phenomenex expands Kinetex F5 HPLC & UHPLC core-shell line
- Agena Bioscience introduces new lung and colon cancer panels
- Bruker's S2 Puma EDXRF now with 21 CRO part-compliant s/w
- Phenomenex unveils new family of Zebtron GC columns
- Agilent launches new 6495B Triple Quad LC/MS system

Investment and Acquisitions

- Eurofins acquires VBM Laboratories in Denmark
- Eurofins acquires Turkish food testing company Gözlem
- 908 Devices secures \$20 million in a growth equity funding round

- Eurofins acquires Mechem Laboratories in Singapore

Collaborations

- Numares and Oxford University to develop NMR-based MS IVD test
- Eurofins and USP collaborate to tackle food fraud
- Waters now offers Proteolabels software from Omic Analytics
- Biodesix and Progenetis announce distribution agreement for Israel
- ChemAxon contributing to European lead factory's success

People

- Samraat Raha to head strategy and corporate development at Agilent
- Agilent Board of Directors elects Koh Boon Hwee as Chairman
- Sartorius appoints Gerry MacKay as new EVP Marketing/Sales of Lab Division

Organizations

- Bruker opens Beijing Center of Excellence
- Eurofins to invest millions in new facility in Scotland

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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.

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What's the Most Dangerous Color?

To 'go green' you sometimes have to run a few red lights. A journey from big to small and back again – and a lesson in how taking risks is one route towards scientific reward.



By Elena Ibañez, Research Professor, Foodomics Laboratory, Institute of Food Science Research, Madrid, Spain.

I have always believed in taking risks – in life and in science. In my experience, most risks bring proportionate rewards. Importantly, you can take risks not only in your actions, but also in the way you think. Do you think conventionally and stick to your comfort zone? Or do you think daringly and take a gamble? Most huge (and small) advances in science have been based on risky hypotheses (often considered illogical or bizarre at the time).

In our laboratory, we move from big to small and vice versa; between chemical engineering and analytical chemistry, between sample preparation techniques and process design, between micro- and pilot scale. What our projects have in common is the desire to develop systems, processes and methodologies that follow 'green chemistry' principles. Ideas about sustainability, environmental impact, green solvents, selectivity, efficiency, and so on, can be applied in all processes and all scales. So why not translate a

sample preparation methodology to a pilot scale process? Why not develop a process at large scale and then use that knowledge to improve sample preparation techniques?

In the Foodomics Laboratory (Institute of Food Science Research, CIAL, CSIC-UAM), we defined foodomics several years ago as "a new discipline that studies the food and nutrition domains through the application of advanced omics technologies in order to improve consumer's well-being, health, and confidence" (1). By definition, foodomics is a 'green' discipline because it gives new answers to important societal challenges; for example, sustainability, food safety and quality, the rational design and development of new foods able to improve our health or prevent diseases. Attaining these goals helps to provide safer foods with lower contamination and chemical risk. But we aim to go further in making foodomics a green discipline (2).

"By definition, foodomics is a 'green' discipline because it gives new answers to important societal challenges."

Two obvious ways to make foodomics greener are the use of green solvents, and switching to integrated processes with less waste and energy consumption. These approaches can be applied to both the development of extraction processes for functional food ingredients and the

"Most huge (and small) advances in science have been based on risky hypotheses."

design of greener analytical methods to measure food quality, safety and traceability. The use of miniaturized sample preparation techniques or greener solvents, and the development of greener separation techniques is a must. By developing green foodomics we can also influence other -omics technologies (mainly proteomics and metabolomics) to cut preparation steps and consumption of solvents, while improving data reliability.

Let's consider some examples. First, from the 'big' point of view (chemical engineering, pilot scale), an important aspect is how functional ingredients are obtained. Traditional extraction techniques (soxhlet, sonication, solid-liquid extraction, liquid-liquid extraction) require long extraction times and large samples, provide low selectivity and, generally, low extraction yields, and need high volumes of organic solvents, resulting in the generation of large quantities of solvent waste. There is enormous interest in more environmentally friendly techniques that can overcome these drawbacks. Among them, ultrasound-assisted extraction and microwave-assisted extraction are versatile approaches that make it possible to use several solvents of different polarities, allow fast extractions and decrease the amount of solvents used. In addition, the development of advanced pressurized extraction techniques

(such as supercritical fluid extraction, pressurized liquid extraction or pressurized hot water extraction – also called subcritical water extraction) perfectly comply with the principles of green chemistry and green engineering, and could represent a key turning point in sustainable development.

From the 'small' point of view, we are developing methods in green analytical chemistry. Analytical methods can be considered processes in which preliminary information and knowledge, solvents, reagents, samples, energy and instrument measurements are used as inputs to solve a specific problem. The outputs of those processes are the qualitative and/or quantitative composition of the analytes. However, analytical methodologies can also have side effects (for example, energy consumption, toxic waste products). Key approaches to mitigate the adverse environmental impact of analytical methodologies are: i) reducing the amount and toxicity of solvents in the sample pre-treatment step; ii) reducing the amount and toxicity of solvents in the measurement step, especially by miniaturization; and iii) developing alternative direct analytical methodologies that do not require solvents or reagents.

Now, what if we – as analytical chemists and/or engineers – focus on measuring the 'greenness' of a process or analytical methodology and on gathering the necessary knowledge so that we are able to better translate the concepts bi-directionally? Then it's just a case of leaving the rest to our imagination!

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Interview with Kevin Schug, Shimadzu Distinguished Professor of Analytical Chemistry, University of Texas Arlington, USA.

As a young assistant professor, I would go to conferences and see presentations from well-established professors, detailing their work on the very best and newest instruments. I asked myself, “How can they possibly have their hands on a new instrument every time one comes out?” Of course, I quickly discovered that many of them have close relationships with instrument vendors, and those companies put the new instruments in their lab. Having access to the newest technology is a massive advantage in a field that’s evolving quickly, and I decided I needed to figure out a way to have that type of connection.

I was lucky enough to have an opportunity to do just that in 2012, when the University of Texas at Arlington and Shimadzu signed a major deal to create the Shimadzu Center for Advanced Analytical Chemistry. It was made possible by forward thinking,

science-minded administrative officers at the university and, when we inked that first deal, it was a game-changer. All of a sudden, we were working with all the latest, greatest and most sensitive instruments – it was instant credibility.

Now, my lab operates almost entirely on what I call non-traditional funding – industry deals and private donations. We work with instrument makers and consumable suppliers like Restek and VUV Analytics, oil and water companies, environmental groups, and others. Industry partnerships have also helped us to break into new and interesting avenues. Soon after the Shimadzu partnership was established, we started looking at environmental analysis. The company has an interest in the area, so they were able to suggest instrumentation to try, and provide additional instruments to support the work. Half of our research now is in the environmental analysis realm, and two million dollars in funding later, we’re leaders in measuring and mitigating the environmental impact of oil and gas extraction.

If you would like to bring industry funding into your lab, my first piece of advice is that you have to be flexible. I’ve often heard colleagues say, “Why would anybody want to give me money to do what I’m doing?” And to that I would reply that you have to be willing to step out of your comfort zone. A company most likely won’t be interested in exactly what you’re doing – you need to find out what their problems are, and see how your expertise can solve them. At the start of the conversation, it should be about what they need, and less about you. If you find after some discussion that you can meet in the middle, then that’s the best of both worlds. Simply going to an industry partner and telling them what you can do, without asking what they need, is not going to be nearly as fruitful.

“A company most likely won’t be interested in exactly what you’re doing – you need to find out what their problems are, and see how your expertise can solve them.”

You have to be open, and embrace the notion that you need to actively seek out these opportunities. Scientists aren’t necessarily the most outgoing people, but you have to put effort into making the initial contact and building the relationship. You need to talk to the right people in the company, and establish a relationship. Spend some time at conferences talking with people from companies and look for a good synergy. If both sides are pulling forward and interested, the collaboration will get off to a good start.

One collaboration often leads to another. On the oil and gas side, we started working with Apache Corporation to assess environmental impacts in West Texas. Since we started working with them, we’ve been contacted by several different water supply companies that want us to test water quality. We would never have got into water quality research at all if our university hadn’t partnered with Shimadzu back in 2012...

Alternative Atomic Spectroscopy

Solution-cathode glow discharge is the answer to atomic spectroscopy's most frustrating traits.



*By Michael Webb, Associate Professor,
Department of Chemistry and
Biochemistry at the University of North
Carolina Wilmington, USA.*

Atomic spectrometry is not a new field – in fact, its timeline can be measured in decades. It's been 19 decades since Henry Fox Talbot linked flame emission spectra to compounds of particular elements. Sixteen decades since Robert Bunsen and Gustav Kirchhoff began extensive studies of atomic absorption and atomic emission spectra. Ten since Niels Bohr linked atomic spectra to atomic structure. Six since Alan Walsh developed flame atomic absorption spectroscopy (FAAS) into a quantitative analytical technique. Five since Velmer Fassel and Stanley Greenfield introduced inductively coupled plasma optical emission spectrometry (ICP-OES). Even Sam Houk's initial ICP mass spectrometry (MS) work is nearly four decades old.

