AUGUST 2015 # 31

the Analytical Scientist

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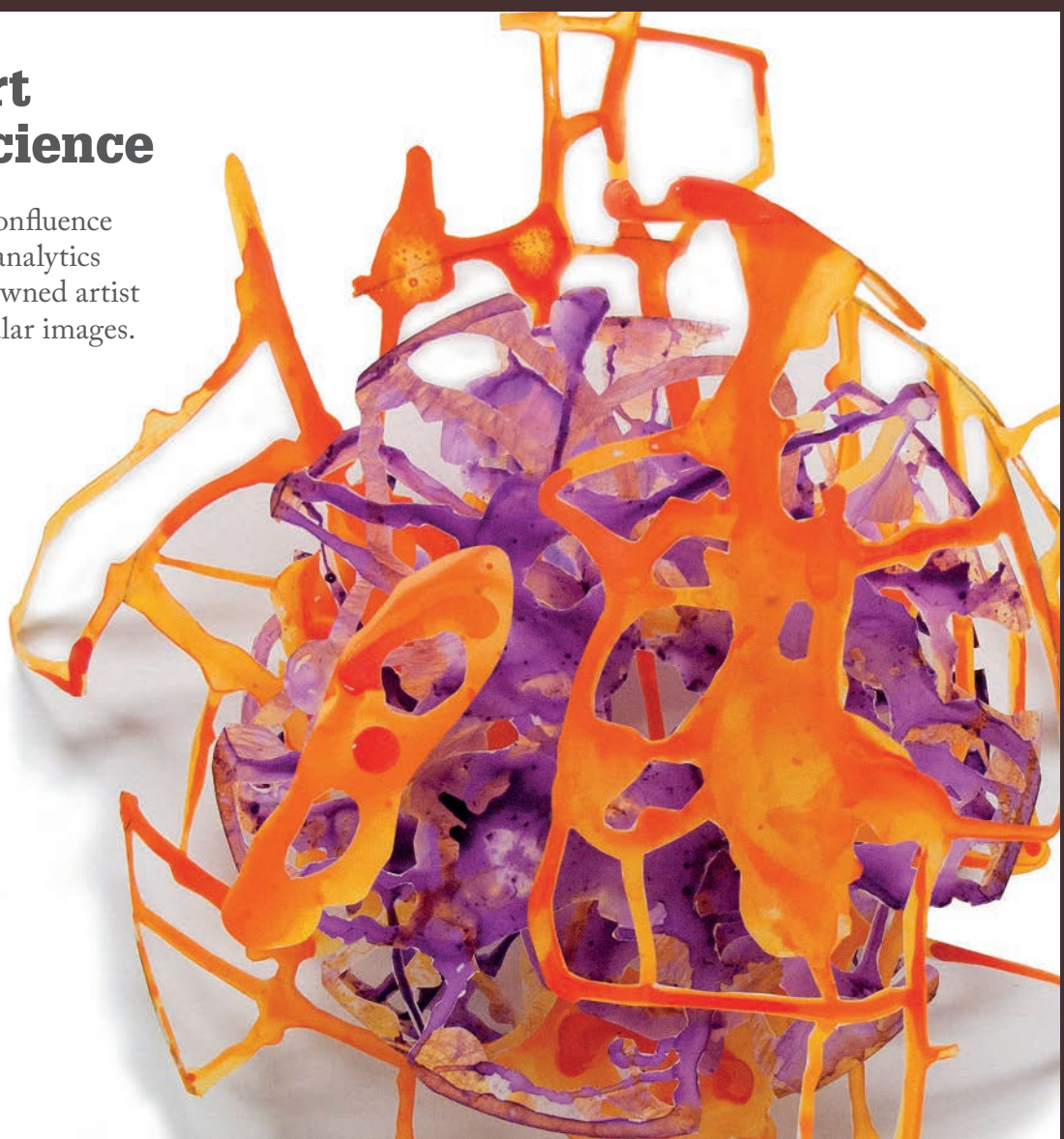

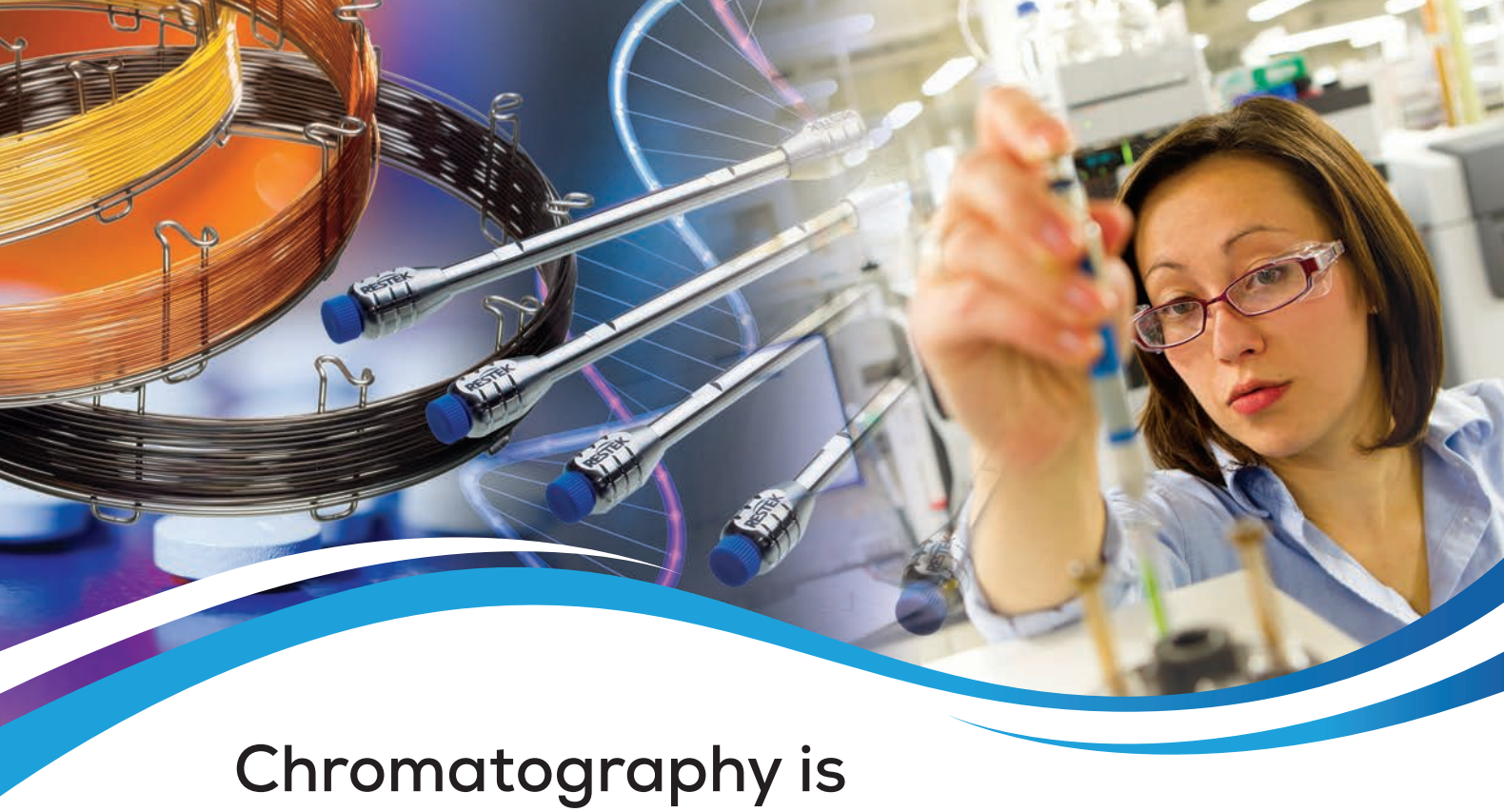

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Tea With Rich...at HPLC 2015 in Geneva.

Watch the trailer now: tas.txp.to/0715/TeaWithRich

Contents

On The Cover

Fluid # 6, © 2010. Acrylic on mylar, fiberglass rods 17"x 13" x 6" The work of Rebecca Kamen (www.rebeccakamen.com)

Upfront

In My View

When Art Meets Science

Reports

Sitting Down With

the **Analytical Scientist**

ISSUE 31 - AUGUST 2015

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2015 Winners
Andreas Seidel-Morgenstern (left)
and Peter H. Seeberger (right),

Who will be the winner in 2016?

Nominations for the 2016 Humanity in Science Award are now open

Analytical science has the power to change human lives for the better, but rarely receives the same fanfare as other scientific disciplines. The Humanity in Science Award was launched to recognize and reward a recent breakthrough in analytical science that has truly made the world a better place.

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Athens 2035

Gazing into a crystal ball is not only fun, it can also stimulate discussion about the road we need to take. And sometimes it can cause controversy or make us reflect on the past.

At HPLC 2015 in Geneva, Peter Schoenmakers made a number of bold predictions for "Athens 2035: a peak capacity of 1,000,000 is commonly achieved; spatial 3D-LC is well established; the Netherlands are finally soccer world champions; some delegates argue that LC is now mature and that major developments can no longer be expected." Some of his ideas were (semi-) serious, some were fun, and a few were controversial. But all of his forecasts shared one thing in common: they got people thinking and talking. Peter also somewhat satirically alluded to the state of the Greek economy (which may have offended some delegates), but who can prove that HPLC 2035 won't be hosted in Athens? A great deal can happen in 20 years; projecting so far ahead should protect us from too much criticism.

Six members of the 2013 Power List joined me for tea in Geneva (watch the latest trailer: tas.txp.to/0715/teawithrich). They all commented, with a smile, on Peter's lecture and the buzz that it had generated. The previous month, we posed a similar question in our feature "Pushing the Limits of LC" – but our gurus only dared predict 10 years ahead. If nothing else, our predictions of the future echo where we would like to be.

To that end, we'd love to hear your vision of 2035. Whether you're in metabolomics, foodomics, lipidomics – or a field with no-omics – please get in touch with your serious or fun predictions. Simply email: rich.whitworth@texerepublishing.com. You never know, collectively we might even get a few right.

Finally, and much more seriously, while looking to the future, we should not forget the past – nor the pioneers who have contributed so much to progress. Late last year, we lost Georges Guiochon, who was honored at HPLC 2015 with the inception of a special Faculty Fellowship. (Next month, we sit down with its inaugural member – Amy Herr.)

On July 8, 2015, the HPLC field sadly lost another highly respected pioneer. Over the course of her lifetime, Phyllis Brown received the Tswett Medal and the Dal Nogare Award among many other accolades. She will not only be profoundly missed by her family, but also by the many students whose lives were touched by her passion and dedication. It reminds us that, at the very least, we should attempt to make a difference over the next 20 years.

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

Unraveling Art with Analysis

SORS meets microscopy to delve deeper into historical art and sculptures

In the past, we've explored how analytical techniques can uncover the secrets of paintings by probing beyond what we see with the naked eye (tas.txp.to/0815/portrait), but what about getting beneath thicker layers of paint at the micrometer scale? A collaboration of researchers from the UK's Science & Technology Facilities Council (STFC) and the Italian National Research Council's Institute for the Conservation and Valorization of Cultural Heritage (ICVBC) have developed a technique that they refer to as a "new Raman imaging modality" – microscale spatially offset Raman spectroscopy (micro-SORS).

"Traditional SORS extends the access of Raman spectroscopy to greater depth within diffusely scattering (turbid) samples. However, one limitation remained – SORS was unable to probe and resolve micrometer-scale layers in highly turbid materials," says Pavel Matousek, a STFC Senior Fellow. "Due to micrometer-scale laser illumination and Raman collection areas, and spatial offset dimensions, micro-SORS can readily resolve thin turbid layers that are beyond the reach of both traditional SORS and conventional Raman microscopy."

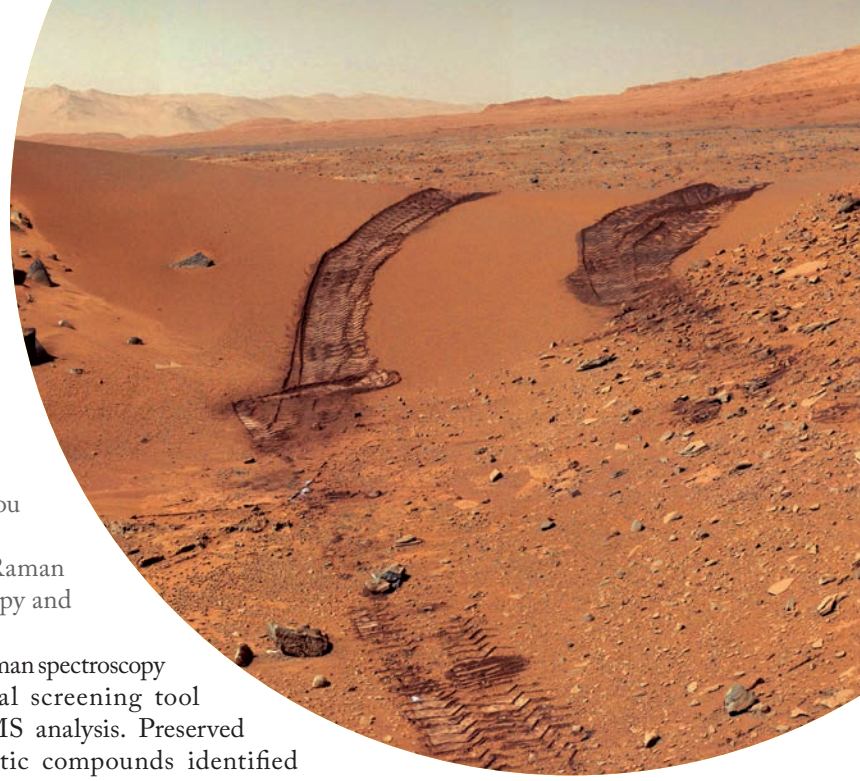
Matousek began working with ICVBC in 2010, after a conservations scientist from the institute, Claudia Conti, approached him when she heard about his work. "One of the topical issues in conservation science is how to obtain chemical information in a non-destructive and non-invasive way. Many such methods available today provide only partial information on the chemical elements so new technologies are needed to achieve full characterization of the concealed compounds," says Conti. "Our research efforts with Pavel and his team ultimately lead to the successful transformation of macro-SORS, enabling its application in the cultural heritage area and the successful demonstration of micro-SORS."

So far, the technique has been demonstrated successfully on both painted sculptures and mural paintings. According to Conti, the most interesting findings came after analyzing the polychrome sculptures originate from the "Sacred Mounts" (UNESCO World Heritage sites) in North Italy. "They consist of a series of chapels containing wall paintings and terracotta or stucco sculptures representing the life of Christ. Due to their religious value, these sculptures were often re-painted to enhance the polychromy, thus their stratigraphy is extremely complex mainly due to the presence of multiple layers. Micro-SORS allowed us to discriminate the pigments used and their position from the surface to the more internal portions," says Conti.

The research collaboration is also investigating the applicability of the technique in other areas, such as polymer sciences, biology and forensics, as well as working on the optimization of the technique both theoretically and experimentally. "Our Monte Carlo simulations indicate that there is a major scope for further improvement of the performance, in terms of penetration depth and sensitivity. The last but not least step is the development of a portable micro-SORS device that can be brought to the art itself," says Matousek. *SS*

Life on Mars?

No confirmed sightings. No little green men. Still hope...



Unmanned probes have indicated that liquid water could have existed on the red planet, and that means there could have been life too. Are fossilized remains waiting to be found? Of course, accurately detecting ancient biology is not easy, particularly on an alien planet. Nevertheless, Alison Olcott Marshall and Craig Marshall from the University of Kansas believe that Raman spectroscopy and GC-MS should be used together to help develop conclusive evidence of extraterrestrial life. We spoke with Olcott Marshall to discover the true challenges of analyzing alien rocks.

How did you get involved in the great search?

Both Craig and I had worked on the problems of detecting and defining life in the Precambrian – the three billion or so years when most of the life on Earth was microscopic and hard to fossilize. Thus, if we want to understand what is happening in the biosphere – or to explore connections between the biosphere and geosphere for over three quarters of Earth's history – it is crucial to delineate the chemical signals that life left in the rock record. Many of the challenges and approaches used in the Precambrian are also relevant to astrobiological exploration, so it was a natural segue to apply our lessons to future exploration of other planets.

