

# the Analytical Scientist

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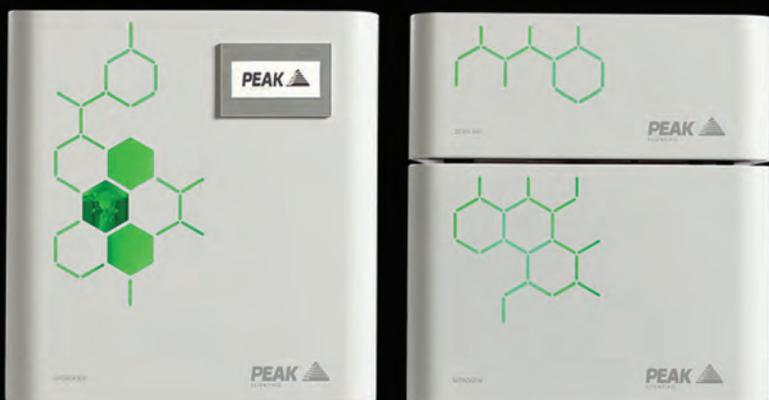


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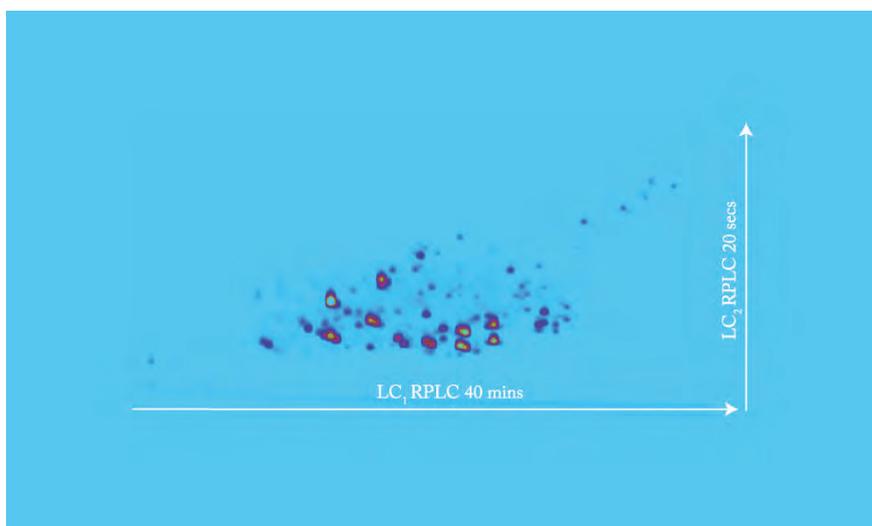
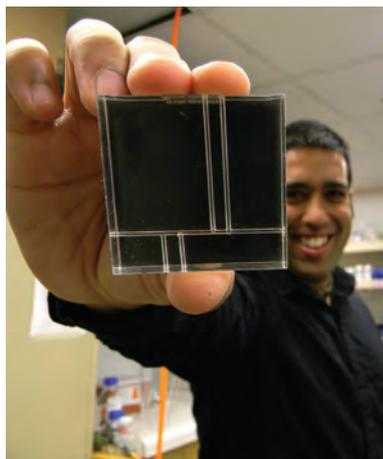
# Online this Month



## *Photos in an Instant*

The majority of this month's magazine is devoted to the celebration of analytical science through the lens of a camera. Of course, space is limited in print, so you can find more photos online. But we don't want the visual feast to end there. We want to see the photos that define your work – why not share them with us on Instagram?

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## *Still Mystified by 2D-LC?*

Last month, we concluded the “Demystifying Two-Dimensional Liquid Chromatography” series in print. Now, we want your opinions and questions to continue the discussion online in advance of a live webinar presented by two authors from the series – Koen Sandra and Dwight Stoll.

Do you have a burning question about the use of 2D-LC in your area? Are you still confused by aspects of the technique? Have you recently started using 2D-LC? Let us know by commenting on any of the following online articles:

- Embracing the Second Dimension: [tas.txp.to/0714/2dlc01](http://tas.txp.to/0714/2dlc01)
- Exploring Chinese Medicine with 2D-LC: [tas.txp.to/0714/2dlc02](http://tas.txp.to/0714/2dlc02)
- Two-dimensional Bioanalysis: [tas.txp.to/0714/2dlc03](http://tas.txp.to/0714/2dlc03)
- Harnessing 2D-LC for Big Pharma: [tas.txp.to/0714/2dlc04](http://tas.txp.to/0714/2dlc04)
- The New 2D-LC Kids on the Block: [tas.txp.to/0714/2dlc05](http://tas.txp.to/0714/2dlc05)

Koen Sandra and Dwight Stoll will answer as many questions as possible during the webinar in September.

To register for the free live event, please visit: [tas.txp.to/0814/2DLCLive](http://tas.txp.to/0814/2DLCLive)



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The Art of Persuasion,  
by Rich Whitworth

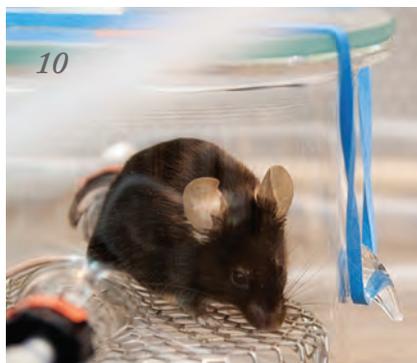
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On The Cover

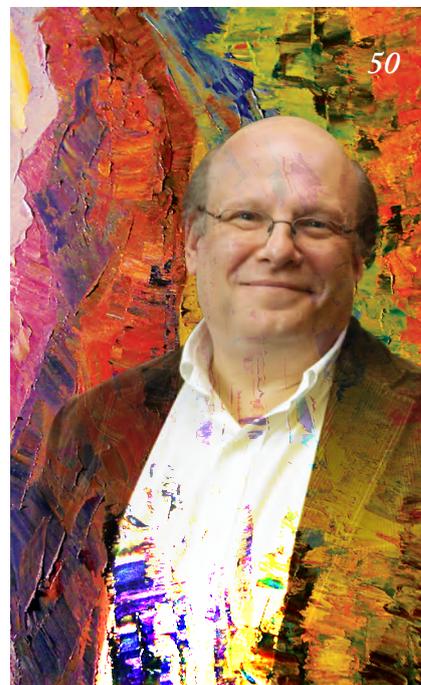
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*Young scientists have their eyes opened to the DRIVE 6 virtual reality cube with Albert Lin. Courtesy of the Desert Research Institute.*



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Old chromatographs (rather like old chromatographers) never die, they just go into a stationary phase, says Ian Wilson.

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# the Analytical Scientist

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## The Art of Persuasion

*This month's focus – The Art of Analysis – also highlights the power of 'self marketing'. What can we learn from the USA and the younger generation?*

Editorial



“Let’s publish a special midsummer photo-driven issue to celebrate analytical science from a fresh perspective,” we stated boldly many moons ago. Well, here it is – and I think the images on the following pages really speak for themselves. That’s not to say that we didn’t have our doubts at first: are there enough great photographs out there? Will people understand what we are trying to achieve? Can art and science happily coexist?

I hope that you will agree that the answer to those questions is “yes!”

But as you casually flick through the six sections, you may not notice at first that there is a strong bias towards one nation. Photos were chosen purely on merit, but the USA is overrepresented, which begs the question: why?

If I were an alien on my first visit to planet Earth, using Google (in English) as my window into the scientific endeavors of the human race, I may well conclude that the USA is streets ahead of the rest of the world. Is that true? I think that the American attitude towards the importance of sharing ‘positive news’ with the rest of the world has a big impact. ‘Marketing’ is no longer a term that applies only to the promotion of products and services; it is beginning to have an impact on our work and even social lives. To get noticed (or ahead), perhaps we need to more carefully consider ‘self-marketing’ – “the act of demonstrating your talent, qualifications, achievements, and likelihood to succeed,” states 99u.com. Certainly, getting published in the ‘right’ journals raises your profile with peers. But wouldn’t it be great to get recognized by the wider scientific community or even the general public? Should you be doing more to promote the fascinating work that you do?

In our fast-paced digital world, great photos and graphics are competing for our attention all the time. Mediocre is no longer acceptable. Think of the rise of Facebook, Instagram or Twitter in combination with 24-hour access to smartphone cameras and clever but simple image-editing software; photos are a fast-rising currency of modern communication. Given the relative novelty of this trend, it may come as no surprise that photos from younger scientists also feature heavily in this issue.

We want the Art of Analysis to be the start of a visual celebration of our field, not the end. You can now share your interesting, beautiful, funny or unique photos via Instagram (@theanalyticalscientist) or Twitter (@tAnaSci) using the tag #artofanalysis.

Oh, and isn’t it time you updated that photo on your biography page? It was taken years ago...

**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*

## Water (E)quality

### **Is ScanDrop the answer to safer water for everyone?**

Water quality control testing at multiple locations along a distribution system is a challenging and time-consuming process, particularly in low-income countries. Standard methods for identifying bacteria in water samples usually take 2-4 days, but researchers from Northeastern University, USA, say they have created a shoebox-sized biosensor called ScanDrop that can do the same thing in just a few hours – and at lower cost.

ScanDrop uses live bacteria capturing, microfluidics and automated fluorescence microscopy in the field and can also work with cloud-based data management and sharing that allows for robotic image acquisition and remote image processing. The biosensor's main components are a droplet microfluidic device for bacteria labeling and a portable fluorescent optical system for signal detection and sharing. The

researchers have already described how the device can be used to detect live *E. coli* in water samples in a new paper (1).

Though other potential applications of ScanDrop include the scanning of biological materials for biomarkers, monitoring live cancer cells and examining bacteria, the drive behind its inception was the need for a low-cost, portable devices for monitoring analyte presence that could be used in low-income countries. "I've previously applied similar technologies to clinical needs in cancer, diabetes and other diseases," says Tania Konry, inventor of the ScanDrop technology, "but making a portable device for water monitoring was more challenging, particularly when costs and an ultra-sensitive detection limit were our main goals." Konry and colleagues are now testing the technology in multiplex mode for the detection of several pathogens.

Konry envisions multiple ScanDrop systems being deployed at various locations along a water distribution network. The cloud-based data management and sharing capability would essentially create a remotely-controlled quality assessment network without the need for support and management typically required for multiple sample analysis – a real advantage where adequate infrastructure is lacking.

One big challenge that remains is getting the technology out into the real world. "We're looking for funding sources that will allow us to move the project from a lab-based set up and into field-testing mode. And we also need investment to create a robust product that can be commercialized," says Konry. SS

#### *Reference*

1. A. Golberg et al., "Cloud-Enabled Microscopy and Droplet Microfluidic Platform for Specific Detection of *Escherichia coli* in Water", PLOS One doi: 10.1371/journal.pone.0086341 (2014).

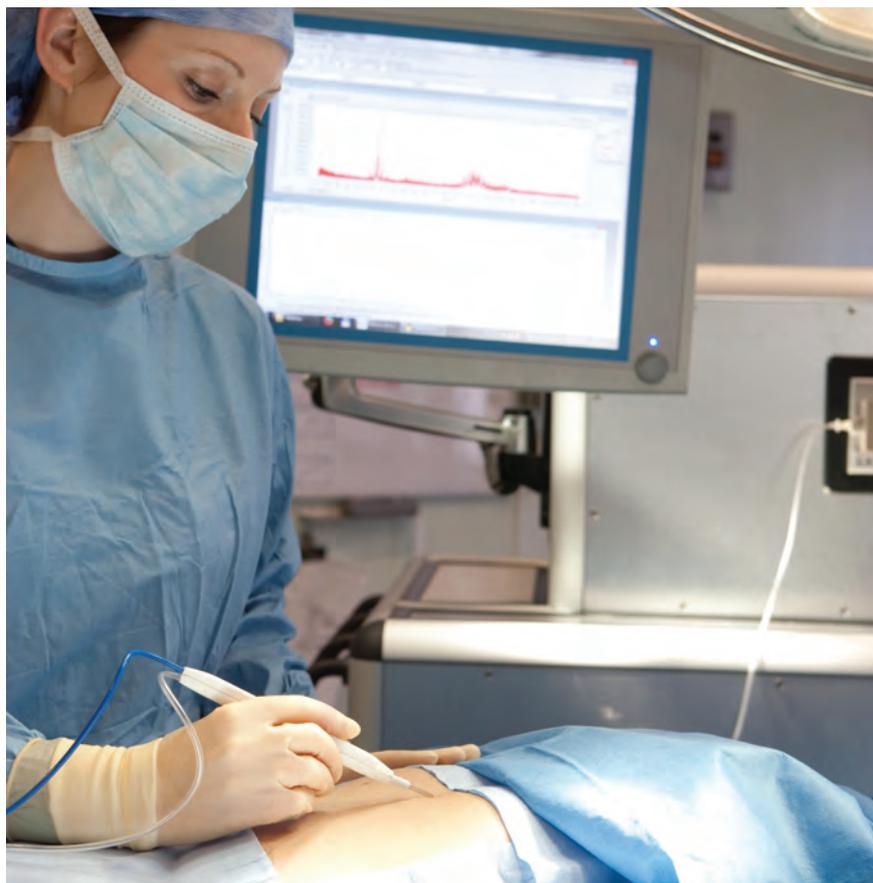
# Surgeons and Spectrometry

**Will further progress in direct ionization technologies kick-start a revolution in surgery – and what does that mean for other fields?**

Back in July 2013, Zoltan Takats' iKnife – the 'intelligent' scalpel – opened people's minds to a new kind of mass spectrometry application (1). Exactly one year later, and mass spectrometry enters the operating theater again – this time without the catchy name, but with the same goal: to monitor metabolites intraoperatively with the aim of distinguishing between normal or cancerous tissue (2).