Despite this long history, ICP-OES and ICP-MS remain the preferred methods for many analyses, and outsiders

to the field could be forgiven for thinking atomic spectroscopy was stagnant. That would overlook enormous progress. ICP torches of today may not look much different from Fassel's torch of five decades ago, but every step from sample introduction to signal processing has evolved, particularly through work that continues into identifying and reducing or correcting matrix interferences. Other authors would be better suited to bringing attention to this research. My interests are in a more radical direction – developing alternative atomic spectrometry sources.

The strengths of ICP-OES are well known – trace-level detection limits, long linear range, mild matrix effects, and good precision. Still, it has disadvantages. It requires around 15 L/min of Ar, 1.5 kW, water cooling, and a high-resolution spectrometer. Most sample introduction uses nebulizers that can be prone to

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clogging with high solid samples. ICP is not practical for on-site industrial or remote environmental monitoring. Solution-cathode glow discharge (SCGD)–OES, on the other hand, is well suited for such applications.

SCGD is one of a growing number of atomic spectrometry sources operating on similar principles. All owe their roots to Cserfalvi and Mezei's electrolyte cathode atmospheric glow discharge (ELCAD), which was introduced in 1993 but got surprisingly little attention at first. In addition to SCGD, sources related to ELCAD now include liquid sampling atmospheric pressure glow discharge, direct current atmospheric pressure glow discharge in contact with a flowing liquid cathode, and alternating current electrolyte atmosphere liquid discharge. These instruments have now been applied to tea, mineral water, brines, tuna fish, aquatic plant matter, oyster tissue, coal

fly ash, groundwater, hepatitis-B vaccine, lake water, soil leachates, spruce needle leachates, colloidal silica, zirconium alloys, and simulated natural water. I'll focus on SCGD, but these other sources have similar advantages.

SCGD does not use any compressed gases, requires only about 70 W to maintain the plasma, does not require cooling, and can use a compact low-resolution spectrograph. 'Solution cathode' refers to the sample, which acts as one electrode of an atmospheric pressure glow discharge that is 3 mm tall and about 1 mm in diameter. With the sample directly in contact with the discharge, there is no nebulizer to clog. The power demands are so low that the instrument could conceivably run on batteries. ICP instruments use high resolution (~10 pm bandpass) to avoid spectral interferences, but SCGD has a relatively sparse spectrum and so can use lower resolution

(~350 pm bandpass), while still avoiding most spectral interferences. A small, inexpensive spectrograph can accomplish this resolution while simultaneously covering a wide spectral range to allow multielemental analysis. SCGD-OES is capable of detection limits and precision similar to ICP-OES.

Of course, SCGD has its shortcomings. Most notably, matrix effects are more severe than with ICP (although generally less severe than with FAAS). The inadequacy can largely be overcome using standard addition calibration, but external standard calibration would usually be preferable. Studies are ongoing to identify and reduce or correct matrix interferences in SCGD.

When considered on the scale of atomic spectroscopy, SCGD and related methods are still youngsters. With more attention? I believe they will mature and play a complimentary role to ICP.

Don't Prepare to Fail

Is sample preparation still the bottleneck of analytical chemistry?



*By Victoria Samanidou, Professor,
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Analytical scientists now have a wide variety of sample preparation techniques to

choose from: solid phase extraction (SPE), solid phase microextraction (SPME), microextraction in packed syringe (MEPS), liquid phase microextraction (LPME), single drop microextraction (SDME), dispersive liquid-liquid microextraction (DLLME), hollow fiber supported liquid-phase microextraction (HFLPME), three phase LPME, dispersive liquid-liquid microextraction (LLME), supercritical fluid extraction (SFE), accelerated solvent extraction (ASE), or pressurized liquid extraction (PLE), fabric phase sorptive extraction (FPSE), microwave assisted solvent extraction (MASE), stir bar sorptive extraction (SBSE), micro SPE (μ SPE), quick, easy, cheap, effective, rugged and safe extraction (QuEChERS), dispersive solid phase extraction (dSPE), magnetic solid phase extraction (MSPE), matrix solid phase dispersion (MSPD), disposable pipette extraction (DPX)... the list is almost endless.

When I go into class and introduce all these techniques to my students, I joke that the reason so many exist is to make their exams more difficult. I am not sure that they are convinced otherwise (that is, until they start working in the lab and encounter a tricky matrix). But why do so many exist?

Well, we all know that sample preparation is an essential step prior to any chemical analysis – and optimizing various aspects for different analytes and matrices has resulted in the plethora we see today. And though sample preparation usually consists of several sub-steps – dilution, filtration, deproteinization, centrifugation, purification, derivatization – the most important step is extraction. Even in cases where a 'dilute and shoot' approach is an option, extraction is still useful in terms of protecting instruments and prolonging the life of chromatographic columns.

Extraction can be either sorbent-based or solvent-based and, as noted, has been applied in many formats and versions through the years, as advances in instrument technology have demanded more efficient sample pretreatment, from liquid-liquid extraction (LLE) and solid-liquid extraction (SLE), to modern microextraction techniques.

SPE can be considered the descendant of LLE. The few hundred milliliters of solvents needed in LLE have been reduced to just a few milliliters. Reversed phase, normal phase, ion exchange, mixed mode and many more selective sorbents - for example, molecularly imprinted polymers (MIPs) - can cover all analytical needs.

The next optimization trend was to further reduce the volume of solvents - the birth of microextraction techniques - and it demanded the use of new advanced materials that were only made possible by the evolution of nanotechnology. Nanosorbents with higher surface area and sorption capacities improved the efficiency of dispersive μ SPE. Meanwhile, the increased sensitivity of instrumentation was able to overcome the resulting drawback: lower overall sorbent capacity. Miniaturized techniques promise to improve sample handling and increase efficiency and accuracy by using low quantities of sorbent materials and requiring no or low solvent volumes together with low sample volumes.

Another important factor behind the popularity of microextraction techniques in sample handling is that they comply with green analytical chemistry demands. Selectivity, sensitivity and lower quantification limits are among the impressive performance characteristics of these techniques, which are required to meet modern legislation criteria. The unique properties of microextraction techniques have also resulted in savings in both time and money.

So, when faced with our long list of sample preparation options, we have



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serious choices to make. And although the best sample preparation would be no sample preparation, the second best choice is 'just enough' sample preparation - a suitable technique that provides selective, fast, cheap extraction - all while following the twelve principles of green chemistry. Choosing a sample prep technique by considering their advantages and disadvantages for the purpose of analysis should be common sense for an experienced analytical chemist (but how often is it forgotten?). For young

chemists? Well, they need to live it before they believe it...

To answer my own question in the opening of this article: "yes, sample preparation is still the bottleneck in chemical analysis!" However, we now at least have many tools in our hands to make it easier and more efficient. Perhaps one day we will be able to dispense with sample prep altogether but, for now, Benjamin Franklin's famous quote remains disturbingly true: "By failing to prepare, we are preparing to fail."



THE CASE OF THE DECAYING CADAVER



*By Pierre-Hugues Stefanuto
and Jean-François Focant*

The sickly sweet odor of a dead body is said to be both immediately recognizable and hard to forget. But what chemical cocktail makes up the distinctive odor? And can GC×GC offer investigators a forensic tool that even Sherlock Holmes would envy – the ability to detect the ‘smell of death’?

In 2002, Arpad Vass and co-workers published the first study monitoring the volatile organic compounds (VOCs) released by decaying bodies (1), sparking a new field of cadaveric VOC profiling (1-5). Seven years later, our colleagues at the entomological laboratory at Gembloux Agro BioTech (University of Liège) were examining the behavior of insects as they colonized decomposing

pig bodies, which involved analyzing VOC profiles of the body headspace (6). The complexity of the VOC mixture released by the decaying animals meant that the entomologists soon ran into problems. Facing peak capacity issues when using ‘regular’ one-dimensional gas chromatography (1DGC) – even coupled with mass spectrometry – they approached us to help them develop a superior analytical approach.

We felt the obvious answer was comprehensive two-dimensional gas chromatography (GC×GC) time-of-flight mass spectrometry (TOFMS), as it would allow us to separate and further identify a greater number of components within the volatile cadaveric signature (7-9). For us, decomposition VOC monitoring was another perfect example of how GC×GC can make an analytical scientist's life easier when working with complex matrices, as it had been the case for us previously in our metabolomics and breath analyses projects.

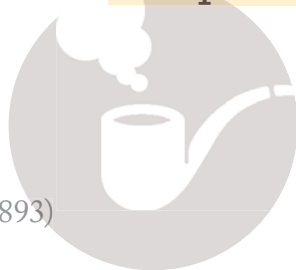
At that time, the trial of Casey Anthony had hit the headlines in the United States, so the issue of decomposition VOC profiling was in the spotlight. Anthony was accused of murdering her two-year-old daughter, and the presence of VOCs "consistent with a decomposition event" in the trunk of Anthony's car was presented as evidence for the prosecution. At the trial, forensic experts were called to testify about the reliability of decomposition odor signatures – in this case, measured by laser-induced breakdown spectroscopy (LIBS). There was intense disagreement between experts, highlighting the need for a more comprehensive description of the decomposition process and its chemical signature. We believed that exhaustive study of cadaveric decomposition by means of GC×GC-TOFMS could help resolve this confusion, thus allowing VOC profiles to be used as evidence in court.