What is the main challenge of identifying ancient life on Mars (or Earth)?

I think the biggest challenge is that we do not have an analytical definition for life, at least life in its simplest form. There is no universally agreed upon collection of chemical evidence that adds up to "life detected".

How do you propose to combine Raman spectroscopy and GC-MS?

We see Raman spectroscopy as an ideal screening tool for GC-MS analysis. Preserved biosynthetic compounds identified by GC-MS can be an excellent sign of life, but the data can be hard to collect; it is a destructive technique, but there is no way of knowing until the end of the process whether the sample is going to contain any extractable compounds of use. Additionally, GC-MS is limited on a Martian rover by its need for sample preparation – a process that consumes materials; the Curiosity rover has GC-MS capability, but there are only nine sample cups dedicated to looking for polar organic compounds; you have to make those nine samples count! In contrast, Raman spectroscopy is a fast, non-destructive technique that can be done from a distance. However, the resulting data cannot offer definitive proof of life. Our hope is that combining the two techniques will increase the chances for success.

We are also investigating how geological context can be used to influence sample selection. For instance, are there morphological signals that can indicate that a rock would be worth the very arduous process of chemical analysis on Mars?

Can you accurately predict how Raman spectroscopy will work on Mars?

That's potentially a big issue. No matter how many Earth-based Mars analogs we examine, Mars is still alien. It has different geological and atmospheric history, and the trace element compositions are very different. It's possible that elements that do not typically interfere with analytical processes on Earth will lead to complications on Mars.

What stage are you at?

We are continuing the process of thinking through potential complications and work arounds, with the hope that when the next sets of rovers deploy, we as a community have a good chance of collecting reliable data. ESA has a rover scheduled for 2018 and NASA in 2020 – both will have Raman spectrometers on board if all goes to plan.

What are your personal predictions about life on Mars?

I believe data will be collected over the next few years that will be interpreted by some as a sign of life, but I cannot see the issue being resolved in my lifetime. We do not yet even have consensus about the oldest signs of life here on Earth, and those are rocks that anyone can examine in their own labs...

Are you fans of David Bowie?

Ironically, we prefer "Golden Years" to "Life on Mars". When things are going well we tend to break out in a chorus or two. Even our girls now know to chime in on the "bomp-bomp-bomp" part.

Boosting Anticancer Selectivity

A smart poly(acrylic) acid shows promise as a carrier to improve anticancer drug action, says Alison Maniego

Who?

I'm a PhD student at the University of Western Sydney (UWS) where I also obtained my undergraduate degree. My advisors are Marianne Gaborieau and Patrice Castignolles, and my research focuses on finding the relation between the branched structure of PAA (a pH responsive polymer) and its binding to and delivery of an anticancer drug (cisplatin). At the start of this year, I was awarded the Young Scientist Award lecture in the 7th International Symposium on the Separation and Characterization of Natural and Synthetic Macromolecules. I also received a student prize for International Polymer Meetings from the Royal Australian Chemical Institute, Polymer Division, for this symposium.

What?

I have investigated a branched pH-responsive smart polymer, poly(sodium acrylate), PNaA, as a potential drug carrier for cisplatin. pH-responsive drug delivery systems are relevant for anticancer research as tumors have a more acidic environment than non-cancer cells. The presence of extensive branching is an ideal property for drug delivery applications as the branching provides better drug encapsulation. I have also developed a new method for monitoring the binding of anticancer drugs with charged polymers using capillary electrophoresis in critical conditions (CE-CC).

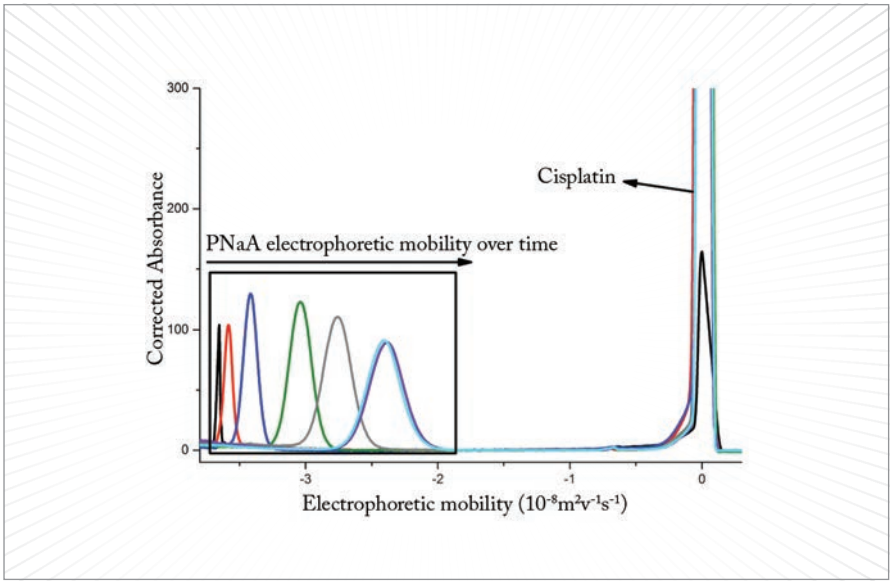


Figure 1. Separation of free cisplatin and linear PNaA. The binding of cisplatin to PNaA was monitored online and over time (as represented in different colors).

Why?

The aim is to bind an anticancer drug and a drug carrier together simply by mixing them in solution (without coupling agents) and to find a novel technique that monitors this binding.

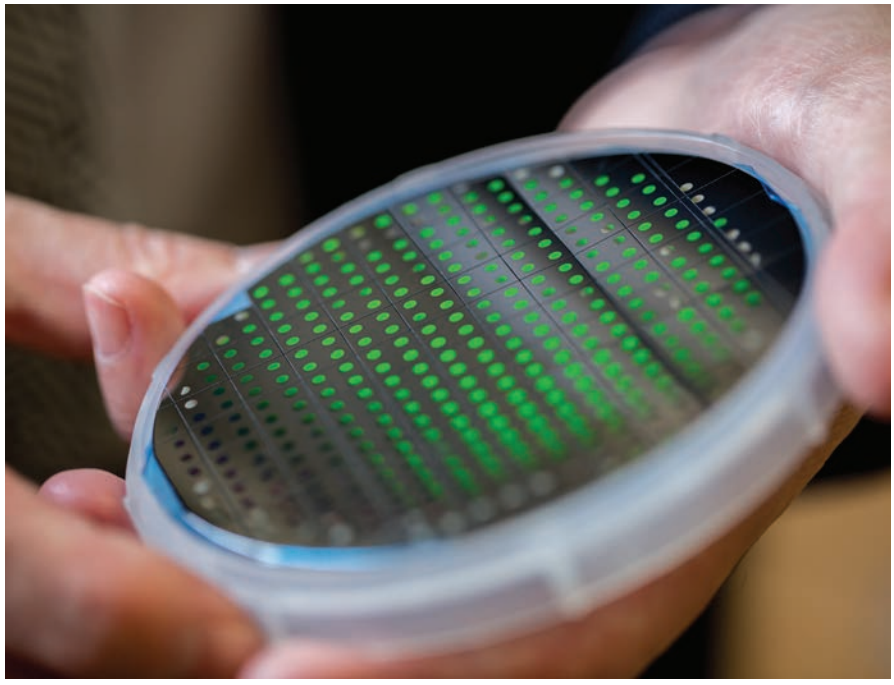
Drug delivery formulations usually involve a tedious synthetic process so inducing binding simply by mixing cisplatin and PNaA in solution and then leaving them to react is a much more straightforward approach. Moreover, promoting the use of CE-CC in terms of online monitoring of the binding and release of a drug to a drug delivery system is a novel idea that could be beneficial for other disease areas. As long as your samples are charged, I don't see why you can't use CE-CC – it's cheap and doesn't use much of your sample.

How?

Online monitoring in CE-CC enables separation of the drug and PNaA during their binding. Free cisplatin, which is neutral, migrates the fastest followed by the negatively-charged PNaA (see Figure 1). The separations in this study are shown as a function of electrophoretic mobility, which depicts the intrinsic velocity of the species traveling in the capillary and corrects for the minor discrepancies the electroosmotic flow may cause from one injection to another. For our preliminary experiments, an increase in the electrophoretic mobility of linear PNaA was observed over time, suggesting that the polymer is binding to cisplatin (boxed region in Figure 1). Both the dissolution of cisplatin and the drug release from PNaA were also monitored using CE-CC. The drug release experiment was initiated once the binding was completed and a decrease in the PNaA's electrophoretic mobility was observed. The activity of cisplatin bound to PNaA is investigated in vitro and other PNaAs with a higher degree of branching are also investigated.

Next?

Since this study, I have been optimizing the conditions for the release of cisplatin incorporated in PNaA. I have also done some preliminary in vitro testing with the PNaA/cisplatin formulation on a cancer cell line.



Get REDI for Matrix-Free MALDI

Could a new nanofabricated surface lower the limit of detection – and remove the need for matrix – with existing MALDI MS instrumentation?

A new surface – the REDIchip – uses nanopost array (NAPA) technology and can identify traces of chemicals as low as 10^{-19} moles, according to its inventor, Akos Vertes, a professor at George Washington University, who has been working on the project for over seven years.

"Initially, we were experimenting with a silicon surface made by a laser process. Our idea was to take the silicon surface and use it for the production of ions. We had some success but there was no way we could get a wide enough range of geometries," says Vertes. At that point, Vertes and his team turned to nanofabrication, which was able to produce nanopost structures with a much wider variety of geometries. The research team tuned the post diameters, post heights, and the periodicity of the posts, and found that the best for producing ions had a 150 nm diameter and a height of 1200 nm.

However, the big breakthrough came when Vertes' students laid down some yeast cells on the nanostructures (1). "To our great surprise, we got very rich mass spectra from our MALDI instrumentation from as few as 100 yeast cells. Even when we used one yeast cell we still got meaningful spectra. And that meant two things: one, the limit of the detection on the surface was exceedingly low; and two, we had a method that enabled us to directly interrogate micro-organisms without sample processing," says Vertes. Resonance-enhanced desorption ionization – REDI – was born.

Other studies confirmed the low limit of detection (2) but one big challenge remained – being able to manufacture the chips or, more specifically, the nanoposts economically in greater numbers; around 27 million posts are needed on each chip. Vertes says, "Producing posts one by one, which is how we started, is not a welcome proposition. Indeed, it was a dead end for commercialization. But Protea Biosciences – a long-standing partner of the university that licensed the technology – came up with a method that helped us to produce a large number of chips in parallel in a relatively short amount of time."

According to Vertes, there are many potential applications for the surface, including trace analysis in biomedical samples and detection of trace contaminants in the environment. "Today, people are also talking a lot about endocrine disruptors and their detection is another potential application," Vertes adds. "Another class of applications will be imaging applications. We can take a tissue section and lay it over the surface of nanoposts to map the distribution of metabolites and lipids. It doesn't take one molecular image, but as many molecular images as the number of peaks you have in the spectrum."

Even though the chip has recently been commercialized by Protea, Vertes doesn't intend to wash his hands of the technology, and is currently working on the next generation. He wants to push the sensitivity even further and discover more applications, particularly in the biomedical field. *SS*

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In My View

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

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

Contact the editors at
edit@texerepublishing.com

Black-Box Data Analysis for Spatial Metabolomics

Automated and reliable tools for spatially annotating metabolites from imaging mass spectrometry data are essential.

By Andrew Palmer and Theodore Alexandrov, European Molecular Biology Laboratory, Heidelberg, Germany.

In recent years, metabolomics has been recognized as a field of major importance that promises to advance our understanding of cell biology, physiology, and medicine. Metabolites are the 'small cogs' in the cellular machinery and consist of small molecules that are ingested, altered, and catalyzed within the cellular machinery, including not only those molecules synthesized within cells but also those gained from the environment, such as vitamins and nutrients. Such molecules are indicative of cellular processes both from the underlying genetics, cell differentiation and the immediate environmental pressures – and they provide a real-time read out of the state of individual cells and cell populations. Cellular activity can be highly spatially localized and so being able to image markers of metabolic activity may provide researchers with new perspectives on biological problems. Traditional methods often treat samples as homogeneous bulk materials, but this risks missing important biological information; for example, the degree of penetration of an anti-cancer drug into a tumor or a secretion of an antibiotic in proximity to invading bacteria.

Imaging mass spectrometry (MS) is essentially a chemical camera that can map the distribution of chemicals across a sample with micrometer precision using highly accurate measurements of the molecules' masses. Its unique feature is that effectively millions of images are recorded showing the distribution of potentially thousands of molecules. Unfortunately, this makes the datasets very large; a single image can be over 100 GB of data and processing the data is currently the main bottleneck in gaining further biochemical and biological knowledge.

What we need to exploit the full potential of such an advanced technique are algorithms for high-throughput molecular annotation of our 'big data' data. Successful algorithms must incorporate existing molecular knowledge databases, efficiently exploit both the mass spectral and spatial information inherently present in imaging mass spec data, but also, importantly, control annotation confidence.

"Our tools will be wrapped up as an online 'black box' search engine to which researchers can directly submit their data."

A large body of knowledge on metabolites and metabolic pathways has been accumulated for specific biological systems and recorded in curated databases (for example, HMDB, KEGG, LIPIDMAPS, ChEMBL). We are developing novel spectral and image analysis tools to assess whether these molecules are present in imaging MS data – and where. In fact, this approach is quite different to the usual methods for analyzing mass spectrometry data, which typically focus simply on individual spectra. Our tools will be wrapped up as an online 'black box' search engine to which researchers can directly submit their data. Users will receive molecular images corresponding to detected metabolites as an output, which shifts the perspective away from MS peak analysis of individual spectra to high-level analysis of metabolic images linked to molecular knowledge bases.

Over the past few years, we have developed the algorithms that form the cornerstone for such a black box system and evaluated them within the biological analysis pipelines of several collaborators. The next step will be to provide it to the community as an open source engine so that everyone can use it online or offline to turn the chemical pictures produced by imaging MS into functional maps of metabolic activity. This is the core aim of the European Horizon2020 project METASPACE we have just launched that unites eight partners from five countries.

For more information, visit: www.embl.de/research/units/scb/alexandrov. And on page 36, enjoy an artistic representation of the future of 3D chemical mapping from Alexandrov.

Vibrational Spectroscopy on Show

Making the case for more use of reflection FTIR and Raman spectroscopy in analyzing works of art.

By Silvia Bruni, Associate Professor of Analytical Chemistry, Università degli Studi di Milano, Milan, Italy.

Visible-near infrared reflection spectroscopy and X-ray fluorescence are by far the most popular point-analysis spectroscopic methods for non-invasive investigations of works of art. From a qualitative point of view, these methods are popular because they are easy to use and give immediate, readable results. But...

Reflection Fourier-transform infrared (FTIR) and Raman spectroscopy are a competitive choice because they are non-destructive and at the same time provide the high specificity needed for identifying chemical compounds, mixtures of pigments or organic dyes, or uncolored substances, such as binders. Conservator-restorers can be skeptical of these techniques, because they output complex spectra – an attitude that's encountered more frequently in museums that don't have on-site analytical laboratories. Additionally, some scientists like to emphasize the disadvantages of both techniques; for

example, highlighting the weak signal intensity and fluorescence emissions of Raman spectroscopy, and noting the presence of peaks due to different components found in the material under investigation (binders, varnishes, fibers, and so on) in FTIR. In my view, however, we ought to be using both of these vibrational spectroscopic methods for non-destructive analysis of cultural heritage materials in the field, and we should be testing them under different environmental conditions and on different sorts of artifacts.

"Conservator-restorers can be skeptical of these techniques, because they output complex spectra – an attitude that's more common in museums without on-site analytical laboratories."

There are challenges of course; the first being how we mount the instruments or probes. The apparatus must adapt to different geometries and, in our experience, a tripod equipped with a counter-balanced extension arm provides a very stable mount. An XY stage completes the mount when using a Raman microprobe with a 50× objective. Our setup enables micro-Raman spectroscopy for in-situ examination, giving satisfying results for a range of works of art – from frescoes to illuminated manuscripts and easel paintings (1). Using the technique we can recognize most inorganic pigments even in the presence of organic binders and varnishes that create fluorescence; for this purpose we use two microprobes with two different laser sources – 532 and 785 nm – chosen according to the color of the pigments or the intensity of the fluorescence background. This equipment is also useful for obtaining laser-excited fluorescence spectra from organic dyes, for example, which are difficult to identify in situ with other techniques.