Although the objectives are the same, the ionization technology behind the two surgical tools is different. Rapid evaporative ionization mass spectrometry (REIMS) is at the heart of iKnife, and essentially enables analysis of metabolites from vaporized tissue released by an electrosurgical blade. The latest research from Graham Cooks and his colleagues at Purdue University relies on a technique called desorption electrospray ionization (DESI, also developed by Cooks), in which a microscopic stream of charged solvent is sprayed onto the surface of the tissue. "In a matter of seconds this technique offers molecular information that can detect residual tumor that otherwise may have been left behind in the patient," says Cooks, "The instrumentation is relatively small and inexpensive and could easily be installed in operating rooms to aid neurosurgeons." Certainly, a very familiar ambition.

But there is something else that links the two technologies. Waters Corporation announced in July 2014 that



it has acquired REIMS technology from MediMass (noting in a press release that REIMS is "substantially all the assets" of the company). The month before, Waters and ProSolia signed an exclusive agreement for DESI technology for clinical mass spectrometry applications. Clearly, Waters are very serious about moving into the clinic.

Jeff Mazzeo, senior director for Waters' health science businesses, says that the move is part of a wider strategy: "We believe that MS and LC-MS technology is at a real inflection point and is going to have a tremendous impact on patient care over the next 5-10 years. That's a real motivation behind our strategy." In terms of applications, Mazzeo cites tissue pathology as a killer application for DESI. "It's traditionally an area that relies on immunohistochemistry staining and microscopy. Such methods are quite subjective," says Mazzeo. "MS has a clear advantage: objective, quantitative measurement of compounds." For REIMS, aside from the aforementioned

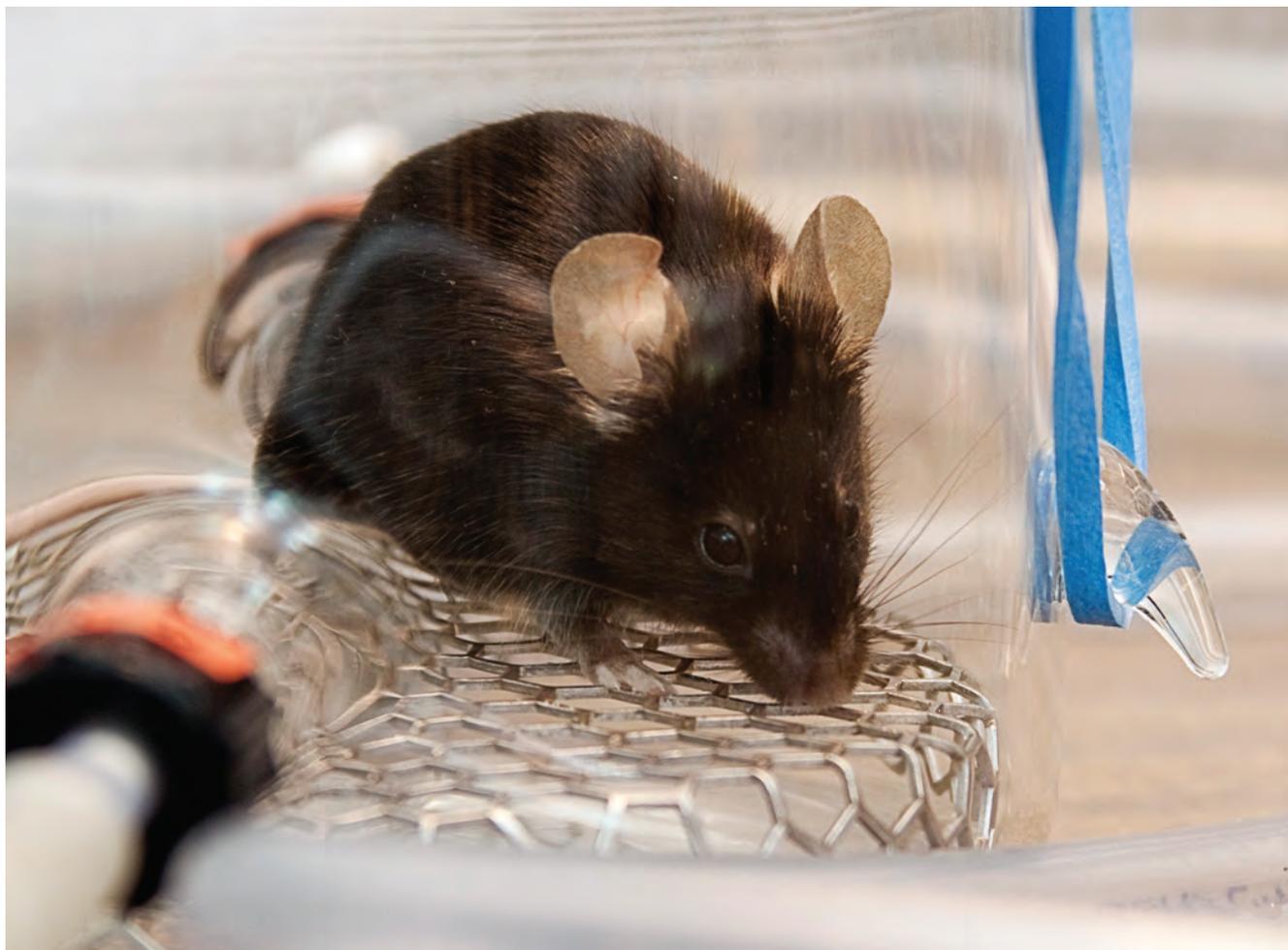
surgical applications, Mazzeo sees potential for it to push aside MALDI-MS in microbiological identification.

Given that both technologies are still very much in the research phase, Waters is keen to push progress. "Much of our work so far has been a collaboration with the Imperial College London," says Mazzeo, "We now plan to actively expand the collaboration to other thought leaders and universities that are interested in helping us develop the technology."

So, how far away are we from an explosion of MS systems in health care? According to Mazzeo, five years does not seem unlikely. *RW*

## References

1. J. Balog et al., "Intraoperative Tissue Identification Using Rapid Evaporative Ionization MS" *Sci. Transl. Med.* 5, 194ra93 (2013).
2. S. Santagata et al., "Intraoperative MS Mapping of an Onco-metabolite to Guide Brain Tumor Surgery", *Proc. Natl. Acad. Sci. USA* 111 (30) 10906-10907 (2014).



## The Aroma of Malaria Infection

### Tracking the volatile chemical profile modifications that attract mosquitoes

The ecology of malaria is complex, involving two different replication cycles of the parasite alternately in humans and mosquitoes, which propagates the disease. Researchers

from ETH Zürich and the Pennsylvania State University wanted to discover how plasmodium parasites change the body odor of its host (in this case, a mouse) to attract further mosquitoes. Penn State's Mark Mescher, one of the authors of the new study (1), explains in more detail.

What kicked off your interest?

Our primary interest is in discovering how chemical cues mediate ecological interactions among organisms. We had already done work on understanding how pathogens influence the attractiveness of hosts to insect disease

vectors – primarily in plant systems. We were also aware of previous work that suggested malaria-infected people were more attractive to mosquitoes (2), although the cues were not identified. When Andrew Read, who works with malaria in a mouse model, joined us at Penn State, we had the ideal opportunity to conduct detailed chemical analyses and behavioral studies.

We thought there was a good chance that we would see increased attraction of mosquitoes to infected mice, and that this might be related specifically to the presence of the transmissible stage of the malaria parasite (the gametocytes).

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We were hoping that this attraction would correspond to clear differences in the volatile profiles of healthy and infected individuals that might even prove useful for diagnosis.

How did you go about the study?

We used a wind tunnel to present mosquitoes with a choice of odor sources to see which they preferred. We tested healthy mice versus infected mice, and we also tested the (extracted) odors of infected mice against the odors of the same mice that were collected before they became infected. Those experiments revealed that mosquitoes were preferentially attracted to infected mice, but only during a specific stage of infection: after the mice recovered from the acute symptoms of malaria but while they still harbored high levels of the transmissible stage of the malaria pathogen. This makes sense from the perspective of disease transmission, but it was not necessarily expected.

We also conducted chemical analyses, which involved placing infected mice (and healthy controls) into glass chambers and collecting volatiles for several hours each day over the course of infection (about six weeks). We analyzed the resulting samples by gas chromatography-mass spectrometry. We also took blood samples each day so that we could track levels of the malaria parasite present, and particularly the levels of malaria gametocytes, which is the stage of the pathogen that is transmitted to mosquitoes.

I would describe the work as logistically challenging!

What next?

I believe this work improves our understanding of the cues that guide mosquitoes to infected hosts and may inform efforts to develop lures and repellents. We also have some hope

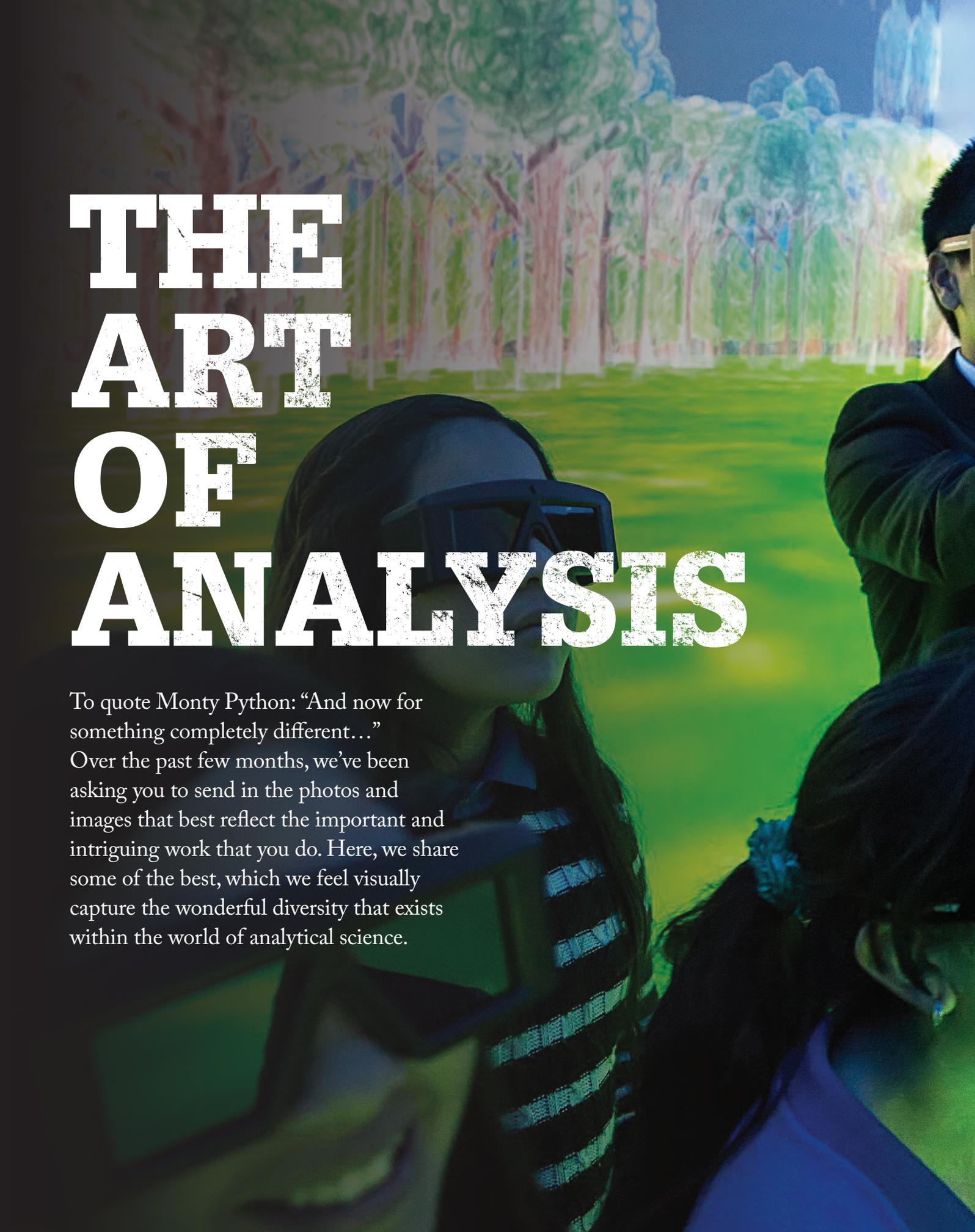
that the malaria parasite, and other pathogens that actively alter host odors in order to attract vectors, may create biomarkers that we can use to identify infected individuals. In particular, identifying and treating asymptomatic infections (people who don't become sick with malaria but can still transmit the disease) is an important goal to combat the spread of the disease.