"You know my methods, Watson"
 – The Memoirs of Sherlock Holmes, A Conan Doyle (1893)

Setting out on our quest for a better understanding of the VOCs of human decay, we soon realized that most previous studies were exclusively focused on the forensic aspect of the decomposition process, while neglecting the analytical aspect

– unfortunate, given that the analytical challenge is immense! The headspace of a decomposing body contains hundreds of different compounds, from most chemical families, and over a large dynamic range. Moreover, the dynamic nature of the decomposition process itself further complicates the design of VOC signature experiments. Thus, our first goal was to optimize our GC×GC-TOFMS method to perform non-targeted screening of the decaying pig headspace at various stages of decomposition.

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In doing so, we came up against the same challenges as GC×GC users in any other field: how do we sample and introduce analytes into the system? How do we optimize peak dispersion into the 2D space? How do we process replicate chromatograms? How do we deal with the large amount of corresponding data? Which statistical methods are compatible? All these questions are still common to all studies in the field of GC×GC – and remain hot topics at symposia like the forthcoming ISCC & GCxGC (www.isccgcxgc.com).

First, we tested three different sampling techniques: solid phase micro-extraction (SPME), solvent extraction, and thermal desorption (TD). TD soon emerged as the most effective method for trapping cadaveric VOCs (10). TD also has the advantage of preserving sample integrity during sampling (tube loading) in body farms, storage, and shipment of tubes to the analytical laboratory. Furthermore, with dynamic sampling and solvent-free extraction, TD allows a representative trapping of the decomposition headspace. In our

first few studies, we carried out chromatographic separation using a classic non-polar × semi-polar column combination, with 5 percent phenyl siloxane as 1D and a 50 percent as 2D (8). We later evaluated many other different phase combinations, such as semi-polar × non-polar, and ionic liquid × non-polar. Ultimately, the most appropriate phase combination came from our collaborators at the Forbes lab in Australia (11), who reported a combination of a cyanopropyle phase (Rxi-624 SilMS, Restek) and a polyethylene glycol phase (Stabilwax,



Figure 1. Typical decay stages followed by the pig carcass in a forest biotope. From (8).

Restek) for the efficient separation of semi polar compounds in complex VOC matrices (for example, cadaveric decomposition and cell culture headspace).

"It is a capital mistake to theorize before one has data."
—The Adventures of Sherlock
Holmes, A Conan Doyle (1891)

Much of our time in those early studies was dedicated to data handling. The first report we published in 2012 involved

days of manual data sorting in Excel spreadsheets before any statistical work could begin – all very well for a proof-of-concept study, but not realistic for the large number of samples needed for forensic investigations. The implementation and use of commercially available alignment tools, such as “Statistical Compare” in ChromaTOF (LECO Corp.) and GC Image package (Zoex Corp.), made our lives much easier. However, simply feeding raw data into the software won’t get the job done. One of the main problems was separating the relevant information from artefact signals and analytical noise. When your sample alignment generates almost 1,000 hits, you know that many of them will not be significant. Based on work by the Synovec group (12,13), we decided to use a Fisher ratio

The Smell of Life

Determining an accurate fingerprint for the smell of death may prove invaluable for the recovery of bodies in disaster areas – but what of survivors buried under debris? Currently, rescuers use highly trained dogs to locate trapped survivors – a dog's nose is a highly accurate VOC detector, and search and rescue dogs have an excellent success rate. However, dogs take a long time to train, can work only for short periods, and cannot be used in highly dangerous environments. Several groups have explored alternative routes for detecting the 'smell of life', using a range of technologies (C-MS, PTR-MS, SIFT-MS, MCC-IMS, FAIMS and sensor-based systems). Figure 1 shows the composition of volatile organic compounds (VOCs) released by living human bodies. A group from Austria classified these compounds, and identified 11 VOCs consistently released in detectable quantities – CO₂, ammonia, acetone, 6-methyl-5-hepten-2-one, isoprene, n-propanal, n-hexanal, n-heptanal, n-octanal, n-nonanal, and acetaldehyde. This information may help scientists find new ways to sniff out disaster survivors, and so relieve the burden on canine search and rescue teams.

Reference

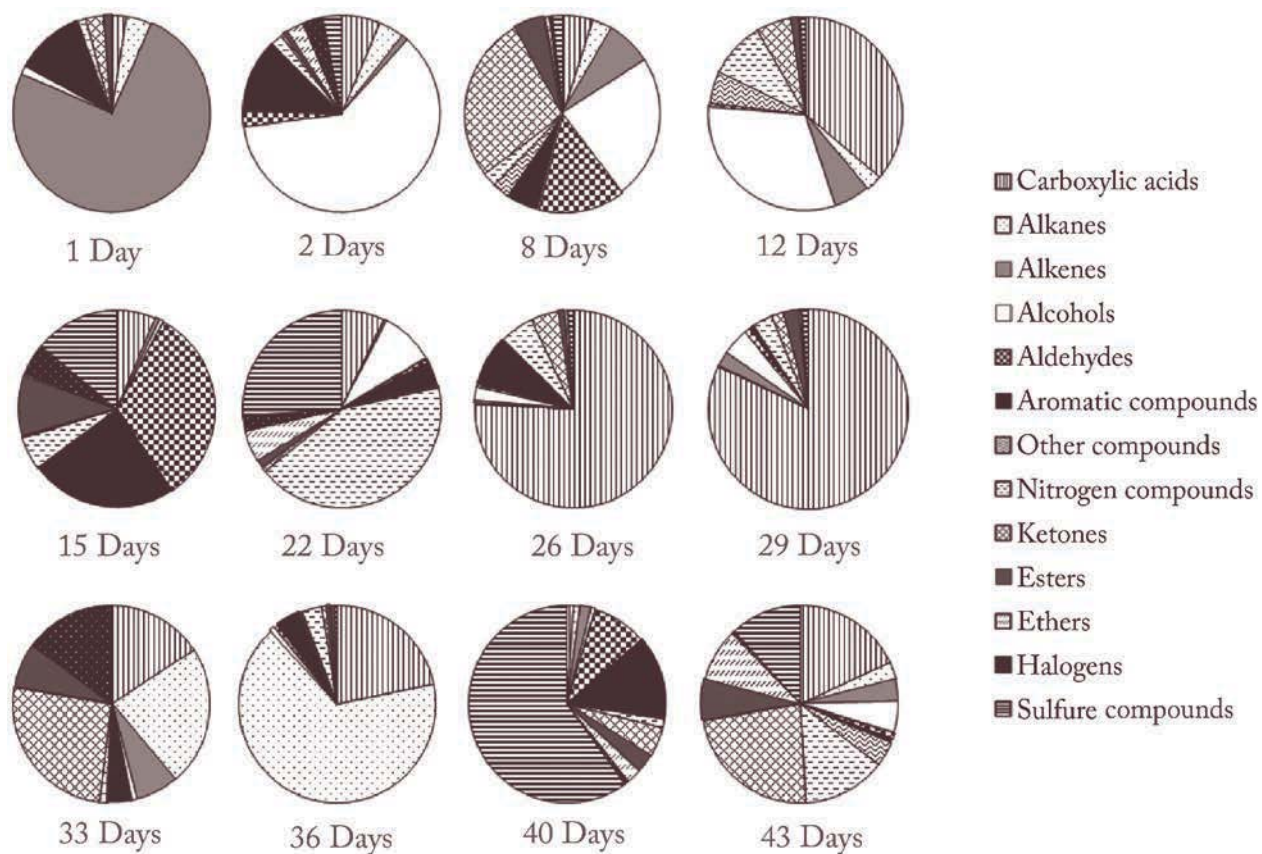
1. P Mochalskia et al., "Potential of volatile organic compounds as markers of entrapped humans for use in urban search-and-rescue operations", *TzAC*, 68, 88–106 (2015).

"The headspace of a decomposing body contains hundreds of different compounds, from most chemical families, and over a large dynamic range."

(FR)-based approach to reduce the size of our data matrix. But where should we set the cutoff to concentrate our statistical treatments on the most significant features? We evaluated a number of different approaches, but settled on the use of F critical values. These values are defined by the degree of confidence we want to apply (for example, 99 percent or 95 percent) and the two degrees of freedom of our analysis (the number of classes and the number of replicates in each classes) (14-16). All compounds with a FR value above such F critical values were defined as statistically significant. The method cuts the number of features by 10–20 percent, allowing us to focus only on the most significant compounds for statistical treatment (14-17).

Multivariate statistical methods (for example, principal component analysis, clustering, partial least squares) are increasingly used to handle data sets issued from GC×GC analyses (18,19). In fact, multivariate statistics have been used and reported in almost every GC×GC paper for the last three years. However, we question the utility of these mathematical treatments. As we see it, one of the important points of concern is data dimensionality. The vast majority of mathematical models used in GC×GC are based on a classical data dimensionality, so that there are three to five times as many replicates (n) as the number of variables (p). Before you apply methods such as PCA, you have to be sure of a good n/p ratio, or risk overfitting of the data (20). The F critical





(Above) Figure 2. Distribution of chemical classes according to postmortem time (days). From (8)

(Right) Prof. J-F. Focant group and collaborators at the ISCC and GCxGC 2016 conference in Riva del Garda

(Far Right) Belgian dog rescue team during a training on a simulated natural disaster event

approach allows us to reduce data dimensionality, with a focus on the most informative variables (12,13). And that's why we believe that this approach will benefit GC×GC users.