As far as reflection FTIR spectroscopy is concerned, the acquisition of spectra is not as critical as with Raman, while their elaboration and interpretation appear more demanding. For example, the contribution of both specular and diffuse reflection to the collected radiation does require you to make a decision whether to apply an algorithm to the spectrum to make it comparable with transmission spectra found in most databases.

We have seen two different situations with illuminations in ancient manuscripts, where mainly specular reflection was obtained, allowing us to use the Kramers-Kronig transform, and with organic dyes found in historical textiles. These reflect diffuse radiation to give spectra that can be compared with transmission spectra of pure dyes, because the fibers "dilute" the colorant. In northern-Italian illuminated codices, dating to the 16th century, both pigments and binders, such as gum Arabic and egg white, could be identified; this information is usually gathered using laboratory-based analyses (2). For ancient Caucasian textiles dating from 17th to 18th century, we used a library-search method based on the correlation algorithm and on the subtraction of the prevailing spectrum from the textile fiber, which allowed us to identify many different dyes ranging from madder to indigo and tannins (3).

In a rather daring application of the technique, we suspended the spectrometer from a scaffolding at a height of more than four meters to obtain FTIR spectra from deterioration patinas (calcium and magnesium sulfates, and calcium oxalates) in a low relief frieze decorating a Baroque arcaded courtyard (4).

I hope these examples of how we use FTIR and Raman spectroscopy for analyzing artistic and archaeological materials encourage you to experiment with these techniques inside and outside your laboratories for obtaining as much information as possible in a non-invasive manner. In my mind, they certainly deserve their place as analytical tools for helping to conserve important works of art – and no doubt, there are applications in a great number of other fields.

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Advancing Water Analyses

Presenting new considerations to evaluate drinking water.

By Lisa Holland, Professor, Department of Chemistry, West Virginia University, Morgantown, West Virginia USA; Vince Remcho, Professor, Department of Chemistry, Oregon State University, Corvallis, Oregon, USA; Susan Richardson, Professor, Department of Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina, USA; and Vicki Blazer, U.S. Geological Society, Fish Health Branch, Leetown Science Center, Kearneysville, West Virginia, USA.

Water is life. Indeed, its existence on Mars has driven the search for life on the red planet (see Art of Analysis page 43). Water is also a powerful solvent, carrying a myriad of chemicals, many of which undergo chemical conversion in the resulting complex mixture. Importantly, the quality of water entering a processing facility can affect the purity of the polished product. But, how much control do we have? Monitoring water and limiting toxic chemicals introduced into our water system can improve the process, and regulations govern what we know to be dangerous. However, there is a struggle to predict what new contaminants should be restricted.

At Pittcon 2015, we presented the conundrum of water quality in our session on emerging contaminants and healthy water. At the University of South Carolina, exquisite analyses based on chromatographic separation and high-resolution mass spectrometry provide powerful insight into the complex and dynamic mixture that is our municipal water. Analyzing water for pharmaceuticals, illegal drugs, food additives, pesticides, herbicides, and consumer products can reveal much. For example, penta and octa brominated contaminants (originating from polybrominated diphenyl ethers once used in flame-retardants) are toxic (1). A deca-brominated contaminant should be safe, except that it degrades to these more toxic constituents (1). So we must ask: "Is this an isolated problem?" Perhaps not.

Iopamidol is an invaluable imaging agent in medicine; it is safe for consumption and improves lives. Yet, when it is excreted by the body and subjected to chlorination, a 200-gram dose of a critical medical chemical becomes a toxic iodinated disinfection by-product (2). How could this have been anticipated? If we put the power of an LC-MS into a wastewater treatment facility, the operator would know, but such equipment and knowledge comes at a cost.

What if we reduced the cost by using non-toxic, disposable microfluidics to

make simple and robust sensors? This would allow the operator to identify those species that are intolerable in the water system, those that can be better removed with changes in processing, and those that are indicators of anthropogenic contamination of natural waters. When knowledge is power, such strategies make sense.

At Oregon State University, researchers use polycaprolactone to build portable devices by printing simple patterns on laboratory filter paper (3, 4). The work – supported by the Bill and Melinda Gates Foundation – paints an interesting picture; colorimetric assays for bromide using the technology, for example, can easily recognize the yellow spots of hydraulic fracturing (fracking) fluid leakage. Paper is cheap and the human eye is the ultimate convenient detector. The measurement can be performed on a tight budget for less than one dollar with no training required. And, for an additional 100 dollars, a stable light source and USB adapter can be added to the device to improve quantification; another option is to use a mobile phone for detecting and data sharing. With these relatively low-cost tools, on-site monitoring becomes achievable for bromide and the principle may be applied to any other contaminant that can be adapted to colorimetric detection.

But let's return to the question about what is not known. There are 800 known endocrine disrupting compounds, but the bigger threat comes from those compounds, metabolites or mixtures for which toxicity is not yet known. In our waterways, for example, dying freshwater fish tell us when agricultural runoff, antibacterial additives in soap, or pharmaceuticals excreted by humans, lead to a toxic recipe for aquatic life. So, we can learn a lot by monitoring wildlife. Population declines or sudden die-offs can be signs of caution, as can indicators of reproductive dysfunction, compromised immune systems, cancer, neurotoxicity and behavioral effects in fish living in these waters. Sediment, water, passive samplers, and fish may hold secrets that led a U.S. Geological Society (USGS) research team to assay 138 chemicals collected from samples at six different sites throughout the Potomac River basin – which supplies water to more than five million people in Maryland, Pennsylvania, Virginia, Washington D.C., and West Virginia in the USA (5, 6).

What can be done when human activities create chemical cocktails in our water system? Researchers at West Virginia University demonstrated the power of analyzing circulating steroids in fish by using a rapid capillary electrophoresis method to separate multiple steroids within five minutes, enabling detection of steroids in individual fish using UV-visible absorbance (7). When adapted for the analysis of a single zebrafish weighing only 1.5 grams, this method generates nanomolar detection limits and provides insight into hormonal responses to chemical exposure that correlates well with physiological endpoints. Monitoring changes in multiple circulating steroids enables researchers to screen chemicals rapidly for endocrine disruption. With information about specific changes in estrogens, androgens, and progestogens, the mechanisms of dysfunction can be better elucidated.

After we presented the above examples in our Pittcon session, we had a lively panel discussion, which increases the likelihood that this topic will be included in other national and international meetings. Being able to show how integrating technologies and how analytical chemistry can tackle such a complex problem, such as water safety, fires debate and, above all, we hope that scientists and citizen scientists will seek answers to these environmental issues with new enthusiasm. Certainly, further research must be supported to address these important questions (8).

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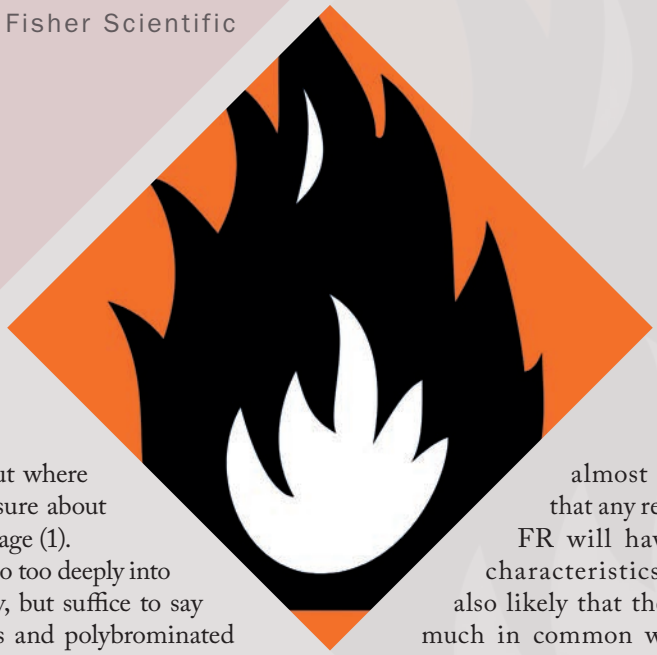
A Burning Issue

Legacy flame retardants (FRs), emerging FRs and dioxins are all infiltrating our environment. How are they linked and how should we assess their impact on human and environmental health?

By Martin Rose, environmental contaminants and food integrity, Fera Science Ltd, York, UK.



Flame retardants (FRs) have been used for decades to help prevent death and injury from fires, but it is clear that some of these compounds are entering the environment and food chain. I believe that FRs – legacy and emerging – and dioxins should not be considered in isolation. Instead, a holistic approach is needed.

But before I delve into the what's, how's and why's, please allow me to apologize for the acronym onslaught and address the potentially confusing issue of terminology in this field:

i) Legacy or established FRs (bromine: BFRs; chlorine: CFRs; phosphorous: PFRs) are chemicals that are extensively documented regarding production and use. Furthermore, we have a significant amount of data on the chemistry, fate, exposures, and environment and health issues, which is to say (eco-) toxicity and/or human health effects.

ii) Emerging FRs are chemicals that are documented in terms of production and use, and that have also been shown to occur/distribute to the environment and/or wildlife, humans or other biological matrices.

iii) Novel FRs are chemicals that have been documented as potential FRs and have been shown to be present in materials or products.

iv) Potential FRs are chemicals reported to have applications as FRs, for example, in patents, but where we are unsure about levels of usage (1).

I won't go too deeply into the history, but suffice to say that PCBs and polybrominated biphenyls (PBBs) are no longer used. As a quick aside, one of the first persistent organic pollutant (POP) incidents occurred in 1973, when a PBB mixture – FireMaster BP-6 – was accidentally (and frighteningly) mixed with livestock feed in Michigan. It led to the quarantining and slaughter of nearly 30,000 cattle and thousands of other animals (1). Polybrominated diphenyl ethers (PBDEs) were widely used in plastics, upholstery, textiles, and foams, and can make up over 15 percent of some products by weight. Tetrabromobisphenol-A (TBBPA) and hexabromocyclododecane (HBCDD) were brought in to replace PBDEs.

The lesson here is that demand arising from the regulation of BFRs will always be met by an increasing number of alternative FRs – after all, industry must still comply with fire safety regulations. Indeed, hundreds of emerging FR compounds have been registered. To put that into perspective, current production of BFRs exceeds 100,000 tonnes per year.

Environmental impact

Why does that matter? Well, as already indicated by the terminology above, emerging FRs have already been found in the environment – and some in foods. As you'd expect, flame retardants must be chemically stable, which is typically embued by halogenated aromaticity and low aqueous solubility. Therefore, it's almost inevitable that any replacement FR will have similar characteristics, and it's also likely that they'll share much in common with other POPs: persistency, bioaccumulation and toxicity.

Many BFRs are being regulated; octa- and nona-BFRs have essentially been phased out in many countries. And the European Commission has asked all member states to gather data on the levels of BFR compounds in foods. The Commission Recommendation (2014/118/EU) recognized that levels of these substances in food of animal origin could be related to their presence in animal feed – expect a further recommendation on monitoring animal feed in 2015.

Why is the European Commission so concerned? It comes off the back of a series of six very comprehensive scientific opinions on the topic from the European Food Safety Authority – an excellent source of background information for those who are interested (www.efsa.europa.eu).

There's a big challenge here; hundreds of compounds pose potential risk, so we decided to prioritize method development using four factors: environmental persistence (our criterion was over 500 days), bioavailability, toxicity, and occurrence in biota and food. We identified a top ten (see box) – and I'd be very interested in anyone's views on our selection.

When it comes to risk assessment – or the impact of exposure on human and environmental health effects – a vicious

circle exists. It's difficult for analytical chemists to get funding to develop methodologies to assess exposure to chemicals if there's no data on toxicology. But toxicologists can't find funding to research the toxic actions of compounds if there's no evidence of exposure. How do we break this vicious circle? Students can certainly help. Otherwise, it's a case of scraping together enough funding to start the ball rolling. I wish we had a more open approach to the problem of emerging compounds...

The dioxin–furan link

Most, if not all, BFRs can form brominated dioxins and furans (PBDD/Fs) when they degrade. They are created by thermal breakdown of brominated organics (burning BFRs in plastics) and are highly toxic and persistent. Moreover, mixed (and highly toxic) chlorinated- and brominated-dioxins (PXDD, PXDF, PXB) may be formed in the presence of chlorine.

How do we deal with these mixtures? We've already done it for chlorinated dioxins, so we're well ahead of the game. We can use the very elegant WHO-TEQ scheme, a simplified expression of the toxic equivalency (TEQ) of the different PCBs and dioxins as one number:

WHO-TEQ = ∑[PCDDi× TEFi] +∑[PCDFi× TEFi] +∑[PCBi× TEFi].

I was fortunate enough to be involved in a review on the toxicity of these compounds in 2013 (2). It was noted that PBDDs, PBDFs, and some dioxin-like biphenyls (dl-PBBs) may contribute significantly to the total TEQ. But we need more data on exposure. Also, other mixed halogenated PXDD/Fs and PXBs are found in foods, admittedly at lower levels; however, as there are many more congeners (a grand total of more than 5000) and only very few are measured, the potential contribution to total dioxin toxic equivalency could be significant.

The key point is that they are present and a lot more measurements need to be done. If we start looking at compounds that we know have the same type of toxic effect, we will get a much more comprehensive view of the risk.

The analytical challenge

The measurement of mixed halogenated and brominated dioxins is challenging to say the least. Mainly, because there are so many congeners and so few analytical standards – and there are even fewer 13C analogs. For that reason, I've only scratched the surface. Clearly there is a lot more to be done and many other compounds also need to be considered, such as polychlorinated naphthalenes (PCNs), which also exhibit dioxin-like toxicity.

To see the whole picture, perhaps we need to revisit our elegant and simple equation from above and make it less simple and elegant:

TEQ = ∑[PCDDi× TEFi] +∑[PCDFi× TEFi] +∑[PCBi× TEFi] +∑[PBDDi× TEFi] +∑[PBDFi× TEFi] +∑[PBBi× TEFi] +∑[PXDDi× TEFi] +∑[PXDFi× TEFi] +∑[PXBi× TEFi] +∑ [PCNi× TEFi] …… + ∑many more?

The truth is, we don't know the importance of these compounds – and we don't know what we're not looking for. Indeed, we start to echo Donald Rumsfeld (US Secretary of Defense, 2002): "... there are known knowns; there are things we know we know. We also know there are known unknowns; that is to say there are some things we do not know. But there are also unknown unknowns; the ones we don't know we don't know." I'm not sure that's a place I want to be. The way out? Well, I believe we need next-generation mass spectrometry (MS), we need to combine MS with measurement of biological effect; for example, using cell based or receptor assays. And we need to be aware of the impact of cleanup methods.

The use of the TEQ scheme for dioxins was the first – and very sensible – attempt at regulating chemicals as mixtures. Why? Because of the similar mode of toxic action through the Ah receptor. But if we acknowledge the value of this approach and can prove that we are exposed to other chemicals with the same mode of action, then surely these compounds should also be included in the scheme. Other environmental chemicals, such as some of the BFRs, do not directly share this mode of action– but they can be converted into compounds that do. All of these factors need to be taken into account when undertaking risk assessment to ensure we sufficiently protect human and environmental health.

