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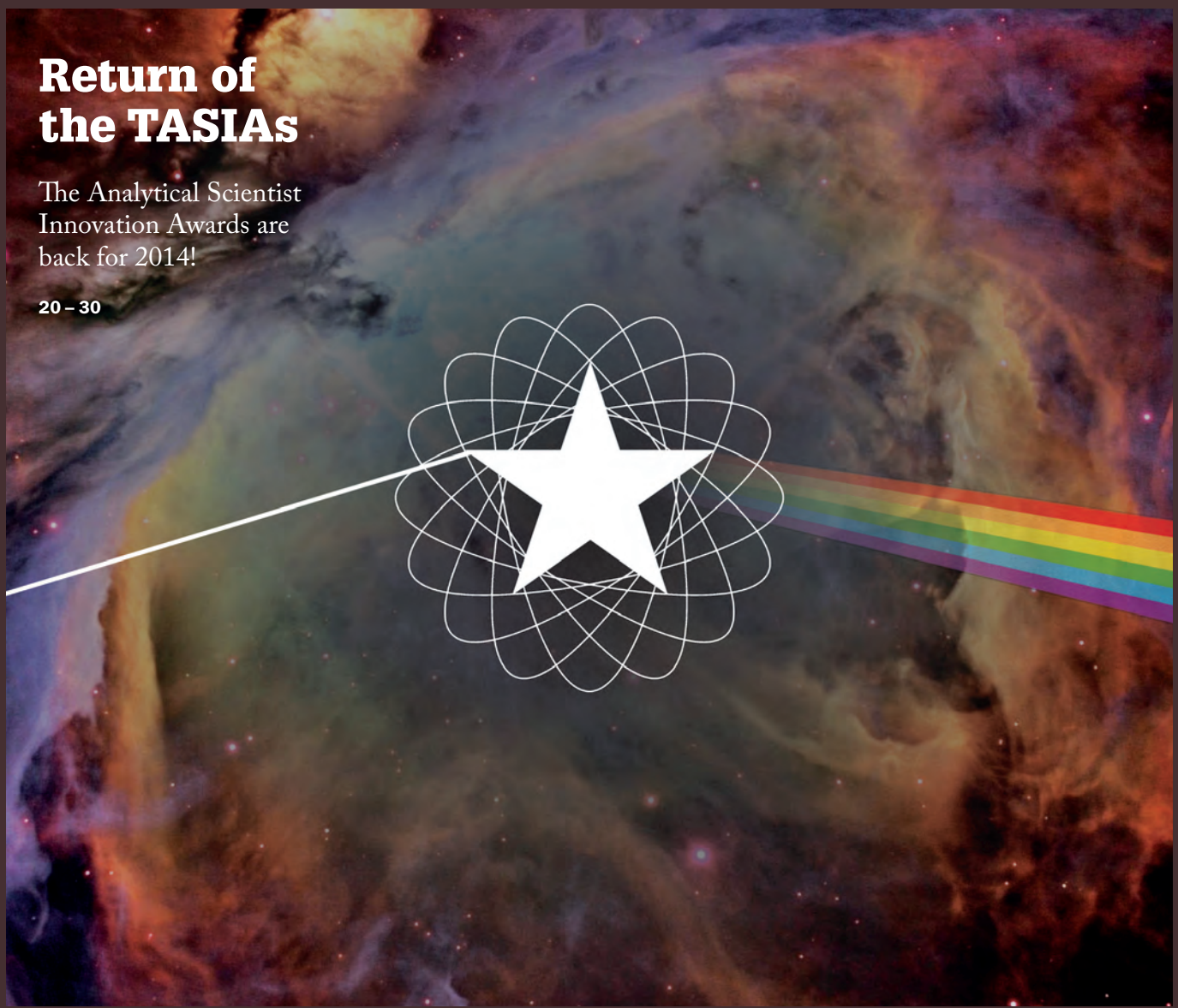

## Return of the TASIAs

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# Online this Month

## *Tea With Emily*

Tea With Rich is back for a second series. In this first episode from the ISC2014 conference in sunny Salzburg, Emily Hilder – one of our Top 40 Under 40 – introduces an exciting and ambitious collaborative project focused on portable analysis. The ARC Training Centre for Portable Analytical Separation Technologies (ASTech) is a recently established center funded under the Australian Research Council's (ARC) Industrial Transformation Research Program (ITRP), and is a partnership between the University of Tasmania and Trajan Scientific and Medical. "It's really exciting because it's about deliberately bringing industry and academia together so that fundamental research is driving technological change in industry," says Emily – before tackling the really big challenge: eternal youth and health.

*Online: tas.txp.to/1214/Emily*

## *Tea With Pat*

Pat Sandra reflects on the prestige of the Pregl Medal 2014 Award from the Austrian Society of Analytical Chemistry and takes an educated guess as to why he is in a long line of impressive recipients. Pat continues to voice concern over the lack of respect paid to sample preparation: "If you don't have good sample preparation - all of your data are wrong…" and then takes us on a whistle-stop tour of other issues in the world of analytical science – including the lack of fundamental knowledge. Pat notes that miniaturized techniques will complement rather than compete with lab-based analytical systems, before finally lighting the touch paper of a debate on the nomenclature of supercritical fluid chromatography.

*Online: tas.txp.to/1214/Pat*

## *Tea With Jean-Pierre*

In the third episode from Salzburg, Rich invites Jean-Pierre Chervet for tea to discuss life after LC Packings – in particular, his focus on electrochemistry (EC) with LC-MS. Ten years ago, Uwe Karst described the coupling of electrochemistry and mass spectrometry as a "great combination". Today, Jean-Pierre believes electrochemistry is really coming into its own. "All the headaches you had in early grad school with electrochemistry suddenly disappeared because you don't do detection – just REDOX reactions." Mimicking drug metabolism is still a key application area for EC, but Jean-Pierre is starting to see other exciting areas open up as well, including 'omics' applications and extended use in pharmaceutical stability testing, as pioneered by Pfizer.

*Online: tas.txp.to/1214/JP*

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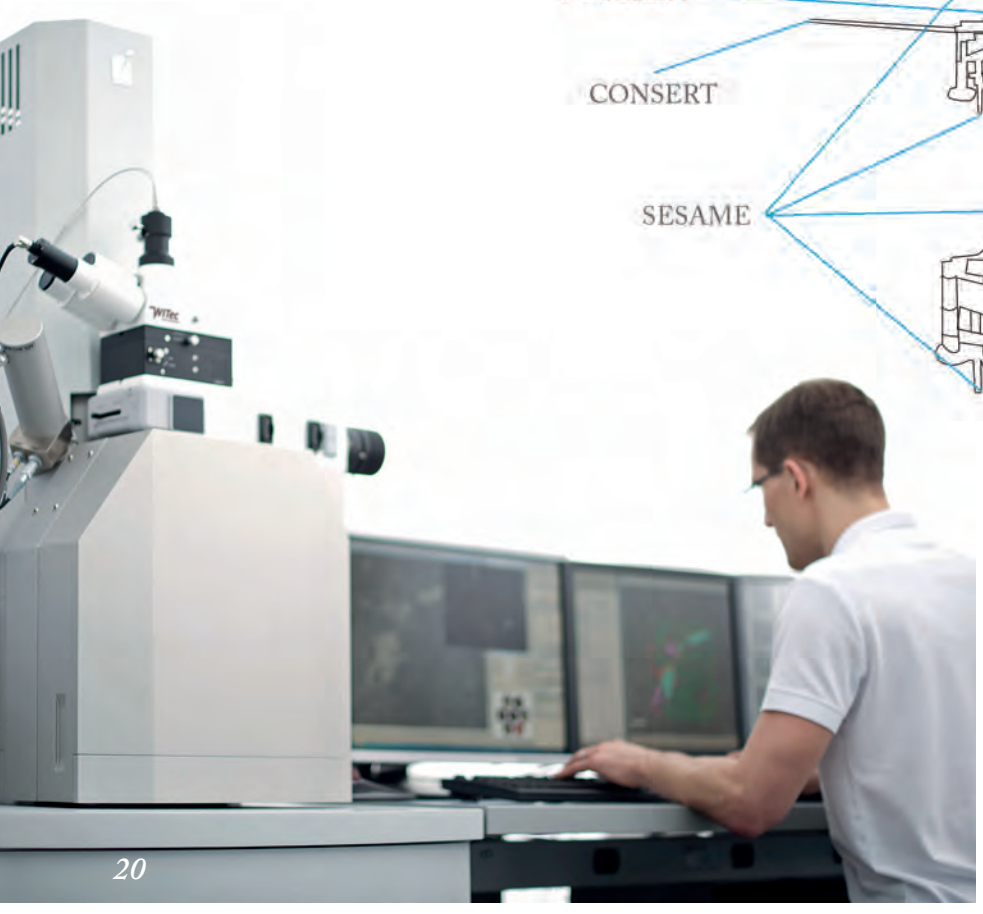

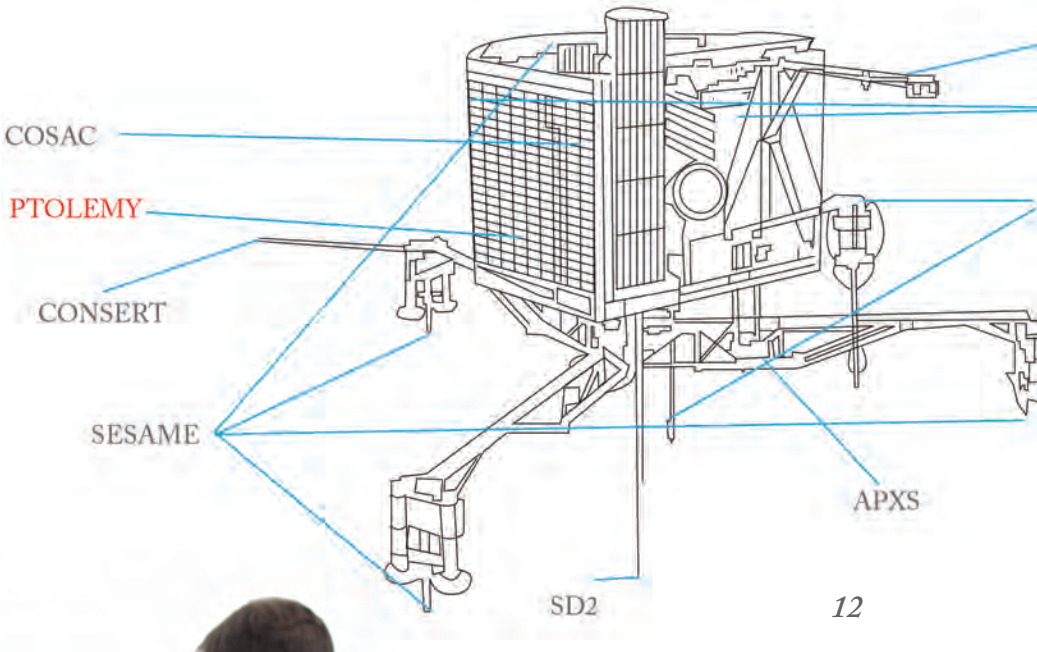


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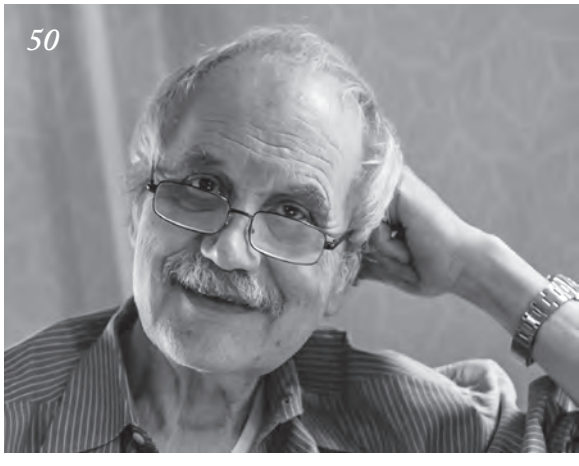

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the **Analytical Scientist**

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# Two Years On

*Including the contents this final issue of 2014, we've published just shy of 350 articles to date, covering all aspects of analytical science. Where next? Well, that's really up to you...*



Has it really been two years since we started our mission to record, scrutinize and celebrate analytical science – or a year since our inaugural 2013 Innovation Awards? Is it a case of tempus fugit (for geneticists: time flies like an arrow; fruit flies like a banana)? Or is the past, present and future just an illusion as Albert Einstein believed? Either way, it's not until I recall the brilliant and engaging scientists who have graced The Analytical Scientist that I realize how far we've come. We covered a great deal – from sampling and sample preparation to paper-based microfluidics to MS imaging (your Top Ten online favorites of 2014 are listed on page 14) – and yet, there is so much left to explore. Was your field left out in the cold? Did we skip your core technique? Have we not even acknowledged your existence? If you are solemnly nodding, then I apologize and invite you contact me to discuss how we can make amends.

We were very clear from the beginning that The Analytical Scientist is your magazine. Earlier this year, many of you helped us stay on track by completing our online reader survey – thank you (there will be another at some point in the new year). We have tried to take as many of your comments on board as possible in 2014 and hope that we are publishing content that is as fresh and engaging for the whole analytical community as it was when we started. Your ongoing feedback is extremely valuable.

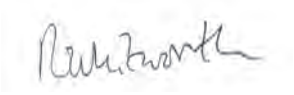
In the spirit of community, I would like to welcome contributions (concepts, text, images or video) from anyone in the analytical sciences with an opinion or exciting work to share. The Analytical Scientist is an open forum for discussion and knowledge exchange; our aim is to drive the field forward just that little bit faster or in subtly different directions. Your views, ideas, debates – and involvement – are what makes The Analytical Scientist tick. If you've already contributed – thank you; the invitation to do so again is always open. If you've not been involved but feel you have something to offer, you can email me directly at rich.whitworth@texerepublishing.com.

And so we return to the present (assuming it is not merely an illusion), which brings with it our annual Innovation Awards. On page 20, we showcase 15 winning combinations of invention, vision and utility that were selected and ranked from your nominations by a judging panel that comprised three leading experts and the editorial team. We extend our sincere congratulations to all 15 TASIA winners.

To conclude, I offer somewhat more digestible words from Einstein: "We cannot solve problems by using the same kind of thinking we used when we created them."

Thank you to all innovators in our amazing field.

Best wishes for the New Year,
**Rich Whitworth**



## Stephanie Sutton

"Making great scientific magazines isn't just about delivering knowledge and high quality content; it's also about packaging these in the right words so that readers can be truly inspired by a topic," says Stephanie Sutton. Steph has spent seven years writing and editing articles for scientific and manufacturing publications, ensuring that the content is engaging and accessible without sacrificing its scientific integrity. "There is nothing better than a magazine with fantastic, readable content." Steph is the Associate Editor of The Analytical Scientist.

## Frank van Geel

Frank van Geel studied analytical chemistry in the Netherlands, ahead of several years of post-doc work in spectroscopy with Jim Winefordner at the University of Florida. Later, he became a science teacher and publisher in chemistry and physics related topics. Frank has developed numerous publications in his time, and knows where the future lies: "Building online communities is the road to take. We need to strengthen the quality of analytical chemistry and we need to strengthen our community by sharing know-how and by sharing our opinions, visions and our views of the future of analytical science." Frank is the Scientific Director of The Analytical Scientist and owner of educational website Chromedia (www.chromedia.org).

## Marc Bird

Marc Bird is a graphic designer with over 10 years of professional experience. "My career began at London lifestyle magazine Dazed & Confused. After several years, I moved to Grand Designs Magazine – the accompaniment magazine to the UK TV series". After relocating to the North West, Marc continued working in design for a classic music publisher and latterly for Live Nation producing marketing materials for their extensive theatre division.
"More recently I set up a Community Interest Company to provide creative support to Third Sector companies based in the North West," he says.
Marc is the Senior Designer of The Analytical Scientist.

## Rich Whitworth

After studying medical biochemistry, Rich Whitworth worked for a number of companies before escaping to Tokyo, where he spent five years at the largest English-language publisher in Japan. On returning to the UK, Rich eventually found Texere Publishing, where he is now Associate Editorial Director. "I feel honored to be part of the team that forged The Analytical Scientist. I owe a huge thank you to everyone – colleagues, readers, contributors, and advisors – for supporting The Analytical Scientist over the past two glorious years."
Rich is the Editor of The Analytical Scientist.

