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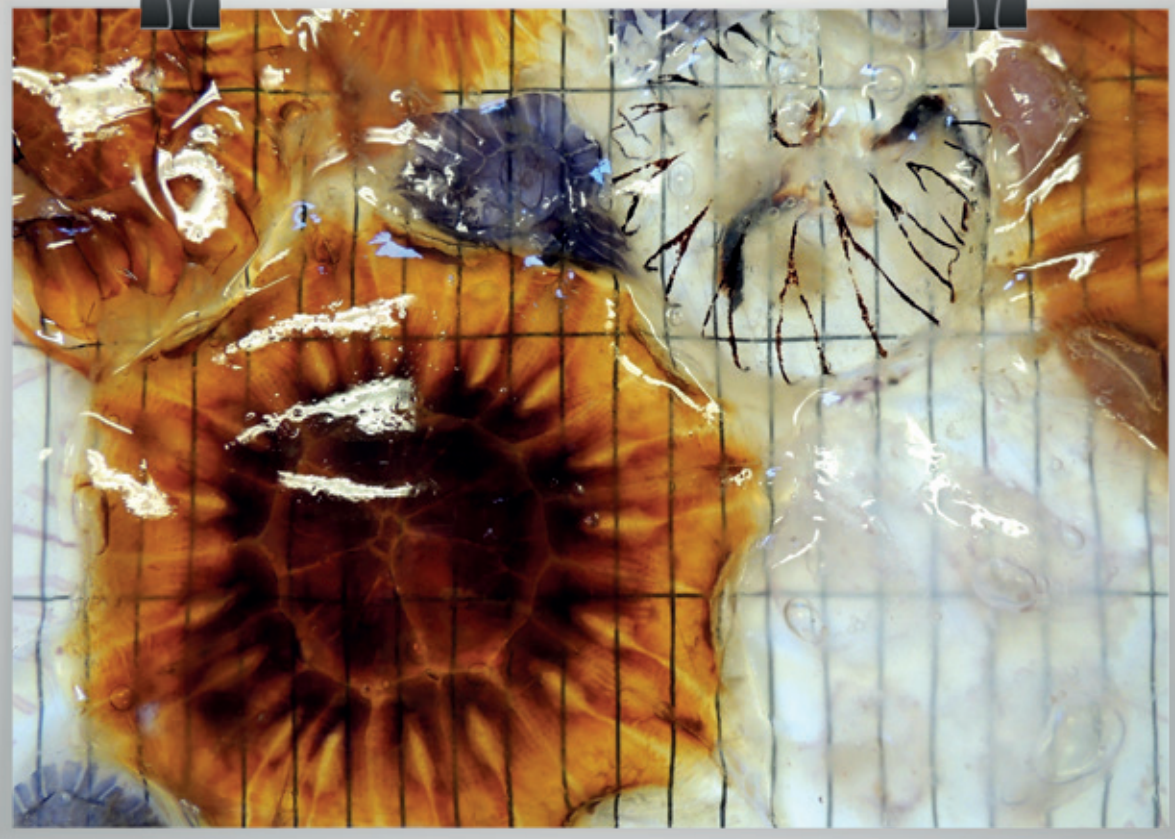
Image of the Month



Where the Jellyfish Roam

Following the path of seafood from 'fisherman to fork' is important for regulating the industry and reassuring consumers – but current analytical methods are limited when it comes to proving claims about origin. Luckily, jellyfish are joining the frontline in the fight against food fraud. Scientists from the University of Southampton recently used the "chemical record" collected from jellyfish to create a stable isotope-based map of the seas (1).

Reference 1. CN Trueman et al, "Stable isotope-based location in a shelf sea setting: accuracy and precision are comparable to light-based location methods," Methods, Ecol. Evol. [online only] (2016)

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

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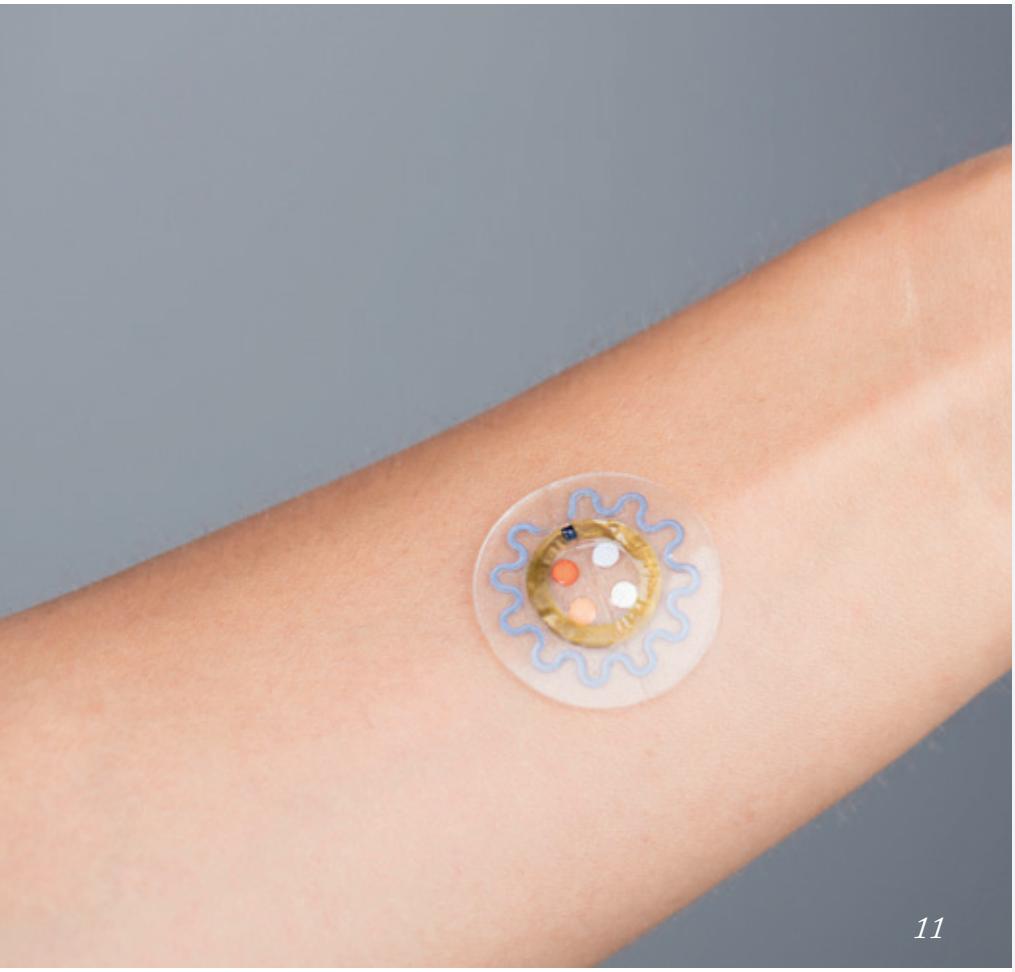

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the Analytical Scientist

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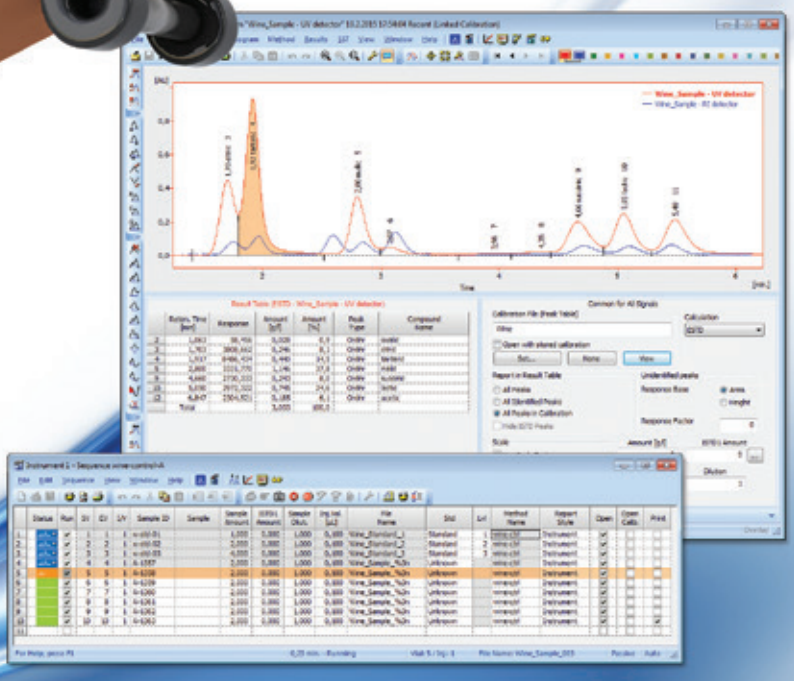

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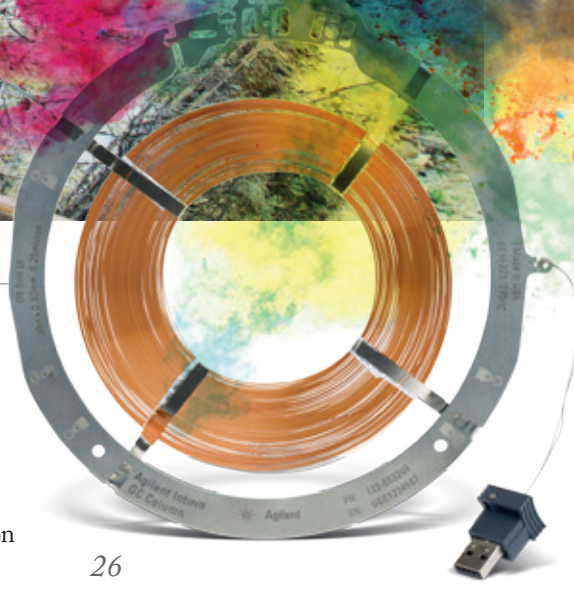

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HUMANITY IN SCIENCE AWARD

2016 Winner
Waseem Asghar

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Combined Wisdom

Twelve brilliant quotes from a year's worth of "Sitting Down With..."

Over the past year, the editorial team has had the pleasure – and honor – of interviewing gifted, inspiring, and often humble analytical scientists. I decided that the final issue of the year was a great time to share their thoughts rather than mine...

1. "Chromatographers are not magicians and separations do not happen by magic (although it sometimes seems like they do)! In reality, you need to understand what you are looking for, which is why it is so important to teach basic concepts."
2. "Who says you can't have fundamental and applied science working together? The one cannot exist without the other!"
3. "I'm helping humanity in some way; there's no greater goal."
4. "What questions are compelling in other fields, and how can you contribute? That's how to stay excited and engaged."
5. "A lot of my ideas come from keeping my eyes open to what's really happening in the chemistry, and not taking as gospel what people think about a particular system. People can sometimes make the mistake of turning speculation into fact..."
6. "I'm not a biologist and a biologist is not an analytical chemist – and we might both need informatics support. In other words, we need to work together. Modern science is very much a team game."
7. "Life will take you where you do not expect. Take advantage of what you have when you have it."
8. "We take our analytical equipment (often instrumentation we have developed ourselves) to the museum, and we really get up close with masterpieces – normally, you are not allowed to touch!"
9. "The feeling that you reached a new level of understanding – that excites me very much. It's a little bit like being the first man on the moon."
10. "How can we measure tiny quantities, in real time, in complex biological systems? It's incredibly challenging, but if we can develop the right tools, a whole new world of opportunities opens up in terms of what we can understand about the world around us."
11. "Some professors don't want their students delaying their research by working in industry for the summer – they should stay in the lab, doing basic research! Eighty percent of PhD students in the USA go into industry, yet 90 percent of grad students are taught that they should become academics. There's something wrong there."
12. "As a community, we need to invest more in the education of our students; they need to be free enough – financially and emotionally – to do the crazy stuff."

Best wishes for the New Year!

1. *Carlo Bicchi*
2. *Lutgarde Buydens*
3. *Waseem Asghar*
4. *Frank Bright*
5. *Chris Pohl*
6. *Jessica Prenni*
7. *Gary Christian*
8. *Koen Janssens*
9. *Albert Heck*
10. *Emily Hilder*
11. *Harold McNair*
12. *Sarah Trimpin*

Rich Whitworth
Editor

Upfront

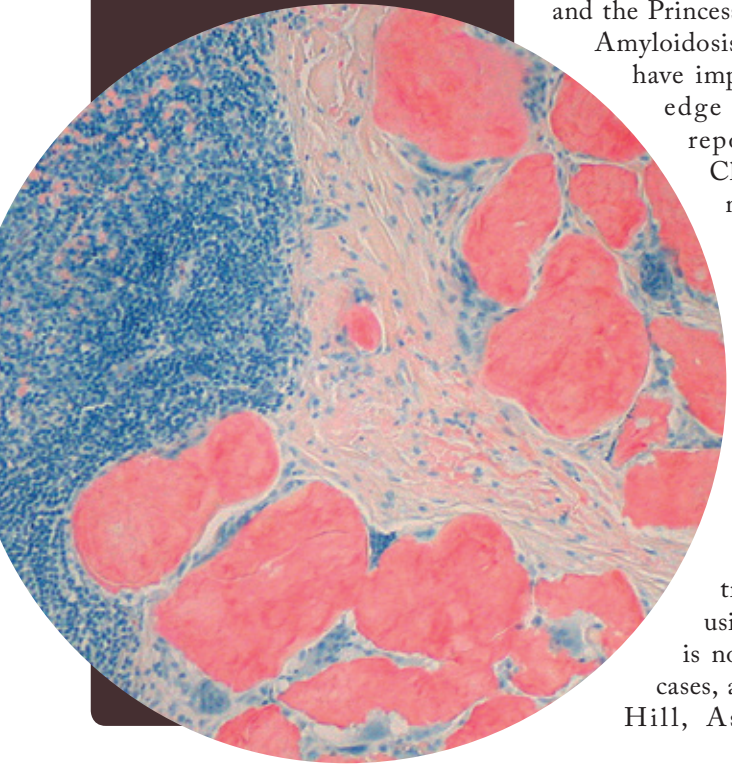
Reporting on research, personalities, policies and partnerships that are shaping analytical science.

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

Detecting Dangerous Deposits

Could tandem mass spec improve detection of amyloidosis-causing proteins?

Amyloidosis is a rare, devastating and potentially deadly condition caused by the buildup of abnormal proteins in tissues and organs. More than 28 subtypes have been identified, each caused by one of a number of possible proteins. And finding appropriate treatment depends very much on correctly identifying the culprit. Moreover, treating the wrong type of amyloidosis can make things worse instead of better – so accurate identification is crucial.



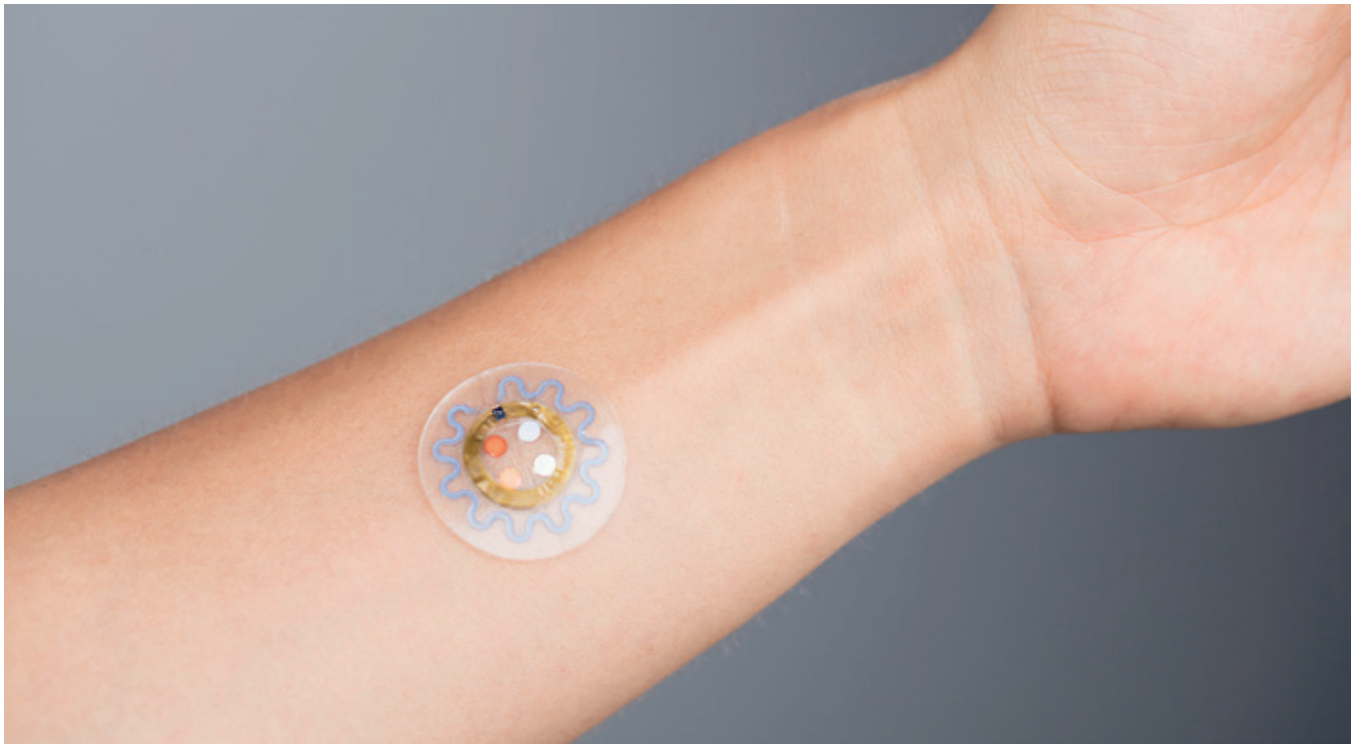
Now, a multidisciplinary team from the University of Queensland and the Princess Alexandra Hospital Amyloidosis Centre, Australia, have implemented a cutting-edge technique recently reported by the Mayo Clinic in an attempt to more accurately detect these amyloidosis-causing proteins. The combination of laser-capture microdissection (LCM) and liquid chromatography-tandem mass spectrometry (LC-MS/MS) offers an alternative to the traditional method of using antibodies, which is not successful in most cases, according to Michelle Hill, Associate Professor from The University of Queensland Diamantina Institute.