Top Ten Emerging BFRs

1. Hexabromobenzene (HBB)
2. 1,2-bis(2,4,6-tribromophenoxy) ethane (BTBPE)
3. 5,6-dibromo-1,10,11,12,13,13-hexachloro-11-tricyclo[8.2.1.02,9]tridecene (DBHCTD)
4. 1,2,3,4,7,7-hexachloro-5-(2,3,4,5-tetrabromophenyl)-bicyclo[2.2.1]hept-2-ene (HCTBPH)
5. Pentabromotoluene (PBT)
6. Pentabromobenzyl acrylate (PBB-Acr)
7. Pentabromoethylbenzene (PBEB)
8. 1,2,4,5-tetrabromo-3,6-dimethylbenzene (TBX)
9. Decabromodiphenyl ethane (DBDPE)
10. Octabromotrimethylphenyl indane (OBTMPI)

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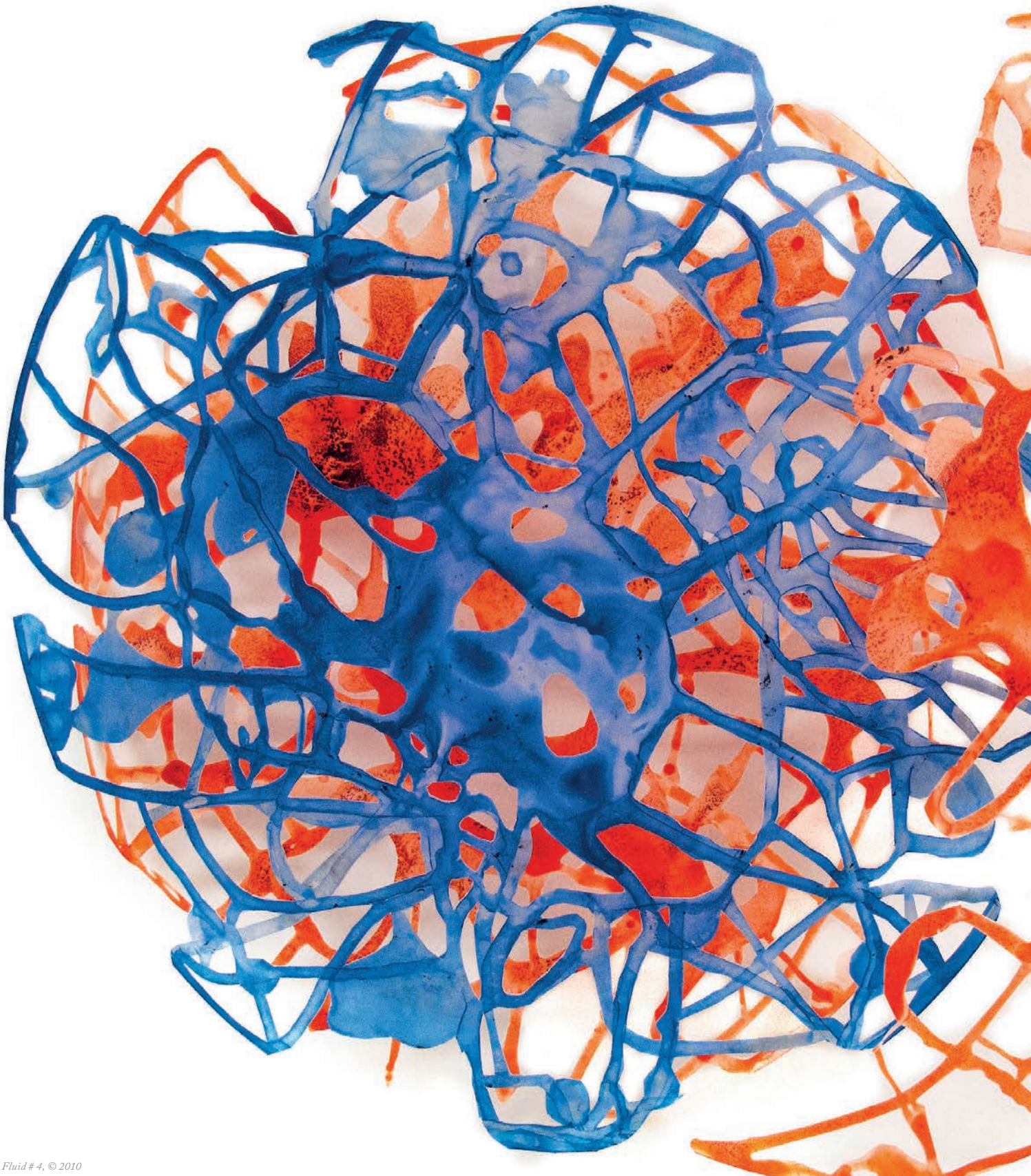
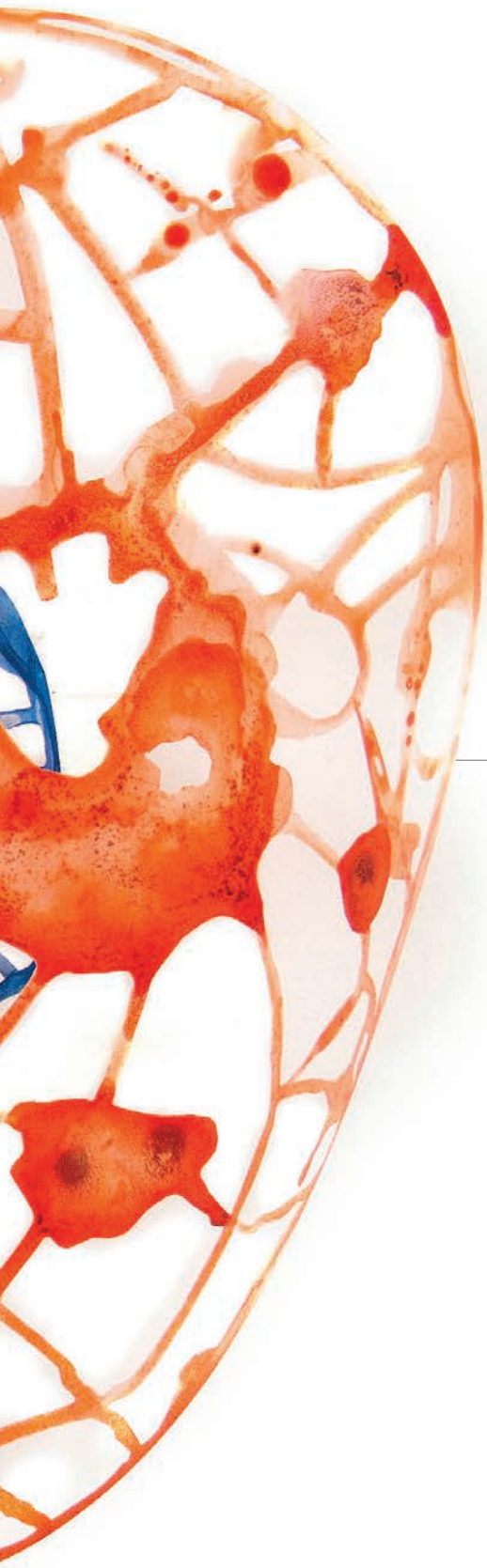
**The opinions and conclusions expressed are solely the views of the author and do not necessarily reflect those of Fera or any other organization.*



Fluid # 4, © 2010
Acrylic on mylar, fiberglass rods 15" x 18" x 5"



When Art Meets Science

Welcome to our second foray into the fascinating confluence of aesthetics and analytics, where we celebrate the wonderful and diverse world of analytical science by sharing your spectacular images.

The Invisible Becomes Visible

World-renowned artist Rebecca Kamen re-imagines and visualizes complex knowledge and the process of discovery – an approach that explores the nexus of art and science in a unique and beautiful way.

Scientific analysis factors greatly in the creation of Rebecca Kamen's work. Through her research into various fields of science and by working closely with scientists, Kamen analyzes what she understands and communicates her observations and discoveries through exciting forms of art.

When did your fascination with science and discovery begin?

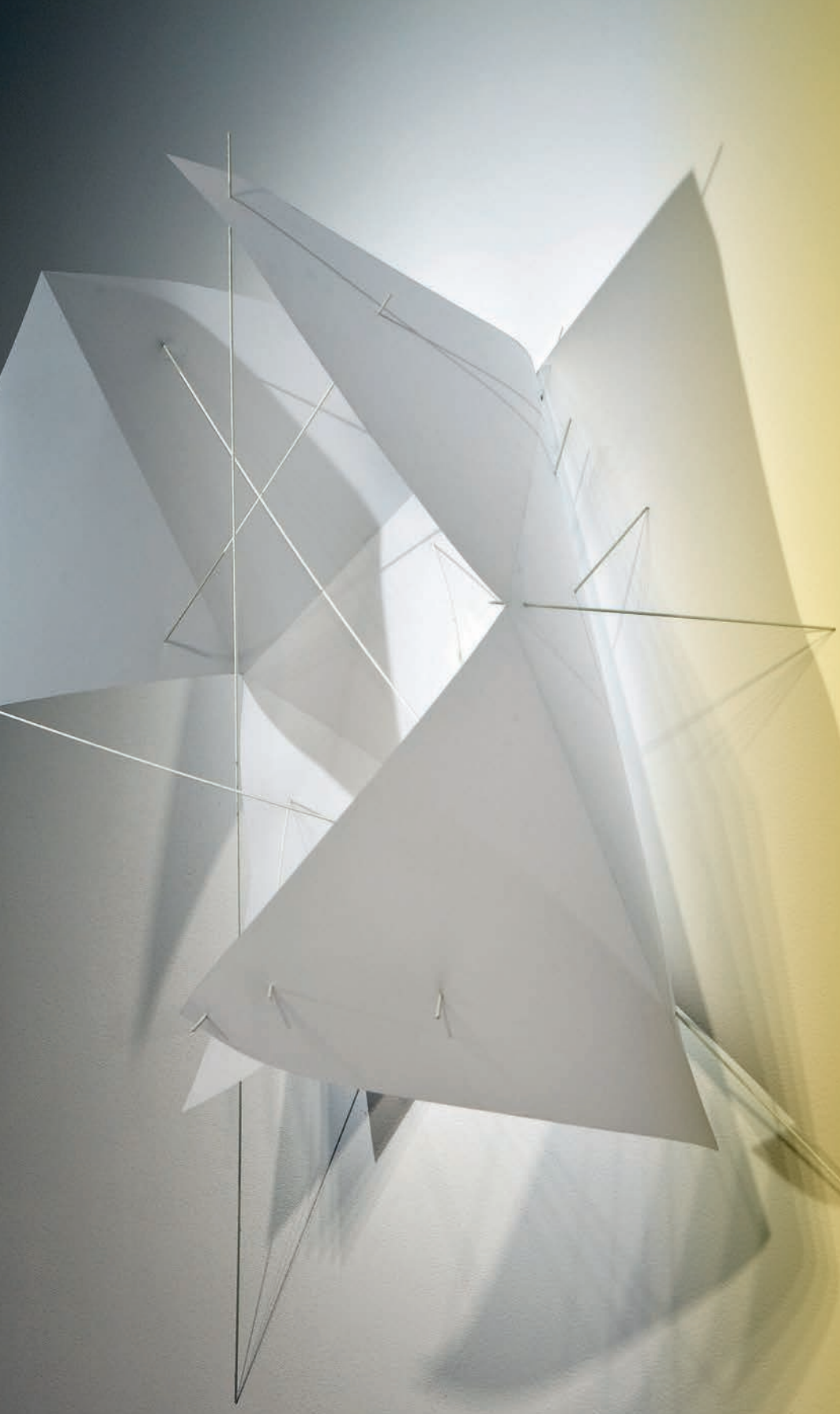
I fell in love with discovery as a young girl. With awe and wonder, I spent much of my childhood investigating the world of elements with a simple chemistry set, and used it to create elaborate science-fair projects. Insatiable curiosity and a deep love of learning created bridges between seemingly unrelated disciplines. As a result, I have devoted my life to an intuitive examination of properties that overlap from discipline to discipline. I remember the thrill when my first cardboard telescope magically connected me with the cosmos, and can still summon my feelings and fascination as I continue to explore its matter and meaning. These discoveries have inspired me to use my artwork to make the invisible visible, connecting common threads that flow across various scientific fields to capture and re-imagine what scientists see.

How can art help explain scientific concepts, principles and processes?

Art enables people to visualize something through different eyes. If, for example, you change a lens on a microscope or a telescope the instrument will reveal something new. A macro lens, for instance, will reveal more detail. When any discipline is able to view something through a new pair of eyes – or apply a new way of thinking – discovery happens. That's certainly been true in my work, as I don't have any formal scientific training. I am an extremely curious person and fascinated with discovery in all fields of inquiry. I create work that is inspired by various fields of scientific research that many think aren't accessible to them. I like to tackle serious subjects, such as the periodic table of elements – something that would typically make people glaze over; when I tell them about my journey of discovery, they perk up. Essentially, I'm providing a new lens for people to look through, perhaps so they can understand something that they previously could not see.

How do you immerse yourself in a topic?

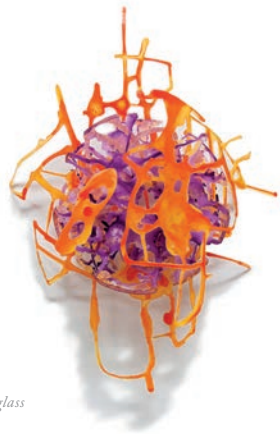
I spend a great deal of time talking to scientists and I research many rare books that record the history of science; they help me to understand the genesis of a discovery. And those historic discoveries explain what we now know in the 21st century. The history of science also provides a sense of a personal narrative; it's one of the significant ways we connect to other human beings through telling stories. For example, my research on general relativity reveals that Einstein began envisioning his theory when he was 14 years of age; wondering what it would feel like to ride on a wave of light. Einstein's "gedankenexperiment" – thought experiment – brings more meaning to his scientific discovery because people can appreciate that general relativity was something he originally thought about as a teenager. I also work with metaphor and try to make my art visually poetic, so people can see it and understand it in a way that is much more accessible to them.



Plato's Air © 2008
Mylar and fiberglass rods 42" x 34" x 19"
Photo Credit: Angie Seckinger

"Rebecca Kamen has great passion for the science and artifacts she studies and her curiosity leads her to transcend her point of origin, producing a response that both surprises and delights. Her creative process is akin to that of the natural philosopher whose scientific investigations sought correspondence rather than differentiation, as do today's scientists. Rebecca practices imaginative participation, seeing layers of relationship that broaden rather than narrow consciousness. She has the capacity to access a wide variety of human thoughts, hopes, beliefs and yearnings embedded in complex scientific artefacts. Rebecca has a gift for bringing out the spiritual dimension of science."

– Marjorie Gapp, Curator of Art and Images, Chemical Heritage Foundation, Philadelphia, USA.



Fluid # 6, © 2010
Acrylic on mylar, fiberglass rods 17"x 13" x 6"

Fluid # 1, © 2010
Acrylic mylar, fiberglass rods 12" x 23" x 3.5"

How did you get interested in dynamics?

I've always been interested in movement and dynamics. I grew up in Philadelphia but I spent my summers in Atlantic City (New Jersey), and I think those seeds were sown while walking on the beach, watching the movement of the ocean, and wondering about how things orbited the earth in space. Another example comes from when I was an artist in residence for the US National Institutes of Health's neuroscience program, where I became very interested in the "avalanche effect" (bursts of neuronal activity) in the brain. I found it interesting how things at the micro level in the brain are really a very small-scale version of what we actually experience at the macro level. The new work I'm currently developing is a dialog between inner and outer space, and the dynamics of what happens in both of those realms.

Scientific discovery really seems to inspire you...

As an artist, one of the things that fascinates and excites me is looking at certain natural phenomena, in outer or inner space, through various instruments that enable one to view things in a different way. For example, with electron microscopes, our ability to be able to see things at a minute level is quite humbling. It's so interesting how diverse scientific instruments reveal very different information about the dynamics of a natural phenomenon. Being invited by scientists to view and see what they get excited about is also inspiring.

I'm trying to understand more about my own creative process, now that I've had a little foray into neuroscience, and to discover what's occurring in my brain that enables me to make unique connections. About 15 years ago, I learned that I am dyslexic, which explains a lot about the challenges I had as a young student. Dyslexia also prevented me from becoming a scientist because I had a difficult time with school tests. But that particular cognitive obstacle turned into an extraordinary opportunity, enabling me to understand the world through making connections. And that contributes to my understanding of how everything in the universe works; I look at one thing and understand how it connects to something else.

You appear to learn intuitively. Does that help with your creativity?

Dyslexic people are often highly creative; we process information in a different way. And we are usually visual people. We learn by creating relationships between forms so that we can understand how things relate to each other. My own ability to see different kinds of relationships – because of the way my brain is wired – enables me to make connections between different scientific fields. When I deliver a lecture to senior scientists, I inevitably get the same response: "You have no formal training in science, so how do you know this stuff?" So, yes – I guess it's intuitive!

I also find it interesting that scientists work on such small parts of a much larger puzzle. It fascinates me that sometimes a scientist in one office will not communicate with another scientist next door because he's doing different research. I am also intrigued that when scientists leave their offices to present research and findings, they do so to other scientists who are doing similar types of work, but no one seems to put all these pieces together. With my work, I embed myself in a diverse range of scientific communities to understand what types of connections exist between areas I've researched already, which creates wonderful bridges between different scientific fields.