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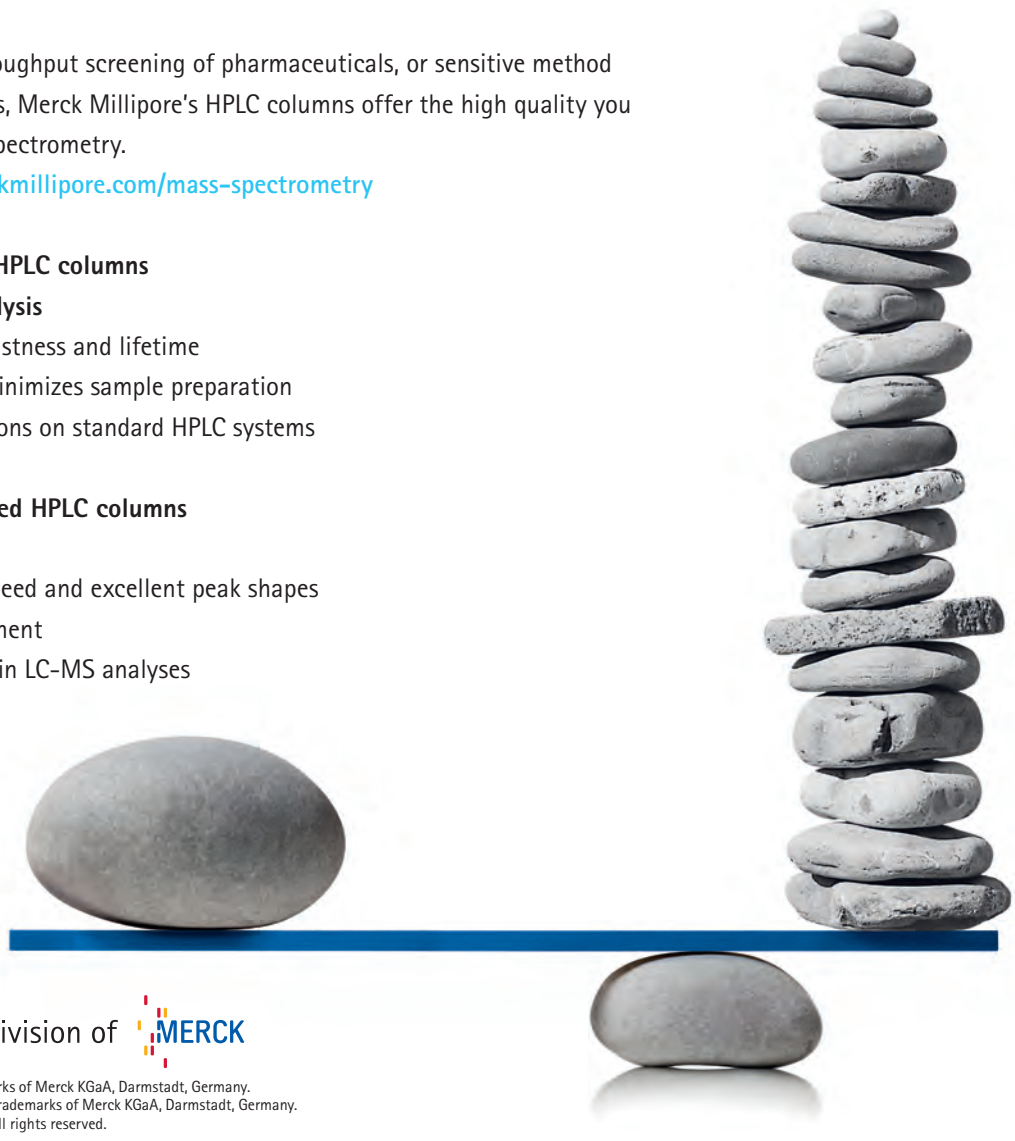

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# Upfront

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

*We welcome information on interesting collaborations or research that has really caught your eye, in a good or bad way. Email:*
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## Smells Like... Blood

**Can the human nose beat analytical instrumentation when it comes to identifying gory components?**

For predators, blood means food, and the scent alone is enough to trigger behavioral responses. Matthias Laska, professor of zoology at Linköping University in Sweden, wanted to identify the volatile compounds that give blood its "alluring" aroma.

"Very few people have analyzed the composition of blood odor – even in humans – except for finding biomarkers for certain diseases. It's not an odor that's commercially valuable; I think you have to be interested in animal behavior for this kind of study," admits Laska, who sent a student to Andrea Büttner at the Friedrich-Alexander University in Erlangen, Germany, which specializes in the analysis of complex odors.

The volatile constituents of pig's blood were isolated and the mixture was separated using gas chromatography. "There are hundreds of volatiles in blood odor, so identifying all the compounds is an enormous task," explains Büttner. "Often it is the substances at very low concentrations that are the most potent, but they are difficult to detect with conventional detectors." And so, the team chose to use a very specialized instrument: the human nose. "To this day, the human nose is more attentive and can detect lower concentrations of odorants," says Laska.

Trained 'sniffers' sat at the outlet of the GC and were able to pinpoint the peaks of most interest. Several odorants were identified in the blood samples, one of which was very potent: the metallic smell of trans-4,5-epoxy-(E)-2-decenal.

"We used the hypothesis that we humans might be able to smell the same substance as the predators," says Büttner. "I had a gut feeling from my

daily sniffing experience that this was a promising substance that might be a potent trigger for the smell of blood."

Laska infused logs with trans-4,5-epoxy-(E)-2-decenal and presented them to animals (1). "The animals performed better than even in our wildest dreams," he says. "They clearly reacted to the infused logs – sniffing, licking, pawing and toying. It will be interesting to continue this line of research to see how this has evolved."

When it comes to practical uses, Laska says that presenting odorant objects to carnivores in captivity can be useful for environmental enrichment. The next step of the study will be to present the substance to other animals, such as prey species.

"I would assume from the development of smell and its genetic base that all mammals react to similar compounds," says Büttner. "For me, it's also important to do further identification and quantification on all the other odorants we detected. I would like to see if this whole bouquet of blood smells works better than the trans-4,5-epoxy-(E)-2-decenal."

*Reference*

1. *S. Nilson et al., "Behavioral Responses to Mammalian Blood Odor and a Blood Odor Component in Four Species of Large Carnivores", PLOS One (2014). DOI: 10.1371/journal.pone.0112694*

# Miraculous miRNA Disease Detection?

**A new microRNA analysis platform aims to detect disease well ahead of symptoms**

A start-up company called Miroculus (www.miroculus.com) is developing a microRNA detection platform (Miriam) that could potentially detect dozens of different diseases using just one milliliter of blood. MicroRNA molecules – whose number vary depending on both internal and environmental conditions – regulate the expression of genes in cells. Given enough data linking microRNA signatures to disease states, the platform could potentially give clues about a person's health – long before symptoms appear.

"Traditionally, medical intervention has focused on the treatment part of disease and not so much on prevention," says Jorge Soto, CTO and co-founder of Miroculus. "Early cancer detection tests are something that other research groups have tried, but in our case we have decentralized the lab using the cloud, which dramatically reduces costs."

The Miroculus and its Miriam platform, which span out of Singularity University (singularityu.org), have certainly captured the attention of the popular media; Soto's TED talk has garnered nearly half a million views in just two months (online: tas.txp.to/1214/TED). "One in three people sitting in this audience will be diagnosed with some type of cancer, and one out of four will die because of it," Soto told the quickly attentive live TED audience.

At the core of the platform is a special 96-well plate that has been pre-treated with patented biochemistry to "trap" specific microRNA. After the plate is inserted into the reaction device, a smartphone records images and sends them to a cloud database, which identifies patterns that may be associated with disease.

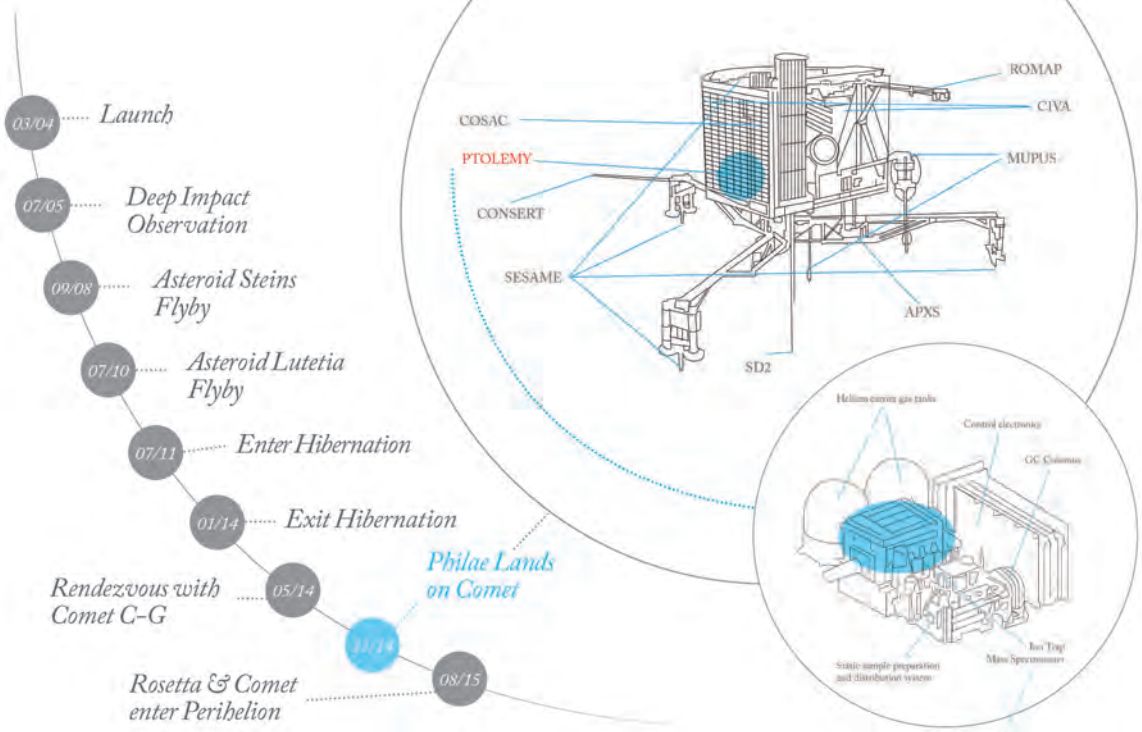
"Specific patterns of expression (or not) of microRNAs correlate to specific diseases, particularly cancer, but also other metabolic and psychiatric diseases," explains Soto. "With this platform we are not directly looking for specific types of cancer; we are looking for the microRNAs circulating in blood."

The problem? MicroRNAs are short in length and not highly differentiated. Nevertheless, Soto claims the

developing (but somewhat mysterious) technology is up to the task, and says that the partially 3D-printed prototype has been able identify microRNA patterns of pancreatic, lung, breast, and hepatic cancers.

It's early days and a huge amount of data will be needed before the platform can be marketed as a diagnostic tool. In the meantime, the company will be targeting the pharmaceutical industry as potential users of the device because it could provide important information about how patients react to new drugs – and allow Miroculus to obtain more robust microRNA-related data.

## Mission Milestones




# The Comet Lander

**Performing GC-MS on a speeding comet certainly sounds like science fiction...**

"The greatest satisfaction will be the return of some valid electromagnetic signals that ultimately have the capacity to convey some new scientific meaning and knowledge," Ian Wright told us back in January 2014 when comet chaser Rosetta awoke from hibernation and phoned home from some 500 million miles away (online: tas.txp.to/1214/cometchaser).

Despite a harpoon system failure and the lack of downwards thruster, Philae – Rosetta's comet lander – finally came to a safe but shadowy resting place, having bounced twice after the initial touchdown.

Wright sent an email in the midst of the exciting activity: "We are, as of 16:56 UTC on the November 14, waiting to find out whether some newly configured telecommands can be uploaded tonight for what might be a last attempt at making some measurements. We already have plenty of data in the bag but are hungry for more."

In fact, in a little over two hours of communication time, the Philae was able to send all of its science data from the targeted instruments, including Ptolemy, the "miniaturized" gas chromatography-mass spectrometry system developed by Wright. Given the lack of solar power available, Philae's power supply faded rapidly...

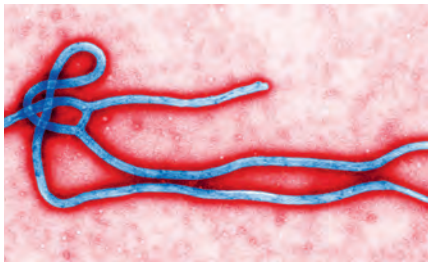
What next for lonely Philae? "We still hope that at a later stage of the mission, perhaps when we are nearer to the Sun, that we might have enough solar illumination to wake up the lander and re-establish communication, " said Stephan Ulamec, lander manager at the DLR German Aerospace Agency.

We look forward to sharing results that are out of this world in the near future.

*For more information on Rosetta Mission: tas.txp.to/0114/Rosetta*

# Outsmarting Ebola While You Sleep

**A new World Community Grid project harnesses excess computational power donated by volunteers to screen millions of candidate drug molecules**



"The Ebola virus outbreak is devastating and heartbreaking. It has taken many of my colleagues who I knew personally and worked with in Sierra Leone," says Erica Ollman Saphire, a Professor at the Scripps Research Institute in La Jolla, California, in a video outlining the "Outsmart Ebola Together" project (online: tas.txp.to/1214/outsmartEbola).

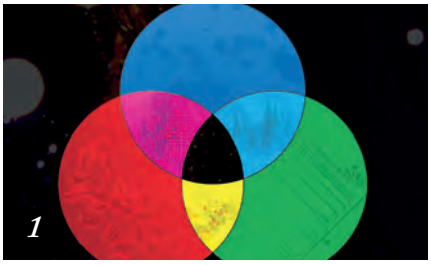
Erica's team have worked on Ebola full-time for the last 11 years. The knowledge of molecular structures gained during that time could hold the key to identifying the most promising drug targets – but only if sufficient computing power is available. "[Our Ebola] molecular structures are like enemy reconnaissance; they tell us exactly where to hit in the virus to stop it from infecting new cells," says Erica.

The World Community Grid uses the Berkeley Open Infrastructure for Network Computing (BOINC), which acts as the conduit between your devices' unused processing capability to provide projects, such as Outsmart Ebola Together, with the computational power they need for complex tasks. Erica puts the potential impact into perspective: "If the hundreds of thousands of people on this grid each do a small piece of the calculation, it will let us do in weeks what would take hundreds of years otherwise."

The BOINC software is available for Windows, Mac, Linux computers and Android devices (for free, of course). You'll be joining (on the last check), 225,966 active volunteers, who are producing a 24-hour average of 8.403 petaFLOPS in computer power – in other words, the ability to do 8,400 trillion floating-point operations per second – give or take (that's a lot).

In addition to the Ebola project, the World Community Grid also enables you to participate in other worthy projects, such as Mapping Cancer Markers, Uncovering Genome Mysteries, and the long-running FightAIDS@Home, which we featured last year (online: tas.txp.to/1214/99percent). Plus, BOINC software offers access to further projects across a diverse range from astronomical particle physics to an attempt to decode three original Enigma messages from 1942...

Why not let your computer do some work while you take your New Year's break?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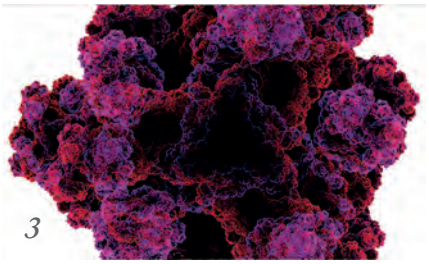
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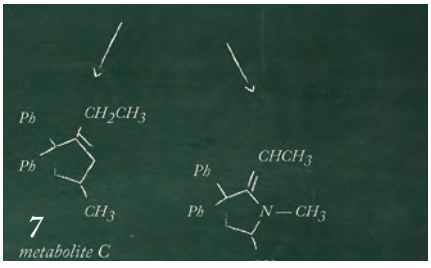

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# What You've Been Reading...