In fact, the new method proved to be significantly more effective in identifying the causal proteins, with a success rate of 92 percent, compared with 45 percent when using amyloid typing by immunohistochemistry. With these superior results, Hill says, the LC-MS/MS test is set to become the new gold standard for amyloidosis subtyping. "Being able to accurately diagnose the subtype, and hence administer the correct treatment in a timely manner, will greatly improve the health and emotional outcome of patients."

Hill, whose team runs tests at various stages of research and development (mainly for diagnosis or prognosis of cancers) expects the current work to have a positive impact on the day-to-day work of hematology and pathology professionals. However, she acknowledges that, because of equipment costs and the complex nature of the procedure, further development is needed to improve access for patients. "The level of expertise required for this analytical technique means that widespread establishment of an LC-MS/MS test may not yet be feasible, and a referral system to a specialist diagnostic center may be required," Hill says. "Currently, my team is looking at simplifying the test, which should also reduce the cost. Imaging mass spectrometry has recently been reported for localized detection of amyloid peptides in situ, and this is certainly something worth evaluating further." *JC*

Reference

1. *P Mollee et al, "Implementation and evaluation of amyloidosis subtyping by laser-capture microdissection and tandem mass spectrometry", Clin Proteom, [Epub ahead of print] (2016).*



Biomarkers, Sweat, and Tears

A novel wearable biofluidic device could noninvasively analyze biomarkers in sweat to help diagnose disease

An eight hour fast, a pin prick, and a blood test. Standard procedure when testing for diabetes, but could the same diagnosis be made by wearing an epidermal patch instead? Researchers at Northwestern University are working towards making that a reality with their "lab on the skin" device which collects, stores, and analyzes sweat in real time (1). Why focus on sweat? John Rogers, Professor of Materials Science and Engineering at Northwestern University, explains, "Sweat is an interesting class of biofluid because it can be captured noninvasively. We were looking to work on a simple type of device capable of performing in situ chemical analysis of sweat, as well as analyzing sweat rates and total sweat loss." Sweat contains an array of biomarkers, so the approach has potential as an alternative to invasive diagnostic tests.

The wearable epidermal device collects sweat through microchannels and displays pH, chloride, glucose, and lactate levels via colorimetric analysis. An embedded NFC coil allows the wearer to optionally connect their phone to the device with a simple tap, then take a photo of the device, enabling the phone to quantitively determine the status of each metric.

"We're focused first on fitness and sport, partly because the application requirements are relatively easy to meet. But we're simultaneously exploring sweat glucose measurements with relation to diabetes patients, and sweat chloride measurements as an assessment of cystic fibrosis," says Rogers. The team also suggest that the device could be modified to noninvasively test other bodily fluids, such as tears or saliva.

The investigators previously developed a whole suite of electronic devices that interface with skin to perform clinical quality measurements. The latest device is an evolution of those projects – cheap, durable, and power-free, but with a stronger focus on fluidics and analysis. "In terms of technology, we're taking the next steps in integrating fluidics with electronic/optoelectronic functions beyond what we've demonstrated with our 'lab on the skin' device," concludes Rogers. *WA*

Reference

1. *A Koh et al., "A soft, wearable microfluidic device for the capture, storage, and colorimetric sensing of sweat", Sci Transl Med, 8, 336ra165 (2016). PMID: 27881826.*

Hongen Jiang

The Grateful Dead?

Cannabis plants over two millennia old have been discovered in Chinese tombs

Dead men don't wear plaid... But they can be shrouded in the leaves of cannabis plants. The recent discovery of a corpse decorated with archeobotanical remains – with some identified as cannabis – has provided archaeologists with an insight into ancient burial rituals in prehistoric Central Eurasia.

The construction of modern tombs in the Jiayi cemetery of Turpan, Northwestern China, recently led to the discovery of several burial chambers, including an ancient tomb where several plants were arranged around the body of a buried male. Radiometric dating indicated that the tombs – as well as the plants – are approximately 2,400–2,800 years old.

To determine the age, three samples from the tomb were selected and sent to Peking University for analysis by accelerator mass spectrometry (AMS) – a stem from the cannabis plant, a femur from the skeleton itself, and a reed straw from the pillow beneath the head of the deceased. "Using AMS is fairly routine for dating the age of plants, and tombs like the one in Turpan," explains lead author Hongen Jiang (1). "I confirmed the plant identification using scanning electron microscopy (SEM), which shows the morphology of the plants in detail, including the surface of the plant organ, and even the structure of the seed cell walls."

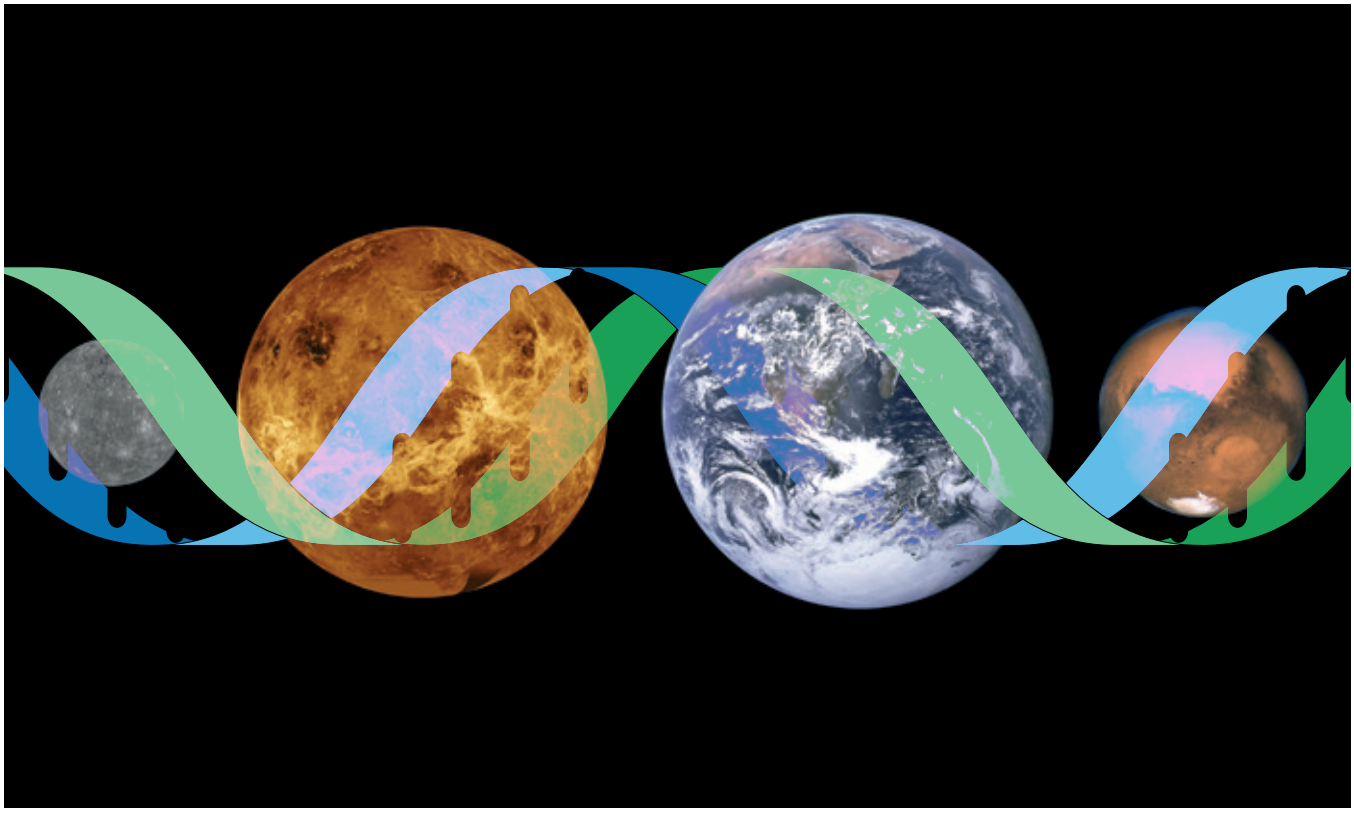
Jiang says it is impossible to say whether the marijuana was used for ritual purposes based just on an analysis of the plant itself. But the arrangement of the plant was significant. "It seemed to have been purposefully placed over the body, suggesting that the plants had some significance to the buried man, or that it was imagined the plants could be of use in the afterlife," proposes Jiang.

According to Jiang, it's the first time that such old whole plants of cannabis have been discovered, which allows researchers to draw some conclusions about how it was used and sourced. "Fragments of cannabis have been discovered in Central Asia and Southern Siberia on several occasions, but nobody knows where they were from, whether they were collected from other areas, or moved via trade," says Jiang. In the case of the Turpan tomb, the fact that whole (rather than fragmented) plants were discovered suggests that they were cultivated or collected locally. It was an amazing discovery."

Based on archaeological excavations – as well as The Histories of Herodotus – it seems that cannabis use was very popular during the first millennium BC, with other discoveries asserting that it may have been used recreationally or for medicinal purposes. "The cannabis discovered in the Pazaryk cemetery was found in containers, with the seeds carbonized due to burning, and in other parts of the coeval Yanghai cemetery parts of leaves, seeds, and small twigs were discovered in leather baskets or wooden basins – very like the cannabis used today," says Jiang. *JC*

Reference

1. *H Jiang et al, "Ancient cannabis burial shroud in a central Eurasian cemetery", Econ. Bot., 70, 213–221 (2016) [published online: 20 September 2016]*



One Small Sequence, One Giant Leap

Gene sequencing blasts into orbit

NASA runs a full program of biomedical research, with this year seeing space studies on the effect of stem cell-derived cardiomyocytes and drug pill properties, amongst others. Now, the agency has sequenced DNA in space for the first time (1), rapidly sequencing one billion base pairs aboard the International Space Station (ISS).

Why sequence in space? Sarah Wallace, project manager of the investigation at the NASA Johnson Space Center, explains, "Right now, we don't have any abilities to diagnose infectious disease or identify any microbial contaminants that are on the ISS. We do monitor though; the crew do take samples, but we have to wait until we get them back to our lab on Earth before we can tell the astronauts what was in the air they've been breathing, the water they've been drinking, or on surfaces they've been touching."

Most conventional sequencing devices are large, power-intensive, and vibration-sensitive – not optimal for transport or operation aboard the ISS. It was the availability of a palm-sized sequencer, the MinION, that made the project feasible, says Aaron Burton, principle investigator of the investigation at NASA Johnson Space Center, "A DNA sequencer like the MinION is really versatile, especially for a task like microgravity sequencing, and no doubt there are people out there who can think of even more creative ways to use it."

As well as the team at the NASA Johnson Space Center, the NASA Ames Research Center, Goddard Space Flight Center, Cornell University, and the University of California San Francisco were all involved with the collaborative project.

"We really hope that this gives us the ability to transform space flight research. We will be making the data from our experiments accessible in the not too distant future, so look out for that," concludes Wallace. *WA*

Reference

1. *NASA, "Biomolecule Sequencer (Biomolecule Sequencer) – 09.21.16", (2016). Available at: http://go.nasa.gov/29ptljd. Accessed September 23, 2016.*

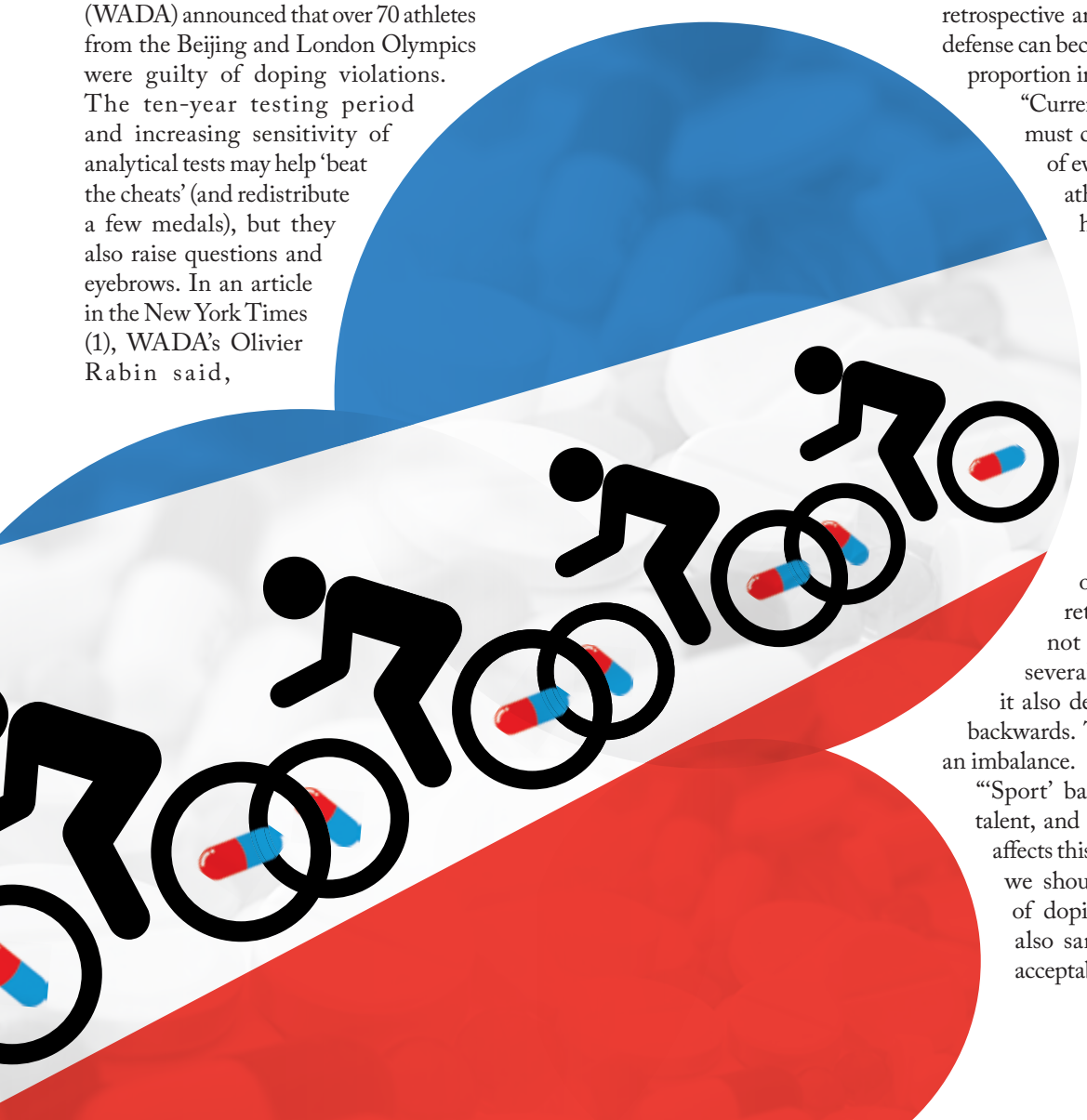
A Decade of Doping – and Analytical Advances

More sensitive methods have stripped 40 Olympians of their medals – but are we on the right track?