Over time, we adopted newer technologies, transposing our approach to GC×GC coupled to high-resolution time-of-flight mass spectrometry (HRTOFMS). HRTOFMS offers mass accuracy below 1 ppm while maintaining signal deconvolution capability, and can be seen as an extra dimension for compound identification. However, this enhanced system dimensionality makes data management even more complex and current data processing tools suffer from significant limitations. GC×GC-HRTOFMS profile data files are large and unwieldy, especially when considering replicate analyses of several sample classes for statistical comparisons. For now, our approach is to first perform all data analyses from GC×GC-LRTOFMS, including data acquisition, data alignment, data reduction, and statistical treatment up to isolation of features of interest. Next, we produce GC×GC-HRTOFMS data exclusively focusing on specific features for proper identification using two dimensional retention time (1tR and 2tR), linear retention time (LRIs), MS fragmentation screening in MS libraries, and accurate mass data for molecular formulae elucidation.

"I am the last and highest court of appeal in detection."
 – The Sign of the Four,
 A Conan Doyle (1890)

GC×GC, especially coupled to TOFMS, has now become the most applied method for cadaveric decomposition profiling. It is no longer necessary to demonstrate what GC×GC can do; instead, it is time for a full validation of the technique, not just for the characterization of parameters that influence the decomposition process, but also for routine applications and evidence in court (11,21).

There is no doubt that the additional information provided by GC×GC will lead to major advances in our understanding

of cadaveric decomposition chemistry. GC×GC-TOFMS instruments are now being installed in analytical laboratories of taphonomy facilities (such as body farms), to be used for large-scale studies on the decomposition of human remains, which will enrich current databases and provide the robustness that has been missing in cadaveric VOC profiles presented in the courtroom.

For the immediate future, we will focus on implementing a quantitative approach for analysis of decomposition VOCs. To date, only semi-quantification has been performed, and a full quantification of biomarker candidates will lead us to a closer understanding of the decomposition process. In addition to

the headspace of dead bodies, we are also chasing these cadaveric VOCs in a broad range of matrices, including (suspected) grave soils, human tissues, and internal cavity gases. Each matrix creates a new analytical challenge in terms of method development and brings new investigative angles to the quest for sample characterization.

"There is nothing like first-hand evidence."
 – A Study in Scarlet,
 A Conan Doyle (1887)

Our internal gas reservoirs project (testing the small pockets of gas inside cadavers) is a collaboration with the Center of Legal Medicine

at the University of Lausanne. Laser-assisted post-mortem computed tomography is used to locate gas bubbles, and samples are taken using gas syringes (22). We then scrutinize the internal gas samples by GC×GC-HRTOFMS to complement the gas measurements performed in Lausanne with our VOC profiles. Preliminary results suggest that not all organs decompose at the same speed, a finding that may help pathologists understand causes of death and make more accurate post-mortem interval calculations (23). We corroborated these findings with further studies on organ-specific VOC production, in which various human tissues were left to decompose in a controlled environment. These tissue-based experiments have the major advantage of allowing for many more replicate experiments than when using a body

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Top: soil samples from underneath a decomposing human body in a forest environment
Bottom: longitudinal monitoring of soil volatile profile underneath a decomposing pig carcass (in collaboration with Dr. K. Perrault and Prof. S. Forbes)



Pig remains in a forest environment after 1 year



farm, where one is always limited by the number of bodies available, and gets us closer to the good n/p ratio we noted earlier as being so important.

"The game is afoot."
– The Return of Sherlock Holmes,
A Conan Doyle (1903).

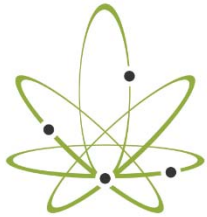
The profiling of VOCs released by cadavers is a continuously growing field. State-of-the-art technologies are allowing us to analyze new kinds of matrices, which opens the door to potential medico-legal applications. Moreover, a comprehensive understanding of tissue degradation chemistry will lead to improved training programs not only for cadaver dogs, but also their counterparts in search and rescue. By pinning down the differences in VOC profile between an injured person and a 'fresh' cadaver, we may be able to improve the efficiency of search and rescue dogs in locating survivors after a mass disaster event. It is these valuable field applications that motivate us to continue to challenge the analytical technology to its extreme.

Pierre-Hugues Stefanuto is a Marie-Curie postdoctoral fellow at Dartmouth College and Jean-François Focant is a Professor at the Organic and Biological Analytical Chemistry Group, Chemistry Department, University of Liège, Belgium.

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THREE. THAT'S THE MAGIC NUMBER

3D printing provides the exquisitely detailed, perfectly controlled structures needed to translate 3D-LC from theory into reality.

By Suhas Narwada

I didn't set out to work in 3D printing. In fact, when I applied to do a PhD with Conan Fee and Simone Dimartino at Canterbury University, New Zealand, it was on a completely different topic. But in the eight months it took for me to receive my New Zealand visa, Conan and Simone had an idea about the capillary-polymer phase fiber columns they were working on: why not just 3D print the fibers exactly where they are needed? In fact, why stop at fibers? Why not just print perfectly ordered particles and open up all manner of possibilities for liquid chromatography? When I finally made it to New Zealand, I was given a choice: either work on the original topic that I applied for – or take on this new area of 3D printing. I was so struck by the potential of the 3D printing approach that I immediately decided to pursue it, despite knowing virtually nothing about 3D printing... or liquid chromatography!

IN PERFECT ORDER

With traditional slurry-packed LC columns, random placement of particles hinders the column's performance. It is possible to create monolithic structures, as Frantisek Svec (E.O. Lawrence Berkeley National Laboratory) and Sebastiaan Eeltink (Vrije Universiteit Brussel) have done. Still, there remains the issue of the random placement of microglobules that are cross-linked. In either case, we end up with column geometry that exhibits inherent randomness. Our initial idea was to make a completely ordered lattice of particles; there are plenty of computational studies that showed the advantages of uniform packings, so our goal was to replicate them experimentally. Another good feature of 3D printing is that we can design and make fittings, distributors and column walls, all in one piece – they are very much plug-and-play.

So far, so good – but turning theory into reality often requires answers to a number of questions. What are the characteristic dimensions? What are the geometries we want to design? What materials should we use and how do we get from a printed structure to a fully functionalized column? Can we use printers that exist in the market or do we need to make our own? Each of these questions is a PhD project in its own right... I decided to focus on the use of inert plastic models to create structures that could replace packed beds. Essentially, I sought to answer the question: what is the best

stationary phase geometry for LC?

But it wasn't just about designing the packing structure – we could also change the flow distributors and column shapes, and we found that it had a significant influence on column performance (1).

A RARE GEOMETRY

We began by making columns with uniformly stacked 'particles'. The particles slightly overlap so they are monolithic structures in the strict sense of the word. We can control the size, shape, arrangement and orientation of these 'particles'. We showed that arranging spherical particles in a face-centered cubic formation is the optimal set-up. And though this fact has been shown many times in computational studies, it was exciting to confirm the theory experimentally for the first time! One result that none of us saw coming was that tetrahedral 'particles' outperform spherical particles when arranged in ordered lattices (2).

We don't need to limit ourselves to packed beds with particle-like elements. Mathematicians have spent whole careers coming up with and studying all sorts of interesting geometries but, until now, there had been no way of physically making them. With 3D printing, that obstacle largely disappears, and suddenly we have access to the best geometries that mathematics has to offer. For example, minimal surfaces – soap-film-like sheets designed to minimize surface tension, resulting in warped, curved geometries, such as gyroids (Figure 1). They have been explored computationally but thanks to 3D printing we could confirm that minimal surfaces beat the best sphere packings by a factor of 6-8 when it comes to separation impedance.

We are only just scratching the surface in terms of the geometries we can build. Minimal surfaces are just one family of mathematically interesting structures; there are many more that we can and should study. Then, we can answer the question of what the perfect stationary phase structure for LC really is.

3D = FREEDOM

One of the things that makes working with 3D printing so enjoyable is the speed with which we can produce alternative designs – we can go from an "a-ha" moment to a 3D design in



“One of the things that makes working with 3D printing so enjoyable is the speed with which we can produce alternative designs.”

an hour and have the new part printed overnight. Next morning, we're ready to test the new part and see if it does any better.

An example of this is flow distribution. The goal is to achieve uniform flow from a single point (the tip of the inlet tube) to the cross-section of the column. Our first design fell down on this point; we couldn't even tell the difference between different packing geometries. We were able to rapidly change tack, and come up with a new flow distributor design based on a Manelbrot H-tree fractal, which was much more successful.

STAMPING OUT SLOW SEPARATIONS

My PhD supervisor Simone Dimartino presented our group's work at HPLC 2016 in San Francisco. Peter Schoenmakers and his team from the University of Amsterdam were also there. And, as part of their work on 3D separations, they were looking for someone with 3D printing experience to join their exciting STAMP (Separation Technologies for a Million Peaks) project; Simone recommended me, and I set off on a new adventure.