**We dived into our analytics to find the most popular online articles. Here, we present a thought-provoking quote from each of the top ten.**

1. "A great deal of scientific literature appears to be invisible to the research community unless it is electronically accessible – certain research projects are therefore in danger of missing critical information or repeating experiments that have already been undertaken. We should not re-invent the wheel."
*– Robert Trengove, Tools of the Metabolomics Trade (online: tas.txp.to/1214/top1)*

2. "It is clear that errors made in sampling, sample preparation or sample introduction (injection) cannot be corrected by using even the most advanced MS systems."
*– Frank David, Three Wizards of Sample Preparation (online: tas.txp.to/1214/top2)*

3. "We need new bioinformatic approaches to combine the proteomic data we generate with other omics data, particularly genomic, but also, metabolomic and lipidomic."
*– Barry Karger, Three Gurus of Proteomics (online: tas.txp.to/1214/top3)*

4. "The Moore's Law-esque advancement in our ability to identify and quantify proteins over the last 20 years is probably one of the few areas where end-users in a field have fully acknowledged the fact that industry has driven much of the progress."
*– Ian Jardine, Building Mass Spectrometry from the Inside (online: tas.txp.to/1214/top4)*

5. "MS imaging technology has matured enough to be applied in the clinic, but small-scale efforts will lead to disappointments; a large-scale infrastructure is needed to take full advantage of the benefits. Investment

is essential, as is the concerted effort of all involved."
*– Ron Heeren, MS Imaging Targets the Clinic (online: tas.txp.to/1214/top5)*

6. "What is especially interesting is that these biomarkers reflect the risk for dying from very different types of diseases, such as heart disease or cancer. They seem to be signs of a general frailty in the body."
*– Johannes Kettunen, Death Card (online: tas.txp.to/1214/top6)*

7. "I've noticed that all around me the 'chemistry' part of my field is less and less obvious – analytical chemistry has become analytical science (as emphasized by the title of this very magazine!). The problem is that you can't simply forget about the exciting and interesting chemistry occurring (nowadays very much in the background) to enable a particular analytical method."
*– W. Franklin Smyth, Back to School for Pharmaceutical Analysis (online: tas.txp.to/1214/top7)*

8. "A specific sampling process can either be representative – or not. If sampling is not representative, we have only undefined, mass-reduced lumps of material without provenance (called 'specimens' in the theory of sampling) that are not actually worth analyzing."
*– Kim H. Esbensen and Claas Wagner, Why We Need the Theory of Sampling (online: tas.txp.to/1214/top8)*

9. "Organic contaminants can undergo bio-transformation once they are in the environment; for example, a pharmaceutical rarely exits the human body in its original form but rather as a more polar metabolite that enters the environment through the sewage system. Such transformation products should get more attention. Are they present and, if so, at what levels and risk?"
*– Annemieke Kolkman, H2OK? (online: tas.txp.to/1214/top9)*

10. "The big change in analytics is the migration from generating analytical data to generating actionable, affordable information."
*– George Whitesides, Using Simplicity (online: tas.txp.to/1214/top10)*

# 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

# Fundamentals, Fun and Funding

**I've been lucky enough to spend time in the grey area between analytical spectroscopy and atomic physics. It's fascinating and enlightening – but is it chemistry?**

*By Nicoló Omenetto, Research Professor, Department of Chemistry, University of Florida, USA.*

Working with lasers – the major tool of spectroscopy research for the last 40 years – I have become very well acquainted with the dangers of being swallowed up by the fascinating subject of atomic physics. But I am a chemist! Getting the balance wrong can have a negative impact on funding if you're unlucky. For example, it's difficult to get funding for research on the coherent interaction of atoms with radiation fields if you're an analytical spectroscopist... they'll tell you it's not chemistry. And they're right – in a way.

Atomic physics is clearly at the root of understanding spectroscopy. Take the diode laser. If you want to do the perfect atomic absorption spectroscopy experiment, you can take a diode laser with an extremely narrow frequency and tune it to the center of an atomic absorption profile of an atom trapped by laser cooling. At that point, only natural broadening is occurring, and guess what: you no longer need to be concerned with the absorption oscillator strength... Suddenly, the language of atomic physics starts to take over.

While having fun with spectroscopy, the ability of lasers to manipulate atoms and molecules has fascinated me most of all, even if it is actually in the realm of atomic physics. It's quite comical that BEC here stands for Bose–Einstein condensate rather than 'background equivalent concentration' as it should for an analytical spectroscopist. But perhaps we should not be too quick to pigeonhole academic interests. Let's consider single atom detection and single molecule detection – those advances come from excellent work done by atomic physicists but also by atomic and analytical spectroscopists, such as James Winefordner.

I for one am certainly very pleased to have an atomic physicist as a colleague; Ove Axner has been following the impressive work in noise-immune cavity-enhanced optical heterodyne molecular spectroscopy (NICE-OHMS) done at the Joint Institute for Laboratory Astrophysics in Colorado. From the theory, one can calculate the signal-to-noise ratio and find that NICE-OHMS is capable of detecting less than one atom – theoretically, of course. With that kind of sensitivity, it's hard to imagine all of the amazing possibilities. Unfortunately, as an analytical chemist you need a practical application. There is a dichotomy at work here. As said by many analytical spectroscopists, it's difficult to develop a fantastic method if it's not driven by an application. But on the other hand, the application would have to be extremely demanding and important to develop such a sensitive method. Sometimes, predicting where the future might lead – or where we should focus our efforts – can be almost impossible.

The NICE-OHMS example clearly highlights the strong connection between analytical spectroscopy and atomic physics, especially with regards to noise. After all, there is no signal without noise. To fully understand spectroscopic noise, you quickly enter the territory of stochastic variables, signal communication theory, and so on. At first, it can appear that such discussions

are outside the scope of analytical spectroscopy, but actually, understanding the fundamentals and characterizing noise is at the very root of improving the quality of our measurements.

Only if we know the characteristics of noise can we devise instrumentation that is capable of improving the signal-to-noise ratio, decreasing the limit of detection, and increasing analytical sensitivity. In other words, we can only improve if we understand. Unfortunately, I don't think we have enough people working on problems with this philosophy in mind. On a more elementary level, I certainly focus on signals and noise, and how they relate to measurement in my spectroscopy classes. After all, there is no algorithm or chemometric program that is capable of superseding a good understanding of data quality, which can only come from fundamental knowledge. For the same reason, I believe that it is very important for students (and academics!) to invest heavily in learning what has been done before. I am absolutely convinced of the need to not only look at papers that have been published in the last four years, but rather the last forty.

It's true that the grey (and yet extremely exciting) border between physics and chemistry can have difficulty attracting funding these days – especially for an analytical spectroscopist – but that doesn't make it in any way trivial. I feel lucky to have been given the freedom to explore so many different facets of my field – and I worry that the current generation will not be so fortunate.

# The Champions League of Measurement Science

**A technique can only make it into the upper echelons of analytical chemistry with a strong, balanced team. And that means bringing together fundamental researchers, application specialists, and instrumentation experts on a well-supported playing field.**

*By Peter Schoenmakers, Professor at the Faculty of Science, van't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands.*

There are numerous physical measurement methods, usually based on fundamental principles and often of great interest to scientists. It is amazing how smart we can measure, how little, and how fast. However, in most cases scientists just amaze each other. The rest of the world remains unmoved – and sometimes completely unaware.

A much smaller number of techniques become truly relevant for analyzing and characterizing products and processes. Consequently, these techniques are adopted and perfected by the (major) instrument manufacturers, with a concomitant proliferation into industry. These elite techniques become part of what is commonly referred to as analytical chemistry. Analytical chemistry, therefore, can be seen as the 'Champions League' of measurement science.

A technique cannot enter the Champions League unless the team is complete. The fundamental principles must be sound and well established. Techniques that rely too much on art – that is to say, the skill of the analyst – without sufficient foundation in science lead to unreliable results, frustration and, ultimately, rejection. The (academic) scientists working on the principles of analytical techniques are not necessarily analytical chemists. They may be physicists, biologists, engineers, and so on. However, based on the nature of their activities, they could all be classified as Analytical Scientists.

An analytical technique in the Champions League must have important applications that are relevant for industry or society, for example, hospitals or food-safety institutes. However, the benefits of the technique must also be recognizable for instrument manufacturers (who form the third pillar of the team) to attract their significant and sustained interest. The true Champions League techniques spiral upwards through a virtuous cycle: increasingly better and affordable instrumentation becomes available, an increasing number of relevant applications are addressed, and the underlying science is increasingly understood.

Meetings on analytical chemistry are showcases of the Champions League, provided they have adequate participation from fundamental scientists, application specialists and instrumentation experts. If the balance is wrong (for example, because too few delegates from industry find it worth the effort, time and money to visit), analytical technology can develop slowly or even in the wrong direction.

The Seventh International Symposium on the Separation and Characterization of Natural and Synthetic Macromolecules (SCM-7) is strongly rooted in industry. The title of the conference reflects an application-driven – or industrial – perspective. The reality is that there is still a great need for better methods

for the analysis and characterization of 'large molecules,' and there is a great deal of potential synergy between groups of scientists applying related sets of techniques for divergent purposes. SCM-7 pulls together many speakers from industry and uses an active industrial advisory board to help the community focus on the most relevant applications. And for the first time, SCM-7 is accompanied by a (partly overlapping) two-day meeting – the International Scientific COAST meeting (I SCM). I SCM will explicitly focus on academic-industrial collaborations, with a view to addressing COAST's overarching goal of facilitating more comprehensive analytical science and technology.

Whichever team you support, a quick trip to Amsterdam offers a prime opportunity to experience what the analytical Champions League is really like.

*The Seventh International Symposium on the Separation and Characterization of Natural and Synthetic Macromolecules (SCM-7), Amsterdam, The Netherlands, January 28–30, 2015. www.scm-7.nl*
*The International Scientific COAST meeting (I SCM), Rhone Congress Centre, Amsterdam, The Netherlands, January 27–28, 2015. www.ti-coast.com*

# CSI: Dust DNA

**Will the future see crime scene investigators collecting nasal swabs or rinses from deceased victims to identify the assailant? In a word: yes.**

*By Bob Blackledge, Forensic Chemist, El Cajon, CA, USA.*

I remember reading an article called "CSI: Breathprint" by Terence Riley and Joachim Pleil earlier this year. They asked the question, "Will the future see crime scene investigators collecting breath samples from potential perpetrators to identify them?" Their answer was "no", and I would have to agree. However, Riley and Pleil were focused on the lung. What if instead we focus on the nasal passages? And instead of focusing on the "breathprint" (total lung contents at some snapshot in time), we focus on just one type of particle?

In her book, "The Secret Life of Dust: From the Cosmos to the Kitchen Counter," Hannah Holmes states, "At least a billion and a half pieces of dust enter your nose and mouth every day, if you breathe exceptionally clean air. Most people inhale many times that number." Like Pig-Pen (the character in the Peanuts comic strip), we all live within our own personal cloud. Each person sheds around 50 million skin flakes per day, and inhale back into their own body around 700,000 of them. In 1998, Miguel Lorente and colleagues looked at dandruff as a potential source of forensic DNA. They showed that dandruff contained some nucleated cells, and that the DNA could be extracted, multiplied by the PCR reaction, and typed. Although interesting, nothing has been done with this information – after all, at a typical crime scene how could you collect either only dandruff particles from the assailant, or collect everything and then somehow separate out only the dandruff particles from a suspect? It appeared to be a dead end.

People close to each other have overlapping personal clouds. If during the course of a struggle that results in the death of an individual and involves more than just momentary contact between the victim and the assailant, it's logical to assume that the last few breaths taken by the victim will contain a comparatively high percentage of skin particles originating from the assailant, especially as the dynamic process of air exchange stops at death. Could the nasal passages of the deceased be a relatively rich source of DNA information, the assailant's 'dust' having been trapped by cilia and mucous? And if these skin particles could be recovered via nasal swabs or lavage for example, could enough DNA be recovered, amplified, and typed?

Certainly, the collected sample would still be highly complex, but we could expect that the most abundant source of DNA would be from the victim, followed by skin particles from the assailant. As Na Hu and colleagues note in their review of developments in forensic interpretation of mixed DNA samples, "Over the last decade, the accuracy and repeatability of mixed DNA analyses available to conventional forensic laboratories has greatly advanced in terms of laboratory technology, mathematical models and biostatistical software, generating more accurate, rapid and readily available data for legal proceedings and criminal cases," but they also recognize many challenges, including stutter, contamination and artifacts of allelic drop-out (4). We're not quite there just yet.

A more manual alternative method could see individual skin flakes being filtered out of a nasal swab solution and selected for separate DNA typing. You may think that such an approach seems completely impractical, and yet it's already been tested with adhesive tapings from skin and clothing (5).

How long will it take for the necessary technology to advance to the point where complex DNA analysis becomes

cheap, easy and infallible? I can't say, but I guarantee it will happen far sooner than some 'experts' would predict. Do you recall how long experts said it would take to sequence the entire human genome?

*References*

1. *T. Riley and J. Pleil, "CSI: Breathprint", The Analytical Scientist, tas.txp.to/1214/breathprint*
2. *H. Holmes, "The Secret Life of Dust: From the Cosmos to the Kitchen Counter" (John Wiley & Sons, 2001).*
3. *Miguel Lorente et al., "Dandruff as a Potential Source of DNA in Forensic Casework", J. Foren sic Sci. 43(4), 901–902 (1998).*
4. *N. Hu et al., "Current Developments in Forensic Interpretation of Mixed DNA Samples", Biomed. Rep. 2 (3), 309–316 (2014).*
5. *H. Schneider et al., "Hot Flakes in Cold Cases", Int. J. Legal Med. 125, 543–548 (2011),*

# Solvent Games in 2D-LC

## How can we avoid band broadening and distortion of high performance liquid chromatographic peaks in the second dimension?

*By Paul G Stevenson, Associate Research Fellow at Deakin University, Australia.*

It is well known that pouring cold water into a hot glass causes a thermal contraction that will form a crack, if not shatter the vessel. The temperature of the water is not to blame, rather it is the change in temperature happening in the glass. If warm water is added to the glass it will survive to live another day.

Similarly, an easy way to lose efficiency from a HPLC separation is to pay little attention to sample preparation, in particular the injection solvent in which the analyte is dissolved. Indeed, if the solvent within the sample vial is only a little stronger than that of the mobile phase (at the initial composition for a gradient separation), peak broadening will start to erode the baseline between closely resolved peaks. If the solvent strength miss-match is even higher, significant band distortion can occur.

In a two dimensional (2D)-HPLC separation, small aliquots of a chromatographic separation (the first dimension) are sequentially transferred to a different separation environment (the second dimension) to enhance the overall capacity to resolve chemical compounds and enhance the resolution of structurally similar molecules. However, trying to complete a 2D-HPLC separation using a gradient in the first dimension is inherently challenging because the concentration of the aliquot transferred between dimensions (i.e., the second dimension injection solvent) is continually increasing. The solvent strength miss-match can deform the peak and remove any ability to extract meaningful data from a separation.

We recently incorporated a third pump into the 2D instrumental configuration to address the problem (1). The aim was to introduce a "counter gradient" to offset the changing mobile phase produced by the first dimension. I found that the second dimension injection solvent could be artificially manipulated so that a consistent composition was sent to the second dimension. The counter gradient has significance in reversed phase (RP) × RP, but also HILIC × RP separations, where the mobile phases are at the opposite ends of the solvent strength spectrum. We also created a free-to-use interactive application that calculates the required counter method for a single step gradient to produce a required transfer solvent strength.