Beyond that, actually using odor cues to diagnose disease is of interest. The question is whether you can identify a reliable signal of infection against the background noise of genetic and

environmental variation. We have some hope that this will be easier to do for vector-borne diseases, like malaria, in which pathogens are actively changing host odors to attract disease vectors, creating a signal that humans may also be able to detect.

#### References

1. C. M. De Moraes et al., "Malaria-induced changes in host odors enhance mosquito attraction," *PNAS*, DOI: 10.1073/pnas.1405617111 (2014).
2. R. Lacroix et al., "Malaria Infection Increases Attractiveness of Humans to Mosquitoes," *PNAS*, DOI: 10.1371/journal.pbio.0030298 (2005).



# THE ART OF ANALYSIS

To quote Monty Python: “And now for something completely different...”

Over the past few months, we’ve been asking you to send in the photos and images that best reflect the important and intriguing work that you do. Here, we share some of the best, which we feel visually capture the wonderful diversity that exists within the world of analytical science.



## Drive Time

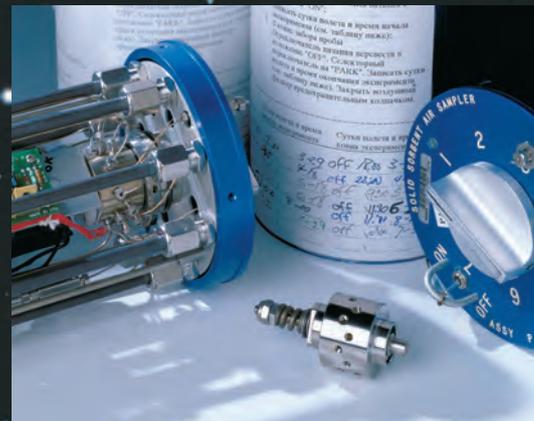
*Submitted by the Desert  
Research Institute, USA*

The DRIVE6 Virtual Reality Laboratory is a cube enclosure with 3-meter sides that uses advanced visual and interactive technologies for training, collaboration and decision support at the Desert Research Institute's (DRI) Applied Innovation Center for Advanced Analytics. Here, students experience DRIVE6 with famed explorer Albert Lin at the 2014 DRI Nevada Medal event – an annual celebration designed to engage students and the public in the world of science and engineering.

Photo credit: Desert Research Institute, Applied  
Innovation Center for Advanced Analytics

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# Extreme Environments

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**Frozen**

*Submitted by Samuel Kounaves,  
Department of Chemistry, Tufts  
University, USA*

*“Analytical laboratories” in Beacon  
Valley in Victoria Land, Antarctica.*

Photo credit: S. P. Kounaves





## Ice Age

*Submitted by Kaitlin Keegan, Dartmouth College, USA*

Here, I am examining the compressed snow layers in the top two meters of the ice sheet at Summit, Greenland, just after the widespread melting event of July 2012. I wanted to know how far meltwater percolated into the snowpack at this site. We used inductively coupled plasma mass spectrometry (ICP-MS) and a continuous flow analysis system to measure black carbon as a proxy of forest fires in Summit shallow ice cores and also on a near-surface sample of firn (compressed snow) core containing the 2012 melt layer.

Photo credit: NSF



### Volcanoes and Dragonflies

*Submitted by Jacob Lowenstern,  
United States Geological Survey*

While sampling waters from a hot pool at Yellowstone in March 2007, I stumbled upon this dragonfly, replaced in its entirety by amorphous silica precipitated from the water. The “fossilized” insect didn't stay visible for long, becoming buried over subsequent years by further deposits.

Photo credit: J.B. Lowenstern, USGS



## Military Coup

*Submitted by Lawrence Berkeley National Laboratory, USA*

Testing a military prototype field version of a laser ablation-based explosives detection system at the Yuma Proving grounds in 2008. The detector was able to discriminate with 85 percent accuracy whether samples contained residues of several types of explosives from 30–50 meters away.

Photo credit: Lawrence Berkeley National Laboratory



**Core Belief**

*Submitted by the Desert  
Research Institute, USA*

Ice inside the drill core barrel following extraction from the West Antarctic Ice Sheet. Desert Research Institute research professor Joe McConnell's projects include ice core chemistry-based studies in Greenland, Antarctica, and the Americas.

Photo credit: Sarah Das

# Make the Connection...From Data to Intelligence



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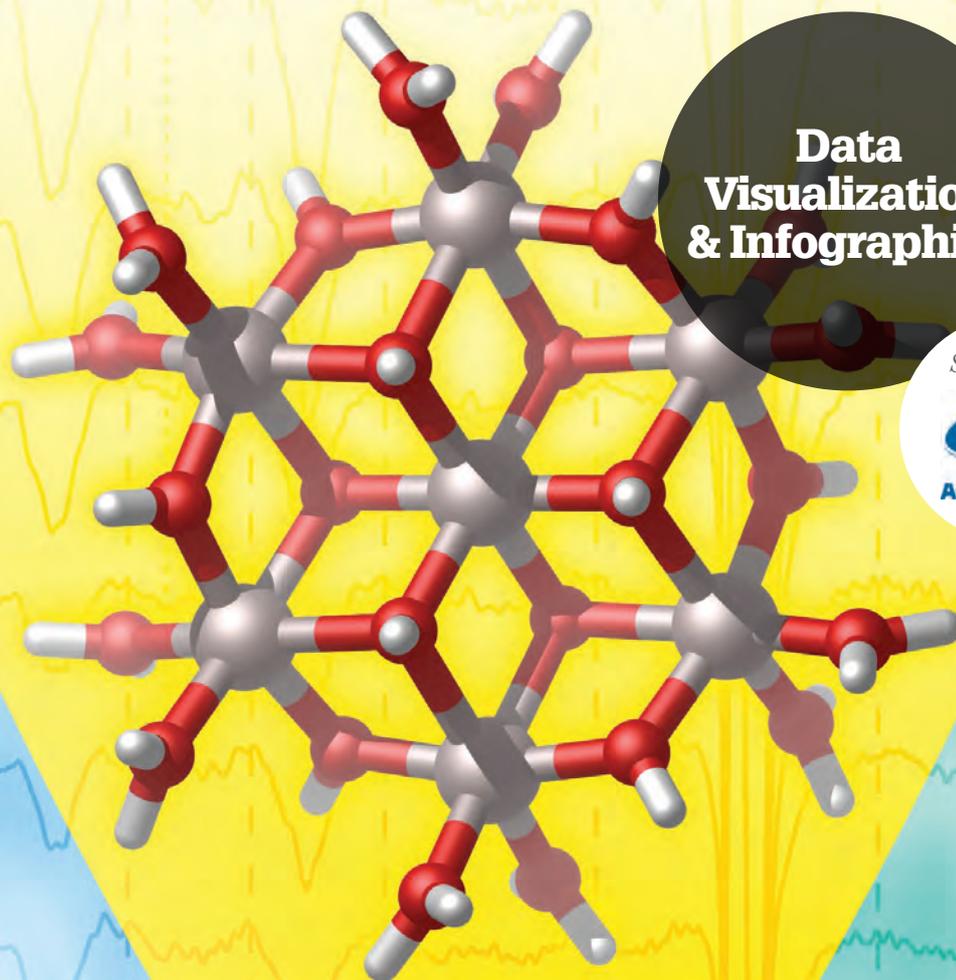
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Al<sub>1</sub>

Aluminum Nanoclusters

*Submitted by Sharon Betterton,  
Oregon State University, USA*

By combining pH-dependent electrolytic synthesis, computational chemistry, and femtosecond stimulated Raman spectroscopy that extends into the low-frequency region, we discovered an intermediate Al<sub>7</sub> nanocluster that is an intermediate species in a three-stage Al<sub>1</sub>→Al<sub>13</sub> reaction. Al<sub>7</sub> serves as a core for stabilization and further condensation to Al<sub>13</sub>, which is a solution precursor to Al<sub>2</sub>O<sub>3</sub> thin films.

Al<sub>7</sub>

Al<sub>13</sub>

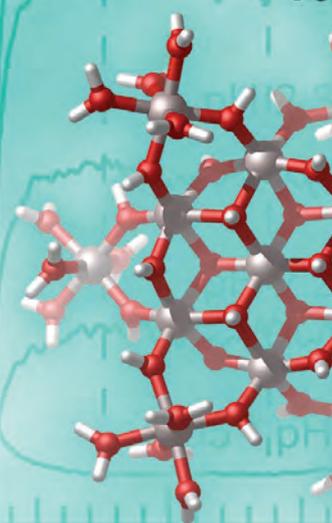


Image credit: Wei Wang, I-Ya Chang, Sharon Betterton, and Chong Fang

600 800 1000 1200  
Stokes Raman shift (cm<sup>-1</sup>)

Stimulated Raman intensity



### DNA Data in Space

*Submitted by Cancer Research UK*

The aim of *Play to Cure: Genes in Space* is to collect Element Alpha, a mist-like substance that can be traded for ship upgrades. It actually represents DNA data, and by collecting it, players are locating genetic variations that may lead to cancer for our scientists.