As everyone in the field knows, one of the main challenges in liquid chromatography is the need to increase separation of very complex samples. Right now, we're several orders of

magnitude short of the peak capacities we need for proteomics and metabolomics. The number of peaks that a single column can resolve has improved over the years, but with steadily diminishing returns. We can make longer columns with smaller and smaller particles but eventually it turns into what Schoenmakers calls “ultra-high patience liquid chromatography” – higher and higher backpressures and very long analysis times.

In the late 1970s, 2D-LC came onto the scene. Fractions from the first column are injected onto a second column with a different retention mechanism, dramatically increasing the resolving power of our overall systems. In principle, 3D separations are no more than an extension (or added dimension!) of 2D-LC; the goal is the same – to achieve greater peak-capacities. That said, with 2D-LC, we typically think of a coupled-column technique, where fractions from the first dimension separation are transferred to the second. The drawback is that the analysis times are long, because fractions of the first dimension are analyzed sequentially in the second.

The alternative? Performing the separations in parallel rather than in series. For this, the first dimension has to be a separation in space. Fractions are also in space rather than time. We can have several perpendicular 2D columns attached to the 1D. This way, these spatial 1D fractions can be transferred to the second simultaneously, and we dramatically reduce the total analysis

times. STAMP aims to achieve radically high peak capacities at short analysis times by carrying out separations in parallel rather than in series; separation in space rather than time.

THREE REALLY IS THE MAGIC NUMBER

As early as 1983, Georges Guiochon et al. described a device for “development in the first two dimensions and elution in the third” – our main working principle (3). They envisioned the device as a single 12x12x12 cm box, filled with particles, where the three separations would occur. Thirty-four years later, we’re still trying to make those principles a reality!

Why has it proved so challenging? For a 1D separation, the ideal shape is a single line; the closest we can get is a long, thin cylinder. For 2D parallel separations, the first dimension has to be a spatial separation, which branches off into several second dimension channels. For this, a planar device is ideal. When we go to 3D, the first two dimensions need to be spatial separations. Bert Wouters has made a first prototype that works in this manner (4) during his PhD research at the Vrije University Brussel and now works

with us on STAMP. As you can see in Figure 2, when we add more dimensions to our separations, the geometries become very complex very quickly!

Effectively, we’re trying to house hundreds or even thousands of mini-columns, complete with valves and distributors in one device. We need to transfer the analytes from the first to the second to the third column in a very controlled manner. And we need to do this without transferring the mobile phases of each dimension to the next. Needless to say, any device of this kind will need to have an incredibly complex structure. Part of what we do at STAMP is to design and optimize these devices.

It might be possible to create these devices with the same methods we use for microfluidic chips (micro-milling, PDMS replica molding, and so on) but there are limitations in terms of complexity. And that’s where 3D printing comes into its own: transforming the impossible into simply very difficult. With 3D printing, there is no upper limit to the complexity of parts we want to build. For me, it’s been an exciting opportunity to work on a ‘moonshot’ project and put my knowledge on 3D printing to good use.

The main application that we’re targeting is proteomics and metabolomics, where extremely high peak capacities are necessary

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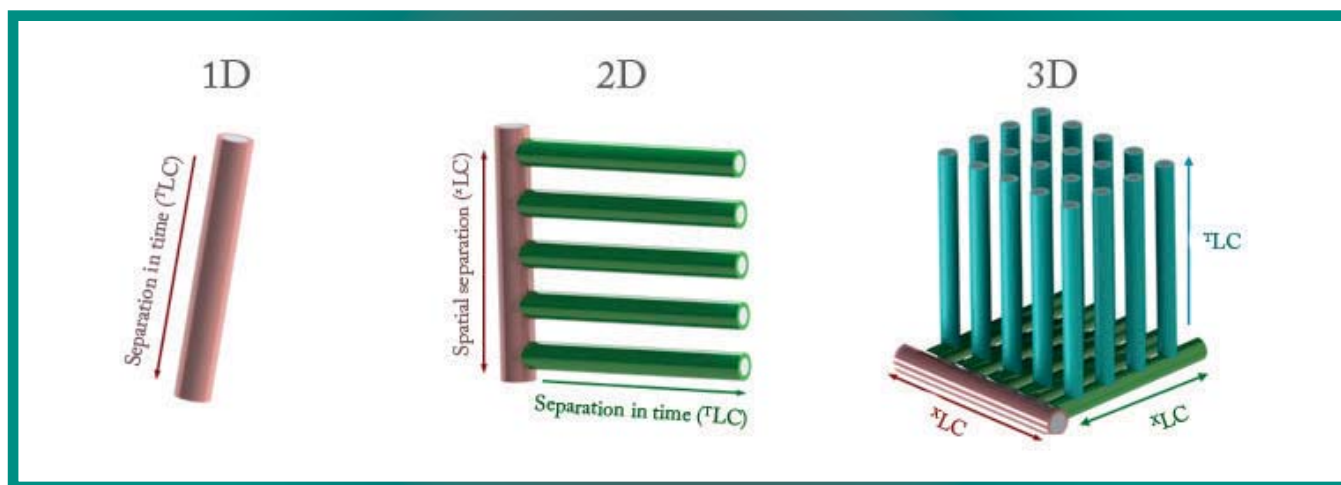
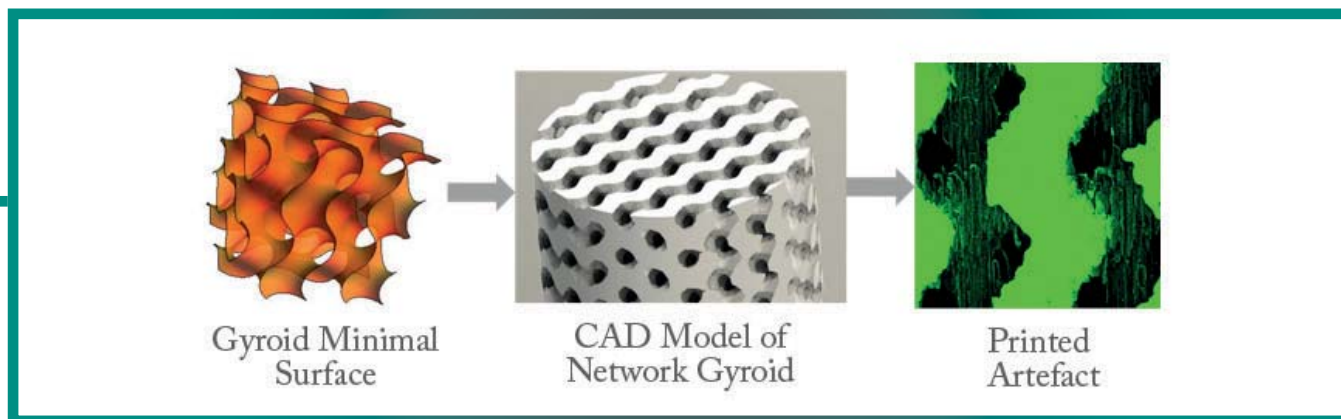
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Top: Figure 1. Printing of minimal surface structures. The initial films are created using trigonometric approximations. These geometries provide highly uniform flows and significantly higher permeabilities Bottom: Figure 2. Typical channel setups for 2D spatial ($xLC \times LC$) chips and 3D spatial ($xLC \times LC \times TLC$) blocks. Parallel separations in the second and third dimensions radically increases the number of resolved peaks per minute.

prior to mass spectrometry (MS). For a good MS analysis, you cannot have dozens of co-eluting compounds with a large range in concentrations.

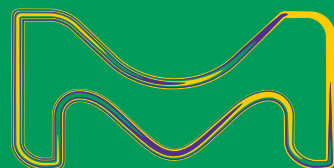
The technology still has a long way to go. As well as the fluid mechanical challenge, there is the difficulty of finding a combination of retention mechanisms that are both compatible and orthogonal. Then, there's the small matter of detection from dozens of eluent streams in parallel. This is why we have five PhD students working on solving different parts of the jigsaw puzzle. These challenges mean that we likely won't see 3D-LC in use for several years. It took column-based 2D-LC a few decades to go from a concept, into academia and finally into industry. We have the advantage that we can piggyback on much of the research that has been performed on column-based 2D-LC – and in the next decade I hope to see 3D devices beginning to appear in university

laboratories for proteomics research. Add another decade or so and we can expect it to seep into commercial research facilities.

Suhas Nawada is a postdoctoral researcher in the STAMP project (Separation Technology for a Million Peaks) at the University of Amsterdam's Van't Hoff Institute of Molecular Sciences, the Netherlands.

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Lessons I've Learned, with Hernan Cortes

Profession

*Leadership
Talent Development
Career Planning*

Hernan Cortes spent three decades at the Dow Chemical Company, where he carried out groundbreaking research in multidimensional chromatography before saying farewell to the corporate world and setting up as a consultant. Here, Hernan shares what he's learned about gaining recognition as an industry scientist, the chromatography 'family', and the secret to true happiness...