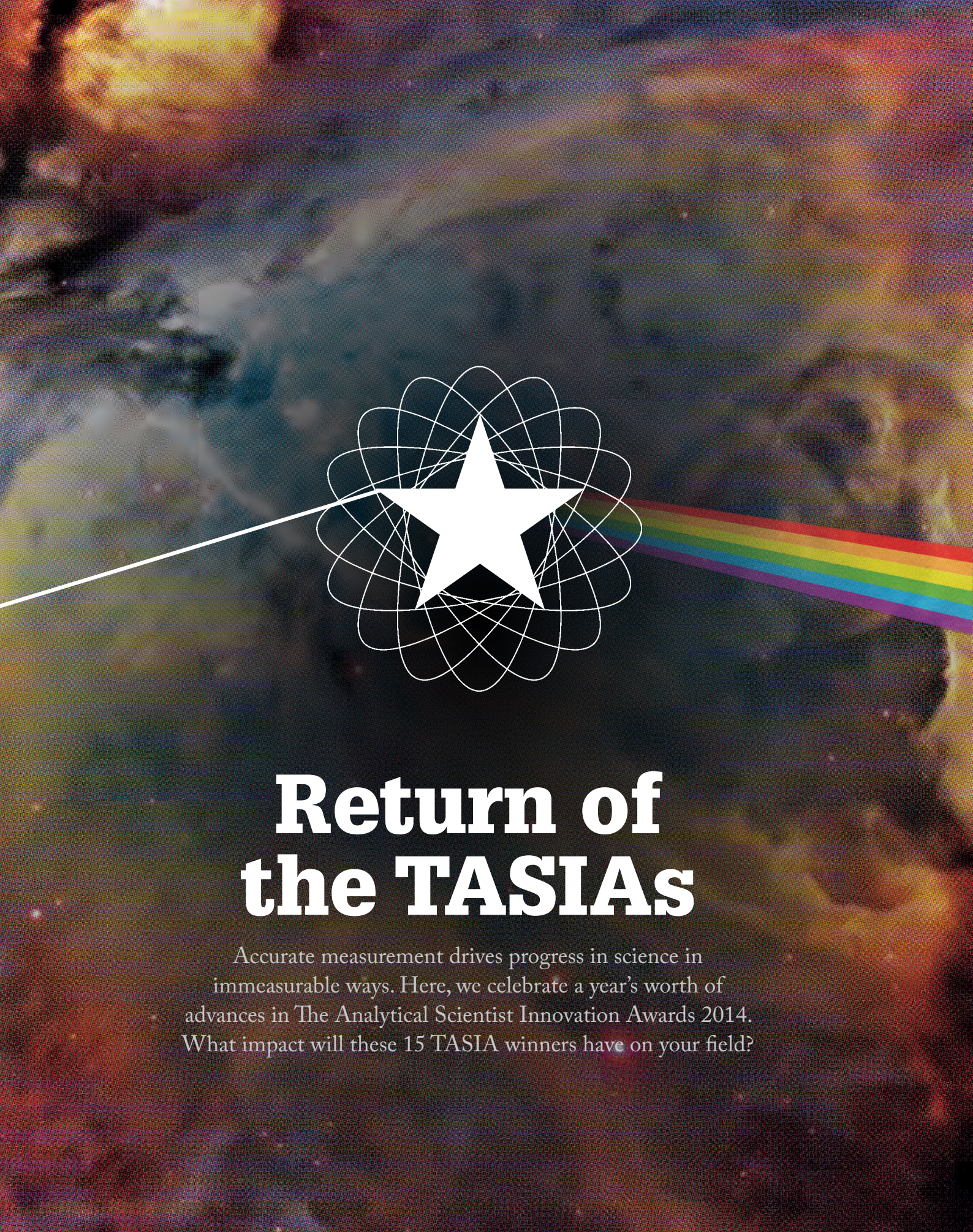
You may be thinking that it would be useful for me to describe the metric that I used to assess the improvement; however, the state of peak shape was so terrible without the counter gradient that a suitable value could not be measured. I can say that the shape of chromatographic peaks in the second dimension were enhanced markedly with the inclusion of a counter gradient, restoring them to a typical Gaussian profile, which allowed for a quantitative 2D-HPLC determination of antioxidant limit of detection (LOD) for the first time.

Unfortunately, the counter gradient approach has its limitations. We found that the mobile phase concentration after the counter gradient was limited to approximately 20 percent solvent component. Below that threshold, several experimental design issues arose, including very slow first dimension times; counter gradient flow rates above instrument max; analytical scale sample loops of insufficient size; and first dimension dilution leading to limited LOD.

We have not used the counter gradient method with reverse and normal phases of chromatography, but I anticipate that the inclusion of a solvent that is miscible in both of these mobile phase environments will improve their compatibility. If successful, it will dramatically enhance the time and space efficiency of 2D-HPLC analyses.

*Reference*

1. *P. G. Stevenson et al., "Improving Peak Shapes with Counter Gradients in Two-dimensional High Performance Liquid Chromatography", J. Chromatogr. A, 1337, 147–54 (2014).*



# Return of the TASIAs

Accurate measurement drives progress in science in immeasurable ways. Here, we celebrate a year's worth of advances in The Analytical Scientist Innovation Awards 2014. What impact will these 15 TASIA winners have on your field?

# 15

## A-Line Quick Connect Fitting

*HPLC finger-tight and reusable fitting stable to 1300 bar*

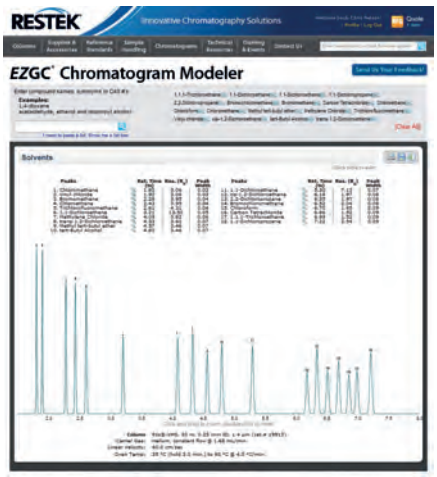
**Produced by:** Agilent Technologies
**Potential impact:** Poor LC connections are a common problem for customers, as traditional fittings require some skill and experience to make successfully. This easy-to-use fitting ensures that every user, regardless of skill level, can get a leak-free connection, so there is less troubleshooting and rework. Moreover, the fact that the connection can be repeatedly remade means that columns are easy to change, further increasing flexibility and productivity in the lab.
**Detail:** Our new fitting is the product of an Agilent R&D initiative to leverage its insights into how liquid chromatography works to address key challenges in the chromatographic workflow, ensuring that customers continually get maximum productivity from their LC systems. These are the only true finger-tight UHPLC fittings that are stable to 1300 bar and they can be used over and over again without loss of performance. The innovative spring-loaded design pushes the capillary tubing against the receiving port for zero dead volume connections with all types of HPLC and UHPLC columns. The rugged design ensures its durability.
**The judges say:** "Handy!"


# 14

## Vanquish UHPLC

*Instrument and columns uniquely designed together to maximize the performance advantages of higher pressures*

**Produced by:** Thermo Fisher Scientific (www.thermoscientific.com)
**Potential impact:** Isn't UHPLC a mature category where improvements are incremental? Actually, it has been evolutionary; when one manufacturer increases the pressure/flow envelope, another company raises it a little higher – and the columns have to evolve to survive the higher pressures. We decided to make a big bet by designing a new platform and columns at the same time, to fully exploit the performance advantages of the industry's highest pressure rating. Scientists have been asking for more performance and throughput with more complex samples, and the rationale was that this new UHPLC platform could have a major impact across a broad segment of the scientific community.
**Detail:** The Thermo Scientific Vanquish UHPLC was designed from the ground up to provide new levels of performance, productivity and usability. It was designed around our new Accucore Vanquish UHPLC columns, featuring 1.5 µm solid core particles to help customers take full advantage of the system's 1500 bar (22,000 psi) maximum pressure and flow rate up to 5ml/min. Ultra-short diffusion path lengths contribute to highly-efficient separations. It features both direct column heating and forced air heating, further enhancing separation efficiency, selectivity and retention time reproducibility. Vanquish UHPLC also combines the ruggedness of an integrated system with the flexibility and serviceability of a modular system.
**The Judges say:** "Good to redesign from time to time. Degree of automation in line with very wide applicability, but some versatility also implemented."




# 13

## EZGC Online Method Development Tool Suite

*Model chromatograms, get column recommendations, translate methods, and calculate flows for free online*

**Produced by:** Restek (www.restek.com)
**Potential impact:** Whether you are developing a new GC method or looking to reliably optimize an application, the EZGC method development tool suite will save you hours of calculations, guesswork, and trial-and-error – without injecting a single sample or even installing a column.

On a PC or Mac, desktop or tablet, EZGC method development tools make it easy to make the most of our chromatographic expertise and tailor a perfect solution for your method development challenges.
**Detail:** The EZGC chromatogram modeler helps you develop GC methods from scratch, including the column and conditions. Simply enter your analyte list to generate a customized, interactive model chromatogram that provides a specific phase, column dimension, and conditions. Zoom in, view chemical structures, and even overlay mass spectra of co-eluting compounds.

The EZGC method translator and flow calculator makes it simple to switch carrier gases, change column dimensions or detectors, or optimize a method for speed or efficiency. Just enter your current method specifications and you will receive a full set of calculated method conditions that will provide similar chromatography. Results include oven program and run time as well as average velocity, flow rate, splitless valve time, and other control parameters – all in an easy-to-use, single-screen interface with seamless transfer between tools.

These free, web-based applications are easily accessible online and Windows users can also download the EZGC method translator and flow calculator for offline use.
**The judges say:** "This tool can greatly reduce the time to (first) results, allowing labs to answer urgent questions faster."


# 12

## Delta Ray Isotope Ratio Infrared Spectrometer (IRIS)

*Solution for the continuous measurement of isotope ratio and concentration of $CO_2$*

**Produced by:** Thermo Fisher Scientific (www.thermoscientific.com)
**Potential impact:** Delta Ray can give climate scientists a deeper understanding of climate change events. It is able to give continuous data at the site of interest, which is dramatically reducing the workload of scientists and also significantly increasing the quality and accuracy of their results.
**Detail:** Delta Ray is a small box that is able to accurately track changes in concentration and source of $CO_2$ plumes. It is having a large impact on the fields of fracking, volcano eruption prediction, greenhouse gas monitoring and carbon storage and sequestration.
**The judges say:** "Although movable (but not yet portable) it takes the lab to the sample. Further steps in sensitivity and miniaturization will unlock this technology for a much wider application area."


# 11

## 1290 Infinity II Multiple Heart-Cutting 2D-LC Solution

*Fully automated 2D-LC system with ability to run long 2D gradients of heart-cuts*

**Produced by:** Agilent Technologies (www.agilent.com)
**Potential impact:** Analytical scientists often question whether they have achieved the full separation of their samples, even if chromatographic peaks look pure. While Heart-Cutting 2D-LC helps to answer this question for one or two peaks, comprehensive 2D-LC gives an overview of the whole chromatogram but has very short 2D gradients. Multiple heart-cutting 2D-LC allows higher resolution for several heart-cuts.
**Detail:** The 1290 Infinity Multiple Heart-Cutting 2D-LC Solution enables users to run longer gradients in the second dimension to increase performance without the risk of losing a peak from the first dimension. Newly designed ready-to-go valves, easy-to-use software, and new data analysis functions make 2D-LC easier than before. The Multiple Heart-Cut Valves all have sample loops installed and can be tested for an installation in 10 seconds. A straightforward 2D-LC method setup easily guides users through all important method parameters and a reference chromatogram allows the user to preview the areas of heart-cuts for the second dimension. Furthermore, the new Heart-Cut Viewer enables fast and easy analysis of multiple heart-cutting 2D-LC data. Changing between 1D-LC and 2D-LC modes can be performed without manual interaction.
**The judges say:** "Good to see that relatively complex/challenging analytical flow technology can be automated in a robust way."


# 10

## Progeny Analyzer

*Handheld analyzer for raw material identification and chemical detection*

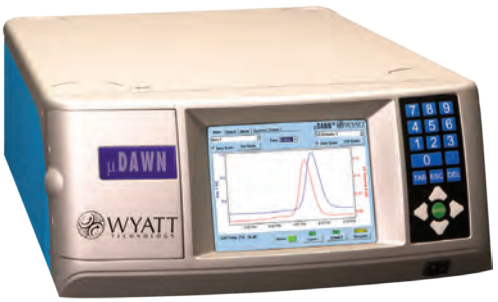
**Produced by:** Rigaku Raman Technologies (www.rigakuraman.com)
**Potential impact:** For pharmaceutical manufacturers, Progeny validates the quality of their incoming raw materials and final products, therefore ensuring that standards and specifications related to product safety and efficacy are met. In addition, Progeny provides emergency response teams with the power to immediately identify suspicious materials and quickly determine threat severity to provide the most appropriate response.
**Detail:** As the first fully sealed 1064nm handheld Raman analyzer, Progeny's ergonomic design and sleek shape allows for easy, single-hand use. Its intuitive, smartphone-inspired software can be used for simple development of new applications, shortening the learning curve. For error-free data entry tracking, Progeny provides 21 CFR Part 11 compliant digital signature capabilities and an integrated camera for sample documentation and barcode readings. Its aluminum housing has an IP-68 protection rating and has been MIL-STD-810G tested, minimizing cross-contamination and ensuring durability. Progeny's use of a 1064nm high-power excitation laser minimizes common fluorescence interferences, and in turn broadens the range of materials that can be measured, such as colored substances, or through thick, colored packaging. In addition, Progeny offers an industry exclusive wavelets-based search algorithm, which speeds up the library search process and ensures confidence in sample identification.
**The judges say:** "Brings the lab to the sample and increases usability with innovative features."

# 9

## OneOmics Project

*Integration of proteomics and genomics data in BaseSpace, a cloud-computing omics environment*

**Produced by:** AB SCIEX (www.absciex.com) and Illumina (www.illumina.com)
**Potential impact:** The collaboration between AB SCIEX and Illumina addresses a bottleneck in biomedical research by helping to securely store, retrieve, and manage large-scale complex data sets, and visualize them in a biological context. The new tools allow researchers to make predictable, actionable, and testable models of disease more quickly and efficiently, which will aid research into diseases such as cancer, diabetes, Alzheimer's, and heart disease. It will also allow these large data sets to be shared globally, making informatics accessible to anyone searching for a truly interdisciplinary systems level understanding of biology.
**Detail:** SWATH Proteomics technology solves the 'missing data problem' that has plagued proteomics in recent years, and makes the reproducible quantitation of thousands of proteins in hundreds of samples possible for the first time. With this capability, it is now simpler to integrate proteomics with next-generation sequencing (NGS) genomics and transcriptomics. To enable this, the SWATH Proteomics Toolkit suite of apps is now available in BaseSpace apps, Illumina's applications store and cloud-based informatics community where genomics data can be routinely stored, processed and shared. SWATH Proteomics data can be processed 25 times faster, making the integration of genomics and proteomics analysis more accessible to the wider community, and allowing new bioinformatics algorithms to be adopted more readily, accelerating multi-omics research. The SWATH Proteomics Toolkit includes the Protein Expression Extractor, Assembler, Browser and Analytics apps for processing of raw mass spectrometry data, protein fold-change analysis, and data quality review. These apps make it easier for scientists to extract biological insight from their data.
**The judges say:** "Good to see acknowledgement of the need to take this data-combination approach beyond the academic level."




# 8

## µDAWN

*First light scattering detector for UHPLC*

**Produced by:** Wyatt Technologies (www.wyatt.com)
**Potential impact:** The transition from standard high performance liquid chromatography/gel permeation chromatography (HPLC/GPC) analysis of macromolecules to UHPLC is in full swing, providing reduced solvent consumption, faster separations and improved resolution, all culminating in a vast improvement to productivity and performance for LC applications. Prior to the advent of the µDAWN, users of UHPLC size exclusion chromatography could not enjoy the benefits of absolute molar mass determination in solution. Consequently, many important applications were forced to continue using standard HPLC/GPC and did not enjoy the productivity and performance increases. Scientists pursuing those applications may now gain those advantages by implementing micro size-exclusion chromatography-multi-angle static light scattering (µSEC-MALS).
**Detail:** The µDAWN is the first multi-angle light scattering (MALS) detector that can be coupled with any UHPLC system to determine the molecular weights and sizes of synthetic and natural polymers, peptides, proteins or other biomacromolecules entirely in solution, directly without resorting to SEC/GPC column calibration or reference standards.

In combination with a UHPLC refractive index (RI) detector, the µDAWN delivers all the advantages of standard SEC-MALS analysis including identification of fragments and aggregates, polymer conformation, and – in conjunction with a UHPLC UV detector – molecular weights for PEGylated proteins, surfactant-bound membrane proteins, co-polymers and similar conjugated molecules.