In November, after a series of retroactive tests, the World Anti-Doping Agency (WADA) announced that over 70 athletes from the Beijing and London Olympics were guilty of doping violations. The ten-year testing period and increasing sensitivity of analytical tests may help 'beat the cheats' (and redistribute a few medals), but they also raise questions and eyebrows. In an article in the New York Times (1), WADA's Olivier Rabin said, "Science progresses every day. Just over the past probably five years, the sensitivity of the equipment progressed by a factor of about 100. You see what was impossible to see before."

On the other hand, Gian-Franco Kasper – a Swiss executive board member of the International Olympic Committee – was quoted in the article as saying, "We need to stop pretending sport is clean. It's a noble principle, but in practice? It's entertainment. It's drama."

We asked three doping experts about the balance between analytics and ethics. Here, we present the highlights; to see their full responses, please visit the online version of this article: tas.txp.to/1216/sportsdoping



Douwe De Boer

Technical lab expert for Hospital Projects, Department of Clinical Chemistry, Academic Hospital, Maastricht

"Retrospective analysis can only be justified if the sanction is proportional to the ways that athletes can defend themselves […] There is also a strong misconception that laboratories never make a mistake. If we increase the period of sanction as well as the period that the retrospective analysis can go back, a fair defense can become impossible and out of proportion in relation to the sanction.

"Currently, the doping authorities must collect a minimal amount of evidence, while the accused athlete is supposed to prove his or her innocence with a maximum amount of effort […] We should perhaps require that the doping authorities collect a maximum amount of evidence, like in criminal justice, while the accused athlete should only be required to prove the opposite with minimal of effort. […] Moreover, retrospective analysis does not only imply a sanction several years into the future, it also destroys a complete career backwards. This creates even more of an imbalance.

"'Sport' basically rewards sporting talent, and the application of doping affects this basic principle. Therefore, we should never accept the use of doping although we should also sanction athletes in a fair, acceptable and proportional way.

Otherwise, we may as well skip other sports rules and principles and revert back to the old Roman gladiator games, where everything was allowed – as long as it added to the 'drama.'"

Herman Ram
Director, Doping Authority, the Netherlands

"The use of doping is unethical, not the detection thereof. There is a clear Statute of Limitations in the rules (presently 10 years) and analytical scientists should do their best to detect doping use within that period. After the Statute of Limitations, no disciplinary proceedings can be started, of course.

"Regarding Kasper's comments, it seems as though he is throwing in the towel – thus abandoning all athletes who want to compete clean. Sport isn't clean, and it will never be completely clean (and I myself certainly have never stated otherwise). But although the fight against doping is far from perfect, it is our duty to protect clean athletes to the best of our abilities. Allowing doping for the sake of the entertaining qualities of sport is an unacceptable infringement of athletes' rights."

Francesco Botrè
Professor, Department of Experimental Medicine, Sapienza University of Rome, Italy

"Not only is analytical technology getting progressively better […] so too is our knowledge of the pharmacological profile of the prohibited drugs, which is perhaps a bigger factor. The isolation of a previously unknown metabolite can prolong the window of detection of a given drug over a very long period – even longer than what could be achieved by targeting an 'old' metabolite using newer instrumentation […] In other words, advances in doping detection is a combination of biochemistry, pharmacology, organic chemistry, protein chemistry, molecular biology – and, of course, analytical chemistry.

"There is no 'end' from a merely analytical point of view; clearly, the discrimination between an actual doping offense (i.e. intentional intake) and accidental doping is more and more difficult as the detected concentration of the prohibited drug/metabolite decreases. The issue of ensuring a long-term retrospective detectability of specific drugs could be overcome by a more frequent testing of the athletes. Should an athlete be tested, let's say, every other week, it would be no longer necessary to ensure a LOD allowing the detection of a drug taken six months earlier..."

Reference

1. *New York Times, "Olympics history rewritten: new doping tests topple the podium", http://www.nytimes.com/2016/11/21/sports/olympics/olympics-doping-medals-stripped.html*

Cytometry, Super-Conductivity, and SOPs

What's new in business?

In our regular column, we partner with www.mass-spec-capital.com to let you know what's going on in the business world of analytical science. This month, column chemistry gets a shot in the arm with products from Waters and Phenomenex, while the International Phenome Centre Network (IPCN) is launched with key partners for the advancement of precision medicine.

Products

- Ionicon launches new PTR-TOF 4000 Trace gas analyzer.
- Phenomenex: new clarity columns for RP and IEX chromatography.
- Fluidigm introduces new Maxpar mass cytometry panels.
- Waters expands Cortecs analytical column portfolio.

Collaborations

- Novasep and Japanese agent AR Brown extend partnership.
- Advion names Accurate Mass Scientific as Australian distributor.
- International Phenome Centre Network launches with Waters as a founding partner.
- Bruker announces corporate partnership with International Phenome Centre Network (IPCN) for NMR Technologies and SOPs.

People

- BioMérieux appoints Pierre Boulud Corporate VP Asia Pacific.
- Danaher promotes Rainer Blair to EVP Life Sciences Business.
- Protea Biosciences promotes David Halverson to President.

Investments & Acquisitions

- Bruker's BEST acquires superconducting wire business of Oxford Instruments.
- Bruker completes acquisition of Oncovision's PET imaging business.

Organizations

- Agilent Technologies opens Folsom, CA, Technology Center.

For links to all press releases and more information, please visit the online version of this article: tas.txp.to/1216/BUSINESS

Mark Viant, Myra Nimmo and Sir Mark Walport at the opening of the Phenome Centre Birmingham – part of the International Phenome Centre Network (www.phenomenetwork.org).

Cheers to GC!

As you stockpile your favorite beverage ahead of New Year celebrations, we ask: what does gas chromatography bring to beer, wine and whisky analysis? Richard Law has the answers...

When I think about key advances in gas chromatography, the birth of the capillary column actually stands out as the biggest game changer – despite the fact that it was a long time ago. I guess some major advances are never superseded (although I know of people who are still working in the 'Dark Ages' with packed columns, believe it or not). The leap in performance afforded by capillary columns really opened GC up to a much broader set of applications; I've personally analyzed everything from Wellington boots to Silly String – both of which may also feature in your end of year celebrations...

Fancy a beer?

Liisa Otama covered the "BeerMaster" Analyzer in an earlier article of this "Cheers!" series (http://tas.txp.to/1216/beermaster), but gas chromatography still has a role to play. For example, diketones are important natural ingredients in beer aroma and characterized by their 'buttery' flavor, but to lager manufacturers, they are considered 'off-flavors' and must be carefully monitored. In 1999, the European Brewery Convention (EBC) issued a method for the determination of vicinal diketones (2,3-butanedione and 2,3-pentanedione) in beers via headspace GC. The EBC method is especially challenging because it demands that samples are incubated at 35°C, which necessitates the use of expensive cryogenic systems (unless you have access to a Thermo Scientific™ TriPlus™ 300 headspace autosampler and its ability to operate at 35°C without such systems...). You can find more information about the autosampler and the use of GC-MS in diketone analysis in an application note devoted to the EBC method here: http://tas.txp.to/1216/beer.

Or perhaps a glass of wine?

To the wine drinkers among you, it's most likely obvious that wine aroma and flavor is dictated by a highly complex mixture of compounds. Notably, certain chemical impurities are key indicators of quality; examples include volatile phenol compounds (from yeast metabolism) and haloanisoles (from cork fungal infections). Though few analytical techniques can compete with the nose and taste buds of an experienced wine guru, GC-MS has proven itself to be an excellent companion. Indeed, the identification and quantitation of maturation tracers and the molecules commonly responsible for taste defects has become an important part of modern day quality control.

In fact, the Thermo Scientific ISQ™ Single Quadrupole GC-MS system is able to detect a number of wine contaminants at lower concentrations than its human counterparts. Couple that sensitivity with ease of use and rapid single-step sample preparation and wineries have a new go-to tool for impurity analysis. Learn more about GC-MS analysis of various critical compounds in wine here: http://tas.txp.to/1216/wine

How about a whisky nightcap?

Delving deeper into increasingly complex samples using GC is an ongoing trend that is only made possible by the increasing accuracy and sensitivity of modern MS systems. The introduction of the Thermo Scientific Exactive™ GC Orbitrap™ GC-MS and Q Exactive GC Orbitrap GC-MS/MS systems take gas chromatography into the exciting territory of high-resolution accurate mass (HRAM) measurements, opening up yet more potential application areas.

Jana Hajšlová (Professor and Laboratory Head, Department of Food Chemistry and Analysis, University of Chemistry and Technology, Prague, Czech Republic) has been applying GC-HRAM MS analysis in an attempt to protect Scottish whisky from fraudsters who go to great lengths to benefit from the expensive spirit. When it comes to tackling counterfeit or adulterated whisky (or any complex beverage sample for that matter), comprehensive 'fingerprinting' using full-scan HRAM data (and advanced chemometrics) is king of authentication, and is able to provide more information in a single run than ever before.

By building up databases and statistical models from whisky samples of known origin using the Q Exactive GC Orbitrap GC-MS/MS, Hajšlová and her team hope to be able to assess the authenticity of unknown samples using HRAM fingerprints. You can read Hajšlová's proof-of-concept in an application note that delves into much more detail here: http://tas.txp.to/1216/whisky.

Although capillary columns have been around longer than most of us have been able to legally enjoy an alcoholic drink or two, gas chromatography (especially coupled with cutting-edge autosamplers and MS systems) looks set to see us through a good few more New Year's celebrations yet.

Cheers to GC and Happy New Year!

In My View

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

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

Contact the editors at edit@texerepublishing.com

Depth Profiling with GD-OES

Glow discharge optical emission spectrometry (GDOES) is now able to shed light on layer thickness thanks to differential interferometry profiling (DiP).

Matthieu Chausseau, Elemental Analysis & Thin Films Product Manager, Horiba Scientific, New Jersey, USA

When I first explored GD-OES some years ago, I was impressed by the capability of the technique to perform depth profiling analysis on solid samples, determining nanometric layers and at the same time going down 150 microns into samples. My background in elemental analysis up until then was limited to inductively coupled plasma (ICP)-OES and atomic absorption, so GD-OES was able to reveal a new world to me. I learnt a lot using GD-OES – not only about the technique itself, but also the added value it lends to material science.

It is unfortunate that, despite many advantages, GD-OES remains a technique that is not well known outside of the material science world. Perhaps because there are more fashionable techniques, such as X-ray photoelectron spectroscopy, secondary ion mass spectrometry or even Auger electron spectroscopy? Or does GD-OES need to bring something over and above those techniques to find its rightful place?

One limitation of GD-OES is the necessity to use an external tool to measure the depth of samples. Having the capability to measure depth directly while performing the profile would definitely attract more users and be seen as a breakthrough for the technique. Indeed, having to use a profilometer to determine the depth looks like a real limitation. Essentially, we must either i) assume that the sputtering rate is constant over the various layers to shorten the total time for the measurement – and that means accepting some bias on depth, or ii) return to the profilometer each time to determine the sputtering rate for each layer, when measuring layer by layer on various locations on the sample. And it's not an easy choice. Moreover, profilometers can be really limited when it comes to the determination of very thin layers.

> *"I learnt a lot using GD-OES – not only about the technique itself, but also the added value it lends to material science."*

Thanks to the continuous work of passionate scientists and engineers, the GD-OES technique has continued to improve over the year. At Horiba Scientific, several different product groups (especially ellipsometry) have been working together for some time – the result? A new invention called differential

interferometry profiling (DiP). For me, this innovation breaks boundaries for GD-OES by allowing real-time measurement of depth during analysis.

DiP is based on the use of a laser source divided in two beams, one focused on the middle of the measured area and the second one directed to the intact surface. The interference between the two reflected beams is measured as the sample is sputtered, which gives a direct measurement of the crater depth. The solution seems simple once summarized in a few lines (don't all good inventions?) but a great deal of development was needed to ensure that GD-OES performance was maintained, in terms of the total amount of light reaching the optics and, crucially, also in terms of ease-of-use. The challenge was to ensure the same accuracy as a profilometer but also provide nanometric layer measurement capability.

Since its development and its introduction, DiP has been successfully tested on many different samples, including Silicon wafer, TiN coating on WC, Au thin films, CIGS solar cells, LED and DLC on Cr steel. DiP performs well on non-transparent layers, being the perfect complementary technique to ellipsometry for thickness measurement, while providing information on the elemental composition. As for the future of GD-OES, we foresee that identifying all the applications of interest will keep us busy for some time...

Inorganic Species Savior

Does the hyphenation of ion chromatography with (inductively coupled plasma)-mass spectrometry represent the pinnacle of species analysis in environmental toxicology? And, if not, what more is needed?

By Rajmund Michalski, Analytical Chemist/Professor of the Institute of Environmental Engineering, Polish Academy of Sciences, Poland.

At the beginning of the twenty-first century, analytical chemistry had to face new challenges. First and foremost, new information about the toxicological properties and forms of elements was appearing and there was a necessity for the detection and determination of gradually lowering analyte concentrations – often in complex matrix samples.

When it comes to living organisms, biological activity and toxicity of elements is governed primarily by the existence of ionic forms. Among the many analytical methods applied for ion analysis, ion chromatography (IC) is perhaps the best suited. It is a well-established regulatory method for analyzing anions and cations in environmental, food and many other samples. IC offers:

- high capacity and selective stationary phases and sensitive detectors
- simple sample preparation
- avoidance of hazardous chemicals
- decreased sample volumes
- flexible reaction options when changing sample matrix to be analyzed
- the option to operate a fully-automated system.

However, at present, there are several areas that must be addressed for ion chromatography to advance, including the need to:

- introduce new ion-exchange stationary phases
- improve the suppressor operation efficiency
- lower the limits of detection and quantification
- introduce new sample preparation methods
- extend the analysis range with new organic and inorganic substances
- increase use in molecular biology and genetics research (genomics, proteomics, metabolomics, transcriptomics)
- further develop new standards and detection methods
- miniaturize apparatus.

As noted above, toxicological tests show that what often decides the element's influence on living organisms is not the total concentration but the participation of the element's individual forms. Consequently, detection and quantitation of the various analytes forms/species (as they pertain to toxicity, bioavailability and reactivity) is the primary goal in environmental and biomedical fields. Because of the inherent challenges, there is an increasing tendency to combine diverse separation methods (for example, chromatography) and detection (for example, mass spectrometry), to which the term 'hyphenated techniques' is often given. A specific hyphenated technique should be selective towards the determined analytes, sensitive in a

"When it comes to living organisms, biological activity and toxicity of elements is governed primarily by the existence of ionic forms."

wide range of concentrations, and should enable the best possible identification of the determined species. The most popular hyphenated techniques employing ion chromatography are IC-inductively coupled plasma-mass spectrometry (IC-ICP-MS) and IC-MS; both are powerful tools when it comes to the unambiguous determination of different organic and inorganic compounds in a single run. The extremely low limits of detection and quantification as well as high accuracy and repeatability of determinations are particularly desirable in species analysis and open up several new analytical avenues.

Unfortunately, like other advanced methods, hyphenated techniques have certain limitations, such as high price and complexity, which means that they do not enjoy common usage in routine laboratories. However, in my opinion, the role and potential of hyphenated techniques in speciation analytics should not be underestimated – indeed, they are invaluable, if we wish to move forward.

I suspect that the next steps for ion chromatography (hyphenated with MS or otherwise) will include the development of new stationary phases with improved separation selectivity and new detection modes, as well as the development of capillary and two-dimensional systems. I would also add that increasing usage of IC with advanced automated in-line sample preparation techniques in species analysis will help extend its application to other complex samples. As to whether it will be a "remedy" for inorganic and organic species analysis... Why not? It simply depends on our scientific courage, curiosity and imagination.

Bring Out Your Data

Questions, questions, questions... A call for community standards and the archiving of exposomics datasets.

By Biswapriya B. Misra, Postdoctoral Scientist at the Texas Biomedical Research Institute, Texas, USA

David Balshaw (Program Director at the Center for Risk and Integrated Sciences, National Institute of Environmental Health Sciences) would rather "not define exposome at all" because of ongoing questions as to what may or may not be included (from pre-birth to death), so I too shall refrain from defining it. At one point, the routine 'food' we intake is also assigned the status of 'exposome' – and rightly so, in my opinion; developmental biologists would see the gut as a hollow tube outside the biological organ system. Given the enormous amounts of exposomics information being generated, it is prime time that community standards – otherwise known as MIAEE (Minimum Information About an Exposomics Experiment) – are introduced and adhered to.