There are great opportunities in industry

I joined Dow in 1978, intending to stay for a couple of years; in fact, I worked there for 31, starting as a chemist and ending up as a senior scientist. My interest has always been in separations, and the company was very supportive of research in the field – Dow scientists invented gel permeation chromatography (GPC), ion chromatography, and hydrodynamic chromatography, among other notable inventions. The company provided the opportunity to do cutting-edge research in micro-column and multidimensional chromatography, to write, edit and publish a book, to publish close to 100 papers, and to interact with academics in the field.

Not many people in industry take advantage of the opportunities on offer. Being part of a large company – particularly working in analytical sciences – one gets exposed to a multitude of areas; I worked on everything from high polymers to pharmaceuticals and agricultural chemicals – and that breadth of experience enriched me.

I retired from Dow in 2009. For me, it was time to step out of corporate America – but it was a very fruitful and rewarding career, and I'm very proud to have been part of that organization.

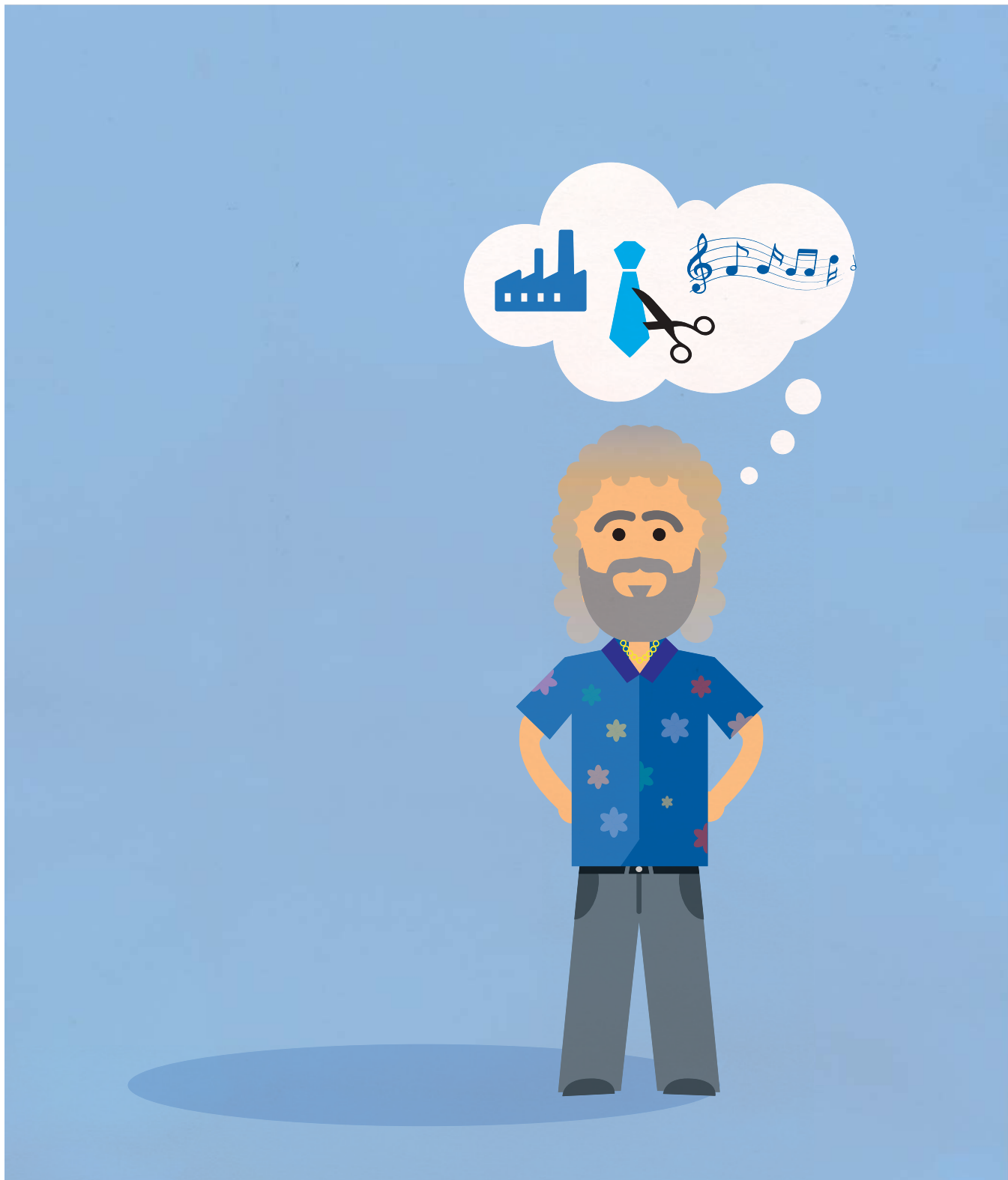
Success means stepping outside your comfort zone

There are many incredible scientists in industry doing state-of-the-art research, but they tend to gain very little external recognition – either because intellectual property restrictions limit their ability to publish, or simply because industrial chemists tend to focus on more short-term problem solving and innovation. I have often worked with industry scientists who are world leaders in their field but aren't widely known outside of that environment...

What I did differently from many industrial chemists was to take the time and effort to engage with academics – and to do independent research. I had the resources to carry out research, but I had to do it in my own time. I put in a lot of extra time at the lab during evenings and weekends so that I was able to conduct research (in addition

“What I did differently from many industrial chemists was to take the time and effort to engage with academics.”

to fulfilling the normal requirements of the job) and publish that work. I couldn't always publish the particular application or problem I was working on, but I could publish the technology that was developed. I'm blessed to have had a supportive partner who stayed at home and raised our children, so that I could work 12–14 hours a day. I missed a lot while our children were growing up, but that sacrifice put me in the position that I'm in today.



Chromatography is a tightknit community

I would compare the chromatography community to a family. As in any family, there is some conflict and dysfunction, but its members have helped me and driven me to do better. People like Cal Giddings, Milos Novotny, Pete Carr, Jim Jorgenson, Milton Lee, Luigi Mondello, Pat Sandra and Mark Schure – among others – have encouraged, challenged and inspired me along the way. I respected them, and wanted them to respect me – and the best way for me to achieve that was by doing good science and demonstrating that I was willing to contribute to the community.

New ideas are often met with resistance. When a disruptive thought or new technology enters the scene, it's been said that the first reaction is usually "it'll never work". The second reaction is "it works, but in very limited cases", the third reaction is "I guess it can be applied to some things" and the fourth and final reaction is "of course, it works – it was my idea!" Some of you have been there...

I've always tried to push the boundaries and explore different ideas. I like to extrapolate from theoretical principles and ask "What if...?" Some of my innovative work occurred when we coupled LC to GC in the mid-1980s. I was collecting fractions off a prep column – incredibly boring work. Automation was not what it is now. I thought, "What if I run this through a miniaturized LC and put the eluting fractions directly into a GC?" To my surprise, it worked well, and opened up a whole new avenue of research for me. We also got into the LC-LC, GC×GC and LC×LC areas relatively early, and used these technologies to solve a number of industrial problems.

If you have an idea, pursue it. In my early days, when I tried to do

something original, I was often told, "We've done this before." And as we get older, it's tempting to think that it's all been done before, but that's something we must fight against. I avoid telling younger researchers that something has been done before; instead, I ask if they have researched the literature thoroughly.

"Even very successful people have some degree of insecurity. It's human nature that we are never really satisfied – there's always that desire for more."

Even if it has been done before, I would never discourage them from pursuing an idea. Why? Because a small variation may produce valuable results. In science, breakthroughs are very few and far between; most progress is incremental. Even a small improvement could be valuable. Look at a gas chromatograph in the 1970s versus one today – it's the same technology, but you wouldn't recognize the instrument; hundreds of incremental improvements in injection, column design, and detection have made today's instruments incredibly powerful.

Don't be afraid to go against the prevailing view

We started doing electro-driven chromatography in the early 1980s, when the field was still in its infancy. We wanted to see if we could get better efficiencies in liquid chromatography with this approach; the theory suggested that you would get a flatter flow profile than you do with conventional flow. After a lot of work, we published a paper in *Analytical Chemistry* that suggested that it was actually not the best approach. Many people are still working in what's now known as capillary electrochromatography, but it has unfortunately failed to enter routine use – for many of the reasons we expressed in that paper. At the time, I faced a lot of criticism but, over 30 years later, it's somewhat satisfying to observe that our conclusions were valid.

Similarly, we did some early work on what are now called monoliths. Some of our catalyst chemists were creating structures made of silica, and it seemed obvious to use them in chromatography. We borrowed the technology from them with high hopes, but our experiments suggested that they were simply not good enough to rival existing technology, so we didn't pursue it. One mistake I made was not publishing that work, because I considered the project a failure. I have since learned that negative results can also provide valuable information! I believe it was the first time that chromatography had been done on those surfaces. Today, I still think it's very difficult for monoliths to compete with packed columns...

To make a difference, you must translate data into knowledge

As an analytical chemist, I would say there are three levels at which you can work: first, generating data (as in quality control); second, translating data into information; and finally, translating that information into knowledge – this final stage is where you get the payoff. You can spend your career running samples, but making the transition from data, to



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information, to knowledge is where one can make a true contribution. Making those jumps requires you to go beyond analytical chemistry – you need to understand organic chemistry, physical chemistry, catalysis, polymer chemistry, and more.