By reducing the conventional light scattering flow cell volume from 63µl to lower than 10µl, a µDAWN/UT-rEX system can accurately analyze the molar mass and size of UHPLC peaks without loss of resolution.
**The judges say:** "Going to smaller flow cells for MALS is just what was needed to further polymer characterization."

# 7

## Nexera-e

*Analysis and identification of unknown compounds in complex matrices by exponential increase of peak resolution and peak capacity*

**Produced by:** Shimadzu (www.shimadzu.com)
**Potential impact:** The Nexera-e comprehensive 2D-LC system achieves high peak capacity by fractionating the first-dimensional eluent and successively injecting the fractions online to the second-dimensional separation system with the dual-loop alternate switching design. This is beneficial in a wide range of research fields, for example, the analysis of pharmaceutical impurities, the analysis of proteolytic digests, food and natural extracts, petroleum components, latex and polymer additives, and residual pesticides.
**Detail:** The "e" means exponential chromatography, exponential increase of peak resolution and peak capacity using the comprehensive LC×LC technology. By combining two orthogonal separation modes (for example, normal phase and reversed phase), the system can separate complex mixtures, such as structural analogues in food and natural extracts, in one analysis. With a conventional 1D-LC system, separations of mixtures containing a vast amount of substances of different chemical classes, such as polyphenols, carotenoids, flavonoids and lipids, are almost impossible to achieve. One injection and sample preparation instead of multiple approaches underline the system's efficiency.
**The judges say:** "Allows spatially resolved analysis using two complementary high resolution techniques. It is no longer just about what is in a sample, but also about where the molecules are, what are their neighbours, etc."

# 6

## BARDS (Broadband Acoustic Resonance Dissolution Spectroscopy)

*Universal comparator to differentiate powders, polymorphs, blends and more*

**Produced by:** BARDS Research Centre, University College Cork (www.bards.ie)
**Potential impact:** BARDS is a new platform technology with broad applications in food and pharma, from R&D to at-line monitoring. It is fast, small, economic and simple to operate. The BARDS team received a Pfizer Award for 'Innovation through teamwork'. The new spectrometer should create a paradigm shift in powder analysis.
**Detail:** We've developed a new acoustic based spectrometer, which detects changes in the compressibility of solvents during the dissolution of analytes. These changes in compressibility are highly reproducible under standardized conditions. This shows there are highly ordered processes occurring during dissolution, which were previously regarded as random and chaotic. The dissolution vessel is induced to resonate using a magnetic stir bar. These resonances change and result in signature time/frequency profiles for a particular analyte. The phenomenon is due to entrained gases in the powder/tablet along with a reduction in the solubility of gases already in solution leading to outgassing in solution.
**The judges say:** "Novel approach, providing relevant information to a large market."

# 5

## VGA-100 Gas Chromatography Detector

*Short wavelength spectroscopic gas chromatography detector*

**Produced by:** VUV Analytics (www.vuvanalytics.com)
**Potential impact:** The VGA-100 is a universal mass sensitive detector that provides excellent sensitivity and selectivity of gas phase molecules. It extends the Beer-Lambert Law into gas phase analysis, providing a very easy-to-use and easy-to-understand technique for the detection and identification of gas phase molecules. The unique molecular absorption cross sections allow for unambiguous identification of compounds, including the discrimination of most isomers. These unique absorption responses and well understood principles simplify the deconvolution of co-eluting analytes and provide a first principle technique that can greatly decrease the need for instrument calibrations.
**Detail:** The VGA-100 is the first new gas chromatography detector technology in approximately 30 years. The instrument is the first commercial instrument to make the vacuum ultraviolet (VUV) regime (120nm to 240nm) available to the general scientific community. The technology extends the very well understood principles of absorption spectroscopy into a region never before utilized. Prior gas phase studies at this energy range have been restricted to synchrotron facilities because of environmental hurdles of working in the VUV. Everything absorbs in the VUV, thus extremely bright sources have been required to overcome these interference difficulties. The instrument provides rapid acquisitions, up to 100Hz, of this full spectral range, which results in unique gas phase absorption spectra that are hundreds of times stronger than in the IR and enable excellent qualitative and quantitative analysis.
**The judges say:** "Nicely complements mass spectrometry where it is weakest: in the identification of isomeric structures."


*2011*

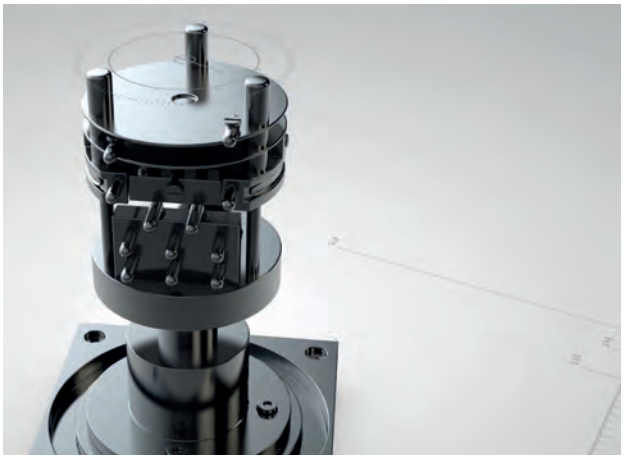
*The first TOYOPEARL mixed-mode biopurification resin, TOYOPEARL MX-Trp-650M, was introduced. This multimodal cation exchanger with unique selectivity and high recovery provides high protein binding capacities and tolerates high conductivity feedstocks*

*2013*

*New solutions for antibody purification and analysis: The new TOYOPEARL AF rProtein A HC media sets a new benchmark for binding capacity in antibody purification. This rigid, alkaline resistant protein A affinity resin offers the largest binding capacity for IgG of all caustic stable protein A media. TSKgel SuperSW MAB columns expand the TSKgel SW (U)HPLC column family by three new (U)HPLC columns, tailored to different aspects of antibody analysis.*

*2014*

*Tosoh Bioscience GmbH celebrates its 25th birthday and prepares to move to a new office. After 25 successful years in Stuttgart, Tosoh Bioscience will centralize offices, presentation and laboratory facilities and the German Diagnostics Business Unit in the Rhine-Main area from January 2015.*



# 4

## Select-eV

*Variable-energy ion-source technology for GC-MS*

**Produced by:** Markes International (www.markes.com)
**Potential impact:** Select-eV allows both standard (70 eV) and soft ionization, so alternative soft ionization techniques, with their associated inconveniences of source exchange and use of reagent gases, can be completely avoided. In addition, at lower energies with Select-eV, the molecular ion is enhanced but structurally significant fragments are maintained. These factors make Select-eV a convenient tool for confirming compound identity, or distinguishing between compounds with spectra that are very similar at 70 eV. The overall impact of these advances is increased ease of use, reduced down-time and enhanced flexibility, at the same time as greater confidence in analyte identification.
**Detail:** Select-eV breaks new ground by allowing electron ionization (EI) energies to be reduced on a sliding scale from 70 eV to 10 eV, without impacting sensitivity, simply by changing a parameter in the software method. This allows the production of reference-quality EI mass spectra with conventional full-fragmentation patterns, and repeatable 'soft-ionization' spectra exhibiting reduced fragmentation and an enhanced molecular ion. This is significant because previous attempts to develop soft EI have suffered from dramatic sensitivity losses, making them all but unusable. In contrast, the innovative design of the Select-eV ion source allows sensitivity to be maintained or even enhanced.
**The judges say:** "Significantly improves lab efficiency by removing the obstacle of having to switch between EI and CI."

# 3

## ionKey/MS System

*Robust, plug-and-play LC-MS platform employing microfluidics to get exceptional sensitivity out of mass spectrometry*

**Produced by:** Waters (www.waters.com)
**Potential impact:** Compared to 2.1 mm chromatography, the ionKey/MS System has been shown to improve chromatographic sensitivity by up to 40 times on sample volumes in the 1- 25 µl range. Simply put, analysts can use gains in sensitivity to uncover information about the smallest concentrations of sample analytes on ever-smaller sample volumes, particularly important when working with pediatric samples or with laboratory mice. Savings come in the form of solvent reduction (90% over 2.1 mm chromatography), fewer laboratory animals sacrificed, and a reduced number of reanalyses.

We expect the ionKey/MS System to have a large impact on reducing time to market for life saving therapeutics and accelerating decision making.
**Detail:** The ionKey/MS System gives every analytical scientist, experienced or not, ready access to an extremely sensitive system by completely removing the complexity associated with using chromatography at this scale. Its performance in terms of robustness and reproducibility equals that of UPLC/UHPLC on 2.1 mm ID columns. Scientists praise the plug and play nature of the ionKey/MS System. They no longer have to contend with delicate fittings and brittle, fused silica capillary columns or concern themselves with extra column dispersion and the inevitable variability and band broadening that comes with it.
The iKey is about the size of a smart phone and contains the separation channel packed with sub 2 µm particles, electronics, ESI interface, heater and eCord Intelligent Chip Technology. It is designed to perform a thousand or more UPLC-quality separations, reproducibly and reliably without a degradation in performance.
**The judges say:** "Micro LC for the masses." "Making instruments smaller and allowing micro analysis using a 'modular approach' is a philosophy that deserves appreciation."


# 2

## RISE Microscopy

*Novel correlative microscopy technique, combining confocal Raman Imaging and Scanning Electron (RISE) Microscopy within one integrated system*

**Produced by:** WITec (www.witec.de)
**Potential impact:** Correlative Raman and SEM imaging accelerates the research workflow significantly as it reduces the time-consuming sample transfer between different systems. The correlative nature can provide new answers and findings for challenging material characterization problems in pharmaceutical, geo, nano-carbon or semiconductor research to name just a few of the potential fields of application.

**Detail:** The unique combination provides clear advantages for the microscope user with regard to comprehensive sample characterization: electron microscopy is an excellent technique for visualizing the sample surface structures in the nanometer range; confocal Raman imaging is an established spectroscopic method used for the detection of the chemical and molecular components of a sample. It can also generate 2D- and 3D-images and depth profiles to visualize the distribution of the molecular compounds within a sample. The RISE Microscope enables the acquisition of SEM and Raman images from the same sample area and the correlation of ultra-structural and chemical information with one microscope system.
**The judges say:** "Allows molecules to be studied in their 'context'".
"A high-tech tool for materials research."


# 1

## iMScope TRIO

*Optical microscope meets mass spectrometer in a unique tool*

**Produced by:** Shimadzu (www.shimadzu.com)
**Potential impact:** The iMScope TRIO acquires images from an optical microscope and MS images from AP-MALDI, featuring the world's highest spatial resolution of 5μm or less. As the only integrated system, it expands the potential research opportunities in a wide variety of fields, including pharmacokinetics analyses (distribution of drugs or their metabolites), toxicity testing, and monitoring the distribution of active ingredients in the food industry. High-speed analysis (6 pixels/sec) shortens experiment time dramatically. Not only limited to imaging, it is also capable of analyzing samples extracted and separated from tissues via connection with liquid chromatography.
**Detail:** Combining an optical microscope with a mass spectrometer, the iMScope TRIO is a unique instrument tailor-made for mass spectrometry imaging. Providing a revolutionary technology, it can be applied to cutting-edge R&D and identifies what users see at the molecular level by superimposing high-resolution morphological images with $MS^n$ images, which identifies and visualizes the distribution of specific molecules.

With the imaging MS solution software designed specifically for iMScope TRIO, optical and $MS^n$ images can be acquired. Additionally, the software allows data analysis by overlay of MS and optical images and provides various statistical data analysis functions (HCA, ROI and PCA).
**The judges say:** "Combine light + MS microscopy = power"

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# Select-eV – Variable-energy electron ionisation technology for GC–MS

*Select-eV allows GC–MS users to vary electron ionisation energies from 70 to 10 eV without loss of sensitivity.*

Select-eV breaks new ground by allowing electron ionisation (EI) energies to be reduced on a sliding scale from 70 eV to 10 eV, simply by changing a parameter in the software method. Previous attempts to develop soft EI have suffered from dramatic sensitivity losses, making them all but unusable, but the innovative design of the Select-eV ion source allows sensitivity to be maintained or even enhanced.

As a result, Select-eV provides both conventional full-fragmentation 70 eV mass spectra for easy library-matching, and repeatable 'soft-ionisation' spectra exhibiting reduced fragmentation and an enhanced molecular ion. All this is achieved while avoiding the inconvenience of conventional soft-ionisation technologies, such as using reagent gases and exchanging ion sources.

These features make Select-eV a valuable and convenient tool for providing enhanced confidence in compound identity across many GC–MS applications, and especially for distinguishing between compounds with similar spectra at 70 eV.



*Markes International (www.markes.com) is a manufacturer of thermal desorption instrumentation and time-of-flight mass spectrometers for the detection of trace-level VOCs and SVOCs.*

MARKES international

Innovation Showcase

*Sponsored Section*

## IonBench MS: Dedicated Benches for Mass Spectrometry

*IonBench is sturdy, movable, and includes a ventilated sound suppressing enclosure, anti-vibration control, storage drawers, computer fixtures, and more.*

IonBench MS enclosures provide:

1. Sound suppression of 15 dBA, a 75% sound reduction.
2. Accommodation for up to three vacuum pumps.
3. Aggressive ventilation to avoid overheating.
4. Audiovisual overheat alarm.

System footprint is reduced up to 30% with additional space saving features, including integration of vacuum pumps.

Other options eliminate a computer desk. On heavy duty solid lockable casters, IonBench may be close to the wall, yet unlocked for safe, easy relocation.

A vibration free work surface is demanded by mass spectrometer manufacturers. The patented IonBench solution?

Dampening springs in the enclosure deliver a 99% reduction in vibration.

*IonBench (www.ionbench.com) is based in Joigny, France. The company was founded in 2009. Products are distributed worldwide by outstanding distributors, especially in North America.*

ionBench

## IonBench LC: Elevator Benches for HPLC/UPLC

*IonBench LC is a unique table that provides safe and easy access to the top of tall stacked HPLC/UPLC systems.*

IonBench LC provides:

1. Vertical resolution within 1 millimeter.
2. Three position memory.
3. Accommodation for any weight and size of HPLC.
4. Electrically powered raising or lowering by 30 cm.
5. Lockable casters for safe transport and positioning.
6. Stable base to eliminate tipping risk.

IonBench LC elevator benches solve the safety dilemma of stacked HPLC/UHPLC systems. These systems are so tall they are challenging to operate safely.

Constructed of chemically resistant materials, IonBench also has sturdy support columns to provide outstanding weight capacity.

Options include solvent waste container, eight power outlets, and in some models, computer fixtures.

*IonBench (www.ionbench.com) is based in Joigny, France. The company was founded in 2009. Products are distributed worldwide by outstanding distributors, especially in North America.*

ionBench

Innovation Showcase

*Sponsored Section*

# ACQUITY QDa Detector

*Separate beyond question by bringing the power of mass detection to your chromatographic analysis.*

Now there's an easy way to add mass detection information to your separations. The Waters ACQUITY QDa Detector has been designed as a synergistic element of your chromatography system. Compact, robust, and requiring few sample-specific adjustments, it seamlessly integrates with Waters' LC, UPLC®, UPC2®, and purification systems to give you more complete separation characterization.

The complimentary mass data provided by the ACQUITY QDa adds certainty to your analysis, giving you more confidence in your results. You can immediately confirm compound identities and identify co-elutions, enabling you to reduce method development times. By enhancing the analytical value of your experiments with the ACQUITY QDa Detector, you minimize the need to perform additional time consuming experiments at the cost of productivity.

The accessible and intuitive design of the ACQUITY QDa Detector gives you the additional mass data you need without the complexity of traditional mass spectrometry.