At the American Society of Mass Spectrometry (ASMS) 2016 conference, an oral session entitled "Exposomics: Targeted, Untargeted and Bioinformatics Technologies" (chaired by Dr. Balshaw himself) and the following "Exposomics Interest Group meeting" (coordinated by Professor H. M. "Skip" Kingston, Duquesne University, and Dr. Anthony Macherone, Agilent Technologies and

"Do we need to set different workflows for metabolomics and exposomics workflows?"

Johns Hopkins School of Medicine) left the audience with more questions outstanding than answers. Most of them are valid and need to be addressed.

Who would lay the foundations for MIAEE? The metabolomics society or the exposomics community? Should there be a formal MIAEE, in the first place? Petabytes of mass-spectrometry (MS) and NMR-based exposomics datasets are being generated and published every year. But are they being archived properly? The answer to the latter question is no, if we look to popular metabolomics community

adopted archives, such as MetaboLights (www.ebi.ac.uk/metabolights/index) or Metabolomics Workbench (www.metabolomicsworkbench.org). Surely, authors could at least take the initiative and archive datasets on their webpages or institutional repositories for community access!

Is it mandatory to go for standard compound-based authentication and validation of detected and quantified metabolites? How is it possible to obtain the plethora of chemical constituents reported in single studies where the number of compounds detected can be a few thousand? How do we know what is noise (from instrument and handling) and what is from environmental/biological systems; for example, does blank air serve as the correct negative control in studies where disease biomarkers are probed in smokers? What about the platform-dependency of the exposome or for that matter geography, socio-economy-diet-genotype-race-gender affected differences in exposomes? How do we account for inter-individual differences in exposome data? Where are the databases for spectral comparisons for exposome studies, especially given that the list is ever-expanding in terms of cosmetics, antibiotics, pesticides, industrial chemicals, petrochemicals, adulterants, heavy metals, phthalates, and unknowns? Existing databases, such as NIST and HMDB, are like drops in the ocean by comparison.

What open source and commercial tools are in place to allow visualization of this peta-byte scale data on a human body or ecosystem? How can we connect exposomes to cell- or tissue-specificity or to the genotype of individuals? How can we make sure that exposure-wide association studies [EWAS] and the resulting biomarkers discovered stand the test of time?

Finally, do we need to set different workflows for metabolomics and exposomics workflows? If so, on what basis and, if not, are they interchangeable? The Metabolomics Standards Initiative (MSI) does not yet specifically mention 'exposome' – and journals do not ask for data archiving in open-access and public repositories. Exposome studies have a history of political ramifications and generate huge commercial interest, as well as playing an enormous complementary role in translational and clinical medicine. Is now not the right time to start answering some of these important but evidently ethereal questions?

Finding Fakes

Looking at the past, present and future of counterfeit drug screening.

By Ravi Kalyanaraman, Associate Director at Bristol Myers Squibb and Varsha Ganesh, Associate Scientist at Bristol-Myers Squibb, New Jersey, USA

Produced and sold with the intent to deceptively represent origin, authenticity or effectiveness, counterfeit drugs are products that contain no active ingredient, inappropriate quantities of active ingredients or other ingredients that are not found in the genuine product. Estimates suggest that the global counterfeit drug market sits somewhere between US$75 and $200 billion and represents 10–50 percent of all drugs sold in some low-income countries (1).

The first step in authentication testing is to compare the packaging and drug product appearance of the 'suspicious' product with the genuine product. However, physical appearance is easily counterfeited, so robust chemical analysis must be used to distinguish between authentic and fake drugs. Needless to say, analytical testing must be both accurate and rapid in this setting.

Traditionally, qualitative and semi-quantitative techniques – for example, disintegration, colorimetry, and thin layer chromatography (TLC) – have been employed to determine if a product is counterfeit (2). Notably, these techniques have been especially useful with regards to taking the 'lab' to the field, providing a simple and inexpensive way of determining counterfeits. Global Pharma Health Fund (GPHF)-Minilab still supplies field test kits with simple disintegration, color reaction tests and easy-to-use TLC tests for rapid drug detection and drug potency verification (3).

When it comes to a detailed characterization of counterfeit drugs, gas and liquid chromatographic techniques (GC and LC) are the most prevalent (4). Coupling mass spectrometry (MS) to LC not only assists in authentication but identifies even low concentration of substitute ingredients in a counterfeit. The drawback with such methods is the sample preparation and high lead time required for analysis. To overcome this, direct-ionization MS methods, such as direct analysis in real time (DART) and desorption electrospray ionization (DESI) are being used to eliminate sample preparation (5).

Spectroscopic techniques, such as benchtop FT-Raman and near-infrared spectroscopy (NIRS) possess a distinct advantage over chromatographic techniques in that they are non-destructive and can rapidly characterize the suspect product in seconds – even without the need to remove the drug from its packaging (6). Such portable spectrometers offer a rapid, accurate and specific means of authentication in-field, as they are able to compare the unique spectral signatures or 'fingerprints' of the authentic drug product against the suspect. Furthermore, they require little to no training, which means they can be used in the field by law enforcement officials, ensuring immediate identification and take down of counterfeit activities (7).

But what about the surge in the number of protein-based drugs on the market? The extraordinarily high costs associated with biologics make them a lucrative market for counterfeiters – as proved by the recent case of counterfeit Avastin (8). Biologics are, of course, large complex molecules, which makes them hard to characterize and fingerprint. We were part of a team at BMS that was able to show that confocal Raman spectroscopy – coupled with a specialized sample preparation technique called drop coat deposition (DCD) – can be effectively used to fingerprint biopharmaceuticals (9). The technique, coupled with peak fitting, could also be used to determine the secondary structure of the biologics and even offer a way to distinguish between biologics and their generic versions (biosimilars). DCD Raman (DCDR) spectroscopy requires limited sample preparation (deposition of a microliter 'drop' of sample followed by solvent evaporation) and yet offers a wealth of structural information (secondary structure can be classified using the Amide I band).

Analytical technology for counterfeit detection has certainly experienced tremendous growth and evolution over time. However, as counterfeiters get smarter and move into the biopharma space, we must arm ourselves with superior authentication techniques. In our view, DCDR spectroscopy is one such tool.

References:

1. *World Finance, Trade in illegal medicine hits pharmaceutical sector, http://www.worldfinance.com/home/specialreports-home/trade-in-illegal-medicine-hits-pharmaceutical-sector*
2. *R Mukhopadhyay, "The hunt for counterfeit medicine", Anal Chem, 79, 2622–2627, (2007)*
3. *The GPHF-Minilab™ Protection Against Counterfeit Medicines, https://www.gphf.org/en/minilab/*
4. *FM Fernandez et al, "Prevalence and detection of counterfeit pharmaceuticals: a mini review", Ind Eng Chem Res, 47, 585–590 (2008).*
5. *L Nyadong et al, "Reactive desorption electrospray ionization linear ion trap mass spectrometry of latest-generation counterfeit antimalarials via noncovalent complex formation", Anal Chem, 79, 2150–2157 (2007).*
6. *Y-P Sacré et al, "Comparison and combination of spectroscopic techniques for the detection of counterfeit medicines", J Pharm Biomed, 53, 445–453 (2010).*
7. *R Kalyanaraman et al, "COUNTERFEITING: Portable spectrometers for pharmaceutical counterfeit detection", Am Pharm Rev, 13, 38 (2010).*
8. *M Chauhan et al, "Screening and detecting counterfeit biologics drugs", BioPharm Asia, 1, 58–64, (2013).*
9. *J Peters et al, "Raman spectral fingerprinting for biologics counterfeit drug detection", Am Pharm Rev, 19, 46–51, (2016).*

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VUV Versus Industry – Part II

In Part I, Hans-Gerd Janssen (Unilever), Pierre Giusti and Gaelle Jousset (TOTAL) considered the potential of vacuum ultraviolet absorption spectroscopy in their respective industries (tas.txp.to/1216/VUVersus). Here, Bill Winniford (The Dow Chemical Company) shares his VUV story and points to a bright future of increasing applications for a shining example of GC detector innovation.

A Vision for VUV

By Bill Winniford, Fellow, The Dow Chemical Company, Houston, Texas, USA.

We started on our vacuum ultraviolet journey about the same time as the University of Texas at Arlington – right at the beginning of March 2010. The experience so far is probably the most useful thing that's ever come out of being on LinkedIn. Sean Jameson contacted me as they were considering the potential of VUV detection for gas chromatography (GC) – even before they had constructed an instrument. They were looking for someone in driving distance of Austin with industrial experience, and found my name. It was a complete cold call, but my interest was piqued by the concept. In particular, I wanted to find out about the potential jump in sensitivity over GC-IR.

And so, Sean and Dale Harrison (the two founders of VUV Analytics) drove down to meet me for lunch. It's not uncommon to be contacted by start-up companies looking for guidance, but in that first meeting I was impressed with the knowledge level of the team – and I acknowledged that there were far worse ways of spending a lunch break...

A rude awakening

Once the VUV Analytics team had a working system in their laboratory, they asked us to send representative samples for analysis. We were particularly interested in catalyst poisons and gathered up a whole set of samples, including a number of oxygenated species – alcohols, aldehydes and ketones, and so on. We assembled a large team of people (all with high expectations) to review the results and I have to say that it was the single most disappointing time of the whole endeavor (which is fortunate, with full hindsight)! We were expecting to see a lot of distinction between spectra for aliphatic alcohols, but it turns out that they are probably the least interesting compounds in terms of obvious VUV spectral features. Looking back, it's funny – we had no appreciation of the excellent spectral reproducibility and, on the other hand, the VUV guys, with their in-depth knowledge, were excited with the results and must have been confused with our initial disappointment. Despite the hiccup, they did demonstrate one very important proof: the VUV detector was capable of good sensitivity at a timescale that gave excellent chromatographic resolution – facts that have maintained our interest ever since.

After that, the team would show up periodically to share their latest results and we'd offer iterative feedback, and in October 2012, we took delivery of the first beta-test VUV instrument. And of all the beta instruments I've worked with, I can say it was by far the best.

Running the full gamut

Once we had the detector in house, we threw every sample class we could at it to see if we could start to make any generalizations about VUV detection. Two important points that may not be immediately obvious became clear:

i. The detector response (if you look at the average response over a range of 140–160 nm, for example) is surprisingly uniform. Those who have worked with LC-UV detection will know that you typically don't expect to get a uniform response. The upshot is that on a first pass, you can do rough quantitation without

By Roy Luck (Dow Chemical plant and railcars) [CC BY 2.0], via Wikimedia Commons

calibration, which is incredibly useful.

ii. Because the spectra don't appear to be very distinct, most people would assume that either they aren't useful, will make library searching difficult or would be sensitive to matrix effects (remember 'Rude Awakening' above). In reality, the spectra are remarkably rock solid. And that means that even if spectra appear to differ only slightly, they can still be accurately library matched, which is a huge – and somewhat unexpected – advantage. Moreover, we have yet to see any matrix effects. Even the temperature of the flow cell, which you might envisage impacting electron transitions, seems to have very little effect on spectra stability.

Over time, another really important point popped out: it does a great job of distinguishing between isomers. And though it has caused a little controversy in certain circles, we've had real success in using computational tools to model spectra to predict differences between isomers; useful trends become apparent when using the system, such as the fact that a conjugated diene will have a certain spectral feature out at a longer wavelength than an unconjugated diene. It's a tremendously powerful tool for investigating trace levels of unknown components in a matrix – say an odor, color or catalyst species. With VUV detection, we can get useful spectra down to part-per-million levels of sensitivity, and we stand to gain information that is very complementary to mass spectral data – especially important when it comes to problem solving.

One of my main roles is to seek out new technology and techniques that can solve the analytical challenges we face – and I can state that we've also found the combination of GC×GC with VUV detection very helpful in this regard. All good news, but any start-up analytical company needs a sponsoring application – either something that no one else can do or something that it does so much better or more cost effectively. In the hydrocarbon world alone, the VUV detector has proven itself with the ability to distinguish olefins and aromatics from aliphatics – that's a killer application given the complexity and time involved using any other technique. The VUV detector's ability to perform a more accurate and much more robust PIONA analysis is an important milestone in its ongoing success.

Process VUV

The utility and robustness of the VUV detector in process analytics is exemplified by the announcement that VUV Analytics are working with Wasson-ECE Instrumentation. Together they will integrate the VGA-100 with Wasson-ECE's enclosures and process chromatography to provide fully automated analyzers that can be used in hazardous locations in hydrocarbon processing. This direction is of great interest to us because the outcome will potentially simplify process GC applications. The VUV detector doesn't require an additional gas supply and it provides a great deal more information than FID. The VUV detector is also far more sensitive than process TCDs (thermal conductivity detectors). And the only maintenance required is the replacement of the deuterium lamp – which you get an automatic warning about. Simplified, more sensitive and more robust is a desirable combination.

Notably, in the world of process applications, we would always choose an optical method over a GC method (if the spectra are different enough that pre-separation is not needed). Why? Because it's a less complex and much more cost effective – and that's why we use IR and NIR spectroscopy a lot. Perhaps it's no surprise then that VUV Analytics has already launched the SVGA-100 for analysis of streaming gases without a GC – another interesting direction...

VUV vision for the future

I've been doing separation science for almost 40 years, and I've lived through many examples of where technology has positioned itself as a game changer – and perhaps overstated its usefulness; people have become wise to this over time. The VUV detector, I believe, will follow a similar path and trajectory to comprehensive GC, where you see the application space steadily growing without any hint of slowing down. Critically, the VUV detector is a high-quality instrument, and will not disappoint scientists who try and fail with applications; reliability has been nailed – and that's essential for wider adoption.

And the faster VUV detection is adopted, the faster the cost can come down, which is another important factor for industry, especially when employing technology at scale. Once VUV detection hits a magic number, I can see its use being very widespread indeed.

Perhaps most excitingly, because the vacuum ultraviolet range is such a new area of the electromagnetic spectrum (aside from people working at synchrotron facilities), people are going to keep finding new applications – there's still so much more to explore. I'm personally very much looking forward to following – and being part of – the continuing VUV journey.

the Analytical Scientist
Innovation Awards
2016

Innovation Explosion

It's time to roll out the TASIAs tagline: "accurate measurement drives progress in science in immeasurable ways" as The Analytical Scientist Innovation Awards return for a fourth year to celebrate creativity and invention. From smarter spectroscopy to simpler separations, we present our Top 15 innovations of 2016.

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HIGH-THROUGHPUT DIRECT GAS ANALYSIS

High-throughput gas and headspace analysis via automated SIFT-MS.

Produced by Syft Technologies and Anatune

In 2016, the automated SIFT-MS solution was commercialized as the outcome of collaborative research and development by Syft Technologies and Anatune, which integrated and optimized the Gerstel MPS multipurpose autosampler system for use with the Syft Technologies Voice200ultra SIFT-MS instrument.

Selected ion flow tube mass spectrometry (SIFT-MS) is a cutting-edge analytical technique for real-time measurement of trace gases with detection limits in the low parts-per-trillion (ppt) concentration range. The high selectivity achieved by this chromatography-free, direct-analysis technique is achieved by application of multiple, switchable chemical ionization reagent ions coupled with mass spectrometric detection.

Automation of rapid SIFT-MS analysis provides unique opportunities for comprehensive, high-throughput sample analysis. The application of direct, ultra-soft chemical ionization enables headspace and gas samples containing routine and chromatographically challenging compounds (such as ammonia, formaldehyde, hydrogen chloride, and hydrogen sulfide) to be analyzed with throughput in excess of 100 samples per hour.

Potential impact

Automated gas and headspace analysis has traditionally been the domain of chromatographic techniques. However, sample throughput with these technologies is limited by the slow chromatographic process itself.

By automating SIFT-MS analysis, Syft Technologies and Anatune have developed a very high-throughput headspace and gas analysis system that revolutionizes gas and headspace analysis, providing new opportunities for both contract and R&D laboratories, from environmental analysis to food testing to pharma. Applications enhanced by more rapid analysis include:

- Residual monomer analysis
- Residual solvent testing in packaging and pharmaceuticals
- Multiple headspace extraction
- Monitoring of polar and reactive species, including ammonia, formaldehyde, and hydrogen sulfide.

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NEXERA-I MT METHOD TRANSFER SYSTEM

Two flow lines enable UHPLC and HPLC analysis in one system.