Do you believe your creative approach encompasses scientific thinking?

Absolutely! Creativity is about problem solving – and those scientists who I've really connected with are those who are creative thinkers. They tend to be universal investigators; they don't limit themselves to one small area, instead they tend to look at what they are doing in relationship to bigger pictures. Creativity in art and science is really about discovery. I can spend hours in my studio trying to solve a problem conceptually before I physically manifest it. It's like chemistry; the notion of transforming materials.

Before the advent of the camera, scientists were natural philosophers who looked more holistically at nature and the universe, using drawing and painting as a way of capturing and recording their observations. My work re-connects scientists to this original way of seeing and experiencing natural phenomena. I have an innate understanding of science and using my art to interpret scientific discovery fascinates scientists. Several have commented on how the artwork captures the aesthetic aspect of science observed in the complexity of a visual pattern or the beauty found in a series of numbers describing a scientific truth.

Many years ago, I was lecturing to a group of chemists and one of them said, "…astrophysicists have all those beautiful Hubble photographs but as chemists we don't have those kinds of beautiful things." I told the group that they had something even more extraordinary as their field deals with transformation. As a chemist, you may investigate how when chemicals come together they transform into something totally different – and that's beautiful. A chemist emailed me after seeing some images from my "Divining Nature: An Elemental Garden" project on the periodic table of elements. She said, "Thank you. I never thought of what I did as a chemist as being beautiful." Her words struck me because many other scientists that I meet do talk about their work in relationship to beauty – a beautiful equation, for example. There is a wonderful aesthetic sense to science that appears when I'm talking to scientists; because they're conversing with an artist, perhaps it's sometimes okay for them to think about their work or explain their work as being beautiful.

Would you advocate that scientists approach work with a creative and aesthetic eye?

I think that anyone involved in a creative field – which includes all sciences – and anyone who deals with discovery can learn so much more about what they are doing by looking at it through a different lens or field. For example, when I'm creating big projects, like Divining Nature, I include other art forms because using sound or dance to interpret the periodic table provides another way of understanding – and to me that's what we do as artists and scientists; we assist others as well as ourselves on our journey of discovery.

A Portrait of Rebecca Kamen

"I never made a painting as a work of art, it's all research." – Pablo Picasso

Not formally trained as a scientist, Rebecca Kamen presents scientific observations through the eyes of an artist. Her presentations to diverse audiences showcase the unique relationships between art and science, including the importance of patterns in both fields. Kamen has exhibited at the Chemical Heritage Foundation Museum, American Center for Physics, National Academy of Sciences, Science Museum of Virginia, and National Institutes of Health. Below, Kamen shares projects inspired by science.

"Matter Series – a series of complex wire sculptures, inspired by Einstein's ground-breaking research, that explores the relationship of space and time."
rebeccakamen.com/gallery/matter

"Fluid – investigates my interest in nature as a mapping system of energy. Informed and inspired by both micro and macro views of the Universe as well as other scientific visualization models such as fluid mechanics and fluorescence microscopy, these acrylic on mylar sculptures, interpret and make visible, the fluid energy of matter, creating a bridge between art and science."
rebeccakamen.com/gallery/fluid

"Divining Nature: An Elemental Garden – inspired by the orbital patterns of the first 83 naturally occurring elements in the periodic table."
rebeccakamen.com/gallery/divining-nature

"Portal – a sculpture and sound installation informed by gravitational wave physics and black holes, created in celebration of the centennial of Einstein's discovery of general relativity."
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In Our Environment

Fuel Gauge

Raman spectroscopy is used to analyze fuel-air ratios in an engine, with a view to understanding efficiency.

Photo: energy.gov

Eruptive Technology

Fei Yan (European Southern Observatory, Germany, and National Astronomical Observatories, Chinese Academy of Sciences, China) operates a UV spectrometer to observe the sulfur dioxide absorption in the plume of Mount Etna.

For more info: http://www.eso.org/~rfosbury/tmp/poster-Etna-trip-2014.pdf

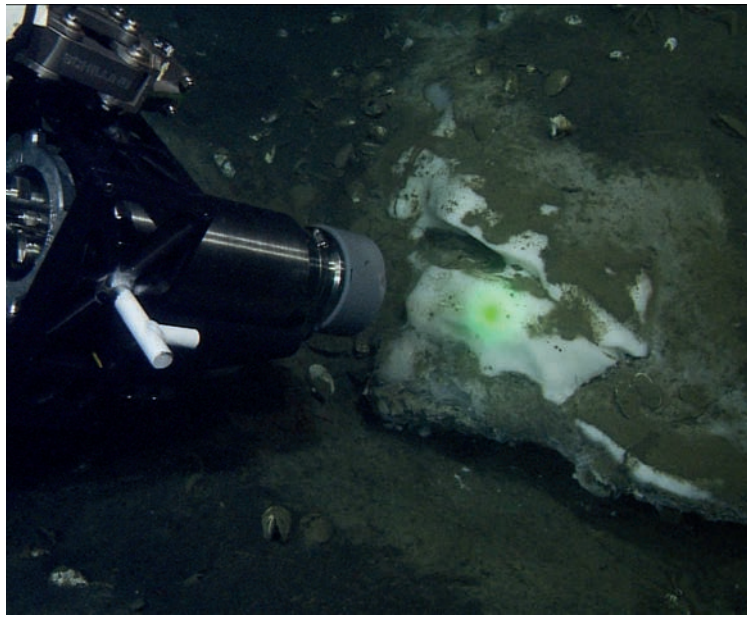
Photo: Leonardo Testi

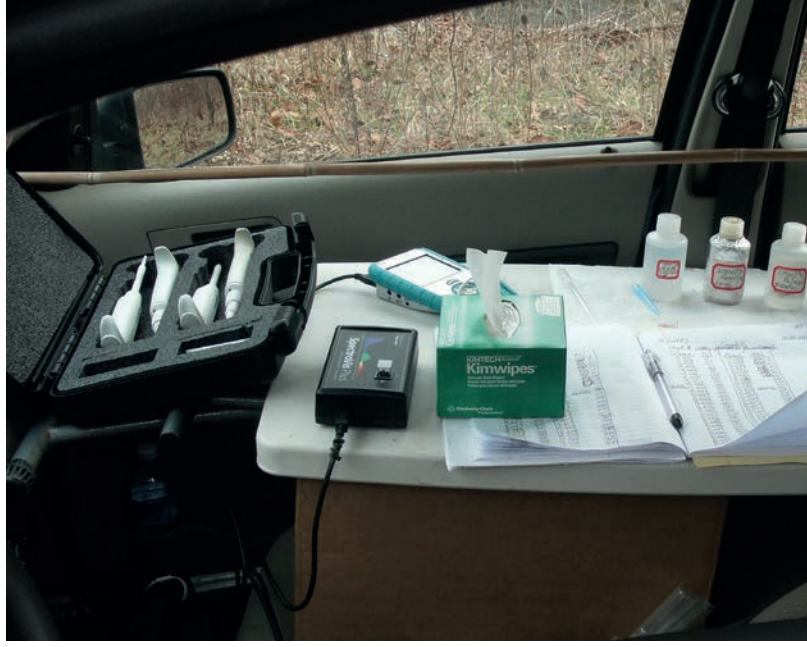
Homemade Spectroscopy

A modern-day John Browning observes the sun's spectrum at Neamt Citadel, Moldavia, Romania.
Photo: Stefan-Constantin Scanteie, Bucharest, Romania

Deep Sea Firing

A naturally occurring outcrop of gas hydrate (off the coast of Northern California, in the Eel River Basin at 1623 meters depth) is examined using an in-situ laser Raman spectrometer by researchers from the Monterey Bay Aquarium Research Institute in California, USA. The laser is held and positioned by the robotic arm of the remotely operated vehicle (ROV) and the Raman signals are collected in real time via Ethernet communications with the ROV.
Photo: Peter Walz, Peter Brewer and Edward Peltzer ©2013 MBARI





A TREATISE ON QUANTITATIVE ANALYSIS.

MISCELLANEOUS EXAMPLES OF

adding nitric acid from time to time so as to destroy ium salts. When sufficiently evaporated, add slight ead acetate, then ammonia in excess, and ammoniu filter, and wash. Acidify the filtrate with hydrochlo rate to dryness, add more strong hydrochloric ac orate, dry, ignite, and weigh the chlorides; calcula and if necessary separate the potassium and sod on p. 35.

To the filtrate add bromine, and estimate the Mn as dire on p. 62.

Estimation of Alkalies.—Dissolve a fresh portion and sepa silica and phosphoric acid as above. Add bromine water, ammonia, boil, and filter. Separate the calcium and magnes and estimate the alkalies in the filtrate as directed for clay on p precipitation with barium chloride.

Sulphuric acid must be estimated in a separate portion.

Carbonic Acid.—May be estimated as directed on p. 34

EXERCISE 11.—ANALYSIS OF LIMESTONE.

obtain a carbonic acid apparatus, fig. 16. Half fill the tube, A, with strong sulphuric acid, and B with dilute hydrochloric acid, weigh about 3 grammes of the limestone, and introduce it into the bulb, C, through the tubule, D; then weigh the apparatus, allow the acid from B to run slowly down on to the powdered sample, the evolved CO_2 escapes through the strong sulphuric acid, and is thus thoroughly dried. When further addition of acid produces no more evolution of CO_2, warm the apparatus so as to expel the CO_2 from solution, and weigh again, the loss of weight is the CO_2.

Fig. 16.

is essentially carbonate of calcium, combine with carbonate of magnesium, and containing We shall estimate calcium, magnesium, manganese, alkalies, sulphuric acid, carbonic acid, water.

Dry a portion at 100°, and weigh; call the

Water.—Weigh about 2 grammes of the pow o a porcelain boat, heat it to dull redness in a collect the water in a calcium chloride tube

and Magnesium.—Weigh about 2 grammes into a covered beaker, dissolve it in dilute ; when solution is complete, rinse it into o dryness, and ignite; take up with dilute , filter, wash, dry, ignite, and weigh be called *silica and insoluble*, if determine its constituents a larger must be treated with acid, and the ated by fusion with alkaline carbo

Organic Matter.—It is sometimes necessary to estimate organic matter; this may be done by dissolving in dilute hydrochloric acid, evaporating to dryness, and determining the amount of carbon by the process of organic analysis descri Chap. VII.

EXERCISE 12.—ANALYSIS OF AN IRON ORE.

trate add ammonium chloride, amm um sulphide, warm, and filter; reject add ammonium oxalate in excess, et it st ine the lime as oxalate. Estimate magnesiu te in the filtrate.

n of Iron, &c.—Dissolve 20 grammes of the ste acid, evaporate to dryness, take up with nit gramme of granulated tin, heat till it is n the precipitate estimate the *phosphe* p. 80.

The princ on ores are oxides or carbonates; th however, generally mixed with quantities of cla and) appreciable quantities of organic matter and necessary to estimate the followi —water, organic matter, insoluble ime, magnesia, carbonic acid, phosphori occasionally copper and other metals.

ure.—Dry 2 grammes at 100°.

mbined Water.—Determine directly as described on ganic Matter.—Treat the sample with dilute hydr

filtrate add ammonia till almost ne acetate, boil, and filter; separate th directed on p. 64.

Laser Chamber

(Top) Forna Fingerprints

In Baccharis trimera, a medicinal plant native to South America, irregular monoterpenes, such as carquejol and carquejol acetate, are considered chemical markers. Studying the species in Centro de Pesquisa e Conservação da Natureza-Pro Mata in Brazil showed us that metabolism differences between the male and female specimens should be also considered.

Photo: Manuel Minteguiaga and Eduardo Dellacassa, Laboratorio de Biotecnología de Aromas. Facultad de Química, Universidad de la República. Montevideo, Uruguay.

(Bottom) Hands on History

A finely-constructed small glass Schrotter reaction vessel (1890s) in front of the laboratory procedure for analysis of carbonic acid in limestone, from Outlines of Quantitative Analysis by A. Humboldt Sexton 1903.

Photo: Andy Brill (via Flickr)

Fourier Transform Infrared Spectroscopy (FTIR) is used to probe the chemical makeup of engine exhaust gases generated in Pacific Northwest National Laboratory's Engine Emissions Laboratory. Understanding the complex chemistry may unlock ways to reduce engine emissions and help the environment.

Photo: Pacific Northwest National Laboratory

Have Lab, Will Travel

A makeshift portable field laboratory for on-site determinations of total iron in mine drainage from several sites in southwestern Pennsylvania. Mark Stauffer (University of Pittsburgh-Greensburg) performed spectrophotometric determination of iron using iron(II)-chelating agent Ferene S, a Vernier Spectro-Vis diode-array single-beam spectrophotometer, a Vernier LabQuest microprocessor, and a plastic cuvet. The best aspect of a lab-in-a-car? Staying dry and warm on a cold December day. Photo: Mark Stauffer

Scent of a Woman

Christine Drea, Professor of Evolutionary Anthropology at Duke University and her student Jeremy Chase Crawford (who has since moved to the University of California) collected secretions from ring-tailed lemurs for gas chromatography-mass spectrometry (GC-MS) analysis. "Chemical richness" decreased with pregnancy, more so for dams bearing male offspring.

For more: tas.txp.to/0815/lemur

Photo: David Haring

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In Our Bodies

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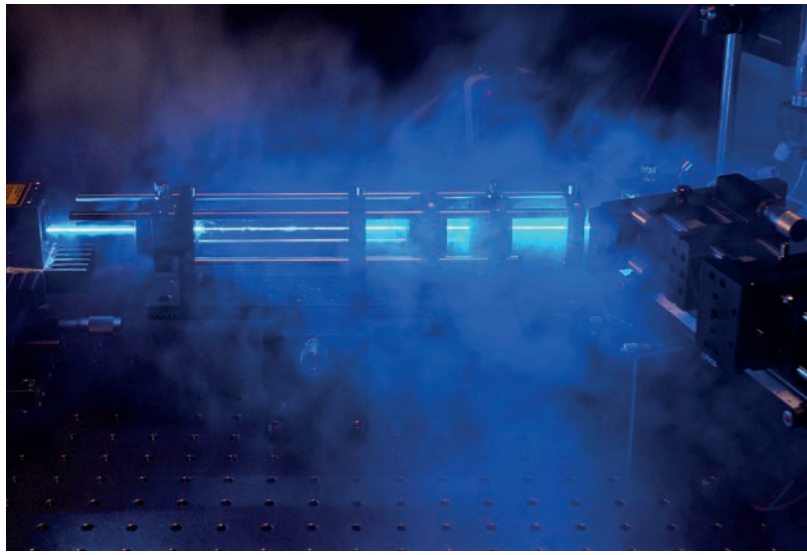
A Nose for GC

We've shown that trained dogs can detect the presence of malignant ovarian cancer tumors using smell. The dogs use odor cues to distinguish blood samples of patients with ovarian cancer from those of healthy women, and even from those with benign ovarian tumors. This is an inside look at the gas chromatography-olfactometry (GC-O) instrument we are using to identify the specific volatile organic chemical biomarkers that the dogs are detecting. Submitted by Katharine Prigge, Monell Center, US.