*Waters creates business advantages for laboratory-dependent organizations by delivering practical and sustainable scientific innovation to enable significant advancement in healthcare delivery, environmental management, food safety, and water quality.*

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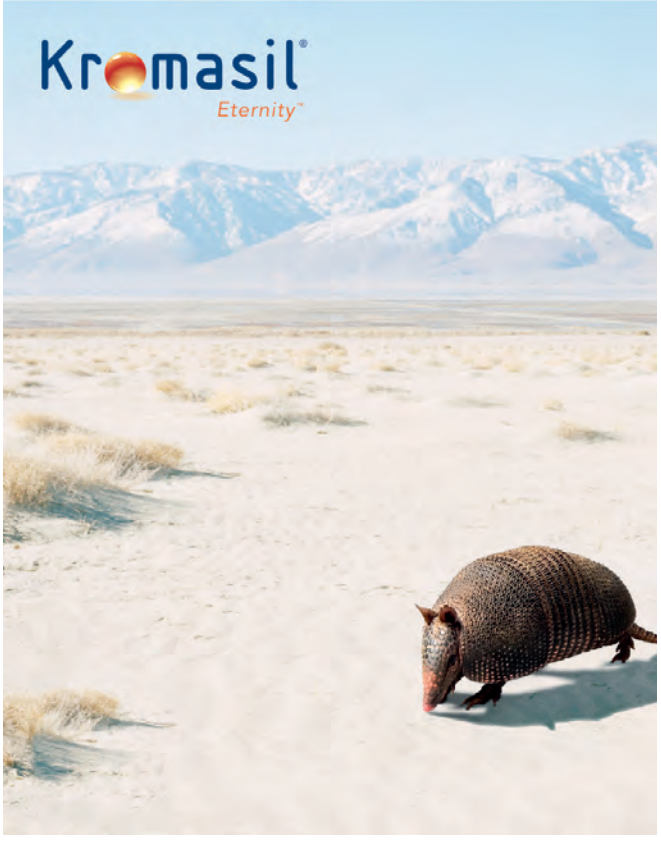
# Kromasil EternityXT, UHPLC/HPLC columns designed for extended lifetime

*Kromasil EternityXT UHPLC/HPLC columns are packed with AkzoNobel's state-of-the-art mechanically and chemically stable phases, for first-rate separations and isolations up to pH 12.*

Under harsh environments, a unique protective structure is required for survival. Kromasil EternityXT UHPLC/HPLC columns are packed with a unique organic/inorganic reinforced silica media that gives these columns an extended advantage under conditions where ordinary silica-based columns would rapidly degrade. It's the EternityXT platform that gives the stationary phases their distinctive resistance to a wider range of pH as well as tolerance to high concentrations of NaOH.

With stationary phase material in particle sizes from 1.8 to 10 µm, you have the flexibility to design and validate analytical methods at the UHPLC/HPLC scale and transfer them seamlessly through your organization to QC, process development, and production.

The EternityXT family of columns is targeted for you to develop and apply methods with confidence in the areas of pharmaceutical and biotechnology, the food and beverage sector as well as clinical and environmental markets.

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EXIT

# When Great Minds Think Alike

The M908 took the top spot in our 2013 Innovation Awards – "Revolutionary technology; will be an inspiration for new generations," said the judges. Here, four co-founders of 908 Devices describe the perfect storm that led to the creation of the world's first handheld mass spectrometer.

## Taming the Perfect Storm

*Kevin Knopp, President and CEO*

I guess it all began for me with a Masters in Electrical Engineering and a PhD in Optics from the University of Colorado. I was funded by the National Institute of Standards and Technology (NIST) and NASA, which gave me an immediate sense of purpose. It was also a lot of fun and extremely interesting. After my PhD, I moved back to Wilmington, just north of Boston in Massachusetts, and joined a fast-growing telecommunications company as employee number 50 in 1999. We grew very quickly up to 250 people and then sold to Nortel for $1.4 billion at the height of the dot-com bubble. I was thrust into many responsibilities that I wasn't trained to do. And it's fair to say I learnt a great deal riding up – and then back down – that bubble as it was bursting. As Nortel worked to stay afloat during the crash, I knew it was time to move on.

### After the bubble burst

Four of us came out of the Nortel experience and founded a company called Ahura Scientific in 2002. Ahura was a fascinating story in itself. We envisaged getting back into telecommunications as we all had optics backgrounds, but the bubble just kept imploding. Our plan was to make the next generation of something that wasn't selling in its current state. It was a pivotal moment for us all.

Fortunately, we found our way into analytical instrumentation. Though we used a lot of the same laser and optical technologies familiar to telecommunications, it was clearly a very different field – especially in terms of how to get to market.

We grew a business in field-portable Raman and FTIR systems for bulk identification of chemicals and ended up selling to Thermo Fisher Scientific in 2010. Thermo is a fantastic company and I actually enjoyed the process of acquisition and integration. It was great to finally have the financial heft of a public company behind us to keep driving along the roadmap of ideas. Thermo was very supportive but also granted us autonomy, which allowed the project to continue to grow.

### The start-up itch

I'd been with the Ahura team for about nine years and I felt that it was time to try to get out of my comfort zone again. I needed to keep my life-long learning alive.

After Thermo, I went scouting for interesting new technology. Trace detection was intriguing to me and mass spectrometry was the obvious candidate – the gold standard. It was also obvious that mass spec was a technique only used in labs with highly trained individuals. I noted that trace detection instruments were out there in airports, the military and fire departments, and so on, but none really working that well. The question of whether we could take mass spec into those application areas really piqued my curiosity.

Chris Brown (page 41) and I, along with a few others, started networking and talking with contacts with the vision of sourcing potential mass spec technology. Mike Ramsey was one of the fellows I knew in the space, and we reached out to him very early in the process to discuss our ideas. It turns out Mike thought the high-pressure mass spectrometry (HPMS) technology he had developed at the University of North Carolina (UNC) at Chapel Hill was about ripe for commercialization.

"The perfect storm" really sums it up. Mike had the technology we were looking for, and we had a good deal of commercial experience. Joining forces was only natural.

We had talked to other groups and realized that there was a lot of good stuff out there. However, Mike's HPMS technology was so clearly differentiated that it gave us the edge to create radically different solutions for our point-of-need mission: designing simple tools for end users.

### Pulling the team together

We reached out to Mike in 2011 and had things figured out by February 2012. One big advantage was that I'd worked with Mike previously on an unrelated NIH project. Our discussions centered on the status of the technology and what gaps needed to be filled. Some aspects were proven academically, but did we have the right resources to negotiate the path to product with enough agility? We came to the conclusion that we did.

I very much enjoy working with others and pulling together great people. I guess one of my skills is being able to bring together the right characters and getting them to gel together as a functional group. I think that resonated with Mike, who's a very applied professor but also very humble – and a great guy to work with.

So right out of the blocks we had highly differentiated technology and a lot of room for innovation. The big challenge? We had to ensure that we steered our ship through the perfect storm in a financially-viable direction. We've all had commercial responsibilities but originally come from technical backgrounds. Collectively, the team at 908 Devices has been mature enough to stay focused on our original mission.

Our aim is to create products that answer particular questions very close to the person who needs that answer. Traditionally, mass spectrometry operates in a core lab and users submit samples; that holds true in forensics applications or in biopharma research. To the contrary, our first product – M908 – is battery powered, handheld and rugged for its particular point-of-need application in the safety and security industry. The "M" stands for multi: multi-threat and multi-phase, incidentally.

### Staying ahead of the curve

Mass spectrometers traditionally rely on an extreme vacuum and the pumps required set limits on cost structure and reliability. Removing the constraints of that extreme vacuum requirement clearly sets us apart; however, on top of that we bring a great deal of expertise on the chemometrics front, which essentially means that we can get the best out of a cool box without shackling the user with complexity. I would say we have a great head start in a new market – but that doesn't stop us looking in the rearview mirror – or looking down the road.

The M908 is our flagship and we're very focused on serving the safety and security market. There's a great deal of opportunity in that space and, of course, we want continued success for M908. I guess to the outsider, we could be considered a "one-product company" at this early stage; however, we consider HPMS very much a platform technology. Every day, we're working towards building the platform out into other markets with new purpose-built instruments. We work closely with great collaborators and have a great group of advisors, who span everything from life sciences to the military, to ensure that we fully understand the customer and the question being asked. Right now, we're working with Schlumberger in the oil and gas discovery field, and have several other interesting applications lined up.

We recognize that in certain applied markets coupling HPMS with gas separations could be very interesting, and in the life sciences liquid-phase separations will undoubtedly expand the reach of technology. Mike was the Science Founder of Caliper Life Sciences and has an in-depth knowledge of microfluidics and separations; he continues to innovate in those areas at UNC, and we're working closely with him on that.

Rapid evolution is occurring in the clinical diagnostics space with mass spec, and we're also keeping a very close eye on that. The big instrument companies are working aggressively towards solutions; generally, they're starting with existing

lab solutions and packaging them for regulatory approval. I believe that evolution will help paint the roadmap for specific tests that our technology could serve. There's a lot of discovery work in metabolomics today – assays and diagnostics are starting to follow behind. As we transition away from needing to measure everything at diverse concentration ranges towards biomarkers that are very well defined, HPMS technology starts to look very interesting.

We've already made a lot of technological progress, but we're really only at the start of our journey. The only thing set in stone is that the future will be exciting.

## Finding the "Secret Sauce"

*Mike Ramsey, Science Founder*

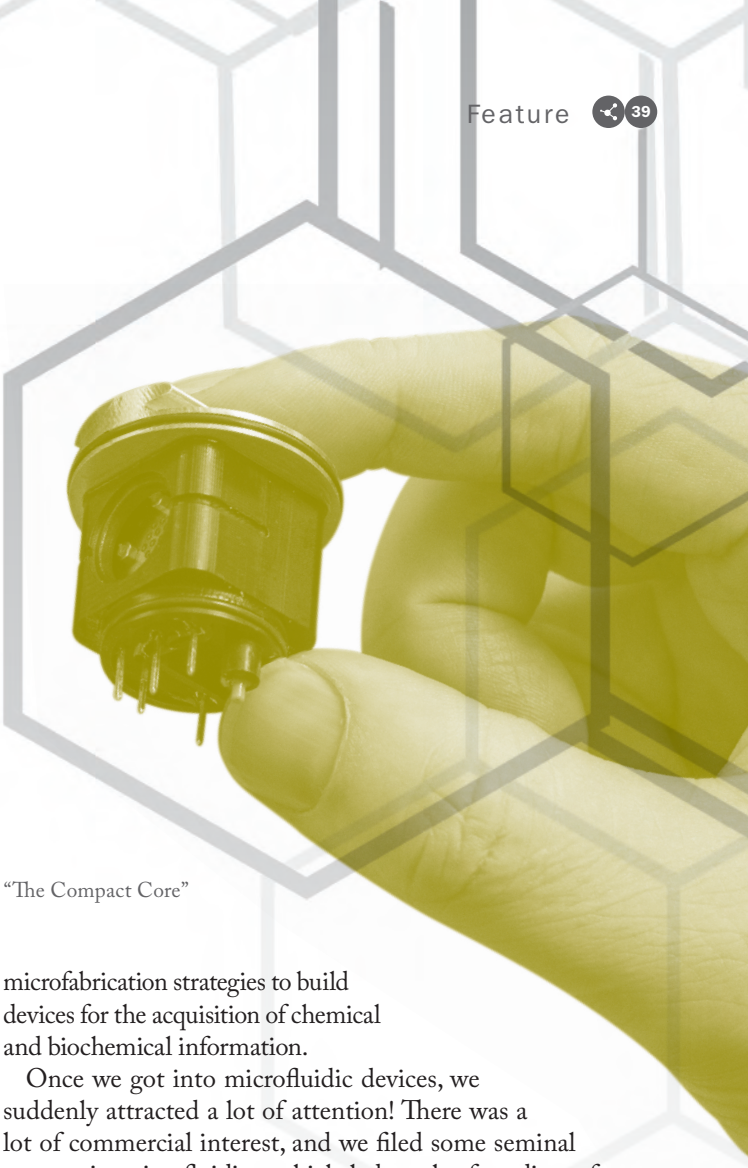
I guess you could say my career in science was an unexpected one. I grew up on a farm in Ohio and I wasn't terribly motivated from an academic point of view in the beginning. I went to a rural high school where I took a two-year course in chemistry. The teacher was good and I seemed to have an aptitude for it. Nevertheless, after high school I wasn't even sure if wanted to go to college. I decided to give it a try and started to get really motivated. In my last semester, my professor said, "Gee – someone like you really ought to be going to graduate school."

### And so... here I am!

Why science? Well, I'm naturally curious and have a good memory – mostly. I've never been one to spend hours with my nose in a book and I didn't like writing either, so that ruled out wordy subjects like History and English. I am fairly reserved, so getting up in a class to perform was not a good experience for me, which ruled out much of the arts. Sometimes the subject chooses you. Somewhat ironically, it now seems that all I do is speak at conferences and write papers.

### All things great and small

It's interesting that most of the senior team at 908 Devices share roots in optical spectroscopy. I was focused on laser spectroscopy in the early part of my career, leaving graduate school for Oakridge National Laboratory. We covered some interesting ground, though we were not very visible back then. One project that put us on the map was the microfabrication of the fluidic structures for capillary electrophoresis. That really kicked off the theme of research that I continue to this day at UNC: using microfabrication strategies to build devices for the acquisition of chemical and biochemical information.



"The Compact Core"

Once we got into microfluidic devices, we suddenly attracted a lot of attention! There was a lot of commercial interest, and we filed some seminal patents in microfluidics, which led to the founding of Caliper Technologies, later Caliper Life Sciences. Our value proposition for the early microfluidics work was the ability to perform faster, more robust measurements at lower cost, using miniaturized laboratory tools rather than engineered electrode-based sensors.

### Honey, I shrunk the ion trap

Given our early successes in microfluidics, we started appraising other analytical tools that could be miniaturized. Mass spectrometry is such a chemically information rich tool that it simply could not be ignored. Looking at the different ion traps and mass analyzers out there, it appeared that the physics scaled very nicely. So in the mid-1990s we set to work on a miniaturized mass analyzer. I wouldn't say we had a full appreciation of how to operate these devices at higher pressures back then. We had a post-doc who did some experiments at pressures over 100 millitorrs ¬– and got some pretty interesting spectra; he didn't even realize that you weren't supposed to operate an electron multiplier at such high pressures. In any case, those early experiments provided the initial spark of inspiration. We also published a theoretical paper on the resolving power

of mass spectrometry that had some big hints as to its ability to perform at much higher pressures.

Interest in small, portable mass spectrometers has been around for well over three decades. Some might find it surprising that even though my basic training is not in mass spectrometry, my team was the first to figure out that if you can't make the pumps smaller, you need to operate at higher pressures. Making that leap is a paradigm shift in mass spectrometry – I'm not sure that we as a community understand yet how powerful it is.

### Time for another start up?

I gained some experience of start-ups with Caliper and that went pretty well, so in 2003, I first set about commercializing the microscale ion trap. I was already connected with some venture capitalists, but the project never got off the ground.

Interestingly enough, Kevin and I first met during a medical diagnostics project when he was at Ahura. We had won some hefty and well-funded projects from the Department of Defense and, at that time, I had put aside thoughts of commercialization. I figured we would take the technology as far as we could with the funding we had.

In 2011, I received calls from two venture capitalist groups wanting to discuss high-pressure mass spectrometry in the same week. On one call, Kevin was helping with due diligence and that's really when our discussions began. A few of the key people Kevin had in mind had already worked together successfully at one time or another, which lubricated the whole process. Analytical people don't like unknown quantities.

### Full steam ahead

It really was the perfect storm. We'd done a decade's worth of research on the technology to make it engineering ready, which was a great starting point. But the impressive speed with which the original research and theory has been turned into a product really highlights the high quality of the team that Kevin pulled together. They are extremely talented and work very well together; we went through two years' of milestones without a single one being missed. That's incredible for a start up.

The M908 is the world's first handheld mass spectrometer. Where do we go now? Well, I think the applications for that basic technology are immense, stretching well beyond security and into the environment, and even clinical diagnostics. The miniature ion traps at UNC have been able to demonstrate sub-AMU resolution at 1 Torr of air. It was a big breakthrough for us, and the new capability opens up a lot of other possibilities.

I have a slightly different mindset than some of my academic colleagues. Analytical science is an applied field and I feel that the projects we work on should have enough societal impact that they lead to technologies that people need or want. I don't run research in my group unless I have a vision for how that could eventually match some unmet need.

I also have some deep-rooted interest in generating patents. I don't really know where that comes from, but I don't want to just publish papers. The work we do should be novel and impactful enough to lead to patents. I'm already working on my next start-ups...

## Innovating Over Hurdles

*Chris Brown, VP and CTO*

I joined 908 Devices from Apple, where I was a platform architect, leading investigations into future-generation hardware and software technologies – what that really means is that I was working on some strange and wonderful strategic technologies that may be many years down the road.