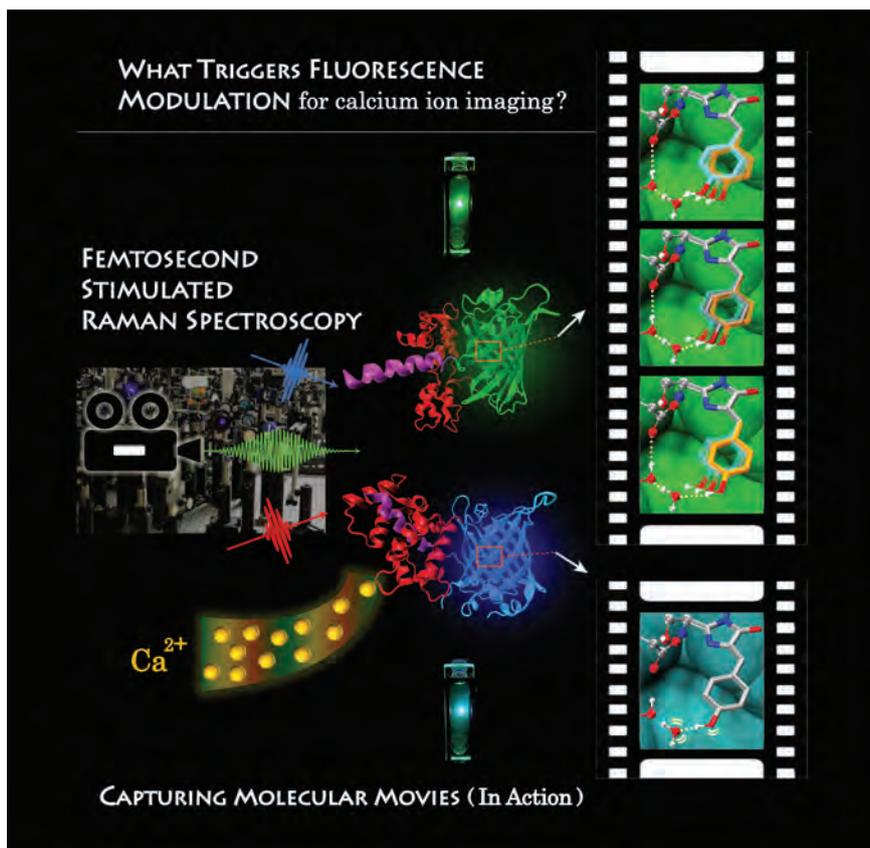
Image credit: Cancer Research UK

### Molecular Movies

*Submitted by Chong Fang,  
Oregon State University, USA*

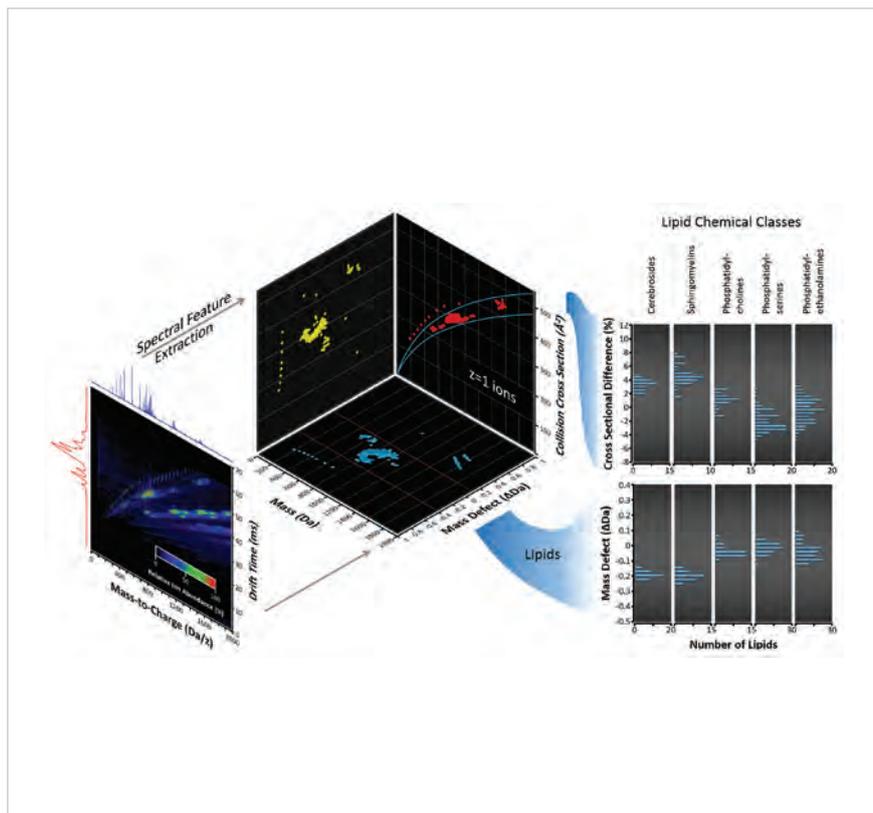
Molecular “movies” of a biosensor called GEM-GECO1 captured by femtosecond stimulated Raman spectroscopy (FSRS). Sequential ultrafast laser pulses unlock the mechanism of the biosensor, which emits green without calcium ( $\text{Ca}^{2+}$ ) but blue with  $\text{Ca}^{2+}$ . The film reel shows vivid structural snapshots of the embedded chromophore that changes dramatically upon  $\text{Ca}^{2+}$  binding.

Image credit: Yanli Wang, Longteng Tang, and Chong Fang (Department of Chemistry, Oregon State University, USA)



## Lipid Map

Submitted by Jody May and John McLean, Vanderbilt University, USA



Visualizing a multidimensional chemical analysis of lipids. Far left: A 2D ion mobility–mass spectrum of a mixture of five lipid classes. The mass spectrum is contained on the x-axis, the ion mobility spectrum on the y-axis, with the heat map corresponding to the relative ion abundance. Middle: Peak features corresponding to singly-charged ions are extracted and projected in a 3D cubic space consisting of mass, collision cross section, and mass defect. Far right: Information can be extracted from the 2D data projections to differentiate the individual lipid classes based on differences in relative size or mass defect.

Image credit: Jody May and John McLean, Vanderbilt University, USA

## We Love Faster BCARS

Submitted by Charles Camp and Marcus Cicerone, Material Measurement Laboratory, National Institute of Standards and Technology (NIST), USA

A form of broadband, coherent anti-Stokes Raman scattering (BCARS) developed at NIST delivers signals that are 10,000 times stronger than spontaneous Raman scattering and 100 times stronger than comparable coherent Raman instruments.

Pictured are false-color images (200 μm across) of mouse liver tissue (left) and tumor/normal brain tissue (right); nuclei are blue, collagen is orange, lipids are red, and proteins (left) and red blood cells (right) are green.