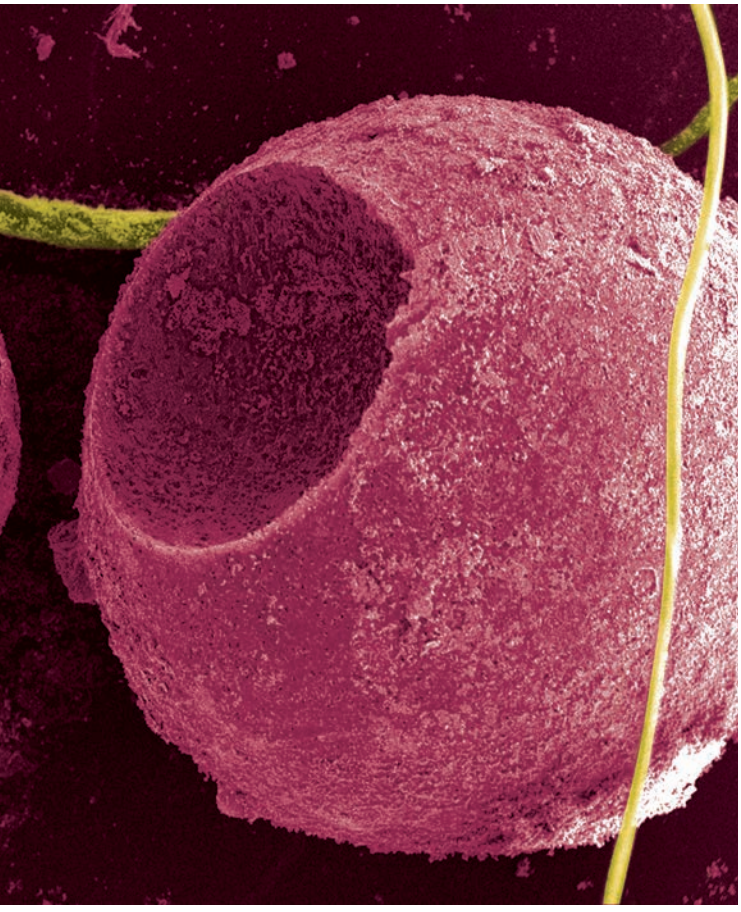
Photo: Nicole Greenbaum



Blossoming Bioassays

Paper is patterned using a craft punch to form a flower-like shape. Every petal is an independent detection zone. Orange petals are for detecting glucose. Through such simple geometry, segmented and multiplex immunoassay for HCV diagnosis could be carried out in an integrated, economic and rapid manner.

Photo: Xuan Mu



Counting Cancer Cells

The PoCyton device developed by researchers at the micro-engineering branch of the Fraunhofer Institute for Chemical Technology in Mainz (IMM) is a cost-effective, small, and automated flow cytometer. Michael Baßler, research scientist at ICT-IMM, says, "Our flow cytometer enables [tumor cell quantitation] to be carried out around twenty times faster [than current technology]. Their cost is also lower by several magnitudes, which takes us into a new dimension that makes these devices much more affordable for clinical applications."

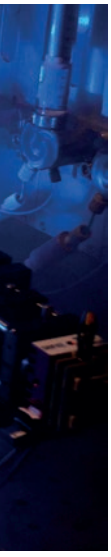
Photo: © Fraunhofer ICT-IMM

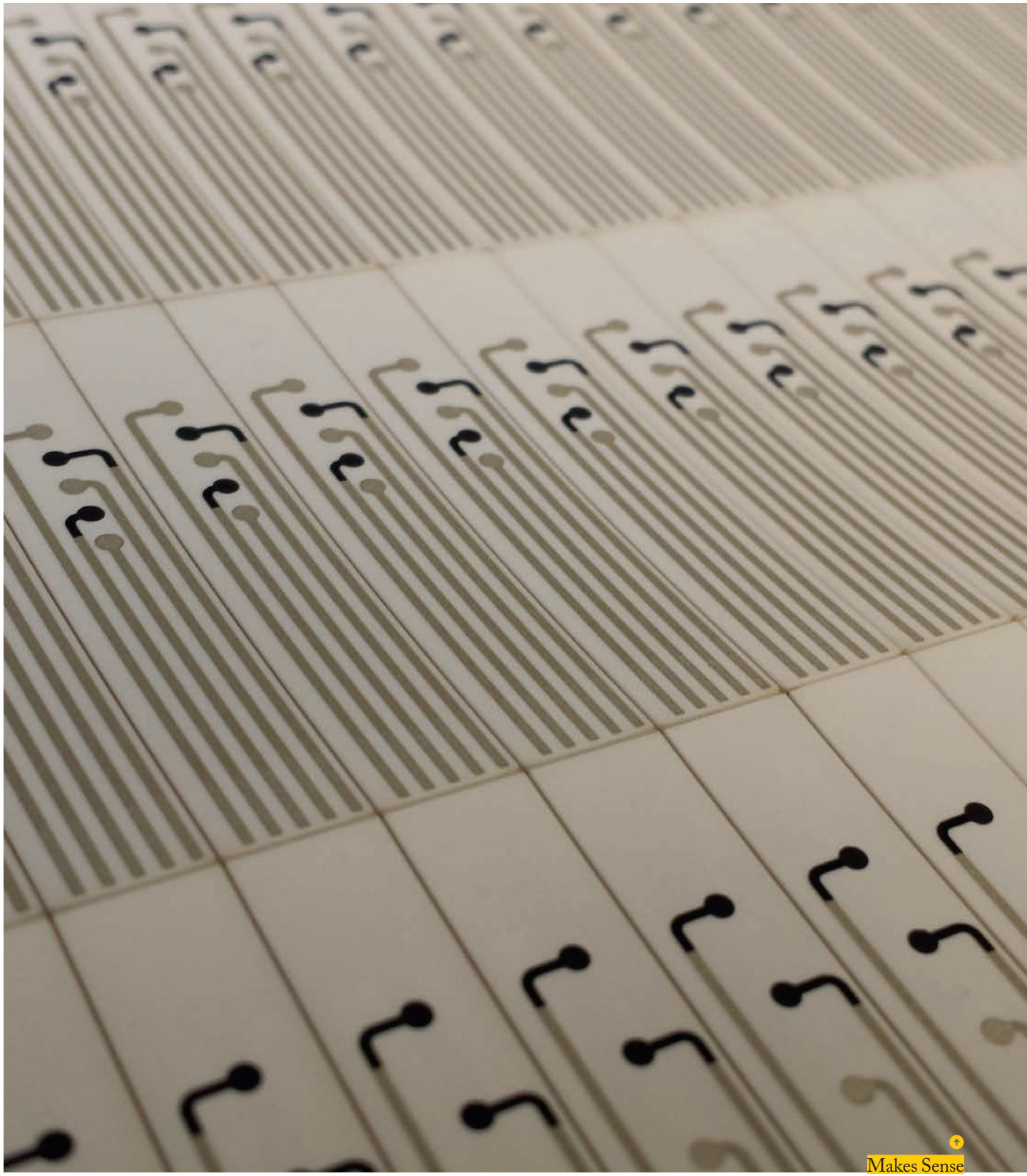
Designing Nano-Potteries

Imaging bio-molecules and cells over extended periods of time is critical to understanding cellular processes. The photostability of cadmium sulfide quantum dots are highly attractive for the real-time tracking of bio-molecules and cells over time. Pacific Northwest National Laboratory researcher Dev Chatterjee provided the image. Other contributors include Matthew Edwards, Paul MacFarlan, Samuel Bryan and Jason Hoki.

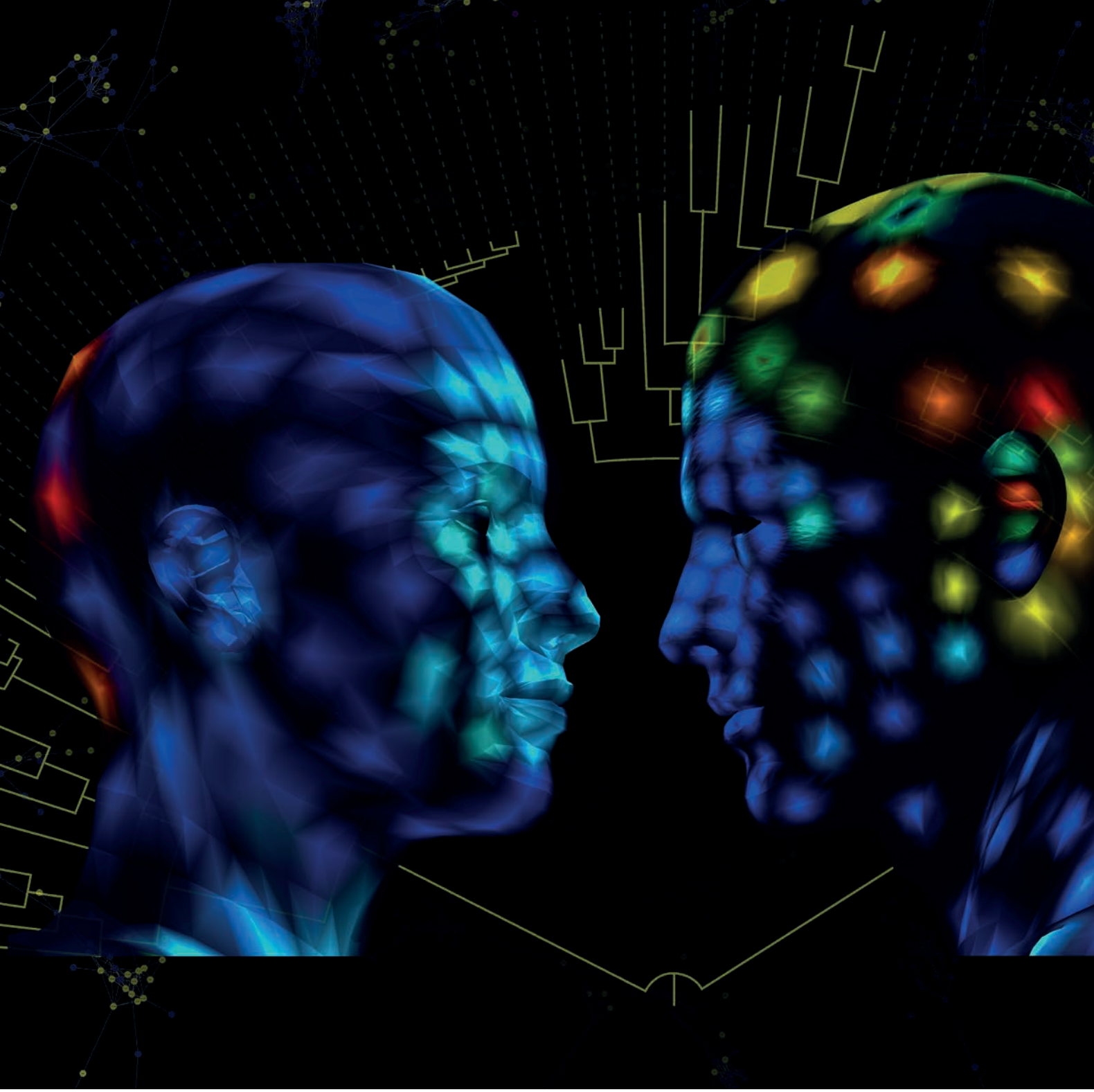
Image colored by PNNL graphic designer Jeff London.

Photo: Pacific Northwest National Laboratory





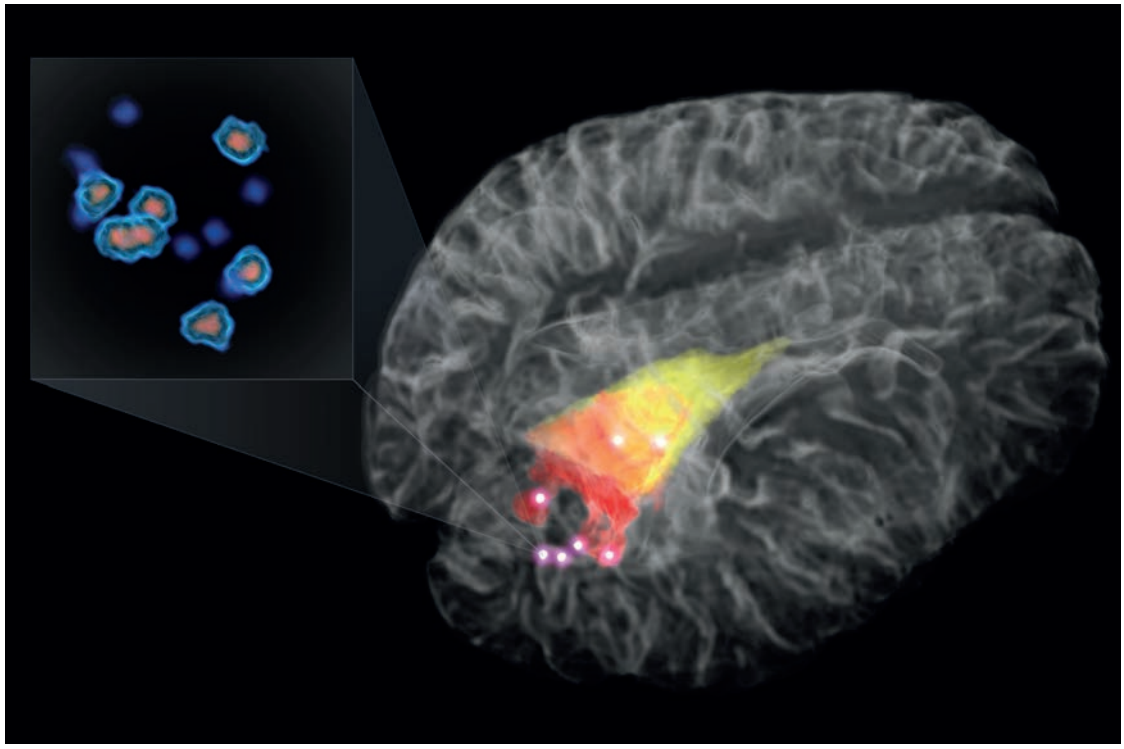
Sheet of printed, disposable biosensor devices for a wearable, wirelessly-enabled sweat analytics platform.
Photo: Electrozyme LLC



Skin Deep Analysis

Artistic representation of 3D mapping of the chemistry and microbes of the human skin. Each of the two renderings shows distribution of yet unknown molecules on the skin of either the female or male individual. Bouslimani et al., PNAS, 112 (17), E2120–E2129 (2014).

Image: Theodore Alexandrov



Multimodal Brain Probe

Post-surgery residual cancer cells are the primary cause of brain cancer recurrence, and result in a poor prognosis for patients. The image depicts a 3D rendering of the brain for a patient with brain cancer (glioma), with the cancer detectable on T1- and T2-weighted MRI in red and yellow respectively. The bright points indicate cancer detected using Raman spectroscopy, as far as 1 cm beyond what is detectable using MRI. The actual cancer cells are depicted in the pop out (based on histology images). By detecting invasive cancer cells, the surgeon should be able to conduct a more complete resection and thereby improve patient survival.
M. Jermyn et al., Science Translational Medicine, 7 (274) 274ra19 (2015).

Image: Michael Jermyn, Kevin Petrecca and Frederic Leblond

Needleless Blood Sugar

EMPA and the University Hospital Zurich have joined forces to develop a sensor that measures blood sugar through skin contact – and without calibration. "Glucolight" will initially to be used in premature babies to avoid hypoglycemia and subsequent brain damage.

Photo: EMPA (www.empa.ch)

In Our Food

Doing the Dishes

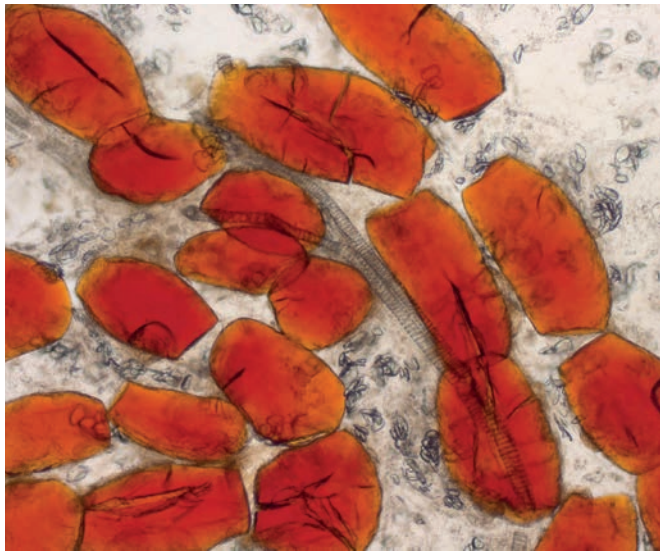
The control of microbes in food is a primary objective across the industry. Whether it be eliminating pathogens, reducing spoilage organisms or encouraging beneficial organisms to grow, an understanding of the microbiology of different food systems is imperative.

Photo: Campden BRI

Class of '64

The first (1964) graduates of the FDA Institute of Advanced Analytical Chemistry are pictured here, a joint venture of FDA and Georgetown University to keep FDA field and headquarters scientists abreast of developments in chemistry.