Of course, there's a back-story. In my graduate school days at Dalhousie University, I focused on applying multivariate statistical and chemometric methods, as well as artificial intelligence techniques to a range of technologies, including mass spectrometry and chromatography. We had two main goals: i) to automate technology in a way that facilitated use by a non-expert, ii) to deliver results in a way that met end user need. In many ways, those objectives have not changed much at all over the years.

After graduate school, I left academia and joined a company called InLight Solutions, which was developing clinical, in-vivo, and non-invasive biodiagnostics across a range of imaging and spectroscopic modalities. I was there for about six years in a number of leadership roles before joining Ahura Scientific in 2004, where I met Kevin. At Ahura, I put together a lot of the embedded software and algorithms that enabled simple push button systems. I saw Ahura Scientific grow from a few people to 150, at which point the wheels were nicely turning and the company had become a different beast. When Ahura was finally acquired by Thermo Fisher, I was in charge of product development and engineering.

### A bite of the Apple

I had a desire to try something new and Apple came calling with an interesting proposal for a strategic role. I wasn't too sure what I would find when I joined, but it more than met my expectations. It was really diverse work, and I like being pushed out of my comfort zone technology wise. Apple is

very focused on prototyping – "try it and show me" – and on practical applications of technology. It was fast and lean, which is how I love to work myself. It was also fascinating from an operations standpoint; watching how a company of that scale manages to transition very early-phase development into product pipeline and then into production was very insightful.

In many ways, Apple functions like a very successful small company. They are both very focused on their "user mission". And they're not dissuaded by bumps in the road on the technology side. For a company to survive, it's got to run through or around those issues.

It's fair to say I didn't expect to stay at a big company for life. I love the fast pace of start-ups too much. I like watching a company succeed and grow from scratch. Kevin and I had kept in touch, and we had been bouncing ideas back and forth for a while. Previously, we had discussed how miniature mass spectrometry was undiscovered country despite various attempts and commentary. Mike Ramsey's approach was highly differentiated and clearly amenable to an entirely different stratosphere of miniaturization, cost and reliability. It provided a light bulb moment that started more serious discussions about a new company.

There was no doubt in our mind that there was going to be a market – and that's a huge advantage for a start up. An amusing road trip with the founding team pretty much confirmed our hypothesis and we were off. This was the first time we were all together in one place and concepts soon became realities. Michael Jobin, our mechanical expert, began looking at industrial design possibilities and pondering component size requirements. Andy Bartfay, our electronics talent studied the drivers and power requirements to make this thing work. While our software guru, Steve Araiza, checked out whether we could fit all the needed processing and control into the box. And Scott Miller, our chemist and analytical expert, studied existing performance.

At that stage it was just a hope, a dream and a twinkle in the eye, but the level of enthusiasm was high.

## Core innovation

The microscale ion trap technology that Mike had done so much work on is absolutely critical to the 908 Devices' platform. But to make a mass spectrometer, you also need ionization, electronics and detection. It's great to have the core technology, but if you can't find solutions to support it, you're dead in the water.

We quickly found that to make the technology work at high pressures in air, we would need an ionizer that could survive under those conditions. Furthermore, a conventional electron multiplier won't survive at high pressures either, so we had to focus heavily on a detector that could give the required sensitivity in a small footprint and in an unusual environment. Innovating our way out of those challenges gave us the "compact core".

A mass spectrometer also requires extremely complex drive electronics. Driving RF voltages of 1000V into these tiny traps at very low power is another trick in itself. In the beginning, we had an RF supply and inductor that was about the size of a shoebox – which is bigger than we planned the entire M908 product to be. That particular problem required some serious head scratching and a lot of sweat and tears. We ended up with something about the size of a matchbook.

*"We were able to avoid several common pitfalls before they even appeared, which not only reduced the risk but also reduced our time to market."*

Essentially, we were creating the market for a handheld mass spectrometer, so many of the components that we wanted to use simply didn't exist. We thought we might be able to at least find a pump – but at our power budget, footprint, reliability requirements and flow rate, we hit another dead end as far as external providers were concerned. It was another "Oh my Lord" moment. In that case, we didn't have any internal experience – so we found someone who did and built our own; another major hurdle overcome.

We were very fortunate to have our experience from the years at Ahura. We were able to avoid several common pitfalls before they even appeared, which not only reduced the risk but also reduced our time to market. The team already knew the constraints of working on handheld systems, and through that, they had a deep appreciation for how important the entire product was rather than being completely absorbed by their piece of the pie.

## Crafting uniqueness

When I think about the critical components in the system

that have an impact on size, weight, power and performance, it's clear that without just one of them, there would be no handheld mass spectrometer. We have an entirely new miniature vacuum pump, a unique detector and transduction system, the ionizer is novel – and that's before we get to the ion trap itself, which has also evolved significantly over the last two years.

The most exciting thing about embarking on this sort of endeavor is that journey into the unknown. The application space for HPMS is undiscovered country. Every week it seems that either one of the engineers or an application scientist learns something new and surprising about what we can achieve. We're constantly uncovering new capability, and that's very exciting from an engineering and scientific point of view.

It's also very encouraging in a business sense – it provides us with a very positive product pipeline. In the coming years, we know we will be rolling out advances that are maturing today.

## Delivering the Dream

*Chris Petty, VP Business Development and Marketing*

Unlike my colleagues, I'm somewhat new to the startup adventure. I received my PhD in chemistry from Southampton University in the UK and focused on optical technologies and spectroscopy in the chemical analysis field. It turned out to be a wonderful grounding; it was a very large and applied group, and I was working mostly on the instrumentation, surrounded by a bunch of chemists who were doing everything from polymers to explosives to analyzing diamonds. I got a real taste for how broadly technology can be deployed.

I moved to the US to start a new job with Nicolet Instruments the day after my thesis defense and started working on Raman and FTIR technology in Madison, Wisconsin. Thermo Fisher Scientific bought the company in 1992, which is where I spent the next 20 years contributing in technical roles, product management and product development. I quickly progressed into General Management where I focused on growth strategy and implementation; finding and understanding successful, innovative startups and running several of those businesses post acquisition.

### The penny drops

For most of my career I was involved with large, flexible, relatively complex instrumentation, so it was an eye-opening moment for me when we acquired NanoDrop and I had the opportunity to run that business. NanoDrop made dedicated bench top instruments that perform straightforward but very specific tasks, such as DNA and RNA quantification. They are very simple devices and don't demand that you know anything about spectroscopy – in fact, many users were not aware they were even doing spectroscopy. Most surprisingly, they were being deployed in the life science space, where all labs already have UV-Vis capability. The difference? NanoDrop applied the technology in a different way. In fact, NanoDrop had managed to do something that I had always been very interested in: it put the measurement tool directly in the hands of the person searching for the answer.

I first worked with Kevin during the Ahura Scientific acquisition – I was the integration manager at Thermo – and my experience with Ahura echoed my reaction to the NanoDrop business. But this time the person looking for the answer might not even be in a lab, so the devices needed to be robust and portable in addition to being simple.

I loved my career at Thermo Fisher Scientific. It's a great company and I credit a lot of my professional growth to the management there. Once I started working with these smaller high-growth businesses I realized I was very much attracted to the entrepreneurial spirit and the speed with which people moved. To be part of the team founding 908 Devices was too good to pass up.

On my last day at Thermo I was responsible for a team of 175 people. In contrast, on my first day at 908 Devices I was building Ikea furniture - and it's been a wonderful experience ever since!

### Checking all the boxes

It's not rocket science to suggest, "wouldn't it be great if this was smaller or more robust". I've learnt that for a successful solution there is a list of boxes that you have to check; it's not enough to be good at just one. Nowadays there are often new developments in technology with a small footprint – but if it's not also robust and simple to use, it makes portability point moot.

We have a fantastic team at 908 Devices and we are all of a similar mindset – so I was confident we could check all the boxes. However, I've been surprised at how smooth the process has been. That's not to say there haven't been challenges. As Chris notes, there were a number of technical issues that we ran into. Many we could not have expected.

Our plan was to launch our first product in two years, and that's what we did; however, to develop so much from scratch is still quite remarkable to me. What's clear is that the right resources are more important than having a lot of resources. Being able to innovate around or over bumps in the road is a testimony to the quality and experience of the team.

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## The Mindset Today

*Kevin Knopp*

This isn't just a story of a start-up or technology breakthrough. It's about making things simpler. Making things that help people do their jobs better. Finding new ways to democratize technology and put it in the hands of anyone. As you can see, the leadership team shares a great sense of passion for making a difference. And our approach is simple: understand the needs of your customers and engineer tools that meet those unmet needs.

Since opening the doors of 908 Devices two years ago a lot has transpired. Our flagship product, M908, launched in March 2014 and was well received by the US safety and security market. Our HPMS technology platform has performed well under rigorous testing and is being further developed for expansion into applications for life sciences, energy, oil & gas and beyond. We have also been honored to win several awards for innovation in technology development and product design.

The success we've seen with M908 and interest in HPMS devices has also fueled further growth of our company. The team has increased from its seven initial founders in 2012 to 30+ employees today with an expected 50 percent increase in 2015. In August 2014, we expanded our office from a 7,000 square-foot R&D space into a 16,000 square-foot full-scale production facility. This new facility allows us to create new concepts, prototypes, and manufacture products in-house, all under one roof – and will enable us to stay actively involved in every stage of development, design verification and manufacturing quality.

We are very proud of how far we've come, but realize this is just the beginning. In the years to come we will hone the capabilities of our HPMS platform even further – and we couldn't be more excited about the possibilities.

### From concept to product to platform

We've had the real benefit of working with great partners in the safety and security space right from the beginning of product development. The honest feedback received about what worked – and what didn't – allowed us to launch a well road-tested product. We've already been through various iterations, correcting design assumptions as we went. A great example is the seemingly innocuous shoulder strap, which we thought was wonderful. The first time we used it with a HazMat team, they couldn't get the strap over their 'space suits'. It's only one example, but it reflects how the details are important in creating a product that is both simple and usable.

M908 is our first product, but there are many exciting developments on the horizon. We're collaborating with other excellent partners, such as Schlumberger in the oil and gas space, where there are clear applications at the point of need. Oil and gas or environmental samples can be collected in inhospitable places, so if we can provide measurements in the field, there's a world of opportunity.

There will be other advancements in a number of different directions – though I'm not at liberty to say exactly when. We will certainly be expanding the capabilities of the M908 to include new target compounds, for example. And the concept of a wearable mass spectrometer may not be too far down the line. We are expanding quickly, and have just moved into a new facility that allows us to scale up our manufacturing capability. All in all, these are very exciting times.

Anything new brings out reservations. With our novel approach to mass spectrometry, there are those people who hear the phrase "mass spec" and are immediately frightened by it, because it conjures up visions of an inaccessible technique. On the other hand, there are those with very deep scientific knowledge of mass spectrometry who tend to react with complete disbelief. Either way, it's completely understandable. The answer to reservations on both sides has been to put the device into people's hands. We also strive to be honest about what we can do; we are not claiming to compete with laboratory-based research mass spectrometers, rather we are offering mass spectrometry in entirely new applications. Scientific Officers in the safety and security space are naturally skeptical. When asked if our two-kilogram device can be trusted for a soldier to detect a chemical weapon release, there is a lot riding on the answer. It is therefore really satisfying when we are able to assure skeptics of our product's capabilities.

The level of scrutiny we were placed under for our first product launch is priceless as we move forward. Do life science laboratories need something that has been tested to military grade standards for reliability and robustness? Perhaps not – but it's a very good place to start.

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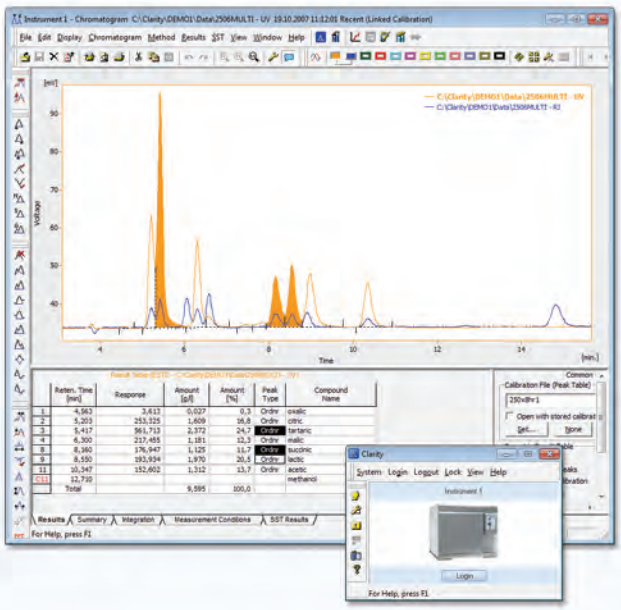

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# How to Get PR Right

How do your customers, your competitors, the press or even the public perceive your organization? Here, I offer my tips, tricks and thoughts on PR – and suggest why you might want to consider a smarter approach.

*By Marcus Lippold*

Over the last few years, I've come to a number of conclusions about the role and usefulness of public relations agencies – and PR in general – in the analytical industry. You may be the manager of a non-listed small to mid-size analytical company that doesn't have its own PR manager or department. Or you might run a mid-size to large research organization that has a lot to gain by establishing professional PR strategies. Or maybe you run a small lab or research group. The point is the same: getting your message out in front of the right people at the right time can pay dividends down the road. Perhaps you're just wondering why your excellent innovation isn't proudly showcased in the TASIAs – did you tell anyone about it?

## Thank you – or not

First, let me describe a normal working week in my office. We get about 200–300 press releases, newsletters and news alerts. We select about 100 of these for archiving, and a selection of those for Twitter and/or manual indexing for inclusion in our database and web portals. From time to time, we send a return email to the company who sent the news: "Thanks for your update, we already tweeted your news!" or "Thank you for your press release, it will soon be online at our web portal!"

Perhaps we send 10–20 of those "thank-you-mails" a week. Why do we do it?

Because we are friendly? No, we are from Northern Germany and an unfriendly bunch of stubborn people. Because it helps our business? Sure. Each email includes our improperly large red logo, which can't be overlooked and will be imprinted in the subconscious mind of the addressee forever, whether he or she likes it or not.

Because it is useful for the person who sends the news to us? Definitely. It helps the sender see immediately that the news has been received and where it has been published. No need for tracking.

Now a question. How many people respond to our thank-you-mail with a return email simply saying, "Thank you!" with their name? Well, approximately one person.

It's very likely that the one person who does respond works for a PR agency.