I use the term ‘measurement science’ rather than ‘analytical chemistry’

In any scientific endeavor, if you can’t measure it, you’re not going to get anywhere. That’s why measurement science is fundamental to all fields – and one must understand the theory to conduct good measurement science. Consider a gas chromatograph – you don’t need to know gas chromatography to use it, you don’t even need to know what’s inside the oven. You can just walk up to the instrument, inject a sample and get data. Anybody can do that, but it doesn’t mean you know what to do with that data, let alone come up with something new. Analytical chemistry gets a bad reputation because essentially anybody trained can do it, but the thing to remember is that not just anyone can do it well – or innovate.

Never stop learning, never stop teaching. Even if you are at the top of your field, you should always be open to new subjects. I think the moment you stop learning is the moment you die. Currently, I am learning about biocatalysis, which previously I knew nothing about. I have collaborated with the University of Tasmania and the University of Messina in both a learning and teaching capacity. I think that passing on our knowledge and experience to the next generation is an important responsibility for scientists as we get older – otherwise it can be lost. There’s nothing I enjoy more than helping a talented young person succeed.

Stay true to yourself

We all have our own personal values – the things that drive us – and it’s

always been important to me that I did not compromise those for any reason. For me, some important drivers are the pursuit of knowledge, the ability to express my creativity, and the quest for spiritual enlightenment – however you choose to define that. Why am I here? What is the meaning of life? Where do I fit? I think it’s important to ask those big questions. In addition, helping other people and continuing to move the scientific field forward are fundamental values that I live by. I have a desire to give to society – I believe in recycling some of the blessings I have been lucky enough to receive.

Success is hard to pin down

Success means something different to everyone, and I don’t think there’s a specific roadmap that one can follow, but I think there are three elements: you have to be intelligent; you have to work hard; and you have to find an opportunity. You can be very intelligent and work really hard, but if an opportunity doesn’t arise, then you may not succeed. On the other hand, you may have all the opportunities in the world, and be very intelligent, but if you don’t apply yourself you are likely to achieve nothing.

Even very successful people have some degree of insecurity. It’s human nature that we are never really satisfied – there’s always that desire for more. And that’s why I tell my kids not to ask “Am I happy?” Instead, I tell them to ask “What is my happiness percentage?” No one is 100 percent happy all the time. If you are in a situation where you are only 40 or 50 percent happy, perhaps you should look to change it. If you are 60–70 percent happy, you’re doing pretty well. If you’re 80 percent happy, you’re golden.

Hernan Cortes is Principal at H. J. Cortes Consulting, LLC, Midland, Michigan, USA.

Joining Forces: Drugs in the Cloud

Business

*Ergonomic drivers
Emerging trends
Business strategies*

As part of our series on academia–industry collaboration, we explore a partnership forged to fight against novel psychoactive substances.

With Petur Dalsgaard, Forensic Scientist, University of Copenhagen and Eric Fotheringham, Director – Centers of Innovation Program, Waters Corporation

Tell us about your project...

Eric Fotheringham: For some years, we have had a collaboration with the University of Copenhagen (Petur's lab) focused on mass spectrometry (MS) applications in forensic toxicology. More recently, this has culminated in us asking him to participate in our Centers of Innovation (COI) Program, working on the monitoring of novel psychoactive substances (NPS).

Petur Dalsgaard: The field of NPS is very fast-paced; there are one or two new compounds hitting the streets every week – so getting the information into your target library is one of the biggest challenges. There is a risk that by the time you finally have the reference standard in your system, the compound has fallen out of favor. So we're trying to build new databases to get ahead of the game. We now have a cloud database called HighResNPS (www.HighResNPS.com); every time a compound is detected somewhere, we can get the reference values to use in our QTOF-MS system. If members find a new tablet or designer drug in Finland, for example, then they post it in the library, and I can use their values in my system, regardless of vendor – without any reference standard. Each member has different instrumentation, but they can still use the information

in the database. At the moment, it's mainly the European countries who are involved, but we're trying to get as many labs as possible to join in. It's free, but everybody has to contribute findings. You could describe it as crowd-building – if everybody contributes, then each party gets back what they need many times over.

*“The field of NPS
is very fast-paced;
getting the
information into
your target library
is one of the biggest
challenges.”*

We are hoping that building a library this way will be faster than the European Monitoring Centre for Drugs and Drug Addiction (EMCDDA). Databases

such as mzCloud (www.mzcloud.org) are really big now – there are 500 NPS compounds (out of a total of 6,500 compounds). The challenge, of course, is how to use these cloud databases...

How did you build the partnership?

PD: I guess it really started ten years ago on our side, when the University of Copenhagen purchased a Waters UPLC TOF-MS system; I was hired to get it up and running – and to conduct forensic toxicology screening. One of the key people I worked with at Waters was Michelle Wood – she did the instrument training and I continued to correspond with her afterwards. Later, I got to know some of the programmers, and it evolved from there. We now have a very close relationship with the company.

EF: The fundamental premise of the COI Program is to carefully select and partner with thought-leading scientists around the world who are already using our technology, whether that's a simple sample prep product, a piece of software or a full-blown LC-MS system. We reached out to Petur for a collaboration because he has access to an incredible range of samples – from police departments and so forth around Europe; there are few people who could claim the same! Petur has





now run many of those samples on our MS-based systems, which has given us some very interesting insights. Not only has it enabled us to further develop the instrumentation but also – even more interesting to us – the software that collects, processes and archives the datasets. It's also enabled us to expand our UNIFI Scientific Information System to include libraries of related drug compounds and their metabolites.

What are the benefits of collaboration between academia and industry?

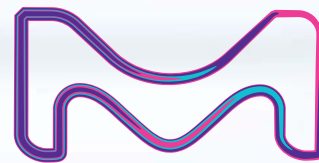
EF: That's a question I'm often asked: "What does the scientist get out of the relationship?" The key word is again 'access'. In April of 2016, we gathered our Program participants together in the UK for a set of workshops. We had them interact with our senior management team – including our CEO and the

Senior VPs – in an open forum. We discovered that our partners greatly valued that access – both to the people in our company, and to new technology. *PD:* It's true – the benefit of collaborating with Waters is that you have direct contact with the people who are programming the software or making key decisions. I have worked with Waters for a long time on software development for MS instruments; in fact, we have been working with them on UNIFI since 2011, doing beta-testing on each new version, implementing it and feeding back to them. I subsequently have a very good relationship with the programmers at Waters. We might feed back some aspects that we would like to see in the next version of the software, and that can be a huge benefit – it's almost like getting custom-made versions for our lab!

Waters have also lent us a new instrument – an ion-mobility QTOF – and we'll be putting it through its paces to see how it performs compared with the older-generation QTOFs.

Although manufacturers have great ideas about how to build the instruments and the software, the truth is that, unless they try it out in the field and see how it works, they won't know how useful a design feature is, or if they've omitted something that should be there. We universities have the ability to do more in-depth work than instrument makers...

EF: I completely agree. We were interested in the science – there's a world of samples that we can't get our hands on directly, and that was a unique benefit for us. The benefit to Petur is being able to give his input, so we can provide him with the software that he really needs for his lab.



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What challenges do you have to tackle?

PD: One of the challenges for Waters is the time it takes to develop everything – to get everything programmed, and wait for the next version. If I ask for a software change today it could be six months to a year before we see it implemented; it's not something that can be written in a day and that you can download and run the next day. One of the challenges with the database is the maintenance – it's 'homemade' at the moment, so we need funding to improve it and make it more professional. It would also be great to centralize support for all the labs rather than having someone from each group updating it.

EF: We always have to be mindful of the workload of our partners. When

you visit Petur's laboratories and see the throughput – the sheer number of samples – it's an eye-opening number! At certain times, they are operating at full capacity, and that's not the time to insert a new request to run a new version of software. It's easy to overreach or over-ask, but I think that can be mitigated by good planning upfront and setting clear expectations.

What makes a collaboration effective?

EF: Trust. As I mentioned, when we choose a partner or enter into a collaboration, there's already a relationship there. It may start with a transaction – they buy something from us – but that's very basic. We want to develop that into a much closer partnership. I think when there is regular

contact, and the benefits are clear to the partner and to us, it's got a great chance of working out.

Want to see your collaboration featured in these pages? Get in touch at charlotte.barker@texerepublishing.com



Determination of Aflatoxin M1 in Milk

Fast and isocratic method with solid phase extraction, fluorescence detection and post column derivatization with an UVE photochemical reactor

By Juliane Boettcher and Kate Monks

Aflatoxins are the best known group of mycotoxins (naturally occurring mushroom poisons) and can accumulate on crops during storage of agricultural products, especially under warm and humid conditions. The maximum aflatoxin M1 level set by the U.S. Food and Drug Administration and European Commission is 0.5 µg/L. The application describes a fast and isocratic method applicable for the required detection limit of aflatoxin M1.