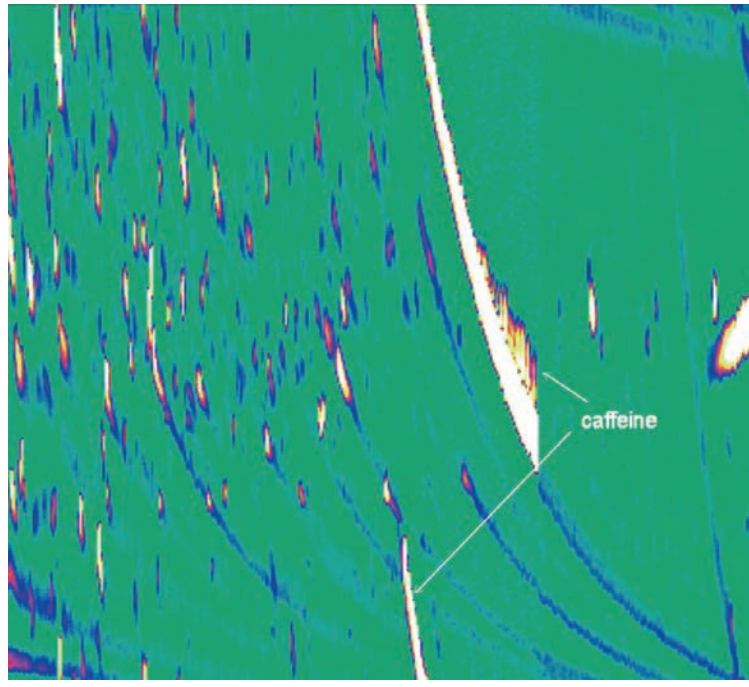
Photo: United States Food and Drug Administration



Have a Banana

Tannin bodies in ripe bananas. Material prepared using cell separation technique. Unripe bananas contain tannins in cells associated with the vascular strands, which are responsible for the astringency of banana flesh. During ripening, the tannins condense into bodies, which means they are no longer astringent.

Photo: Mary Parker, Institute of Food Research, UK



Old Ale

One of two bottles of beer from an 1840 shipwreck that were selected for in-depth analysis.
For more info: tas.txp.to/0815/beer
Photo: VTT Technical Research Centre of Finland

Tea With... Caffeine

The neutral basic fraction of a Solvent-Assisted Flavour Evaporation (SAFE) extraction of a commercial tea product. (First dimension: 25 m, 0.25 mm ID, 0.25 µm DB1; second dimension: 1 m, 0.10 mm ID, 0.1 µm BPX50; carrier gas: helium; temperature: 30°C > 4°C/min > 220°C; detector: ToF-MS.)
Photo: M. Adahchour, Vrije Universiteit, Amsterdam

Dr. Maisch

Columns made in Germany

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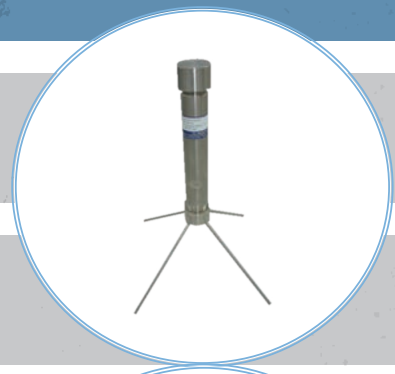
Packing: Reprosil-Chiral-AM, Chiral-OM, Chiral-NR

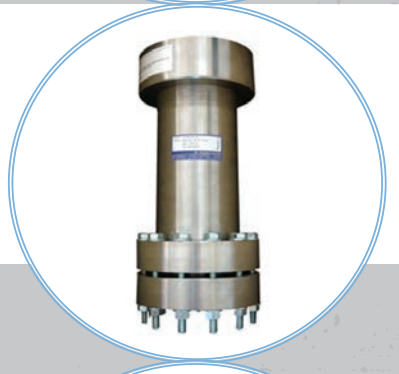


Reprosil Chiral-AM (USP-L51)

Amylose tris-3,5-dimethylphenylcarbamate

Reprosil Chiral-OM (USP-L40)

Cellulose tris-3,5-dimethylphenylcarbamate



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250 x 10 mm	5µm:2950,-	10µm:2550,-€
250 x 20 mm	10µm:6500,-	20µm:5500,-€
250 x 30 mm	10µm:11000,-	20µm:9000,-€
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Switzerland:
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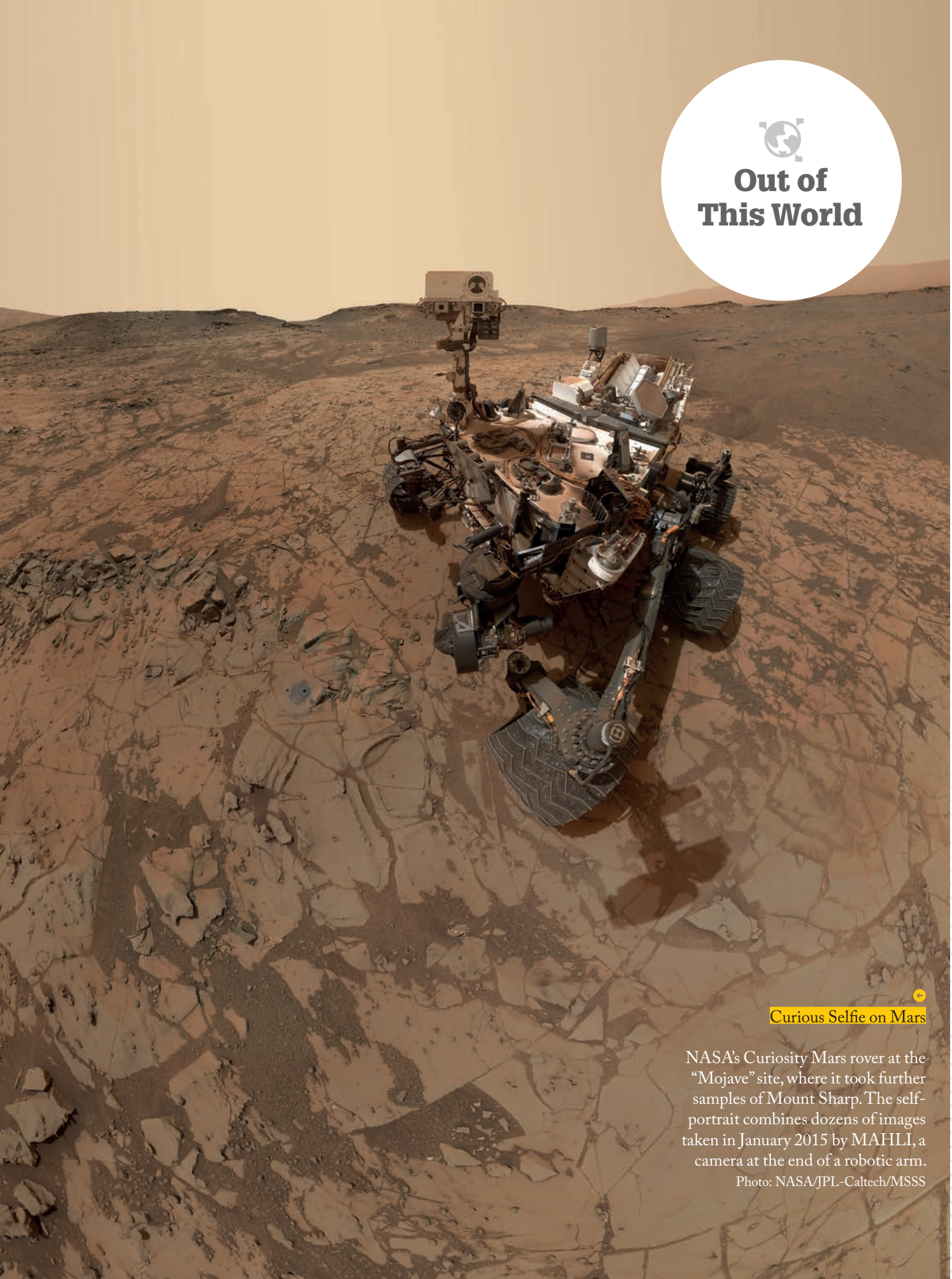
email: morvay-analytik@balcab.ch, www.morvay.ch

Out of This World

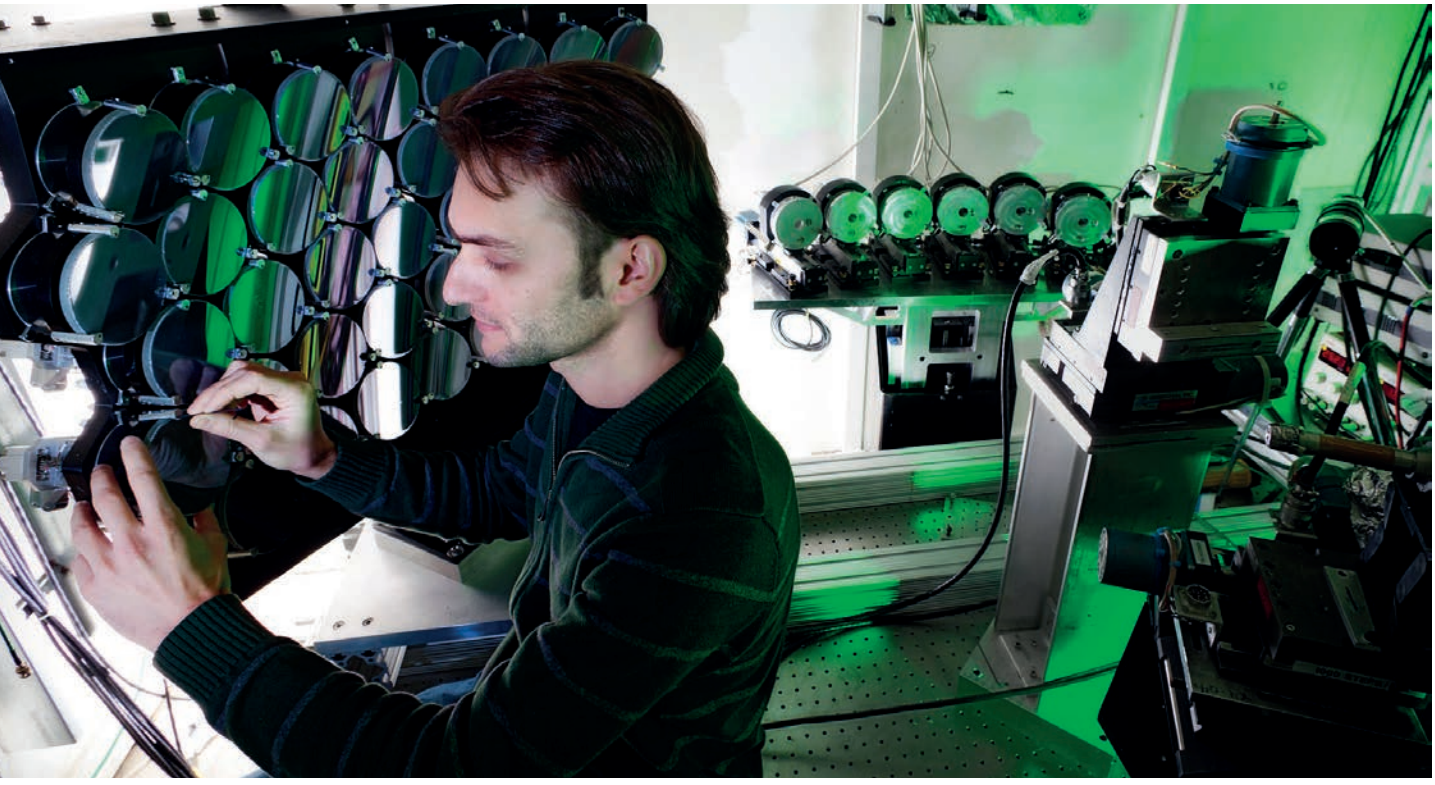


Curious Selfie on Mars

NASA's Curiosity Mars rover at the "Mojave" site, where it took further samples of Mount Sharp. The self-portrait combines dozens of images taken in January 2015 by MAHLI, a camera at the end of a robotic arm.
Photo: NASA/JPL-Caltech/MSSS

The Lab That Time Forgot

An analytical chemistry laboratory that has been lost in time.
Photo: Gumpe (via Flickr)



The Raman King

Dimosthenis Sokaras, scientist at Stanford Synchrotron Radiation Lightsource (SSRL), adjusts the focus mirrors on the X-ray Raman and X-ray emission spectroscopy instrument on its Beamline 6-2.
Photo: Brad Plummer

Distant Analytical Horizons

Image of Pluto, backlit by the sun, taken by NASA's New Horizons spacecraft from a distance of 1.25 million miles. "With flowing ices, exotic surface chemistry, mountain ranges, and vast haze, Pluto is showing a diversity of planetary geology that is truly thrilling," said John Grunsfeld, NASA's associate administrator for the Science Mission Directorate.

Photo: NASA/JHUAPL/SwRI

Plasma Nebulization

Light scattering from a red diode laser reveals jets of liquid aerosol ejected from a solution in contact with a low-power plasma, the solution-cathode glow discharge. Research being conducted by Andrew Schwartz, Steven Ray and Gary Hieftje of Indiana University, US.

Photo: Andrew Schwartz

Analytical Scribblings

A legal "cheat sheet" becomes art – after the exam.

Photo: Ashour Rehana

Food (Analysis) for Thought

Driving the quality and scope of pesticide residue analysis forward is a constant and global endeavor. Is it time to embrace full scan, high resolution and accurate mass?

By Amadeo Rodríguez Fernández-Alba, Professor of Analytical Chemistry and Director of the Department of Chemistry and Physics, University of Almeria, Spain.

To watch the online presentation, visit: http://tas.txp.to/0815/pesticide

Originally from Madrid, my deep interest in food analysis and control actually began when I came to Almeria 20 years ago. Almeria is the main producer and exporter of fruit and vegetables during Europe's winter; focusing on pesticides control made a great deal of sense to me as an analytical chemist. And over the years I've been fortunate enough to collaborate with a number of regional institutions and producers to ensure that Almeria is at the leading edge of pesticide analysis and control. We recognized that one of the most serious issues in pesticide control was unacceptable discrepancies in the results obtained by different laboratories – and that can have a big impact on trade. We began to focus on analytical quality control and method validation procedures for routine pesticide control laboratories.

Harmonizing quality

It was also clear back then that a forum for knowledge exchange would help address those same challenges, and in 1996 the first European Pesticide Residue Workshop (EPRW) was held in Alkmaar, the Netherlands. I presented results from the procedures we had developed, which in some ways was the starting point for cooperation between the whole network of routine laboratories.

Another important step to get us where we are today came in 2006, when the European Commission's Directorate-General for Health and Consumer Affairs made an open call for four European Reference Laboratories (EURLs) for residues of pesticides. We became the EURL for fruits and vegetables (EURL-FV), and I've been its head ever since. We work together with the three other pesticide EURLs (cereals and feeding stuffs; foods of animal origin; and single residue methods).

In a nutshell, our main duties are to harmonize results and improve the quality of the whole network. Today, I am proud to say that the European Union has the world's best network of routine laboratories for pesticide residue analysis, at least in my opinion.

The role of technology

Much of my research is dedicated to the development and validation of new and improved analytical methods. Part of that responsibility means ensuring that National Reference Laboratories are kept up to speed on the latest advances in instrumentation, including mass spectrometry. New technology can have an impact on development of more appropriate or comprehensive methods, and ultimately improve the quality and equivalence of results between laboratories.

There have always been two main issues in our field: sensitivity and scope, both of which have grown in importance as international trade has increased. Go back 20 years, when I first joined this field, and the limit of quantitation (LOQ) was typically close to 1 mg/kg and the typical scope was 20-50 compounds in each run. Instrumentation in an average lab was a GC-single quad MS and LC with UV and florescence detection – and laboratories would spend half a day on very few samples. Today, laboratories must now routinely monitor hundreds of pesticides at very low detection limits – very rapidly. In terms of technology, it's a totally different world; today's instrumentation has risen to help analysts meet the challenges.

The most notable recent advancement in technology comes in the form of high resolution, accurate mass (HRAM) mass spectrometry, which I believe will play a big role in increasing scope and capacity. Introducing such technology for GC and LC into routine laboratories for pesticide residues is the next step, but obviously represents a significant change throughout our network and will take time to implement. We are very much involved in this process, and the instrument companies also have a role to play – and that includes making such technology affordable; after all, pesticide

control laboratories, by their very nature, need high-throughput, broad scope, and cost-effective analytical methodologies.