Produced by Shimadzu

The Nexera-i MT features two independent and dedicated flow lines, one for UHPLC and one for HPLC analyses. Newly developed Analytical Conditions Transfer and Optimization (ACTO) technology minimizes the effect of system volume differences on analytical results. In addition to improving the efficiency and quality of method development and transfer efforts in quality control departments, Nexera-i MT's dual flow lines also boost operational efficiency. They allow a single instrument to run both HPLC and UHPLC analyses, as opposed to separate dedicated instruments for each.

Potential impact

Nexera-i MT achieves excellent analytical reproducibility when switching from a system with large volume to a system with smaller volume – or vice-versa. It also allows matching of existing HPLC or UHPLC methods run on competitive instrument platforms, automatically compensating for differences in system volume. New software features offer support with transfer of existing HPLC methods to faster UHPLC analyses while assuring high cross-compatibility between old and new method conditions. It can also be used for quick method development in UHPLC mode followed by seamless conversion to HPLC methods (using the incorporated conversion program) for broader applicability.

What the judges say:

"Greatly increases the flexibility of laboratories while reducing complexity. More methods can be done with fewer instruments."

THERMO SCIENTIFIC EXACTIVE GC ORBITRAP GC-MS

Powerful GC-MS system for sensitive analysis of targeted and non-targeted compounds.

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Produced by Thermo Fisher Scientific

The Thermo Scientific Exactive GC Orbitrap GC-MS system is designed to provide sensitive, routine grade performance for both targeted and non-targeted analysis, along with powerful quantitation. The system offers the quantitative power of a GC triple quadrupole mass spectrometer combined with the unique advantages of Orbitrap's high resolution, accurate mass technology, allowing new options for routine laboratories to advance their workflows. With the Exactive GC system, users can now acquire high-resolution scan data, mine data, perform retrospective analysis and look for compounds that would otherwise be undetectable with traditional targeted analysis.

The system's capabilities bring additional new benefits to the routine environment, including ease of analytical set-up, broad scope, efficient automatic data processing and retrospective data analysis. In addition to technologies such as time-of-flight and quadrupole-time-of-flight mass spectrometry, the Exactive GC provides other analytical options to scientists – allowing selective, quantitative and qualitative analysis from within the same injection, routinely.

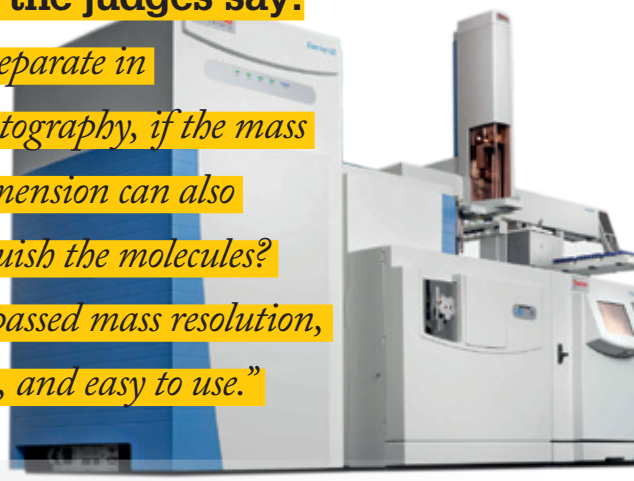
Potential impact

Routine laboratories in the fields of food safety, environmental, forensics and anti-doping commonly need high selectivity and sensitivity to detect and analyze increasingly challenging compounds and matrix combinations, which to date has required a range of techniques to accurately screen and quantify compounds.

Harnessing the power of the Orbitrap technology, the new system is designed for scientists working in these routine environments who are looking to increase their reach beyond targeted quantitation throughout analysis. Through uniquely high resolving power, mass accuracy, linear dynamic range and sensitivity, the Exactive GC allows researchers to gain a deeper understanding of their samples.

What the judges say:

"Why separate in chromatography, if the mass spec dimension can also distinguish the molecules? Unsurpassed mass resolution, reliable, and easy to use."



AIM-9000 INFRARED MICROSCOPE & AUTOMATIC FAILURE ANALYSIS SYSTEM

Unique concept for micro sample and failure analysis.

Produced by Shimadzu

The AIM-9000 offers automation of all necessary steps involved in failure analysis and micro sample evaluation: observation, definition of measurement spots, measurement and identification.

The main features of this grade of automation are:

- a unique wide field camera for automatic zoom-in from eye-size (10 x 13 mm) to contaminant-size (300 x 400 µm)
- Automatic Contaminant Recognition Function to set aperture on measurement spots automatically
- Contaminant Analysis Program to identify the spectrum automatically.

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The AIM-9000 is controlled by AIMsolution software, which unifies all operations for sample observation, measurements and analysis. A large choice of accessories complements the instrument, including objectives, polarizers, a pressure sensor and a TGS detector. Combined with the IRTracer-100 platform, the AIM-9000 can reach a S/N ratio of 30,000/1. Furthermore, it uses high-speed mapping measurement with imaging presentation.

Potential impact

With the AIM-9000, Shimadzu provides an analysis system for all users for quick and easy microanalysis. It targets various industries, including electrical and electronics, machinery and transportation, pharmaceuticals and life sciences, petroleum and chemicals.

Enhanced sensitivity and increased ease of operation enable a completely new user experience.

MULTI-CUT AND HIGH-RESOLUTION MDGC SYSTEM COUPLED TO IRMS AND TRIPLE QUADRUPOLE MS

11

Multidimensional GC (MDGC) coupled to an optimized C-IRMS/triple quad-MS system for accurate δ13C, qualitative and quantitative analysis.

Produced by University of Messina and Chromaleont s.r.l.

A multidimensional GC-combustion-isotopic ratio mass spectrometry/triple quadrupole MS prototype (MDGC-C-IRMS/QqQ-MS) was developed and optimized to allow highly accurate δ13C measurement after high-resolution separation using two different GC stationary phases. The low dead-volumes of the C-IRMS system drastically reduce the extra-column band-broadening effect that usually affects commercial GC-C-IRMS instrumentation. The multi heart-cut Deans switch used poses no limitation to the number of 1D peaks that can be transferred to the 2D column and subsequently measured. Finally, the prototype allows the identification, quantification (in MRM mode) and δ13C measurement of target compounds in a single analysis thanks to the simultaneous IRMS/QqQ-MS detection.

Potential impact

The enhanced performance of the prototype system overcomes common issues of commercial monodimensional and bidimensional GC-C-IRMS systems that have so far limited the widespread use of this technique. Monodimensional systems are affected by the low chromatographic resolution arising from the extra-column band-broadening produced by dead volumes in the combustion oven, as well as in the IRMS flow path. δ13C measurements of impure peaks lead to incorrect values, hampering GC-C-IRMS applications for antidoping, geographical origin and natural/synthetic evaluation. Commercial multidimensional systems suffer from a limited heart-cut number per analysis because of retention time shifts. The prototype combines the high resolving power of the multi-cut MDGC with the low IRMS dead-volumes, resulting in accurate δ13C measurements. The qualitative and quantitative capabilities of the QqQ-MS in MRM mode produce an "all-in-one" high-performance instrument that reduces the time and cost for routine applications.

What the judges say:

"This new MDGC technique improves on commercial systems that limit the number of second dimension fractions that can be analyzed, while also reducing the extra-column band broadening that can limit traditional IRMS performance."

LIQUID-EI (LEI) ATMOSPHERIC PRESSURE MECHANISM

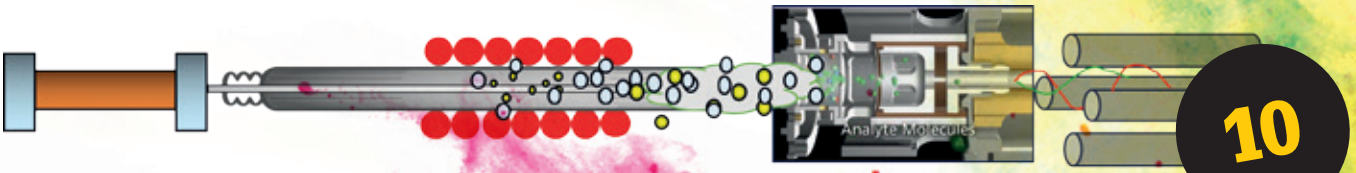
Effortless introduction of liquid streams into an unmodified electron ionization source of a mass spectrometer.

Produced by the University of Urbino, Italy

We have combined, for the first time, an atmospheric pressure gas-phase conversion mechanism with new ceramic coatings to create an innovative interface, called Liquid-EI (LEI). LEI is based on electron ionization (EI) but differs from previous attempts; the vaporization of solutes and mobile phase takes place at atmospheric pressure into a specifically designed region, called the "vaporization micro-channel", before entering the high-vacuum ion source. The interface is completely independent from the rest of the instrumentation, and can be adapted to any gas chromatography-mass spectrometry (GC-MS) system, as an add-on for a rapid LC-MS conversion. A ceramic liner, placed inside the vaporization micro-channel, acts as an inert, 'non-stick' vaporization surface, speeding up the gas-phase conversion of large molecules while lessening possible memory effects.

Potential impact

EI is an unparalleled, well-established tool for the identification of unknown gas-phase molecules. Its extension to a liquid phase, without the drawbacks and limitations that troubled this hybrid combination to date, provide the same unique advantages (library searchable mass spectra, robustness, negligible matrix effects) to LC amenable compounds, opening the door to new, challenging LC-MS applications. Ceramic coatings help to release the heaviest compounds to the gas-phase, improving vaporization efficiency and reducing high-temperature contact time for the most labile substances, bridging the gap between the world of classic LC-MS and GC-MS.



10

09

CLAM-2000

Fully automated sample preparation module for LC-MS/MS.

Produced by Shimadzu

The CLAM-2000* (Clinical Laboratory Automated sample preparation Module) automates the pretreatment of blood or other biological samples before LC-MS analysis.

By simply placing blood collection tubes in the system, the CLAM-2000 performs all processes through to LC-MS analysis automatically. Unlike dispensing systems based on batch processing 96-well plates, the CLAM-2000 is completely automatic from pretreatment to analysis, and processes individual samples successively in parallel.

This results in uniform pretreatment times between samples without slowing processing speed, and improves data reproducibility and accuracy.

Available pretreatment processes include dispensing samples, dispensing reagents, stirring, suction filtration, incubation, and automatic transfer of sample vials to an autosampler after pretreatment.

Potential impact

The new CLAM-2000 is the world's first system able to fully automate all steps from pretreatment of the sample to LC-MS analysis. It requires only the simple task of placing the blood or biological fluids collection tubes, reagents, internal standards and specialized pretreatment vials in the system. The user-friendly management functions provide a dramatically improved workflow with better safety for clinical research along with higher reproducibility.

**For Research Use Only. Not for use in diagnostic procedures. Not available in the USA, Canada, or China.*

ALLTESTA HPLC-BASED ANALYZER

Compact HPLC system: portability, simplicity, affordability, and precision.

Produced by SIELC Technologies

The Alltesta Analyzer is compact and lightweight (200 x 330 x 180 mm and under 10 kg), and is operated by a user-friendly touch-screen interface that requires only a tablet for operation – no desktops, monitors, or cables. The analyzer features a patented wash system, adjustable needle depth, and a flexible communication protocol (RS485/RS232/CAN). Its LED-based detector delivers a narrow, intense bandwidth, and uses a long-lasting, low-noise light source for high sensitivity. The short internal flow path volume minimizes band spreading, and only very stable materials (PEEK, PTFE and quartz) contact the fluid. The Alltesta pump precisely delivers fluid at flow rates from 0.10 ml/min to 4.0 ml/min using up to 5000 psi (350 bar) of continuous pressure. The Analyzer comes preloaded with over 1,000 methods for a diverse array of compounds and does not require comprehensive knowledge of chemistry or chromatography. It is backed up with lifetime free method development screening.

Potential impact

The Alltesta Analyzer overcomes the challenges of downscaling hardware and reducing solvent consumption, which have previously hindered the development of a portable LC system despite advances in stationary phase chemistry, flow rate hardware, and particle miniaturization. The Alltesta Analyzer represents a novel approach to compact HPLC. Targeting applications in pharmaceutical, agricultural, and consumer goods, the Alltesta Analyzer has the potential to transform how chromatography is performed in myriad fields and industries.

08

What the judges say:

"Simplifies HPLC analysis for non-specialists working in key applications."performance."

RAMTEST

07

Advanced handheld Raman analyzer with superior performance.

Produced by BioTools, Inc.

The RamTest is a state-of-the-art handheld analyzer that utilizes the most recent advances in Raman technology. This easy-to-use, lightweight, and ergonomic unit offers best-in-class analytical performance and unmatched cost-effectiveness. The superior performance is achieved by combining 532 nm laser excitation (unique for handheld Raman) with the breakthrough methodology to reduce the impact of fluorescence on Raman measurements. RamTest benefits include:

- 5–16 times faster analysis, improved analysis accuracy, dramatically reduced detection limits
- two-fold reduced unit cost
- best-in-class spectral resolution (4–6 cm^{-1}) and spectral range (120–4000 cm^{-1})
- Superior performance in water and most organic solvents
- Ability to measure delicate (for example, carbon nanotubes) and dangerous (for example, explosive) samples by utilizing up to 5–16 times reduced laser power (compared to conventional 785 and 1064 nm instruments) without compromising analytical quality.

Potential impact

RamTest enables dramatic improvement of Raman analysis business cases for a great deal of applications in the field, laboratory, quality control, process measurements/PAT.

The RamTest opens up new applications areas for Raman spectroscopy, including:

- analysis of biologics/biopharmaceuticals in aqueous solutions
- characterization of complex multicomponent mixtures
- automated quantitation of analyte concentrations in aqueous solutions using 3200–3400 cm^{-1} OH-stretching bands of water for normalization (unattainable with the other handhelds on market)
- detection of ammonia and other compounds previously considered 'hard- or impossible-to-detect' with handheld Raman
- carbon nanotubes structural characterization/ quality control.

VGA-101

06

The next generation VUV spectroscopy gas chromatography detector.

Produced by VUV Analytics

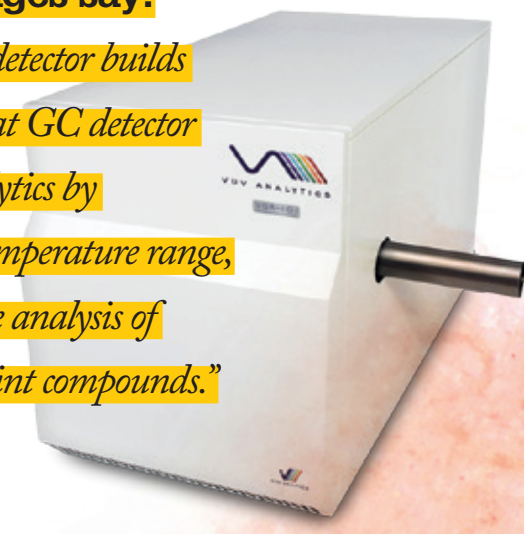
The VGA-101 is a next generation vacuum ultraviolet (VUV) benchtop spectrometer engineered to meet the needs of customers with advanced gas chromatography applications. The VGA-101 features an expanded wavelength spectrum and a higher allowable maximum operating temperature. An expanded wavelength spectrum of 120–430 nm provides unique selectivity for complex structures, such as polyaromatic hydrocarbons (PAHs). The ability to operate the VUV detector as high as 450° C allows GC×GC analysis of high boiling point compounds. Engineering advancements have also enabled the VGA-101 to be placed in-line with other GC detectors for new data correlation and analytical insight.

Potential impact

The VGA-101 provides new analytical capabilities to a number of industries including oil and gas, forensics, fragrances and flavors, petrochemical, specialty gas, and life sciences. Customers in the oil refining and petrochemical industries now have a reliable tool for analyzing high boiling point fuel samples containing complex hydrocarbon mixtures. The expanded wavelength spectrum opens new possibilities in characterizing isomeric compounds with extensive branching or ring structure that are difficult to distinguish with alternative methodologies. Hyphenating with mass spectrometry and other GC detectors opens the door to building rich data sets that are correlated unlike any in the past.

What the judges say:

"The VGA-101 detector builds upon the last great GC detector from VUV Analytics by expanding the temperature range, which enables the analysis of higher boiling point compounds."



ZIPCHIP

Provides high-quality capillary electrophoresis (CE) separation capabilities as a front-end for mass spectrometry.

Produced by 908 Devices

ZipChip allows for direct analysis of complex biological samples providing sample preparation, capillary electrophoresis separation and direct electrospray for MS detection, all on an integrated microfluidic device. ZipChips are compatible with a broad range of analytes from small molecule metabolites and amino acids, through peptides and intact proteins, antibodies and antibody-drug conjugates.