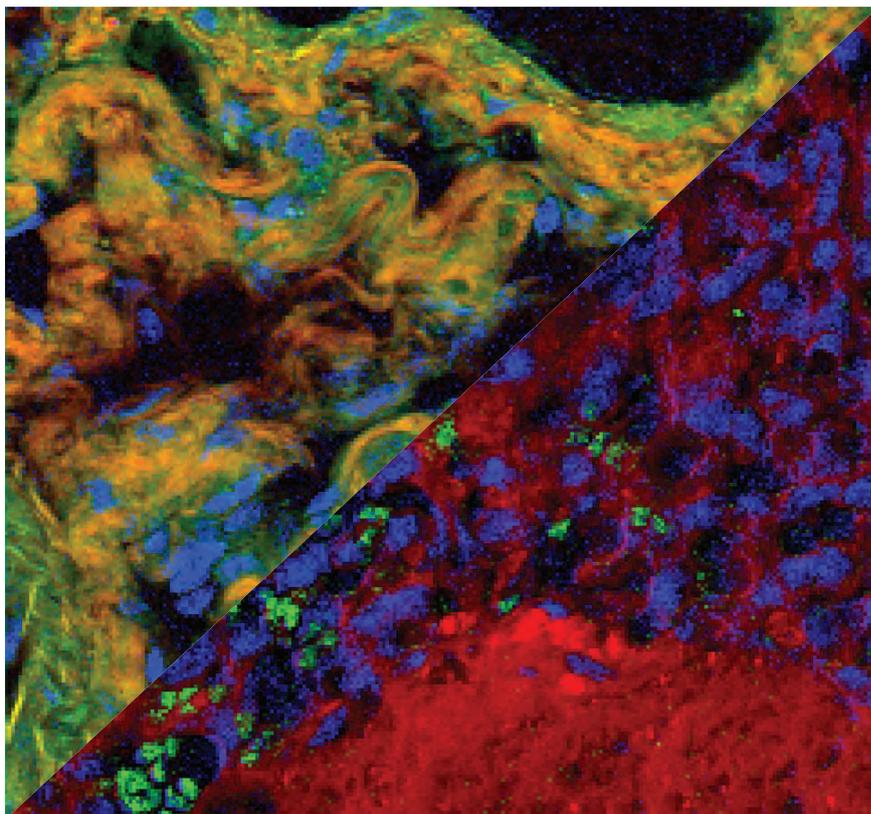


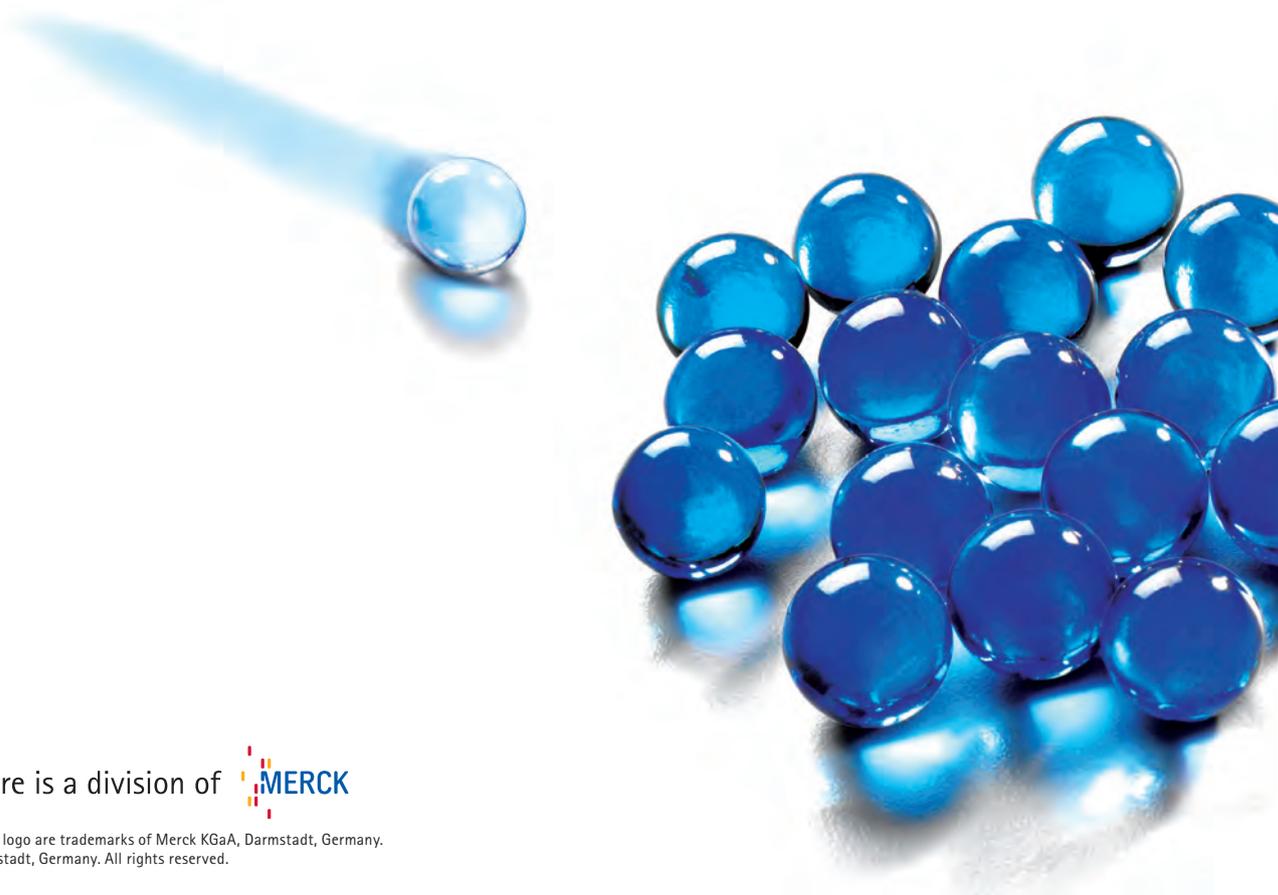
Photo credit: Camp/NIST

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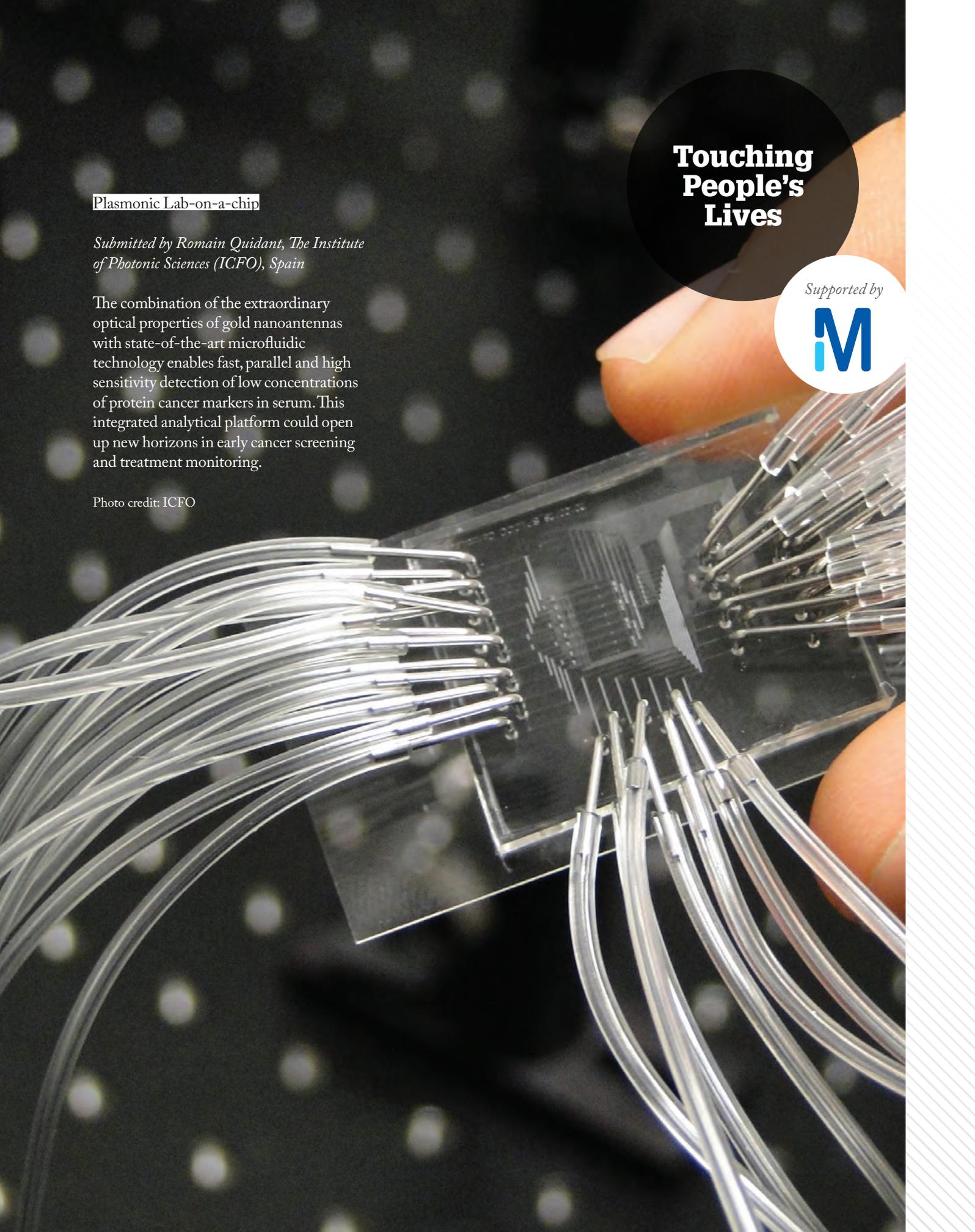
## Plasmonic Lab-on-a-chip

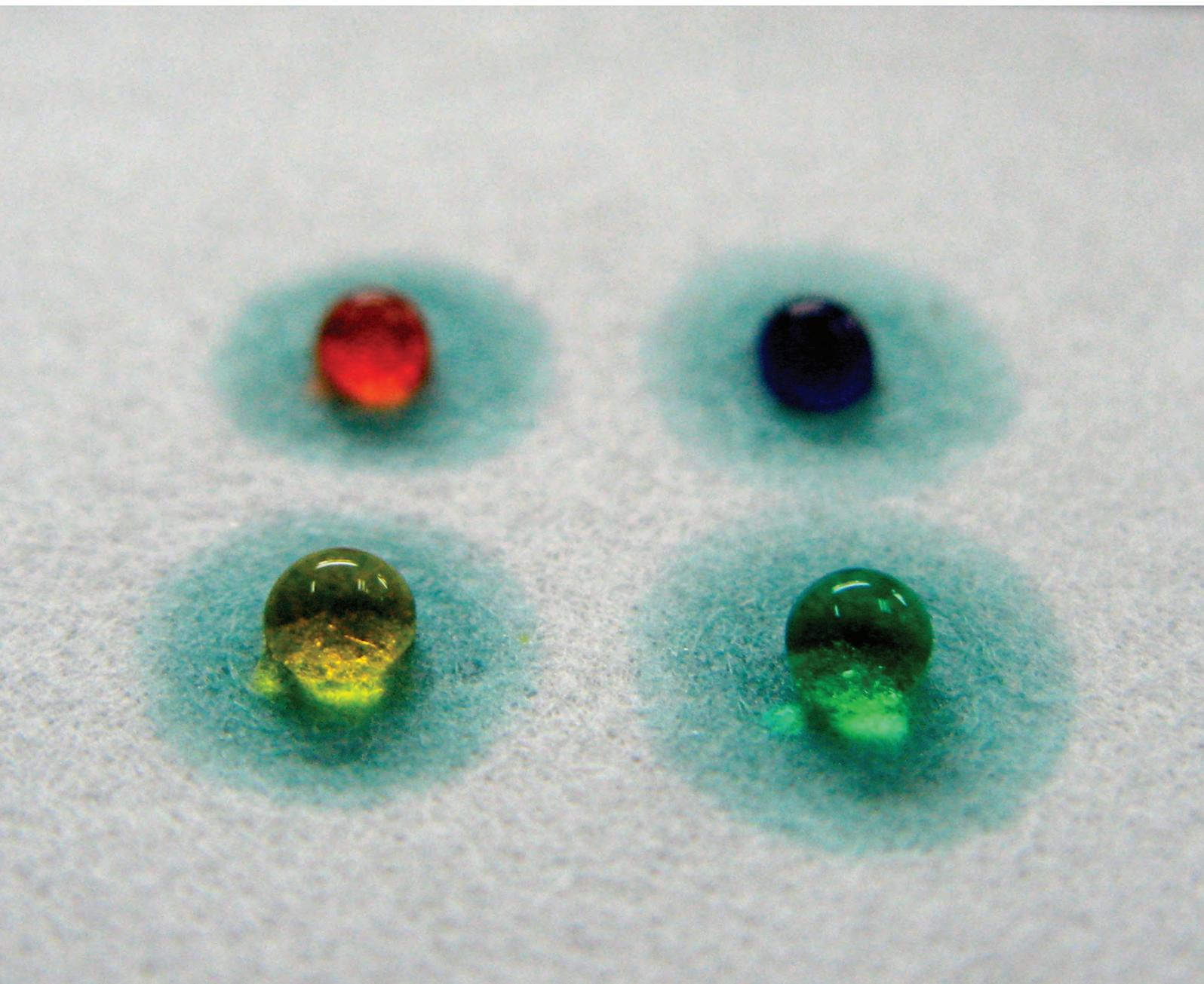
*Submitted by Romain Quidant, The Institute of Photonic Sciences (ICFO), Spain*

The combination of the extraordinary optical properties of gold nanoantennas with state-of-the-art microfluidic technology enables fast, parallel and high sensitivity detection of low concentrations of protein cancer markers in serum. This integrated analytical platform could open up new horizons in early cancer screening and treatment monitoring.

Photo credit: ICFO

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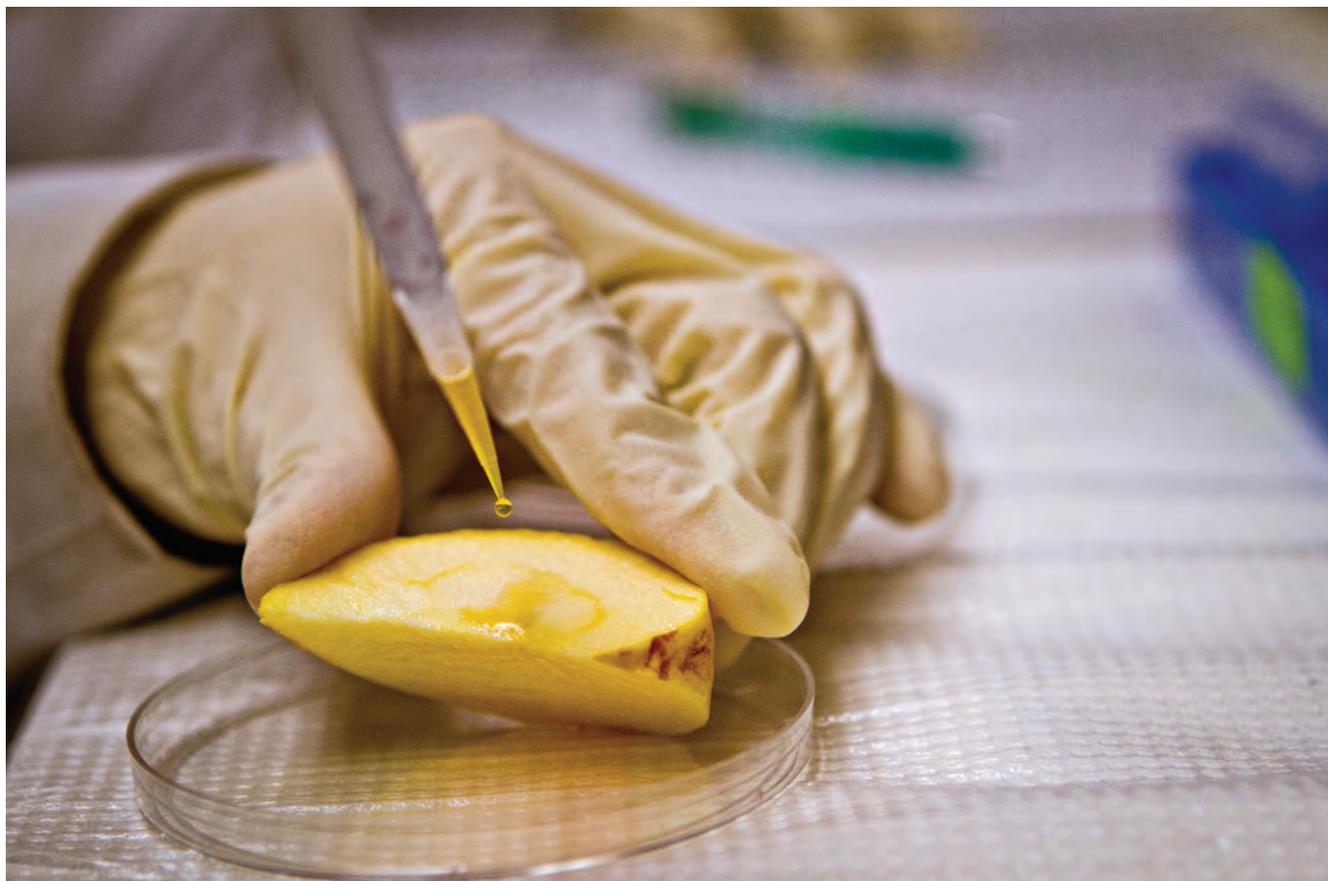


## Just a Drop

*Submitted by Xuan Mu, Institute of Basic Medical Sciences,  
Peking Union Medical College, China*

Four aqueous droplets are pipetted on hydrophobic parts (blue) of a hydrophilic and fibrous paper. The hydrophobic ink is adsorbed on the paper to form a circle shape. Such basic principles are at the heart of many paper-based diagnostics that allow integrated, economic and rapid analysis for the whole world.

Photo credit: Xuan Mu



### An Apple a Day

*Submitted by Missouri University, USA*

As part of Mengshi Lin's study on how toxic nanoparticles may enter our food supply, Missouri University (MU) graduate student Zhong Zhang applies silver nanoparticles to an apple. Mengshi's food science study has found that these particles could pose a potential health risk to humans and the environment. Thanks to the new study, a reliable method of testing foods for the harmful particles has been found.

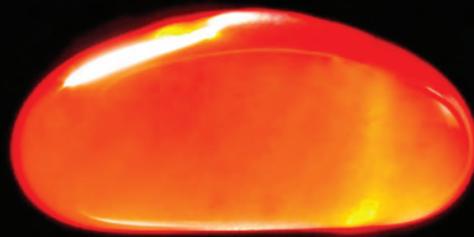
Photo credit: Kyle Spradley/MU College of Agriculture,  
Food & Natural Resources

## Biospectroscopic Magic

*Submitted by Bayden Wood, Monash University,  
Melbourne, Australia*

Biospectroscopy uses the interaction of light with biological materials to provide information on molecular structure. Here, we are using an acoustic levitation device to levitate a suspension of malaria-infected red blood cells and simultaneously probing it with a laser, providing a new way to diagnose this devastating disease.