A new way to fish

My university is close to the sea, so you can see fisherman at work – sometimes fishing with a rod and line, sometimes with a net. I can draw an analogy to mass spectrometry. Line fishing is targeted – you select your line weight and appropriate bait to catch the right size and kind of fish, tossing away rogue catches. In triple-quad MS, we target selected ions using the quadrupole filter. Fishing with a net is a completely different approach – as is full-scan MS – as it captures all fish (or ions). With full-scan MS, the software determines detectability, as the hardware collects all information, and that means that we have the opportunity to not only investigate thouasands of compounds of interest, but also to revisit data for retrospective analysis – something that is very useful in unusual cases or amidst food scandals. It's essentially a much more flexible analysis concept – and it really opens the door in terms of identification. When it comes to pesticide control, there are two important aspects: i) enforcement of regulations and ii) assessment of risk. And an increase in scope allows us to gain a better understanding of current and future risks.

When they were first introduced, full-scan HRAM instruments were considered complementary to triple-quad instrumentation in routine analysis – sensitivity was an issue, as was cost, so they were reserved for challenging samples. But over the last few years, the sensitivity of Orbitrap-based instruments has increased, software has become much more powerful, and cost is coming down. Such instrumentation is no longer simply complementary – rather they are viable contenders to be the workhorses of routine analysis.

New, more affordable technology, such as the Thermo Scientific Q Exactive Focus mass spectrometer, allows us to conduct routine analysis as we would with a triple quad instrument; there are no major differences in analytical performance in terms of sensitivity, reproducibility, and linearity. And though the analytical performance is similar, the advantages in selectivity are significant.

One main advantage is that the identification capability is higher than triple-quad instruments, which is especially notable in dirty matrices with many endogenous compounds, such as tea or orange. In such complex samples, retention time and transition ratio overlaps can lead to false negative or false positive results. The production of false positives and negatives using accurate mass is much lower, because you're not working with nominal mass transitions; you have two or three ions at accurate mass. In a recent presentation (see sidebar), I offered a particularly good example, involving a false negative of linuron in coriander. A second major point is the overarching fact that information is not missed with full-scan MS – everything is collected by the instrument. Of course, advanced software is required to extract that information – but nothing is lost.

Embracing change

The switch to full-scan HRAM instruments is not going to happen overnight – but I do believe that we've reached a tipping point in pesticide analysis. Comparable performance – and price – coupled with the advantages of full scan mode and accurate mass for identification make more widespread adoption almost inevitable.

I'd like to conclude by quickly thanking all of the National Reference and official laboratories in Europe for their past and continued cooperation. Four years ago, we conducted a proficiency test on screening methods and many laboratories have participated voluntarily. I am very proud of our network, which is very motivated to introduce new methods and technologies to increase analytical performance. And that makes my job a lot easier.

Evaluating Q Exactive LC-MS

Amadeo Fernández-Alba presented at the 1st International Symposium on Recent Developments in Pesticide Analysis in Prague. You can view the full presentation online: http://tas.txp.to/0815/pesticide. Here, we present a brief summary.

Four main evaluation areas:
- Sensitivity
- Reproducibility
- Resolution
- Linearity

"In food analysis, quantification is a very critical issue. The results of our analysis can mean the exclusion of a consignment."

Evaluated four different commodities, representing a range of challenges:
- Tomato
- Pepper
- Green tea
- Orange

Considered a number of factors:
- Influence of resolution on detection
- Influence of resolution on peak shape
- Number of points per peak at different resolution

Pilot Study (full scan + MS/MS)
- 100 samples
- Over 180 pesticides
- Mass accuracy (full scan) <5 ppm
- Mass accuracy (MS/MS) <10 ppm
- Sensitivity = 0.01 mg/kg
- Linearity = no saturation
- Reproducibility + linearity < 20% + 10-500 ppb

Conclusions:
- Similar level of quantification to triple quad MS
- More robust identification; no false positives or negatives

Introducing the Pesticide Explorer Collection

Simplified workflows to support pesticide analysis from start to finish.

Conscious of the increasing demands placed on routine pesticide control laboratories, Thermo Fisher Scientific has developed the Pesticide Explorer Collection, comprising four complete solutions that cover all levels of pesticide analysis. Here, we share details of the first: the Triple Quadrupole "Standard Quan" solution.

The standard quantitation configuration – just like its stablemates – includes all the workflow components needed, from consumables and hardware through to software and built-in instrument and data processing methods. Dipankar Ghosh (Director, Enviro & Food Safety, LSMS, at Thermo Fisher Scientific) says, "The Pesticides Explorer Standard Quantitation configuration is designed to meet the complete needs of high throughput laboratories running routine targeted quantitation of pesticides. It provides the analyst the complete tools from sample preparation and analytical methodologies to reporting templates to achieve the desired results fast."

Pre-configured and pre-tested to get you up-and-running as soon as possible, the standard quantitation solution features a TSQ Endura triple quadrupole mass spectrometer to ensure compliance against regulated levels of detection in a routine environment.

Standardized sample prep and separations

Irrespective of the depth of analysis, accurate results are essential. To that end, all configurations of the Pesticide Explorer Collection include the QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) sample preparation reagent kit and HPLC columns, both of which facilitate more accurate pesticide determinations in high moisture samples. QuEChERS is rapidly becoming the method of choice in food sample preparation and clean-up because of its high recoveries, time-savings, and simplicity. Moreover, QuEChERS generates minimal solvent waste but retains the power to cover a wide pesticide range, including polar and pH-sensitive compounds.

Regarding column choice, Mike Oliver (Product Manager, Sample Preparation and Accucore LC Products) says, "Pesticide analysis requires the separation of highly complex samples. In order to quantify and qualify accurately and provide confidence in analysis, highly reproducible and robust separations are required. To meet this challenge, the Pesticide Explorer Collection contains Thermo Scientific Accucore solid core HPLC columns, which deliver greater separation efficiencies in combination with robust formats."

Software that works with you

Pre-configured methods are simple to access on the included USB drive and can be easily set up and adapted in just a few steps.

Compounds can be selected from the database to automatically create the instrument and processing method. But flexibility allows you to upload, create or modify pre-configured methods with SRM transitions and retention times with ease.

Once the optimized data acquisition has been completed, the color flagging features in the bundled TraceFinder software enable you to quickly review data. The final step? The generation of high-quality standard or custom reports that turn your data into results.

Ed George, Senior Application Scientist in Environmental and Food Safety at Thermo Fisher Scientific, was heavily involved in the development of the Pesticide Explorer Collection, and believes the solutions reflect the constant drive for reproducible and robust results in pesticide control. George highlights the key goal of the Standard Quan solution: "The package for the TSQ Endura includes proven multi-class pesticide methods with compound databases and consumables to help you save time."

the Analytical Scientist

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Multidimensional Champion

Sitting Down With... Jean-Marie (John) Dimandja,
Branch Director at the Food and Drug Administration (FDA), USA.

What triggered your interest in science and chemistry in particular?

I was born into a family of academicians – my father is a retired university history professor, and my mother (also retired) was a high school principal –so learning was very much part of growing up. From a very young age, I dismantled things to find out what was inside and how they worked, including my father's Seiko watch and Toshiba radio... And the neighborhood pharmacist impressed me. I liked the fact that he was not an MD but was able to provide "chemicals" to cure people's ailments. So "pharmacist" was on my list of things I might aspire to in later life. I was also interested in agronomy and how you could improve crops like onions and corn. Everything I was interested in related back to science or applied science – there was never any doubt in my mind where my passions lay.

Why did you go into teaching?

I admired my parents greatly for their mission to mentor the next generation. And even though they trained in America and in Europe, they went back to Africa. My father said it was because he wanted to teach the children of his school friends; the connection made it more meaningful. His words stayed with me. When I had the opportunity to teach at Spelman College, I thought about what he said.

You'll have noticed that people who look like me are in the minority at the conferences we all attend. By the time I retire, I would like to have made a small dent on that problem. My mission involves getting more people who look like me into science and my field. There is no reason for a discrepancy in the numbers of people participating in science. It's not a matter of ability, I think interests and conventions need to change. Today, the problems we tackle are worldwide. Whether it's global warming, food production, or health surveillance, we need global solutions and expertise.

You're a great promoter for the college...

It's a pleasure to introduce the concept of schools like Spelman College to my colleagues. For example, the workshop I gave during the second ever GC×GC conference took place in my classroom. Today's leading lights in the field, such as Peter Tranchida (Italy) and Francisco Neto (Brazil), were in attendance.

Notably, Spelman is for undergraduates only, and was not equipped to handle the advanced research and development I wanted to do. For example, we could not afford to pay a post-doc to help me with my research. However, I did manage to find a workaround solution. Clark Atlanta University is right next door and I became an adjunct professor there.

Why is the college so important?

It's a place where students with similar ethnicity can build confidence before moving on to graduate school and beyond. They meet many people like them, who are just as smart as they are, and they can share similar career and life aspirations. When they go back into the world as part of a minority, they have a network of friends they can lean on. In a racially biased society, it's nice to have that sort of blanket or oasis. Perhaps one day, the concept of Spelman will become obsolete. But we'll have to wait for the biases in society to disappear first...

What was your most precious moment?

I was developing a method for drugs in hair with a student called Miranda Hallett. We were making such good progress on the Friday, she did not want to stop. Spending that Saturday with her in the lab was wonderful because it was her idea. When Miranda presented the project at an American Chemical Society meeting, an old colleague from NASA turned to me and said, "I thought you told me that Spelman was only for undergraduates? That's a graduate student up there!" And that was the level of confidence our students had in their work. In my 13 years at Spelman, I mentored 86 students and each one is a story. Those are my proudest moments.

What are you doing at the FDA?

I'm the director of the tobacco branch. I manage a group of scientists charged with developing new methods for tobacco regulation in line with President Obama's "Family Smoking Prevention and Tobacco Control Act". It's a unique opportunity for me and my team to bring in advanced technology, such as multidimensional GC and LC and radical sample preparation, for a new generation of targeted and non-targeted methods.

As you know, GC×GC has been around for nearly 25 years, and yet there is always a question about when is it going to take off! I sometimes say it suffers from "Anna Kournikova Syndrome". GC×GC chromatograms look great – people can't get enough of their beauty – but the elegant proof-of-concept work has not successfully translated into routine analysis methods.

How can its reputation be improved?

Although GC×GC has been demonstrated in many applications – environmental, food, bioanalysis, petroleum, industry, and so on – method validation has not been rigorous enough. In fact, the only regulated GC×GC method I know of is by Eric Reiner at the Ontario Ministry of Environment in Canada. His method uses GC×GC-electron capture detector (ECD) for organohalogen compounds. Now, the good thing is that we know GC×GC will work – we just need to further demonstrate it for a variety of other sample mixtures. So I am going to take my skill as an emerging technologies leader and combine it with the need for routine regulatory analytical work to develop this new era of methods that are not only better but also validated. It's very exciting and I am going to be looking for the best talent to expand our team of 22 to 65 over the next three years.

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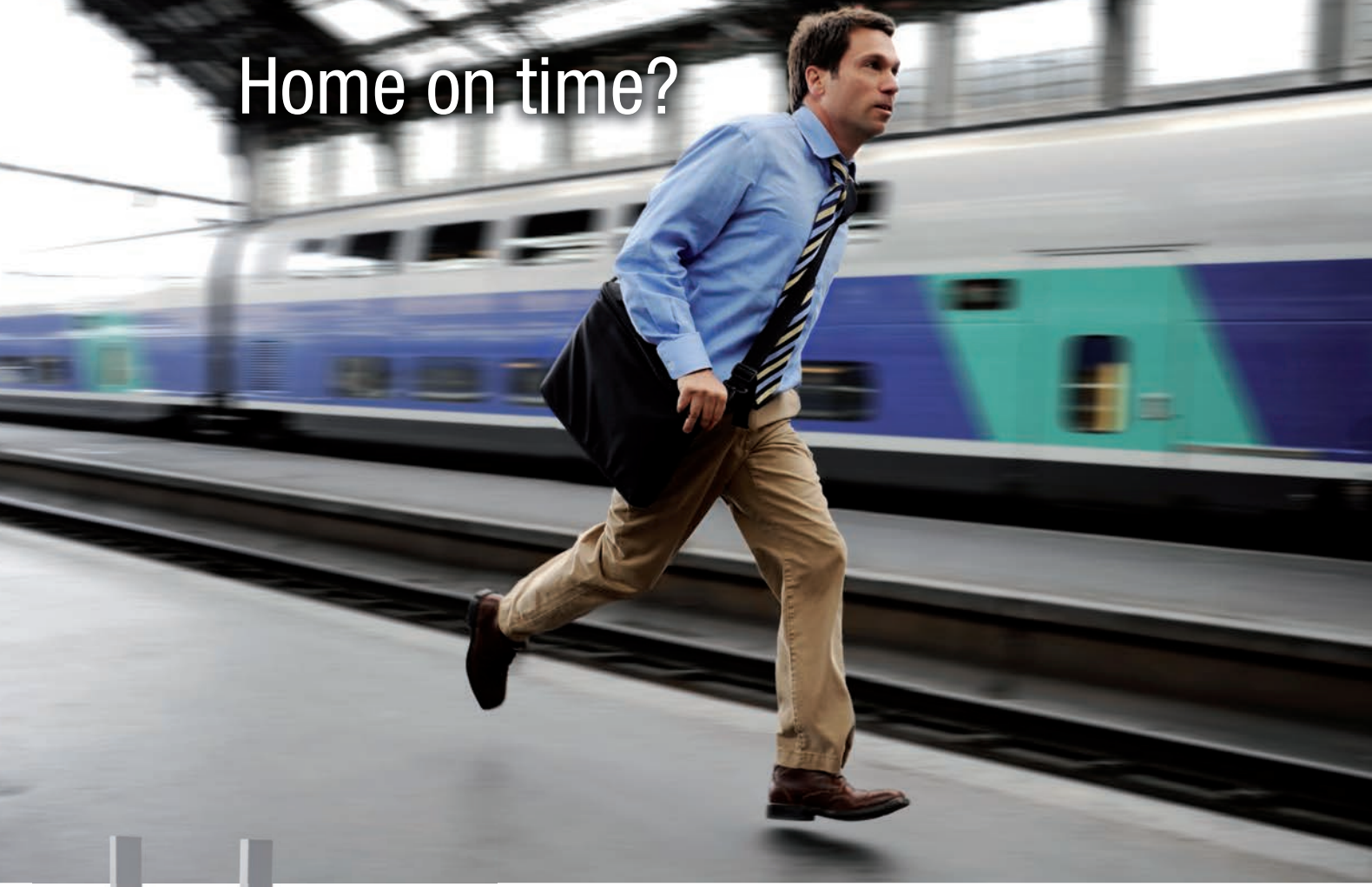

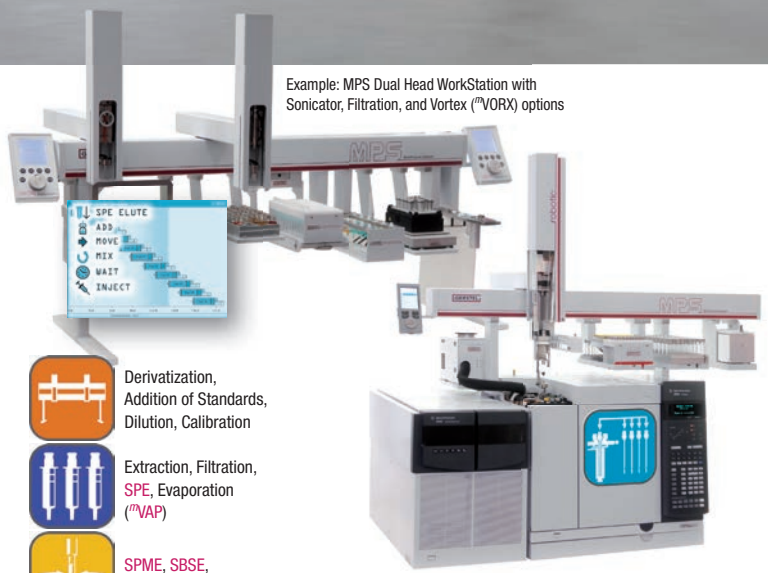

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