First, the analytical method was developed using a standard solution: standard concentration of 1 µg/mL aflatoxin M1 with fluorescence detection and post column derivatization using the UVE photochemical reactor. To make sure that the legal limit value is detectable, a milk sample was spiked with aflatoxin M1 to a concentration of 0.5 µg/L and pretreated with online solid-phase extraction (SPE). Figure 1 shows an overlay of the spiked milk sample after sample preparation and the aflatoxin M1 standard. Although matrix effects occur through SPE pretreatment, it was possible to quantify aflatoxin M1 in the measured milk sample spiked down to 0.5 µg/L. For sample pretreatment the following SPE procedure was conducted: 20 mL of the spiked milk was diluted with 30 mL distilled water. A CHROMABOND® C18 ec SPE column was conditioned

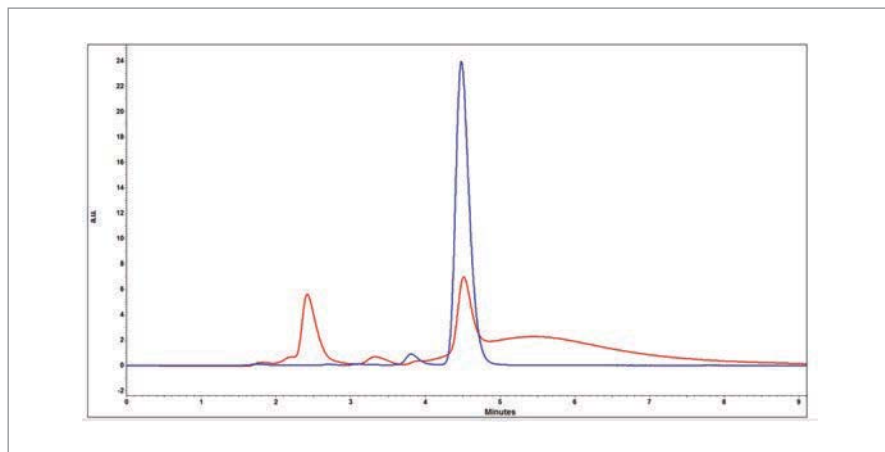
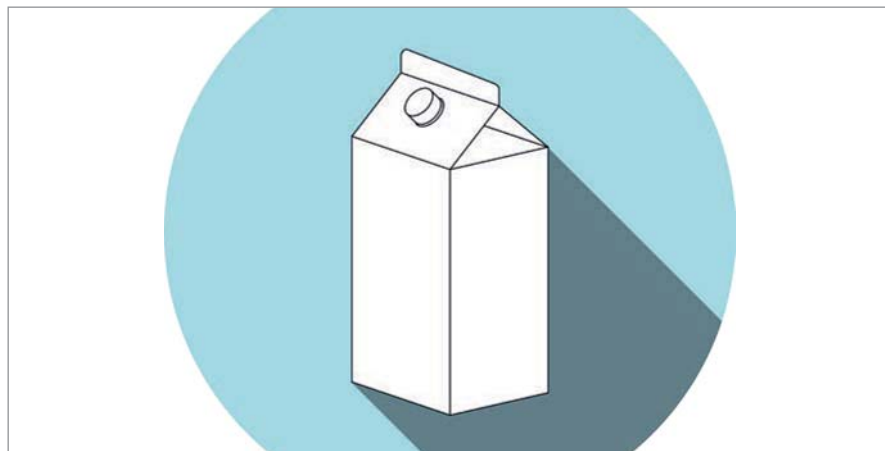


Figure 1. Overlay of spiked milk sample with M1 after SPE (red) and standard (blue).

with 10 mL water and 10 mL n-hexane. Afterwards, the column was dried for 10–20 min at 50°C or overnight at ambient temperature. After drying, the sample was eluted with 3 mL acetonitrile.

An AZURA® Analytical HPLC Plus system was used for this application. It consisted of an AZURA® P 6.1L low pressure gradient pump, an autosampler 3950, a column thermostat CT 2.1, the UVE photochemical reactor and fluorescence detector RF-20Axs. The analytical method was run isocratically at a flow rate of 0.8 mL/min with a mixture of water, methanol and acetonitrile 60:25:15 (v/v/v). The column thermostat was set to 30°C and the detector was set to excitation 365 nm/emission 455nm.

The sensitivity was adjusted to 'high' with a gain of 16. The used column was filled with KNAUER Eurospher II 100–3 C18 silica.

Using the UVE photochemical reactor for post-column derivatization in combination with the AZURA® Analytical HPLC system and fluorescence detection, the valid maximum limit values of 0.5 µg/L for aflatoxin M1 in milk and other dairy products could be quantified.

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[http://www.knauer.net/de/
applikation/determination_of_aflatoxin_
m1_in_milk.html](http://www.knauer.net/de/applikation/determination_of_aflatoxin_m1_in_milk.html)

A man in a light blue dress shirt and a blue and orange striped tie stands in a laboratory setting. He has his hands on his hips and is smiling at the camera. The background shows laboratory equipment and blue storage bins.

Texas Titan

Sitting Down With... Kevin Schug, Shimadzu Distinguished Professor of Analytical Chemistry, University of Texas at Arlington, USA.

Did you always know you'd be a chemist? My father was a chemistry professor, and I grew up running around the halls of Virginia Tech – I don't think that was the deciding factor in my becoming a scientist, but it certainly helped. At one point, I thought I might become an archaeologist – I wanted to be Indiana Jones – but a 'D' in my "Intro to Archaeology" class meant those hopes were dashed! I played football in college and a lot of other football players started out as chemistry majors and switched to less demanding disciplines, but I went in the other direction; I gave up football and stuck with chemistry.

Why specialize in analytical science? In my sophomore year, I contacted three or four professors at Virginia Tech in the hope of getting a summer internship. Harold McNair was the first to get back to me and had the best funding offer, so I decided to go and give this chromatography thing a try... It was a great experience; I participated in the short courses the group taught, got to do some research and gained hands-on experience. The next summer Harold arranged an internship for me at SC Johnson & Wax in Racine, Wisconsin, as a quality assurance technician. I suspect he did it to trick me into going to graduate school! By the end of the summer, I had learnt a lot, but the work was repetitive, and I was ready to move on and pursue a graduate degree in analytical chemistry in Harold's lab.

Harold's been a big influence on you... Harold's lab was a fantastic environment for a graduate student – a diverse group of people, great training, and interesting science. He taught us how to connect with people, and to value both research and teaching. The way I run my group is very much influenced by how I was managed by him, and also by my postdoctoral adviser, Wolfgang

Lindner at the University of Vienna. Their mentorship was exceptional. From them I learned humility, to treat people with respect, and that the old adage "there are no stupid questions" is true at any level. I also gained the ability to communicate with a variety of people from professors, to the person on the street – the importance of being able to explain your work to any audience is something I now preach to my own team.

How important have industry partnerships been for you? I consider them a real strong point of our group – we've had some great industry partnerships with Shimadzu, Restek, VUV Analytics and others. In fact, the vast majority of our support is from non-traditional funding sources – industry contracts or private donations. It's been absolutely essential for our environmental analysis, because there just aren't traditional funding mechanisms available to research things like the environmental impact of oil and gas extraction. I'm lucky that my university considers industry involvement a big positive, so the fact that I don't currently have government funding has never held me back.

What are you focusing on right now? Our 20-strong group has three main research areas: the first and biggest is CLEAR (the Collaborative Laboratories for Environmental Analysis and Remediation) – assessing the real or potential environmental impact of industrial processes. The second area is our work with VUV Analytics, and involves GC-VUV for environmental analyses, but also petrochemical, biological... you name it! Essentially, we're exploring the application of new technology, trying to prove where they have novel utility. The third area is bioanalysis, focusing on LC-MS and on-line sample preparation, and now

moving to multidimensional separations. We're trying to push the envelope on dimensionality for preparing samples and resolving complex mixtures – with a strong focus on analyzing intact proteins.

And where do you see the future of the group?

I think we're already heading in the right direction, and will continue to pick up momentum. We're ramping up our efforts in multidimensional HPLC. I went to Italy and spent a semester with Luigi Mondello at the University of Messina to learn about this approach and to bring it back to the US, because it's a largely underutilized but very powerful technique. There are great opportunities to apply it in the protein analysis realm.

On the environmental front, we're starting to make some important connections across the board. We hope to be a bridge between the environmental and industrial lobbies and be trusted as an independent voice. We must find common ground if we're to provide best practices and recommendations to keep things clean, whilst also maintaining the extraction of energy that has become so important. We're even organizing a conference in April in Dallas, called "Responsible Shale Energy Extraction", bringing the different sides together.

Our relationships with Shimadzu and VUV are ongoing – they will keep releasing new instruments, and we will continue to relish the opportunity to play with them first!

What drives you?

I'm easily distracted by shiny objects! I'm motivated by curiosity, and by the prospect of doing something new. Analytical chemistry is a wonderful field in that there's a vast array of unanswered questions and ways to approach them – that makes it very exciting to develop new technologies and methods.

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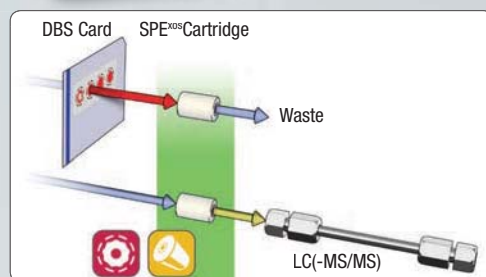
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