Photo credit: Steven Morton (Faculty of Science, Monash University)





### Recruit 'em Young

*Submitted by Ellery Frahm,  
University of Sheffield, UK*

A (very) young analytical scientist in-the-making (four-year-old Liev Frahm) helps his father analyze obsidian artifacts from Armenia using a portable X-ray fluorescence (pXRF) instrument.

Photo credit: Ellery Frahm

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# Historical Analysis

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## Glass Chromatography

*Submitted by Ian Wilson,  
Imperial College London, UK*

Before instrumental LC and GC there was paper chromatography (and awesome it was too). This is the lid of a Shandon glass chromatography tank designed for running paper chromatograms. Through the glass knob on the top can be seen the inverted image of a Hewlett Packard 5710AGC, complete with its 7672A autosampler.

Photo credit: Mark Hillen

## The Rest Home for Analytical Artifacts

By Ian Wilson,  
Imperial College London, UK

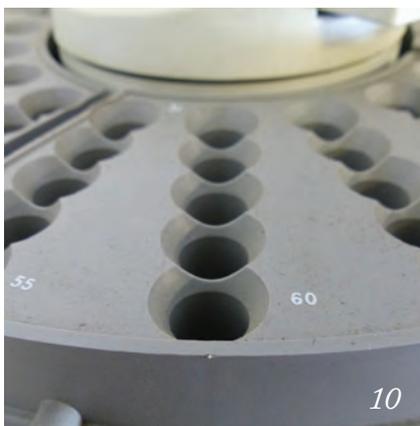
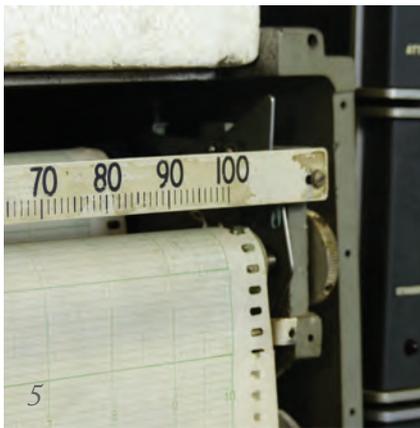
Some years ago, I noticed that the history of separation science was being unceremoniously dumped into the skip. My basement, otherwise known as the (tongue firmly in cheek) “National Museum of Separation Science in Knutsford,” became a refuge for a few survivors that are occasionally visited by the cognoscenti.

Warning: it is likely that there will be a strong correlation between the number of photos that look strangely familiar and your age...

Photo credit: Mark Hillen

1. A Pye 104 gas chromatograph, which came on to the market in 1964 (UK price w/single FID and temperature programmed column: £590). It was very successful and could be found in university labs everywhere, being reliable and robust (or student proof and almost indestructible). It had an oven that could go up to an astonishing 500°C, which was well beyond the capabilities of the GC stationary phases of the day but made it ideal for warming up pies (many students thought that it was indeed the Pie 104...) This one was collected from the University of Keele.
2. A vacuum meter on the AEI MS10 mass spectrometer. The part of AEI that made mass spectrometers became Kratos, which was then taken over by Shimadzu.





3. Another Pye 104, this time equipped with a thermal conductivity detector (TCD). The GC is decorated with the sort of clutter that was common on any flat surface in a GC lab, such as bottles of stationary phase, and situated next to a rather fine Pye chart recorder. Just visible to the right of the chart recorder are the blue boxes of the next generation: Pye 204 (can you guess what the 204's successor was called?)
4. A gas flow controller for Pye 104, this was for one of the hydrogen supply lines to the dual FIDs on this instrument, hence the red spot in the middle.
5. Detail of the chart recorder from image 4.
6. Control boxes for the Pye 204 have moved from the dials and switches of the 104 to push buttons, proving how technologically advanced it is.
7. Believe it or not, this is part of an early gas chromatograph, manufactured entirely in glass by the imaginatively named "Gas Chromatography Limited" on the Brompton Road, London. Apparently, they had a demo lab in a cellar that backed onto the local underground rail line, so had to time demos carefully otherwise the vibrations ruined the chromatograms being recorded on the chart recorder. This round bottomed flask (and glass tube sprouting from it) is the GC "oven".
8. A Perkin Elmer F11 GC (sandwiched between a Pye 304 (congratulations on your answer to caption 4!) and a Perkin Elmer F17. The F11 has a remarkably small footprint for a GC, with the only disadvantage being that the column oven is at the rear, which made column changes tricky. Also, even though its column oven could operate at up to 500°C (like the Pye 104) this layout, and the small size of the oven itself, made it a lot less useful for heating up lunch.
9. A genuine Perkin Elmer twin pen chart recorder.
10. The autosampler tray of the mighty Hewlett Packard (Agilent) 5890 gas chromatograph – a classic of its age. "Not so much a GC, more of a religious experience! The most reliable GC I have ever used. I have had some going virtually non-stop for nearly 20 years [...] The 7673 autosampler was/is still also amazingly reliable" – from 'Chromatography – is it just a box?'



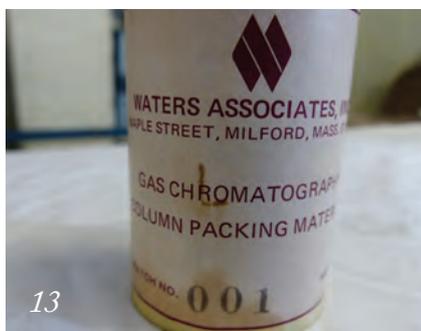
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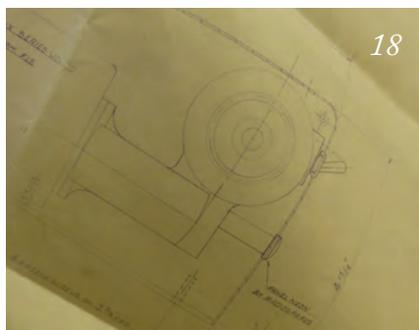
11. The injection port and FID assembly of a Shimadzu GC-9A with stickers celebrating the company's 50th anniversary in the UK.
12. Control panel of the GC-9A
13. Batch 001! Many people don't remember that Waters also used to sell packing materials for GC. The container still has some of Porapak type P stationary phase in it (100-120 mesh).
14. Controls for the AEI MS 10.
15. A range of sample bottles sealed with Vici Mininert valves. The smelly volatile contents date back to 1990/91 and include oil of almond, peppermint and blackberry (as well as the ubiquitous "unknowns"). A portable GC is visible in the background of unknown manufacture. It's a "GC 11" – I would love to know more about it (please comment online with any information).
16. The gradient controller of a Waters system, comprising two M6000A pumps, with the 10 preset gradient programs available shown in the little black panel in the middle of the controller.
17. The business end of the AEI MS 10 mass spectrometer, where the volts come from to accelerate the ions.
18. A small section from an ICI Pharmaceuticals Division blueprint (now sadly yellowed with age) dating back to April 1970 for a device to automatically spot samples onto a TLC plate.



16



17

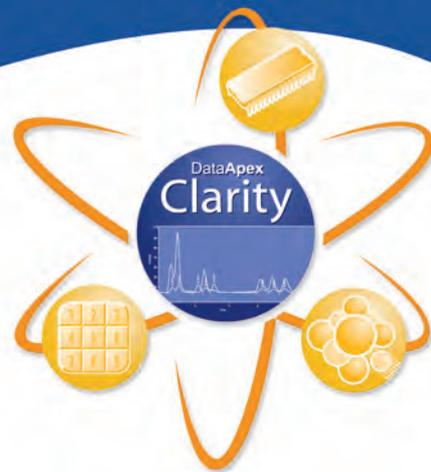


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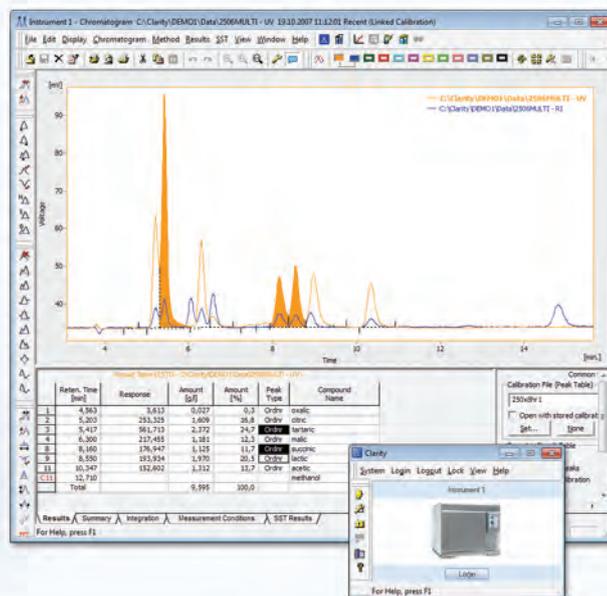
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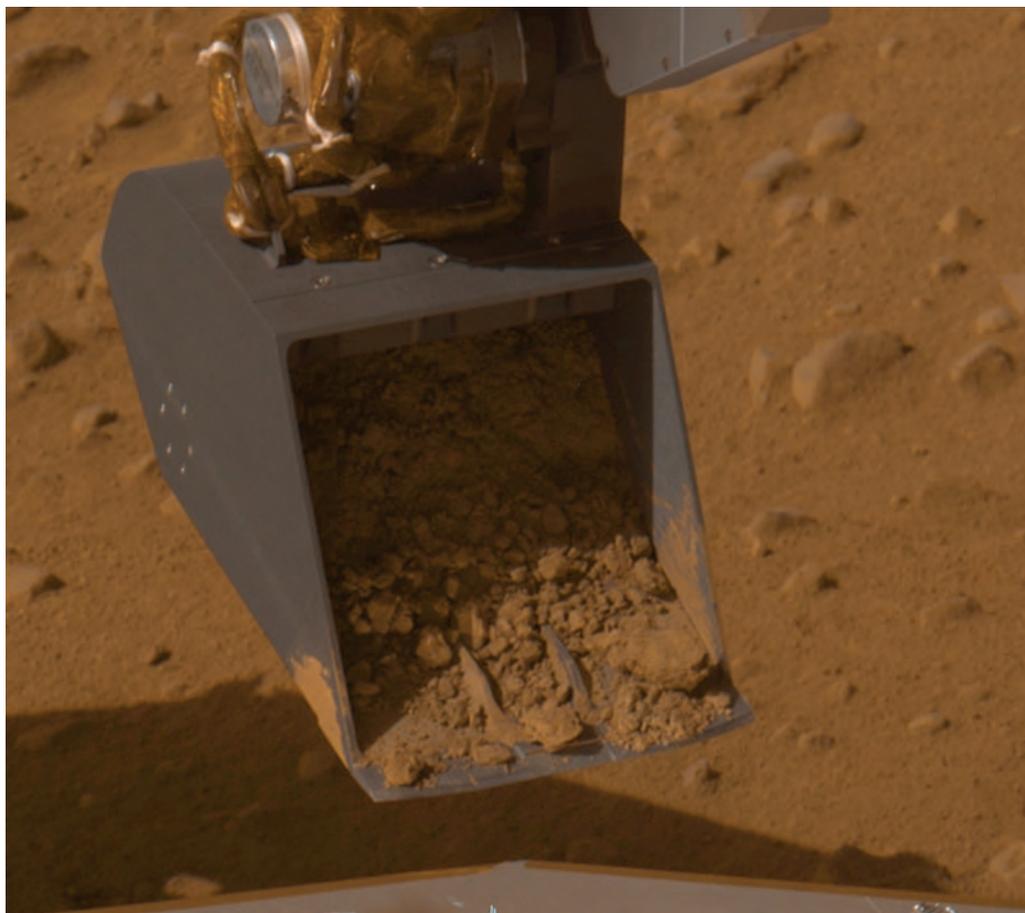
## Surprising Samples

### Scent of Cerumen

*Submitted by Katharine Prigge,  
Monell Center, USA*

Earwax – or cerumen – comprises secretions from specialized sweat glands and fatty materials produced by sebaceous glands. Until now, it has been a little-studied human secretion. We analyzed, for the first time, the volatile organic chemicals in earwax using gas chromatography–mass spectrometry. Differences were detected in the earwax of East Asians and Caucasians, suggesting that earwax is an untapped source of personal information.