ZipChip is deployed from fundamental academic research as well as in the biopharmaceutical industry from early stage research through to monitoring of growth media and final biotherapeutics in production. With intact proteins and antibodies, ZipChip gives characterization of intact molecules in a near native state that is unique and not presently available with other MS-compatible techniques.

Potential impact

The rapid expansion of the life sciences market over the past few decades is driving the demand for increased analytical capabilities. ZipChip addresses some of the most essential areas, from analysis of complex intact proteins to the burgeoning science of metabolomics. Its simplicity of analyses, minimal sample preparation, and delivery of unique data is creating demand from research labs through each critical step in bio therapeutic development through bioprocessing for production.

ZipChip's end-to-end speed, combining minimal prep with analysis times of 2–3 minutes suggests dramatic productivity enhancements and the study of processes that would have been impractical with traditional techniques. By incorporating ZipChip into the life science analysis process, we are dramatically improving what users can see with their MS instruments; transforming time-consuming sample runs into fast, everyday analyses.

05

What the judges say:

"An integrated front-end CE solution for MS, including portable MS."

LIVETRACK

Real time focus-tracking technology for Raman imaging.

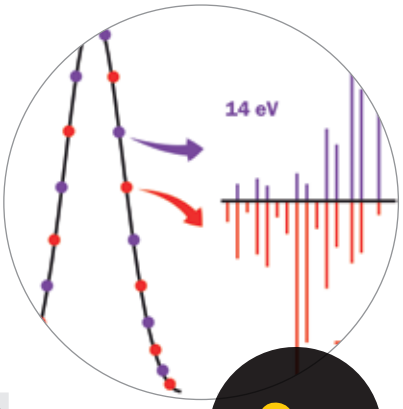
04

Produced by Renishaw

Typically, Raman microscopy needs to be performed on flat surfaces. With Renishaw's LiveTrack technology – incorporated in Renishaw's new inVia Qontor confocal Raman microscope – this is no longer the case. LiveTrack removes the need for manual focusing, pre-scanning or sample preparation (to give a flat surface). Uniquely, LiveTrack provides continuous feedback to the sample stage, which adjusts to follow the height of the sample. Users can track the surface of a sample, live, while acquiring surface or subsurface Raman data. The resulting Raman image and surface topography is viewed in 3D. The range of focus travel is exceptional and can be used across the whole horizontal and vertical travel of the microscope stage. LiveTrack opens the door to a new era of applications and measurement simplicity.

Potential impact

LiveTrack technology significantly reduces overall experiment times and makes analyzing even the most complex samples easy. Now, Raman imaging is no longer limited by a sample's topography. Efficiency is improved and reliable. Reproducible spectra can be rapidly obtained from a whole range of samples, covering a diverse range of application areas, including those not previously possible. Example application areas include rocks and minerals, pharmaceutical tablets and tissue biopsies. Focus is maintained during dynamic measurements, such as heating, cooling or melting, expanding the range of measurements to which Raman spectroscopy and imaging can be applied.



TANDEM IONISATION

03

Technology for simultaneous acquisition hard-ionization and soft-ionization

Produced by Markes International

Tandem Ionisation technology for time-of-flight mass spectrometry (TOF-MS) means that a single GC or GC×GC run can provide all the information needed to fully characterize a sample for target compounds and unknowns. Tandem Ionisation works by generating two electron ionization (EI) mass spectra from a single peak by rapid switching between conventional 70 eV 'hard' ionization and 'soft' ionization at 10–16 eV. Crucially, acquisition of the soft ionization spectra is not associated with the inherent loss of sensitivity historically associated with soft EI, and unlike other soft ionization approaches does not require switching of ion sources or use of reagent gases. In addition, operation of Tandem Ionisation is fully automated within the software package for Markes' BenchTOF-Select time-of-flight mass spectrometer, meaning that laboratory workflow is unaffected.

Potential impact

Tandem Ionisation allows regular library-matching of 70 eV spectra against commercial libraries, such as NIST or Wiley, alongside all two key benefits of soft ionization – discrimination between structurally similar isomers, and confirmation of the identity of compounds with weak molecular ions at 70 eV. Providing these capabilities within a single GC run has the potential to change the way that analysts approach GC and GC×GC analyses – it is already proving valuable for identifying long-chain alkanes in petrochemicals, and for discriminating between structurally similar terpenoids in fragranced products.

What the judges say:

"Tandem Ionisation technology allows two different MS spectra to be collected simultaneously, which should greatly enhance the analyte identification capabilities of the technique."

UNISPRAY SOURCE

02

Novel ion source for mass spectrometry with increased ionization efficiency.

Produced by Waters

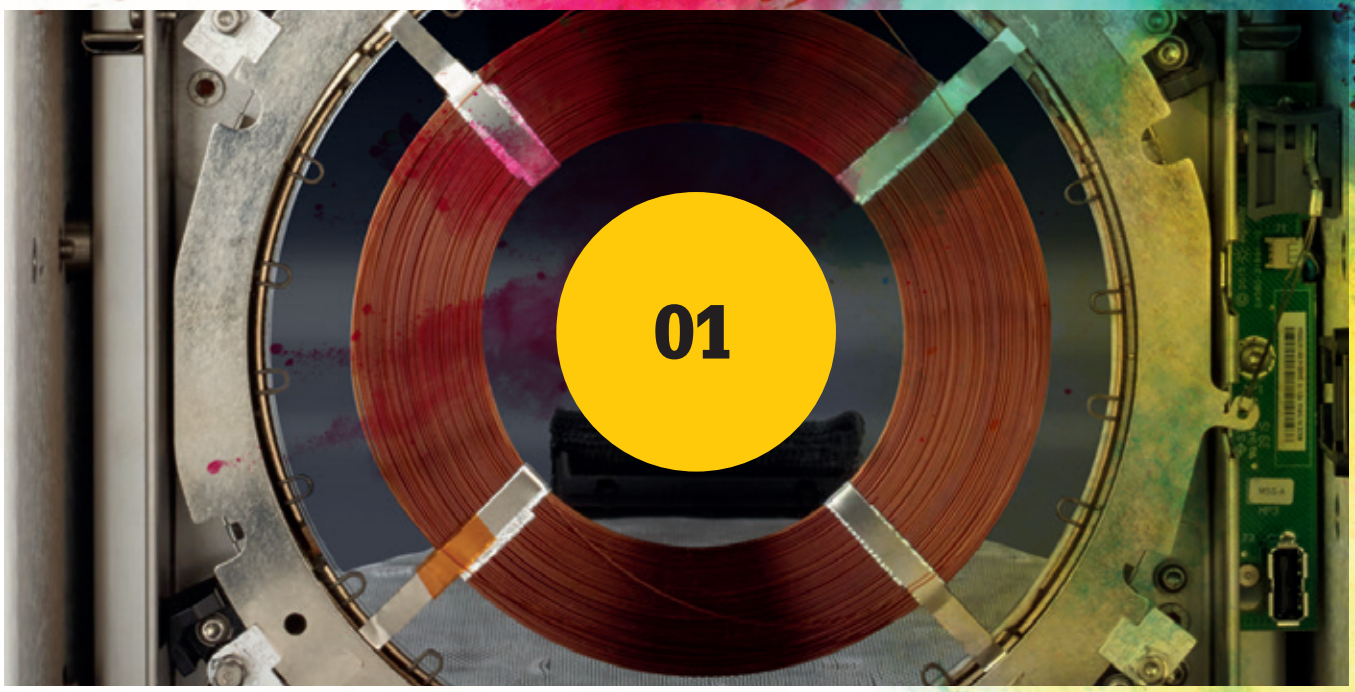
High flow rate ESI remains the preferred ionization technique for LC/MS analyses because it offers the most facile coupling for a wide range of analytical flow rates. However, when compared to nanospray ionization, ESI is known to suffer from poor ionization efficiency at high flow rates. UniSpray is a novel ion source for mass spectrometry that incorporates unique aerodynamic features. The resulting "cylinder in cross-flow" geometry demonstrates significant enhancements in both ionization efficiency and compound coverage when compared to conventional, nebulizer-assisted ESI sources.

Potential impact

UniSpray has the potential to increase the number and type of compounds that can be detected by mass spectrometry in a single run while simultaneously enhancing sensitivity. Therefore, Unispray could allow the consolidation of multiple methods into a single analysis, giving laboratories the opportunity to optimize efficiency, as well as allowing users to see a more complete picture of what is present in their samples.

What the judges say:

"Improves ionization efficiency of ESI, which is key to improving performance of ESI-MS."



AGILENT INTUVO 9000 GC SYSTEM

Designed to simplify the way GC is performed.

Produced by Agilent Technologies

The Agilent Intuvo 9000 GC System changes the paradigm in GC, comprising hardware, software, consumables and supplies. Intuvo embodies three transformational innovations:

- Direct conductive heating is used to temperature program the entire flow path and analytical column. This uses less than half the power of a conventional air bath oven, takes about half the laboratory bench footprint, and heats and cools much faster, improving throughput.
- Intuvo's click-and-run, leak-free connections replace traditional column nuts and ferrules. An audible and tactile 'click' indicates when the correct connection has been made. Unplanned downtime and associated business disruption, so often encountered from leaks arising from incorrect connections, are eliminated.
- Intuvo's no-trim columns are designed with a simple, disposable Guard Chip, which serves as a retention gap. The Guard Chip traps unwanted material from depositing on – and potentially damaging – the head of the column. Column trimming is eliminated altogether, enhancing productivity.

What the judges say:

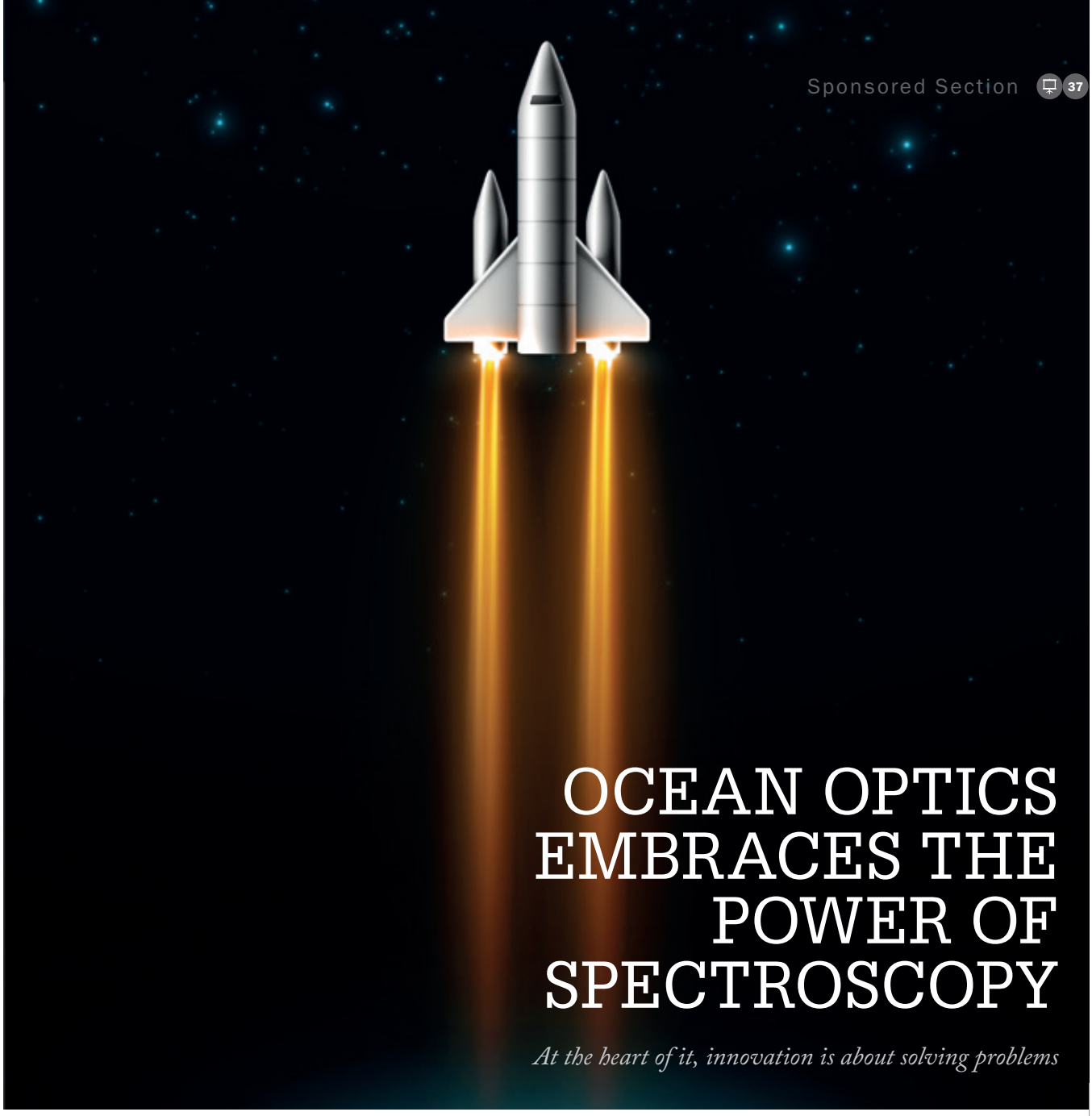
"Eliminates three major instrumental hurdles for GC. Opens the way for use of GC by inexperienced operators in the field, by the hospital bed or at borders. No compromises, easy to use."

Potential impact

Intuvo delivers features and benefits not seen with other GCs, significantly improving operator experience, laboratory operation and business success. The Intuvo offers faster heating, reducing sample time, and column replacement that's over 10 times faster, improving uptime. Fewer leaks and the elimination of column trimming mean that mistakes are reduced, avoiding costly reruns and delays. Intuvo helps to drive sustainable operational improvements, including on-time delivery, number of priority samples, cost per billable sample, and resource and asset management. By streamlining the GC experience, including installation, setup, operation and maintenance, Intuvo is transforming the way GC is performed.

THE INNOVATORS 2016

From detecting hazards to ensuring food safety, from the lab to the field, from the resolutely robust to the cutting-edge... Meet the innovators defying limitations and driving analytical science forward.



OCEAN OPTICS EMBRACES THE POWER OF SPECTROSCOPY

At the heart of it, innovation is about solving problems

After decades of innovation, modular spectroscopy has become a powerful technology for use in compact, reliable instrumentation across various applications. Today, Ocean Optics (www.OceanOptics.com) is a leader in modular spectroscopy for needs ranging from lab testing and turnkey measurement solutions to field analysis and custom OEM analytical systems.

Ocean Optics offers a portfolio of market-leading miniature spectroscopy equipment - modular, highly customizable building blocks that offer a fundamental method of measuring and interpreting the interaction of light with matter. We combine these tools with the knowledge to solve measurement problems, providing assistance to our customers in utilizing spectroscopy in ever-evolving ways.

This drive has led us on many journeys with our R&D and commercial partners. We have supported NASA on space missions, summited Mount Everest with researchers measuring ozone, and partnered with developers on systems that monitor food safety.

Ocean Optics has built a solid infrastructure of spectrometers, accessories and know-how to help provide solutions for a wide range of dynamic and demanding measurement challenges.

info@OceanOptics.com, www.OceanOptics.com

SEPARATE YOUR SCIENCE FROM THE STATUS QUO

How chromatographic boundaries are being shattered: UHPLC innovations that help scientists solve their toughest analytical challenges.

In scientific research, the need for instrumentation that is newer, faster, and better, is not innovative. Scientists have long looked for ways to break down traditional chromatographic boundaries that have stifled research from realizing that next big discovery.

Traditionally, companies have tackled advancements in liquid chromatography through incremental advancements, but these minor improvements have failed to provide the tangible results researchers need. As Jeanine Pippitt, Global HPLC Marketing Manager for Thermo Fisher Scientific, points out, manufacturers have focused on a baby-step approach through frequent small improvements instead of true instrument innovation. "If you fix one problem at a time or you are constantly releasing small upgrades, you often cause more problems than you originally had. I think a lot of the improvements that we've seen in UHPLC systems were actually more like a series of Band-Aids," says Pippitt. "We wanted to do better."

With this mindset, the engineers at Thermo Fisher stepped back, looked at what was currently possible and asked themselves: what are the true limitations facing scientists with modern UPHLC systems? They focused on seven big challenges:

1. Pressure and flow rates limitations
2. Sample delivery precision
3. An easy to use UHPLC, without sacrifice on performance
4. Detector capabilities
5. A lack of easy method portability
6. Run-to-run reproducibility
7. Robustness of system, preventing frustrating maintenance and downtime

They imagined how an instrument that could be versatile for a variety of chromatographic needs – from small molecule analysis to large molecule analysis. How an instrument could be simple-to-use and integrate easily into any lab, and how this instrument would be robust enough to handle the most challenging separations with confidence. The result of these efforts is the award-winning Thermo Scientific™ Vanquish™ UHPLC platform.

As Pippitt states, "When I first saw the data, I almost didn't believe the chromatography presented in the literature. I thought it was just marketing fluff. It's not."

The new Vanquish platform uses an ultra-precise piston drive that has the highest pressure pump on the market, without restricting flow rate. At 1500 bar, up to 5 mL/min, and a 1000 bar system that runs up to 8 mL/min; the new platform can now open new avenues to scientists and researchers in a variety of fields. Both pump types, binary and quaternary, use Thermo Scientific™ SmartFlow™ solvent delivery technology; this ensures excellent flow and gradient precision, independent of eluent composition and an improved retention time precision that is up to 11 times better.

Method portability is simple and the Vanquish platform's hardware and software can be configured to replicate delay volumes and column environments of other UHPLC platforms, including competitive systems. One unique hardware feature is the active and passive heating and cooling, providing unique separation refinement and precision.

Thermo Scientific™ Viper™ Fittings are used throughout the entire system. These are "finger tight" tool-free, virtually zero dead-volume connection systems; that allow scientists to quickly connect LC modules, valves and columns and improve chromatographic results.

Engineers constructed robust valves with unique coatings so that scientists would only need to perform minimal preventive maintenance.

The completely new design of the Thermo Scientific™ Vanquish™ Diode Array Detector (DAD) HL incorporates Thermo Scientific™ LightPipe™ Flow Cells, which provide the best signal-to-noise (S/N) performance through the combination of lowest baseline noise, a very long light path, and minimum peak dispersion. The ultra-wide dynamic range is ideal for simultaneous detection of highly concentrated main compounds and impurities down to trace levels.

Other detectors include the Thermo Scientific™ Vanquish™ Fluorescence Detector offering selectivity and sensitivity, as well as, the Thermo Scientific™ Charged Aerosol Detector technology to measure analytes that cannot be detected by UV and consistent response independent of chemical structure or quantity.

The high-throughput Charger module is an intelligent, fully integrated robotic unit for environmentally controlled sample management and automated sample loading of up to 23 well plates into the Vanquish system with sample tray barcode reading.

The Thermo Scientific™ Vanquish™ Horizon UHPLC system and Thermo Scientific™ Vanquish™ Flex UPHLC system have both been recognized as innovative products by R&D Magazine. The Vanquish platform is in a unique position to take chromatographic research to the next level. Learn more about the Vanquish platform at www.thermofisher.com/vanquish.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INNOVATIONS COME TOGETHER TO SET THESE SYSTEMS APART

With over 75 years of experience in the industry, PerkinElmer is no stranger to innovation. This year is no different. As 2016 draws to a close, here is a look at the innovations from PerkinElmer.

Patented Technologies Deliver Improved Efficiencies

The QSight™ triple quadrupole LC/MS/MS is an end-to-end solution designed to deliver maximum sensitivity and exceptional uptime for meeting both your industry and operational requirements. Inside and out, QSight comes together with unique patented technologies in a compact, easy-to-use form factor. And it gives you 15% more uptime due to a self-cleaning source that requires virtually no maintenance.

High sensitivity, even higher productivity

- Unique StayClean™ technology employs hot-surface induced desolvation (HSID™), a multi-orthogonal sampling interface that can significantly increase your uptime.
- Instrument drift and frequent reoptimization and cleaning are eliminated, for better productivity, thanks to the systems Laminar Flow Ion Guide™.
- For standard methods or regulatory compliance, the QSight triple quad can do both - while giving you more time to run more samples reliably and confidently. It's LC/MS/MS done right.

Portable Innovation for Faster Results

PerkinElmer's Torion® T-9 portable GC/MS brings new meaning to innovation and portability. You can take this one-of-a kind GC/MS to your samples wherever they are. Torion T-9 is the lightest, fastest and most portable gas chromatograph toroidal ion trap mass spectrometer – and provides reliable, reproducible results. At a weight of only 32lb, the Torion T-9 GC/MS is ideal to carry in the field for rapid screening of chemicals such as environmental volatiles and semi-volatiles (VOCs/SVOCs), explosives, chemical threats, and hazardous substances.

Get Actionable Results in Less Than 20 Minutes

With the Torion T-9 GC/MS, first responders can act rapidly and reliably to unexpected critical incidents. The system is fully self-contained, easy-to-operate and ready for sample analysis in under five minutes. Simply, collect, analyze, and identify samples on site with virtually no degradation, transport and processing, which significantly reduces the time it takes to get actionable results – by more than 70 times faster than conventional lab analysis.

The Best Answers Happen When Great Technologies Connect

Materials get more complex all the time. So the need for their precise analysis has never been greater. PerkinElmer's TGA and STA systems coupled with FT-IR, MS, or GC/MS systems represent the industry's most complete and advanced hyphenated platforms for answering how materials degrade and gases evolve – revealing new information not available to single systems working alone. Because of this experience, PerkinElmer is the only company capable of making, supporting, and servicing a combined system.

Are you interested in how a material responds to a non-standard test environment like high UV levels or humidity changes? TG-DMA or UV-DSC can give you the answer. Do you want to better understand how a material degrades or what gases evolve when that material burns? PerkinElmer's TG instruments can be coupled to several FT-IR, MS, or GC/MS options to provide you with greater knowledge, gain better insight and advance your laboratory.

Hyphenation with PerkinElmer provides pathways for innovation and scientific understanding because the more you know, the more you can do.

New Level of Performance and Flexibility

PerkinElmer's new Avio™ 200 is a compact ICP-OES that combines a vertical plasma design with a host of unique hardware features to handle even the most difficult, high-matrix samples without dilution, delivering a whole new level of performance and flexibility to ICP.

The smallest ICP on the market, the Avio 200 offers the most efficient operation, reliable data, and lowest cost of ownership with:

- The lowest total argon consumption of any ICP: only 9 L/min, compared to 21 L/min required by other systems;
- The fastest ICP startup: spectrometer ready in just 10 minutes from power on (versus up to 2 hours);
- Superior sensitivity and resolution for all elements of interest;
- The widest linear range;
- Plus, Avio 200's unprecedented performance comes with unparalleled ease-of-use. Unique hardware features combine with the industry's most intuitive software to make multi-element analysis as easy as single-element.

NEW SERIES OF THERMAL DESORPTION INSTRUMENTS

Dependable, highly sensitive pre-concentration of organic volatiles for GC–MS, for everything from routine analysis to cutting-edge research.

The new 'xr' series of thermal desorption instruments from Markes International builds on Markes' 20 years of experience and reputation as the global leader in TD technology.

The series includes the flagship TD100-xr™, a 100-tube thermal desorber that allows the quantitative re-collection of both inlet and outlet split flows, meaning that valuable samples can be re-run, and that complete desorption can be easily validated.

Markes' TD instruments pre-concentrate VOCs and SVOCs from air and materials, enabling the detection of these compounds using standard GC–MS equipment. None of Markes' instruments use liquid cryogen, reducing operational costs and ensuring fast sample processing.

Other members of the 'xr' series include instruments for analysis of single tubes (UNITY-xr™), on-line air streams (Air Server-xr™) and continuous air sampling (TT24-7xr™). Also available are a 100-tube autosampler (ULTRA-xr™), and the Kori-xr™ system for removing water from humid air sampled on-line or using canisters.

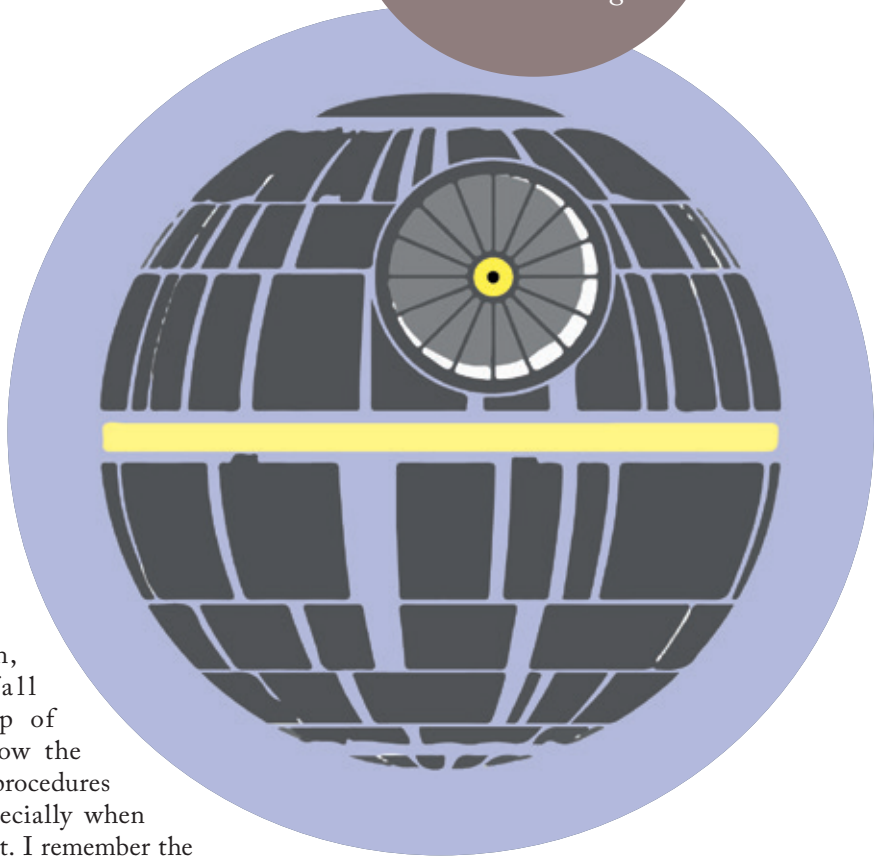
Profession

Leadership
Talent Development
Career Planning

Good Job Hunting

How to make the leap from graduate school (or janitor at MIT) to a permanent and rewarding career.

By Anthony Stender



If only the professional job search was akin to an experiment in freshman-level general chemistry. Remember general chemistry lab? Just follow these 10 clearly-written steps for success! At least in theory – for the lucky few. I was not one of them; I was a math major, and struggled in general chemistry. And yet, somehow, after taking a very circuitous path (1), I ended up with a PhD in analytical chemistry, then a postdoc, and now a tenure track position in forensic chemistry.

When I was looking for my first job after graduate school, I would ask faculty members, "How did you get your job?" One told me he applied to 150 different positions and got a handful of interviews. Many of the others simply said, "I don't really remember." A question I often ask people in management is, "How do you decide which candidates to interview for a job?" A common answer is, "It's a black box that I don't understand."

Now that I am on the proverbial 'other side', I can more clearly understand why it seems so mysterious to get a permanent position, but it needn't be that way.

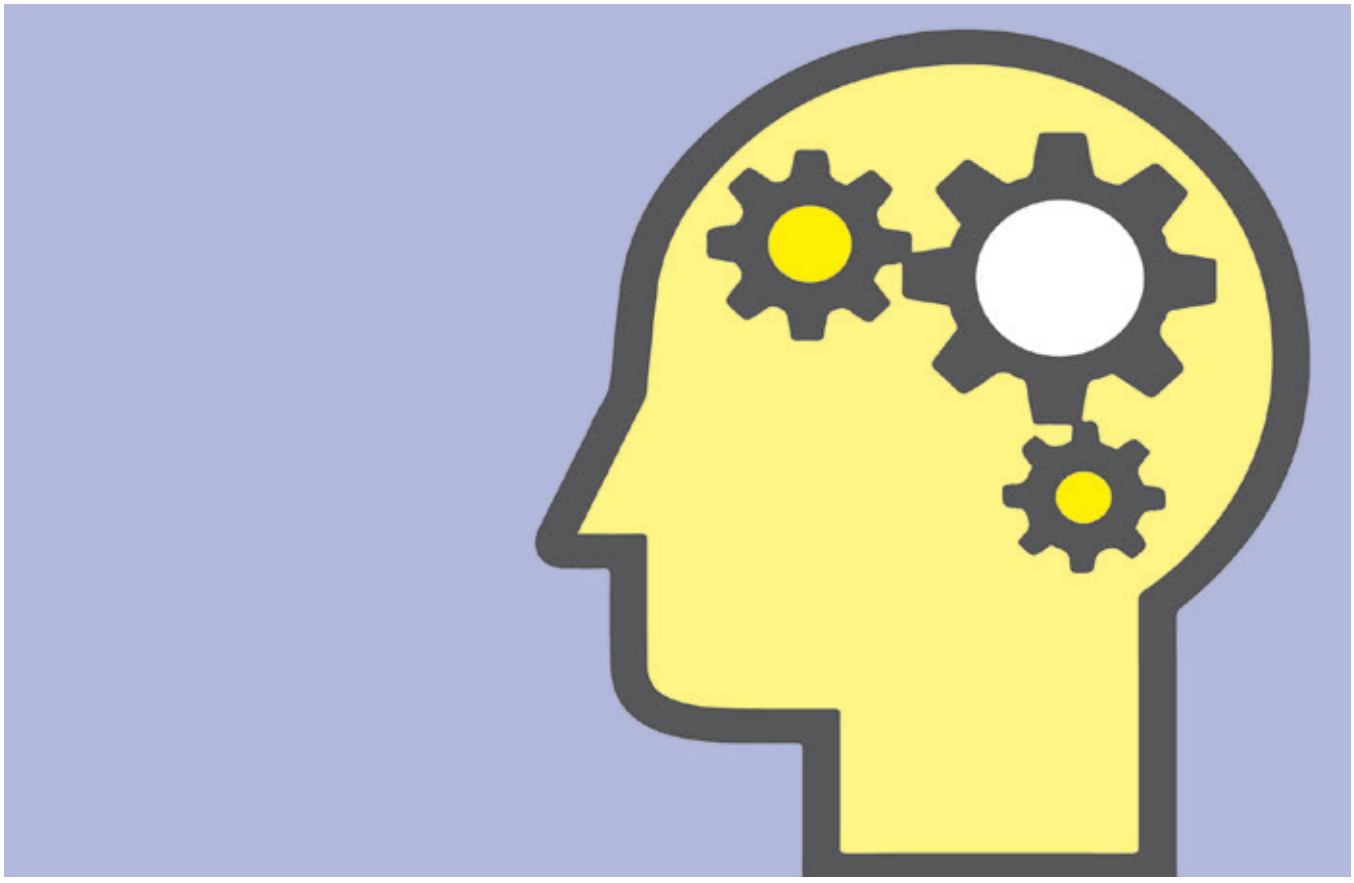
"It's a Trap!" (2)

All too often, scientists fall into the trap of trying to follow the experimental procedures of others, especially when on the job hunt. I remember the era of looking for jobs in the weekly newspaper and having to fill out an application by hand. Nowadays, you elect to have your email inbox inundated with daily job listings and apply to every single one online. The process can feel very much like total information overload, or it can feel depressing if you go a day without any new openings to apply for. Postdocs, on the other hand, can be hard to find, because very few are advertised online.

Another modern approach is the overhyped and ambiguous world of "online networking!" To me, it seems to have all the 'qualities' of online dating: a few random people get lucky while 99.99 percent of people do not. But there is some truth in the adage 'in it to win it' – and I guess the more people you know (or know you), the better your chances of wonderful serendipity... Social media is also rumored to be a place for finding jobs, but I am unaware of any scientist positions that are only posted on social media. I personally use LinkedIn only as a cloud-based Rolodex to keep track of colleagues and HR professionals, but many scientists can't be found there. So what's a sensible approach to securing a permanent job as a scientist?

"Know thyself" (3)

This simple wisdom has myriad interpretations, but it is advice that



shouldn't be taken lightly by job seekers. Everyone imposes their own criteria and barriers when looking for jobs, just as they did when selecting a graduate school. Common considerations include: location, distance from family and friends, the 'two-body problem' (what about your partner's career?), cost of living, pay, benefits, student debt, opportunity to advance, start date, type of job, altruistic vision, whether it's your dream job, and so on.

Before entering the throes of a job search, it is crucial to carefully outline your priorities. For example, in today's economy, it's easier to find a job if location is a low priority. Willingness to relocate can also open doors to move up the ladder. And yet, many job seekers limit themselves by making location a top priority. The key is to be open-minded to the possibilities during the seeking stage, but also to be strategic.