Photo credit: Chelsea Lewis



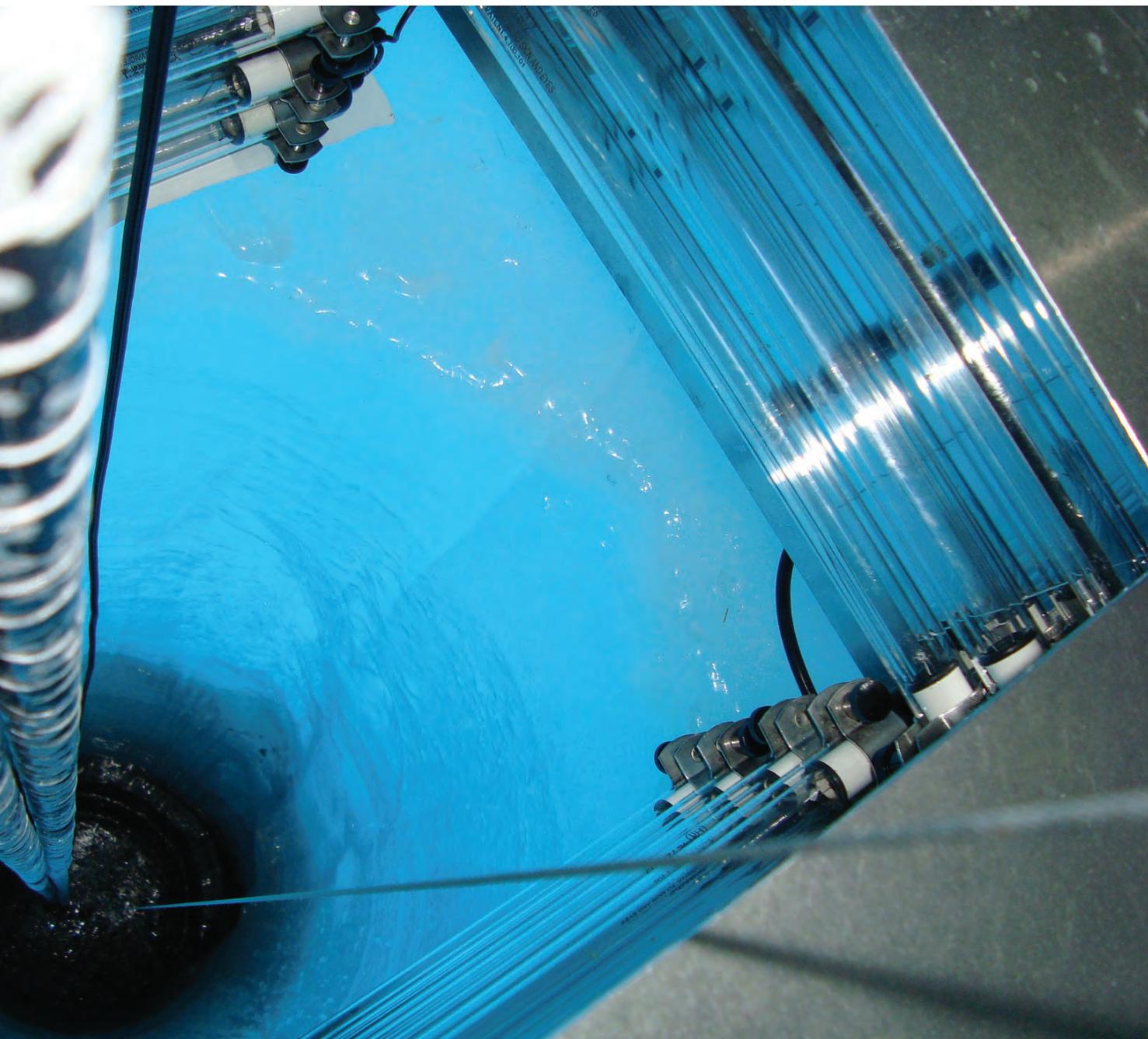
### Soil on Mars

*Submitted by Samuel Kounaves,  
Tufts University, USA*

The first sample of martian soil that the Phoenix Mars lander analyzed in 2008 contained almost 1 percent perchlorate. This unexpected finding has changed the analysis of Mars soil and has wider implications for organics, past and extant life, human exploration, and habitability.

Photo credit: NASA/JPL/University of Arizona/Texas A&M University





Germ Welfare

*Submitted by the Desert Research Institute (DRI), USA*

During Desert Research Institute's (DRI) Lake Vida project, a temporary camp was erected for one month in McMurdo Dry Valleys of East Antarctica to support scientific efforts to study the lake's ice, brine and underlying sedimentary layers. In November of 2012, a pioneering study co-authored by DRI's Alison Murray and Christian Fritsen revealed, for the first time, a viable community of bacteria that survives in a dark, salty and subfreezing environment beneath nearly 20 meters of ice.

Photo credit: Emanuele Kuhn, Desert Research Institute



**Inside Amber**

*Submitted by Jennifer Poulin and  
Stephanie Vuicic, Government  
of Canada, Canadian  
Conservation Institute*

Characterization of Canadian amber has revealed the structural role of succinic acid. Fragments of the amber polymers were broken away with their succinyl cross-linkages intact. The work was performed using a novel method of pyrolysis-gas chromatography-mass spectrometry.

Photo credit: Government of Canada,  
Canadian Conservation Institute,  
CCI 123773-0025





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## Miniaturization

### Short Circuit

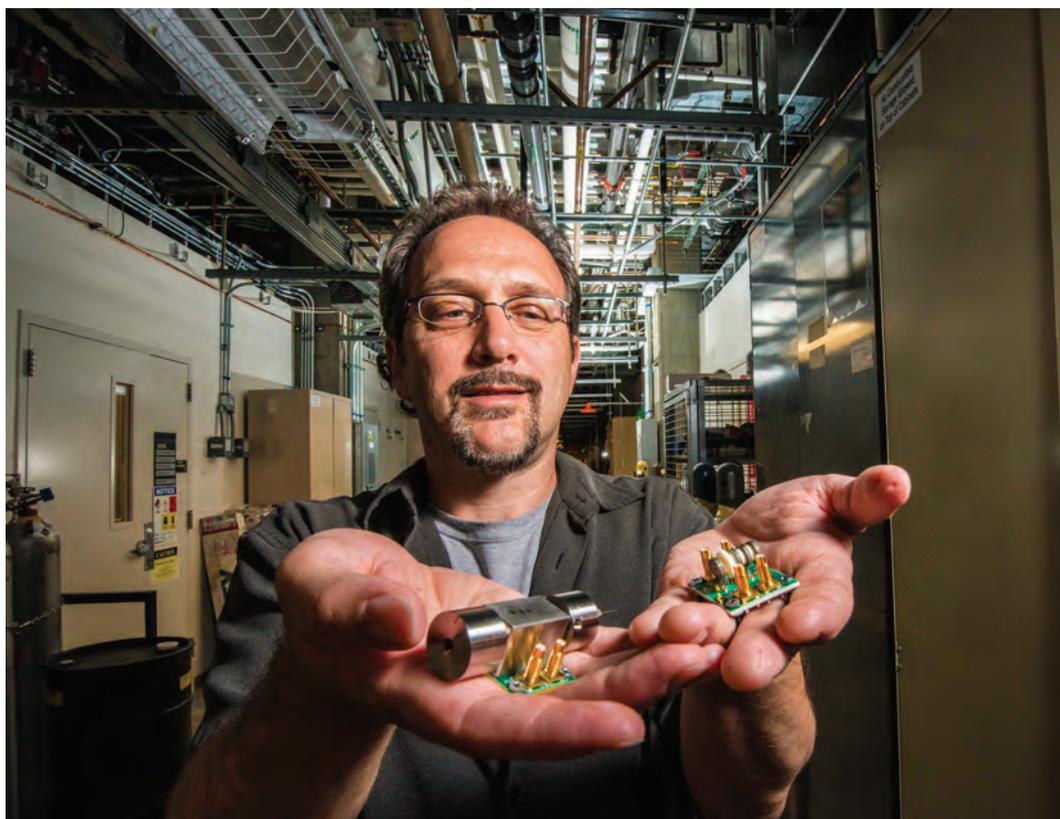
*Submitted by John Rogers,  
University of Illinois, USA*

Advanced electronic materials enable fabrication of integrated circuits, sensors and power supply systems that dissolve, completely and with controlled rates, in water or biofluids. Potential applications range from resorbable medical implants, to degradable environmental monitors, to compostable consumer devices.

The image shows one such device in a state of partial dissolution.

Photo credit: J. Rogers,  
University of Illinois  
and Beckman Institute





### Detection in the Palm of Your Hand

*Submitted by Sandia National Laboratories, USA*

Sandia National Laboratories researcher Ron Manginell displays new miniature pulsed-discharge ionization detectors (mini-PDIDs) that he is developing with colleagues. The tiny detectors have broadened the scope of chemical targets for Sandia's microanalytical detection technology to toxic industrial chemicals, biological volatiles, greenhouse gases and more.

Photo credit: Sandia National Laboratories/Randy Montoya



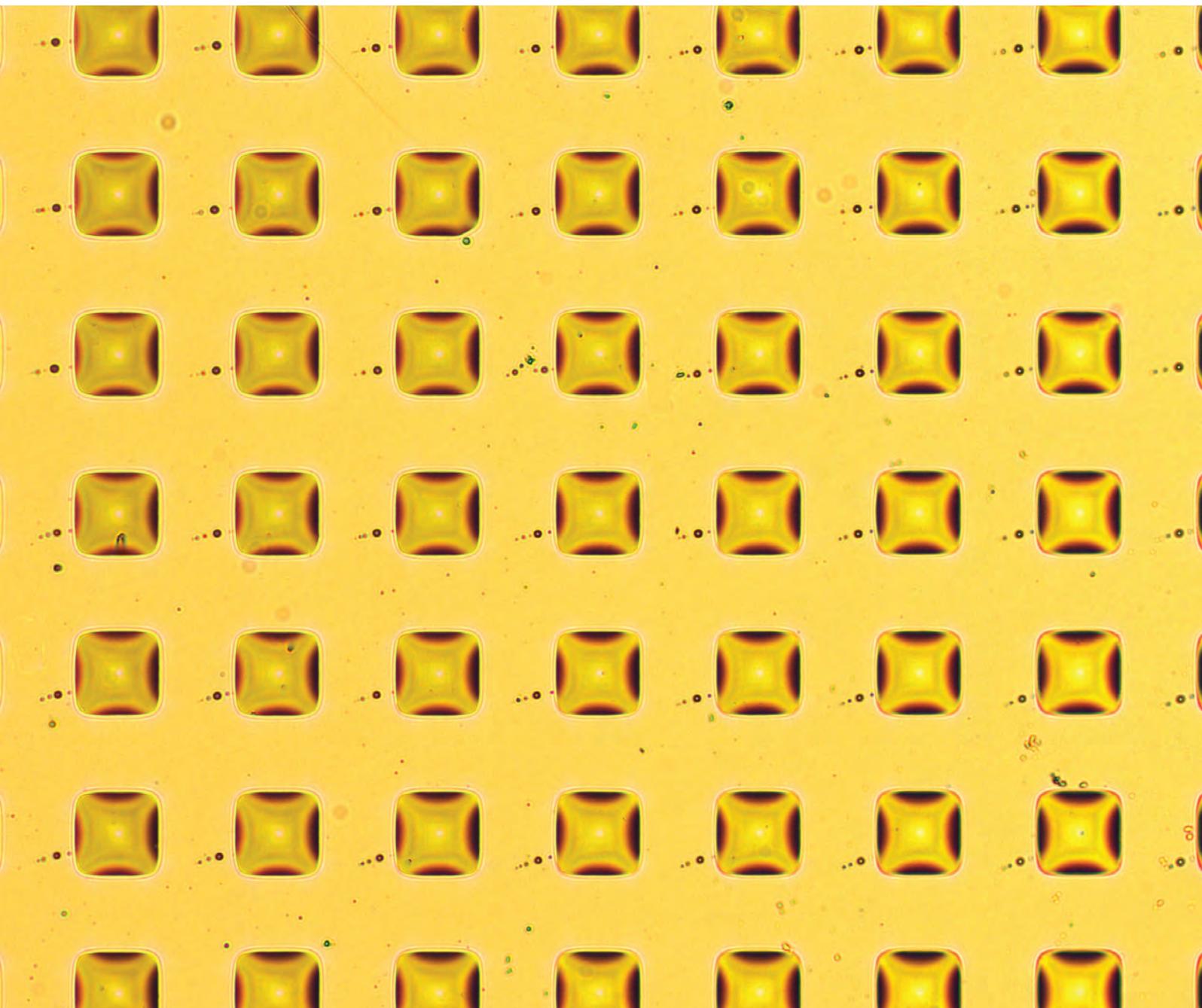
### Low Voltage Plasma

*Submitted by Gary Hieftje  
and the Hieftje Group,  
Indiana University, USA*

The solution-cathode glow discharge (SCGD) is under investigation by the Hieftje group.