A useful exercise to understand yourself better is to write your criteria down on paper before your search begins and revise it later as necessary. It is also worthwhile to consider contingency plans in case of a slow job hunt. Some students are fortunate enough to take extensive time off after graduation, but that leaves a gap on your resume and in your bank account. Taking on a temporary position – teaching at a small college, for example – can grant you more time to look for permanent work while providing you with experience and money.

Knowing yourself is critical in attaining job satisfaction over the long

"Willingness to relocate can open doors to move up the ladder. And yet, many job seekers limit themselves by making location a top priority."

run. As Mike Rowe so eloquently explained (4), don't expect to get your dream job, and don't let the idea of a dream job prevent you from taking a good job. Focus on applying to jobs within that central sliver of a Venn diagram, where your expertise and job opportunities overlap. You're more likely to stand out from the crowd and find satisfying employment if you study the job market and understand your personal selling points. Furthermore, your work should enable you to grow and change over time. As a result, you will prepare yourself for new roles and more responsibilities.

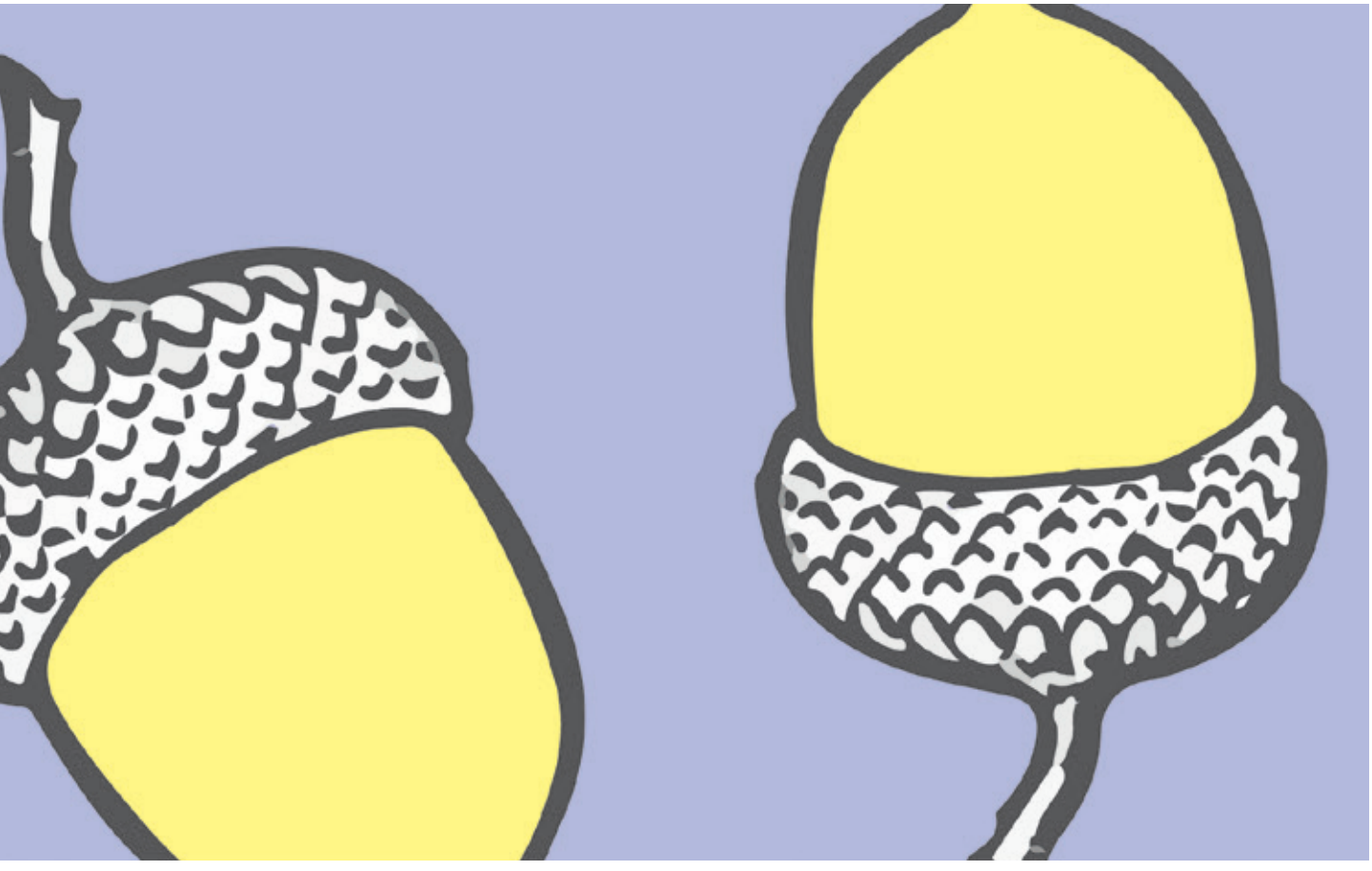
"Big things have small beginnings" (5)

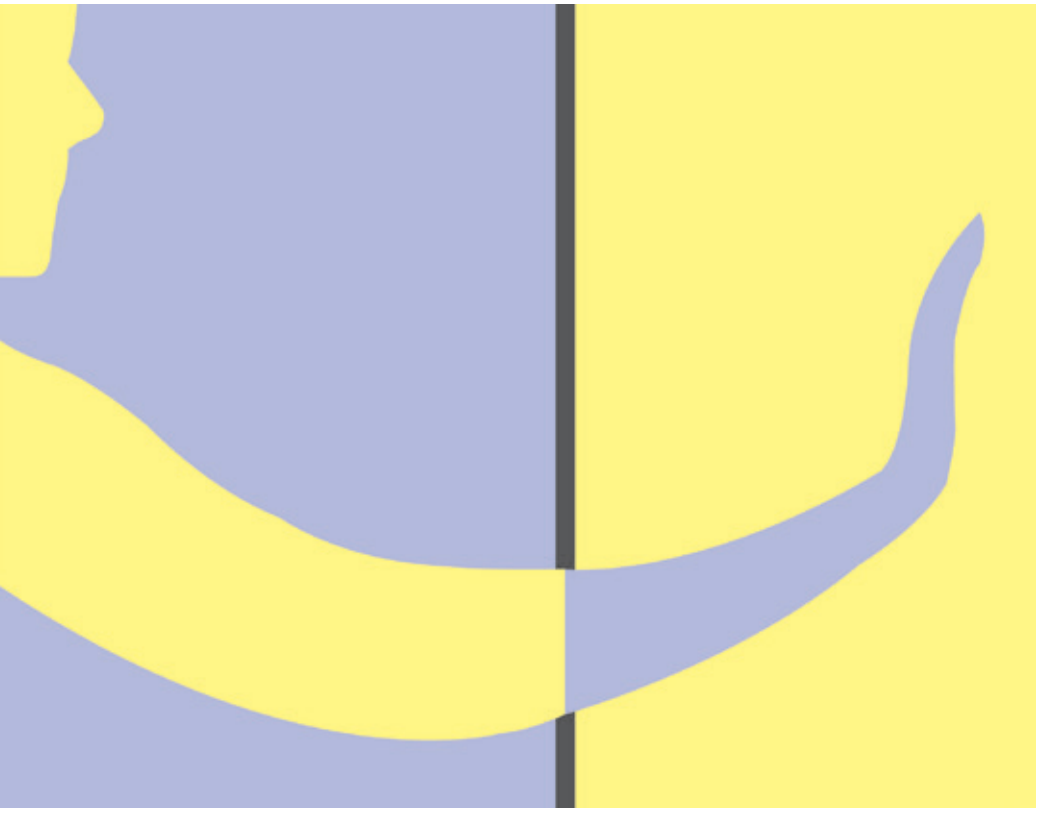
Prepare early. Have a resume and CV on hand before filling out an application. Once you have a standard resume prepared, you can update it and apply for an industry or government position at a moment's notice. If you are leaning towards a career in academia, prepare by writing out your teaching and research statements. The earlier you begin, the more time you will have to perfect these documents.

Talk to lots of people – preferably in person (old-school networking!) – and build relationships with them. But don't overly rely on stalking strangers on LinkedIn, aka "online networking." It's important to have real conversations with people outside your immediate circle of colleagues, and the earlier you start those conversations, the better. If you have met someone face-to-face, then it's easier to turn to them for practical help when you enter the job search.

Few graduate students spend time speaking to non-academic scientists while in school, but look for opportunities to meet people who work outside of academia. Professional scientists can offer you a different perspective on life as a working scientist. They can often provide you with job leads and more professional connections. In some cases, you may even be able to ask them for a facility tour or resume advice.

Similarly, it's easier to secure a postdoc with a professor who knows your work. Every professor gets spammed with emails from students wanting a postdoc. I once saw a student chase





"Don't expect to get your dream job, and don't let the idea of a dream job prevent you from taking a good job."

down a professor who was about to speak at a conference, just to hand over a resume. Whether you reach out to a professor by email or in person, be kind, be courteous, and keep your message short. Explain why you are interested in the professor's research and provide a snapshot of your current work. If your current advisor knows the professor, ask your advisor to introduce the two of you. Securing a postdoc is often about timing and funding, so consider applying for research fellowships while also looking for a position.

But is a postdoc truly necessary? This is the million-dollar question on everyone's mind. If you see an appealing job posted, apply for it, whether you have a postdoc or not. Typically, you won't need a postdoc to work in industry or at a teaching college. And yes, sometimes it's even possible to get hired at a research university without a postdoc.

However, if you really want to work as a postdoc, first understand your reasons why and avoid the traps. A postdoc is not a miracle cure for securing a permanent job, nor is it a good place to hide from an economic downturn. It's a brief layover where you should grow and prepare for your next position. As soon as you start, you need to be thinking about your exit strategy, but you also have to conduct research. Many people use a postdoc as a time to learn lab management and grant writing, but it should also be a time of meeting more new people and developing your own research ideas.

"Through the Looking Glass" (6)

As a parting thought, when I was in graduate school, I spent many Saturdays with a friend who works as a glassblower. He would start each new piece with a plan sketched on paper, but oftentimes he had to adjust his plan on the fly. Hot glass has a mind of its own. After he finished a major piece, we would share our thoughts about the experience. It actually makes for an excellent analogy for the job search. You hone your skills in school, make a rough plan about the future, and see where the process leads you. Sometimes your skills or your curiosity will lead you, and at other times, opportunities will show you the way. It's a different journey for everyone, but it's a better journey if you involve others and permit yourself to be open to the possibilities.

Anthony Stender is Assistant Professor of Analytical Forensic Chemistry at Ohio University, USA.

Reference

1. *After finishing a BS in Math, an MS in meteorology, a certificate in forensic science, 10 years in retail, and a lifetime of hauling manure on the family dairy farm, I decided to get a PhD.*
2. *A quote from Admiral Ackbar in Star Wars: Episode VI – Return of the Jedi.*
3. *A saying that pre-dates Socrates but is often attributed to him.*
4. *"Don't Follow Your Passion," by Mike Rowe and Prager University (https://youtu.be/CVEuPmVAb8o)*
5. *A quote from Mr. Dryden in Lawrence of Arabia.*
6. *The title of Lewis Carroll's sequel to Alice's Adventures in Wonderland.*

Enlightened, Empowered: The Ion Magician

Sitting Down With... Sarah Trimpin,
Professor, Department of Chemistry,
Wayne State University, and CEO
at MSTM, Michigan, USA.

You tend to stir up controversy...

It is true that I have been controversial (though not intentionally and less so nowadays) – somehow, our research accomplishments stirred the pot. I guess it's because we tend to do some crazy experiments that other people don't do because they are worried about failure.

"Crazy experiments" and funding models don't always go hand-in-hand... How do you find a balance?

I was extremely lucky. I did my initial crazy experiments when I became assistant professor at Wayne State; I still had plenty of money in the bank, so to speak. But I didn't have my own mass spectrometer back then (I was waiting for a second generation instrument) – I made my first discovery because I twisted the arm of a colleague and used his instrument to test a laser-assisted ionization concept that I'd had in mind for two years ... and it worked! I made the discovery in spring 2009, wrote my first grant on the topic in July 2009, and received a National Science Foundation (NSF) Career Award... I was off to a good start! I guess there was a whole bunch of luck that just came together at the right time, but it meant that I was able to create more and more evidence, which led to more discoveries and more funding. To answer your question: I think the funding agencies are interested in the crazy (step-change) stuff, but they also want to play it safe – so you need at least some evidence... and a plan.

And did everything go to plan?

We had lots of ideas about what we had discovered, and what the next steps should be – and guess what? We applied our knowledge, and it was plain wrong! Nevertheless, I saw a great opportunity, and others wanted to join me on the journey of discovery. One of my students, Ellen Inutan, performed an experiment that delivered something totally unexpected: we discovered that we didn't need to use anything for ionization with our matrix – no laser, no voltage, no heat, no desolvation gas. If you simply put the matrix:analyte close to the vacuum of a mass spectrometer, you create ESI-like ions with exceptional sensitivity – it's what we now call matrix-assisted ionization (MAI). It went against everything we (and everyone else) knew – I sometimes refer to it as "magic" ionization, poking a little fun at early criticism (1).

How have you dealt with criticism?

In the beginning, it was a tremendous problem – we got one rejection after another. Not even the 'lower level' journals wanted to publish our manuscripts. It was particularly concerning because we knew how important it was and how easily it could have been reproduced and published by another group. On one occasion, I was told by an associate editor from a high-end journal, "A reviewer sent me a personal note, stating, 'the investigator is a woman, she's only from Wayne State University, she is young... and she's only out for big hype." I replied, "Do you honestly think I work this hard just for one big-hype paper?" Nevertheless, she stuck with her decision not to publish. Several months later, the article in question and three more on different aspects of MAI were published in other journals. The community now accepts our work – and my students and I have been honored with numerous accolades, despite or because of the previous criticism.

It certainly paid off – you started MSTM to commercialize MAI with Charles McEwen...

Right. Up to now, we've been working with MS systems that are optimized for ESI and MALDI. Imagine what we could do if we have a source that is tuned to do this new ionization process. Charles McEwen and I are inventors of several issued patents on ionization, so it was a natural fit. We applied for NSF funding and went through STTR Phase I right away, and we are now in STTR Phase II. The NSF has been extremely good to us; they provide opportunities and I've been very happy to play a part in commercializing fundamental research.

"I not only try to pass on knowledge – but also the strength to be confident and open-minded."

How do you motivate your students to follow "crazy" ideas rather than staying on the tried and tested path?

I try to take away some of the fear. Ellen Inutan was actually my first graduate student, and I remember how scared she was about "destroying" our first mass spectrometer – she didn't want to touch it! It's actually mind-boggling how intimidated some students can be – especially women. As a community, we need to invest more in the education of our students; they need to be free enough – financially and emotionally – to do the crazy stuff. Many discoveries have been made by students who didn't follow the 'script.' If we can encourage students (and their mentors) to take chances, we will absolutely make more progress in science. I not only try to pass on knowledge – but also the strength to be confident and open-minded. Good role models are essential. I had very strong women in my family; my mother, my aunts, my grandmothers – they all followed expectations only as much as they needed to... The apple did not fall far from the tree.

Reference

1. *S Trimpin, "'Magic' ionization mass spectrometry", J Am Soc Mass Spectrom, 27, 4–21 (2016). http://tas.txp.to/1216/magicMS*

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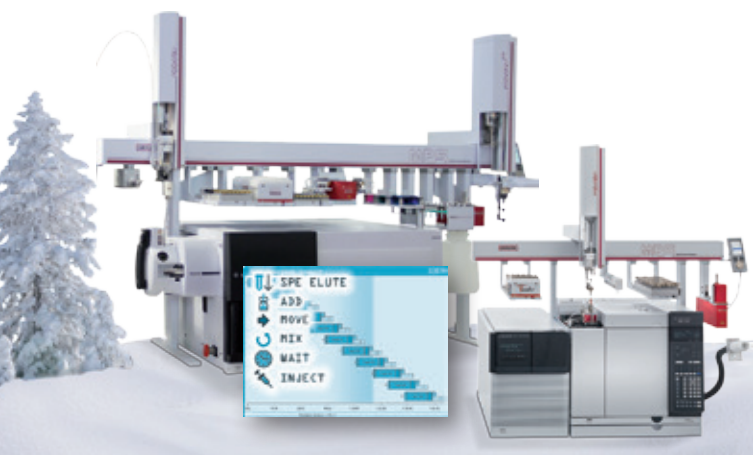

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