Unlike most plasmas used for atomic-emission spectrometry, the SCGD requires no flowing gas, nebulizer, or spray chamber – and it only requires about 75W of power. Yet, it provides detection limits that rival those of inductively-coupled plasma. Work conducted by Steven Ray and Andrew Schwartz.

Photo credit: George Chan



## The Midas Touch

*Submitted by Chuan Zhao and Christian Gunawan,  
The University of New South Wales, Australia*

Micrograph of ionic liquid microarrays fabricated on a gold surface. Each square droplet has a 50  $\mu\text{m}$  length and can serve as an individual sensing unit or microreactor, providing a promising platform for various analytical, sensing or microfluidic applications.

Photo credit: Christian Gunawan

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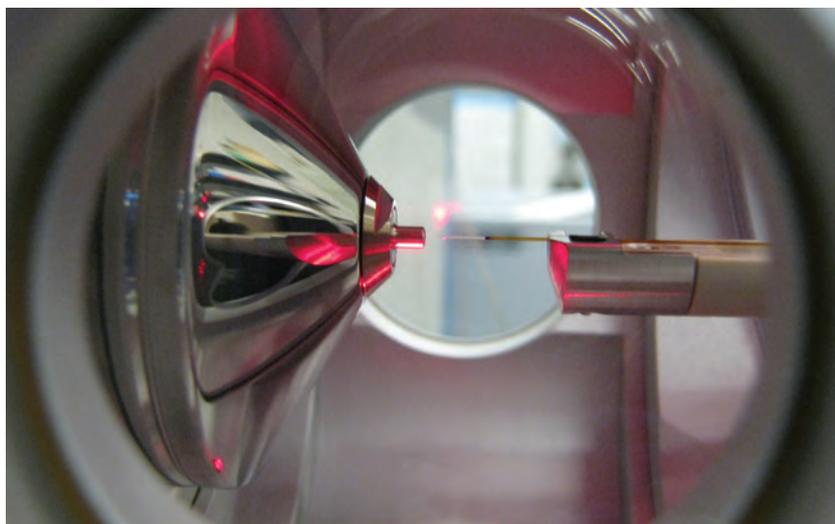
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*Date: Sept 25, 2014,  
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### Space Dust Ionization ▲

*Submitted by NASA, USA.*

Analyzing tiny samples of space dust is very challenging, so we used nano-electrospray ionization (pictured) after nanoflow liquid chromatography to send molecules to a high-resolution mass spectrometer to measure meteorite organics.

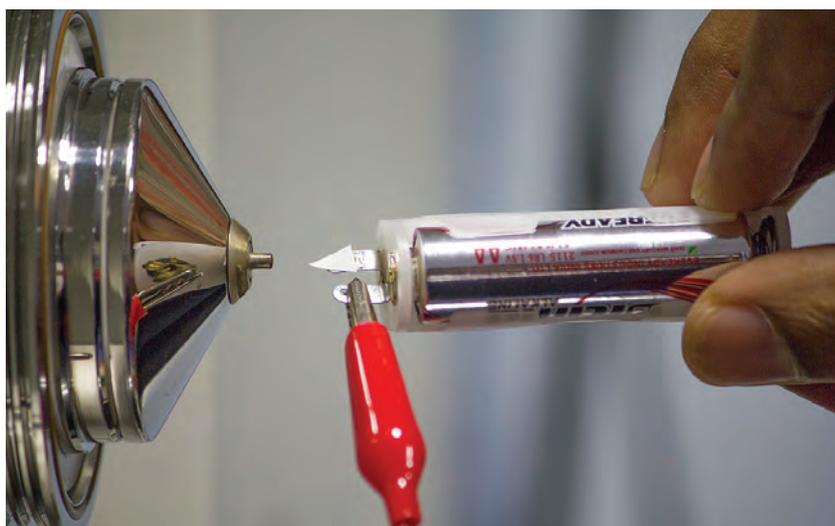
Photo credit: Michael Callahan

### Nanotube Mass Spec ▼

*Submitted by Thalappil Pradeep,  
Indian Institute of Technology,  
Chennai, India, and R. Graham Cooks,  
Purdue University, USA*

Ambient ionization: carbon nanotube-coated paper cut in triangular form and mounted on the positive terminal of a battery assembly.

Photo credit: Thalappil Pradeep/  
R. Graham Cooks



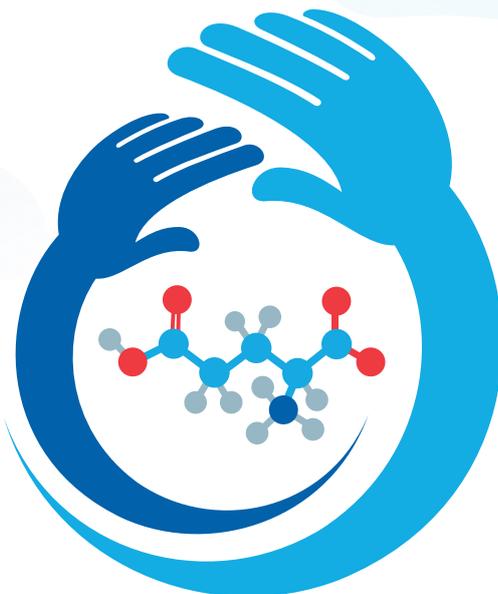


## Portable Paleolithic Preview

*Submitted by Ellery Frahm, University of Sheffield, UK*

Just a few of the 20,000 obsidian artifacts, excavated from a 40,000-year-old Neanderthal site in Armenia, awaiting analysis by portable x-ray fluorescence (pXRF) in a field laboratory. The elemental composition of the artifacts can reveal which volcanoes produced the obsidian.

Photo credit: Ellery Frahm



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# Portrait of a Scientist

Sitting Down With...

John Delaney, senior imaging  
scientist, National Gallery of Art,  
Washington D.C., USA.



How did you find yourself imaging masterpieces of art?

I was actually doing biophysics at graduate school when I had a conversation with a student who was trying to help a conservator image a painting with a vidicon tube with little success. I was experienced in fast spectroscopy and had some knowledge of infrared imaging so I offered to help. I quickly realized that the technology being used was very much out of date – this was back in 1990 – so we decided to build a mockup system with a single diode detector and worked with the conservator to find the right spectral range by scanning test panels. At the same time, new solid-state imaging arrays were coming into use, and I figured they would be perfect for our needs. We convinced Kodak to modify one of its camera systems to work in our spectral range and it worked like a charm! In fact, the results were so great that the research camera was donated to the gallery despite its rather significant cost.

And you were hooked?

Right. That got me hooked for life. Throughout my postgraduate studies and beyond (I worked in the aerospace industry for about 9 years), I found myself consulting more and more for different museums and galleries. I got into multispectral imaging and moved onto using reflectance spectra to analyze art materials with Jack Salisbury's group at Johns Hopkins University – Jack is one of the pioneers of measuring material reflectance spectra. In particular, we were interested in pigment identification. We leapfrogged off work from the geophysics community, who were using airborne hyperspectral cameras to search for rocks and minerals – that's got to be more efficient than a geologist with a Munsell color chart and a pickaxe!

Can you walk us through the main technological advances in art analysis?

Actually, much of the progress seen in the art analysis community echoes advances in the biomedical and material science fields. Good examples include scanning electron microscopy (and its dispersive capabilities), HPLC and MALDI, all of which have been exploited by the community. The concept of scanning a whole painting to gain a general characterization has been developing since the early 2000s. Multispectral reflectance imaging is now commonly used and scanning x-ray fluorescence (XRF) is proving to be invaluable; working with these two different imaging modalities has been extraordinarily helpful in the last couple of years.

What does a good day at work entail for you?

On a good day, I'll be discussing a project with a conservator or art historian. Usually, they will have drawn some inferences about modifications made to the painting and the compositional elements used in terms of pigments. With that information in mind, I hit the lab and start collecting data. But the really fun part is the data exploitation, looking at the maps and making sense of chemical patterns. Finally, I share my conclusions with the conservator and gain their insight. It's an iterative and interdisciplinary process. That's clearly more than one day's work – but you get the picture (no pun intended)!

What's the most exciting piece of art that you've worked on?

Well, the Pablo Picasso 'Blue Period' paintings are rather fascinating in terms of the amount of change that he makes and how quickly the paintings are executed. However, the paintings by Jan van Eyck are unbelievably spectacular in both the

final composition and the underdrawings. It always fascinates me that such painters often deviate substantially from very elaborate underdrawings in the final form. Those in our field (especially the scientists) are often looking for the technical 'hook' that allowed the creation of such a phenomenal piece of work. I get the feeling that these artists knew exactly what they were doing – it is raw proof of their tremendous ability.

Which is most rewarding – the science or the art?

Conservators ask basic questions of very complex, layered materials – it's my job to address those questions using the analytical techniques at my disposal. Meeting that often substantial intellectual challenge is the most rewarding part for me. The artwork is very often breathtaking and beautiful, but I'm a scientist at heart!

Are you artistically inclined?

Many of the people who I work with do paint, draw or do photography – and I can see the desire to get involved. However, I'm satisfied with being an avid appreciator. From that perspective, I find it intriguing that when you spend several weeks with an abstract painting (for example, a piece from Picasso's synthetic cubism period), you start to realize what's so amazing about it, slowly growing to love and understand something you may not have initially liked.

Where is art analysis heading?

We have a lot of single-point analysis methods that work very efficiently, from reflectance spectra to XRF to x-ray diffraction. How best to fuse those datasets spatially and come up with something that doesn't end up with three PhD students arguing over data they all know very well? That's the next big thing.

# JULY 2014 – JULY 2015 CALENDAR OF EVENTS

For all program updates, on-line registration, abstract submission, information on exhibiting and/or sponsoring, please visit the CASSS Web site at [www.casss.org](http://www.casss.org).



## **CMC Strategy Forum: Effective Management of Contract Organizations: Keeping the Product Pipeline Moving, Compliant and Available**

July 21-22, 2014, Gaithersburg Marriott, Gaithersburg, Maryland



## **CMC Strategy Forum LATAM 2014**

21-22 August 2014, Allia Gran Hotel Brasilia Suites, Brasilia, Brazil



## **11th Symposium on the Practical Applications of Mass Spectrometry in the Biotechnology Industry**

September 9-12, 2014, Silverado Hotel, Napa, California

ABSTRACT SUBMISSION DEADLINE: June 13, 2014 oral presentation

August 8, 2014 poster presentation



## **CE in the Biotechnology & Pharmaceutical Industries: 16th Symposium on the Practical Applications for the Analysis of Proteins, Nucleotides and Small Molecules**

October 12-16, 2014, Hyatt at Olive 8, Seattle, Washington

ABSTRACT SUBMISSION DEADLINE: July 18, 2014 oral presentation

September 12, 2014 poster presentation



## **CMC Strategy Forum Japan 2014**

8-9 December 2014, Hotel Okura, Tokyo, Japan



## **CMC Strategy Forum**

January 26, 2015, Mayflower Renaissance Hotel, Washington, DC

## **WCBP 2015: 19th Symposium on the Interface of Regulatory and Analytical Sciences for Biotechnology Health Products**

January 27-29, 2015, Mayflower Renaissance Hotel, Washington, DC

ABSTRACT SUBMISSION DEADLINE: November 26, 2014 poster presentation



## **Bioassays 2015: Scientific Approaches & Regulatory Strategies**

March 23-24 2015, Sheraton Silver Spring Hotel, Silver Spring, Maryland

ABSTRACT SUBMISSION DEADLINE: February 28, 2015 poster presentation



## **4th International Symposium on Higher Order Structure of Protein Therapeutics**

April 13-15, 2015, Courtyard Boston Downtown, Boston, Massachusetts

ABSTRACT SUBMISSION DEADLINE: January 16, 2015 oral presentation

March 13, 2015 poster presentation



## **CMC Strategy Forum Europe 2015**

4-6 May 2015, Radisson Blu Scandinavia Hotel, Copenhagen, Denmark

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