## Do I really need a PR agency?

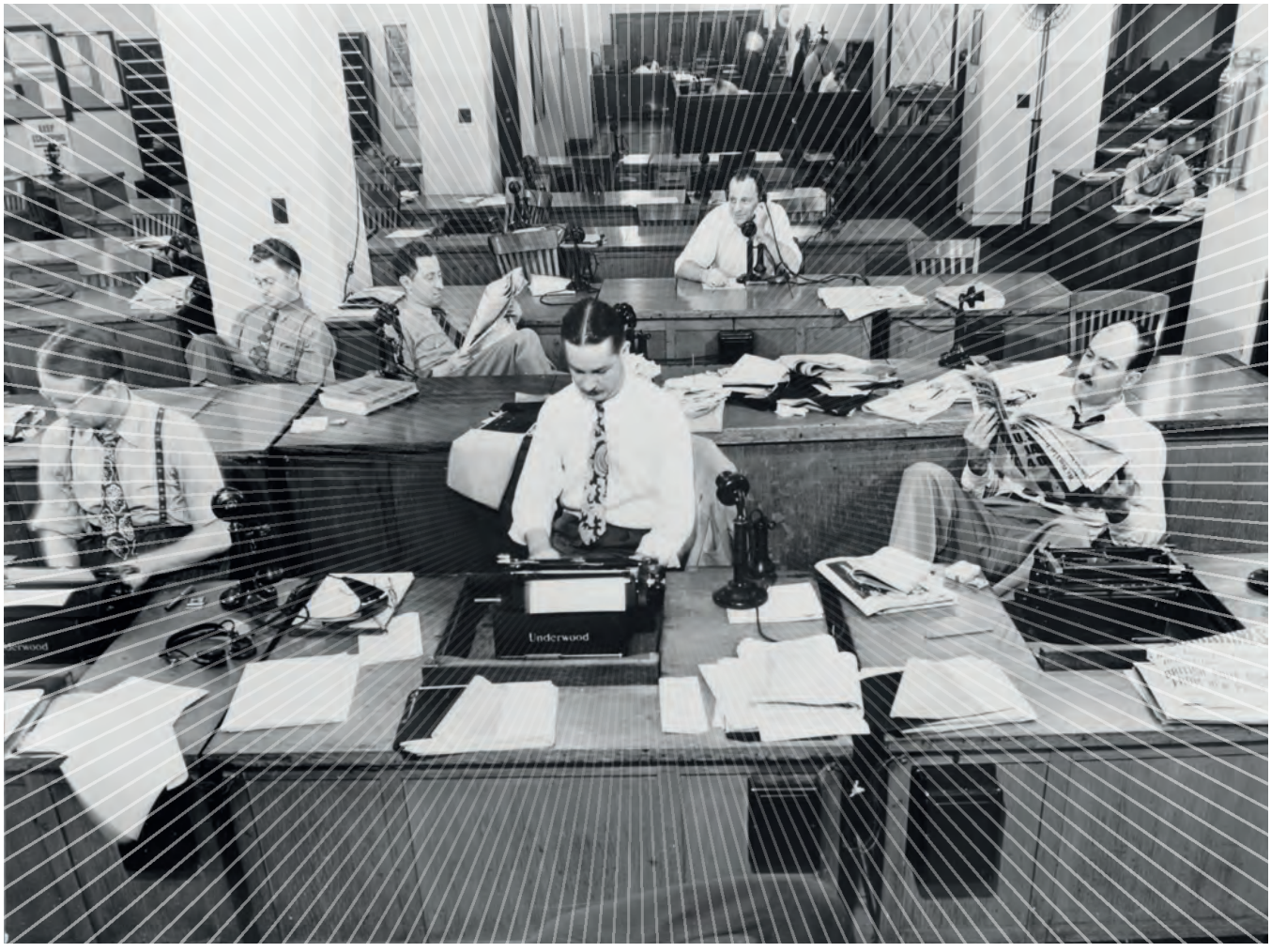
PR agency personnel take PR very seriously and know the essentials; it is the way they make their living, after all. Therefore, if you take PR efforts seriously and know the 'basic' essentials you may not necessarily need an agency. If you don't, then you probably do.

The press release is a cornerstone of PR – do you know the bare essentials? It must:

- Have a short and interesting title
- Use a subtitle to provide a very quick overview of the main message in plain language
- Include a date (and place)
- Include at least three paragraphs: i) the main message, ii) some more interesting and supporting details, iii) a quote from relevant person(s)
- Include the name of a contact person (including email address)
- Provide a short profile of the company/institution.

That's it. If every press release we received followed these basics, we would be delighted.

I urged the inclusion of a quote above, but I would strongly recommend not using more than two. And please don't write, "Ms. A and Mr. B said, 'We are proud of this achievement'". It brings




tears to my eyes when I imagine both parties trying to say the words in unison, standing side by side.

### Beyond the basics

If your company or research institution strives to go beyond the bare essentials in analytical science, why not go beyond the bare essentials in terms of PR to represent your organization accordingly?

i. Put a PR strategy in place. In other words, choose the right format and media outlet for the right message. For example, we at [iito] Business Intelligence are interested in business topics. If you send us great and exciting news about a new sample preparation technology for MALDI-TOF-MS with a detailed scientific description, it will probably end up in our office dustbin. However, if you license that technology to one or several of the big MS players, it will surely end up at the top of our web portal and in our newsletter. On the otherhand, it may be the other way round in The Analytical Scientist.

ii. Pay attention to professional branding (for example, logos, lettering, style).

*"If every press release we received followed a few basic rules, we would be delighted."*

iii. Try to understand words as well as molecules. In other words, produce intelligent text to represent your intelligent chemical analyses.

iv. Try to get to know and understand your (PR) customers (in general and in person).
v. Say "Thank you"

No doubt, there will be somebody within your organization who has the capabilities to perform the basics and even go beyond the basics, but it certainly takes time, especially if you plan to issue many press releases each year.

## Taking the PR plunge

So, you've decided to outsource your PR. Which type of agency is right for you?

Start small? There are many small PR agencies around, simply because starting a PR agency has low barriers to entry; there is no need for large capital investment, patents or copyrights. Such agencies may be single person ventures, or they may have up to twenty people. If you only want to publish a few press releases a year but need good advice and some PR work done in a professional way, a small agency may be the best fit. They will be close, and willing to act in a fast and flexible manner at lower cost.

Go specialized? Industry specialized agencies tend to employ 20–50 people, handle more clients, and charge higher rates. However, they have the critical mass to provide you with a complete package in your niche market that goes far beyond issuing a few press releases a year. Such agencies are often very close to your market and can be partners for many years as your company grows, even worldwide – especially as it is common for such agencies to have partners of the same size in other regions.

Dive straight in at the deep end? Other agencies act as arms of the largest PR business groups in the world. Very often these groups are big players with billions of dollars in revenue. In most cases, you will deal with a special brand of these groups, active in the life sciences or laboratory equipment market, and not the corporate brand of the large business group. The big PR firms can provide anything you need to place your offering on worldwide markets – along with a price tag that may reflect their stature. They certainly have the critical mass, and if time matters, it can make a big difference.

In the online version of this article, you will find a (non-definitive) list of PR agencies and the companies they work with – you can access the full article and table here: tas.txp.to/1214/PR

*"Being fast, competent, funny, smart, friendly, a little bit 'pushy', and paying attention to details – as well as having stamina – is a recipe for success".*

## Personal PR highpoints

Apart from the basics, sometimes it's the small but memorable things that set certain PR agencies apart. In the end, everybody is playing the same chords, but some do it better or differently than others, in either case, a special touch always does the trick. I should note that the following three 'special impressions' are very personal – other journalists and editors may have totally different perspectives and experiences. *

### *The woman at the door*

At my first Analytica, I was at a press conference for one of the largest players in the mass spectrometry and chromatography industries. A small, but very "present" woman drew my attention. She was the boss and founder of the PR agency who invited me, and she stood guard at the main door when the press conference had begun. When somebody wanted to leave the room during the press conference, she opened the door for them and closed it behind them as silently as she could. I was deeply impressed. She was the boss but kept her finger on the door to avoid any disturbance. Over the last few years, her agency has grown to nearly 50 people and also expanded regionally. My compliments.

### *The press dinner*

I don't know why I got invited or who invited me, but I visited my first press dinner of a major analytics firm at Analytica 2012 in Munich. There were a dozen or so top and middle managers from the company, a handful of people from the PR agency, and about 20 colleagues from the press. A nice place, good food and wine – and not soon forgotten.

In fact, it was the best PR event I have attended to date. The right people to talk to; not too many, but not very few. We were able to speak to managers and thereby get first-hand information from decision makers. We chatted with the PR people as well as our colleagues and competitors. You know, sometimes your best competitors are also your best colleagues and business partners. I've attended this event three times in the last three years and actually met the guys from The Analytical Scientist at the second press dinner. Now I am writing this article for them, and some of their articles are regularly featured in our [MSC] Newsletter and on our

web portal at Mass-Spec-Capital.com. Yes, certainly not to be forgotten; all the managers and people from the agency are on our mailing list. Perfect.

*The funny, smart guys & girls*

One day, I received a news release from a UK agency that I have never heard of before. It had a funny introduction and was followed by that all important thank-you-mail. I visited their website and it made me smile. So, I made some fun about how clever and smart they were, and that we Germans seemed to be lagging behind. A woman on the team replied, "Yes, we are a clever bunch!" I could not describe it any better myself – very clever and nice people. The agency owner has been sending me news of his life science clients ever since and, if I don't immediately respond, he just reminds me, "Marcus, did you get my news – has it not been of interest to you?" You can bet that, after his reminder, I try to tweet his news as fast as I can (no payment involved!). This is a small, young agency that will most likely succeed.

To sum up: being fast, competent, funny, smart, friendly, a little bit "pushy", and paying attention to details – as well as having stamina – is a recipe for success.

## The best strategy?

One conclusion stands out: take care of the essentials. Everything else is an extra option, but not necessary. Simply take care of the bare essentials and we will always be happy to receive your news!

In general, I would not recommend for or against a special type of agency – it always depends on your needs and preferences. It is also possible to have a mix: you could have a small company by your side (as some type of external-internal consultant) while you're talking or working with bigger agencies.

Remember that PR work does not end with the concept of your news release and the concrete text. It also includes the design and the corporate branding and style. If you include a 'lousy' logo in a fine press release, the release will suffer – and the other way round.

It's like a chemical analysis: everything – from the concept, over sample preparation, the instrument used, the test run on the system, the software analysis, to the documentation – is important.

PR is a serious business supporting the critical commercial mission of your company and not a weekend hobby for the managing director. The weekend would definitely be better spent with family.

So, if the news you are trying to bring to the market is serious – and indeed, it should be – try to bring in a professional "operator" to place your call, unless you can do it all by yourself to (nearly) the same standard, with the same speed. It has all been sung before...

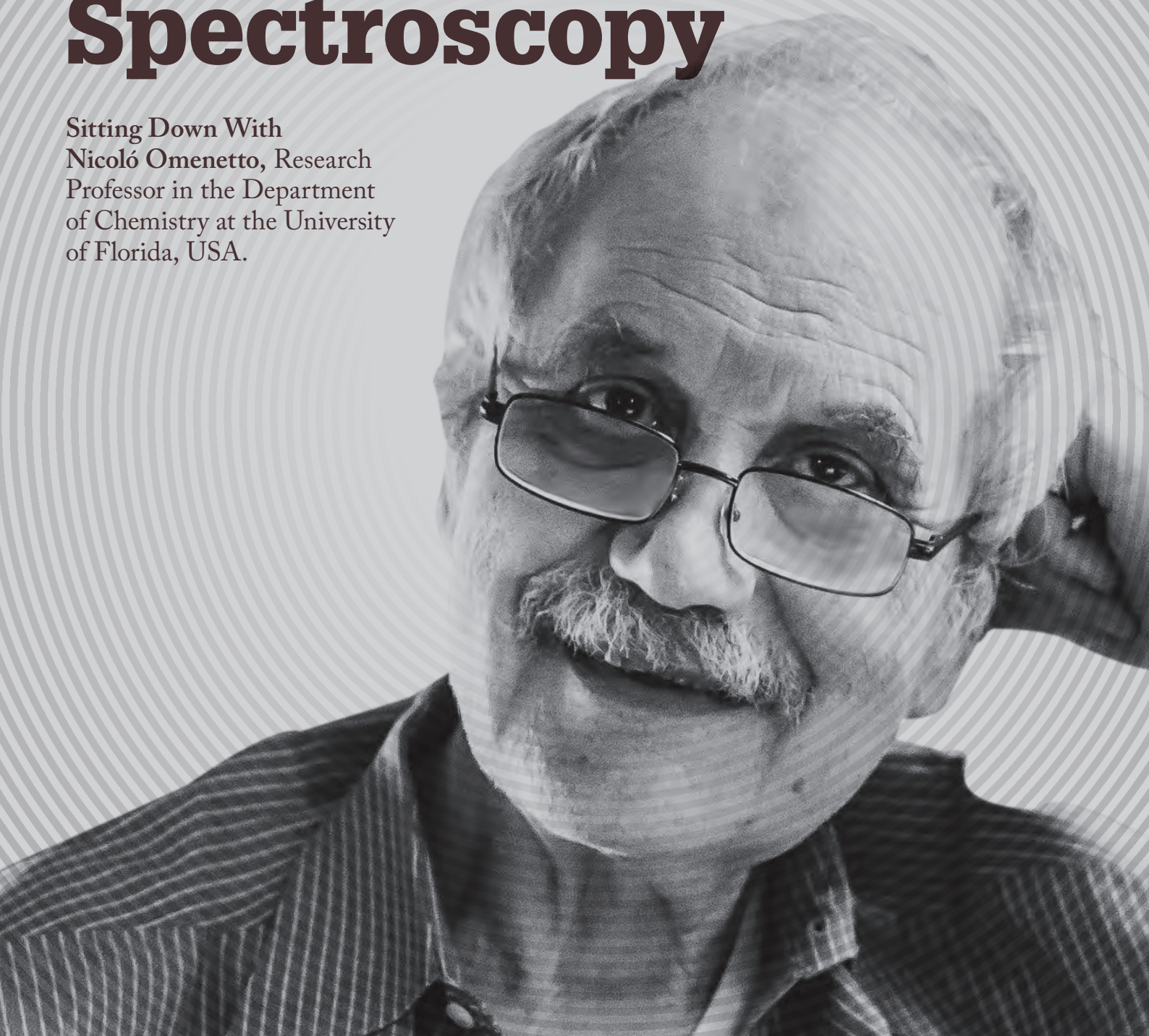
*Long-distance operator,*
*Place this call, it's not for fun.*
*Long-distance operator,*
*Please, place this call,*
*you know it's not for fun.*
*I gotta get a message to my baby,*
*You know, she's not just anyone.*
*– "Long Distance Operator",*
*The Band (lead vocal Richard Manuel, written by Bob Dylan).*

*Marcus Lippold is an Economist and Head of [iito] Business Intelligence as well as Editor-in-Chief of Mass-Spec-Capital.com, the free business web portal for the worldwide mass spectrometry industry. [iito] Business Intelligence is based in Bremen, Germany.*

**Conflict of interest declaration.*
*I hereby confirm that there is no conflict of interest. The PR agencies mentioned in the examples have never placed an order with [iito].*

# For the Love of Spectroscopy

**Sitting Down With Nicoló Omenetto,** Research Professor in the Department of Chemistry at the University of Florida, USA.



You were recently honored in a special issue of Spectrochimica Acta Part B...

It was an absolute surprise. And that's really quite amazing; as editor, I should have suspected something! I didn't even realize that we'd skipped from volume 99 to 101... You know, I love working in my field, but it's really rewarding to get such a boost in credibility from colleagues (not to mention the emotional pleasure of receiving a 'happy birthday' from my son Fiorenzo) and the wider community – that makes me love it even more. It's recognition that I did it right and that I should keep going.

How did you get into atomic spectroscopy?

I fell in love with atomic spectroscopy when I was a chemistry student. I remember an exam where electrons were flipping up and down. I had to put the correct angular momentum to derive the spectroscopic term. I was able to do it easily and that was that; I knew that I wanted to do spectroscopy. I also realized that I only wanted to go down the academic path of research and teaching. And that's what I did.

How do you split your time between research and teaching?

When I was 30 years old, I felt that I couldn't spend too much time teaching because I needed to do research – I was too busy publishing papers and writing proposals. Now, I feel that teaching is absolutely essential. If you teach and are able to get students to understand, it is the only way to approach research and to solve analytical problems. Only then are you fulfilling your role. If you can see the eyes of your students sparkling with interest, you are winning.

Who inspires you?

I would love to try and give credit to everyone who has had an impact – but the list would be too long. It includes collaborators, colleagues – and students. However, one great spectroscopist who always comes to mind is Kees Alkemade, who I had the pleasure of knowing well. He had an incredible intuition for explaining the intricacies of spectroscopy and for making statements that had a great number of scientists thinking, "I wish I'd said that..." One of Kees' favorite topics was noise, a fascination he shared with James Winefordner, who is another spectroscopist I deeply admire. James and I have been working together for over 45 years, which has been an incredible experience for me. I've learned a lot from his 'indefatigable search for knowledge' not only scientifically but also about life more generally. Gary Hieftje is another scientist who is constantly engaged in the development of new ideas and experiments. We must always try to "look around the corner" as Kees often said – for me, that means: if you have a crazy idea, try it.

Could you elaborate?

Well, you can only discover whether an idea is worth pursuing if you get the chance to test it. I can define much of my work over the years as Toccata and Fugue (by Johann Sebastian Bach). Why? Because in Italian, it's called 'Toccata e Fuga', which translates as 'touch and go' – in other words, try an idea and get to the next one! I can give you a very long list of projects that I tried purely out of curiosity. I admit that such an approach is slightly detrimental to being an analytical spectroscopist or an analytical chemist (and funding) – but I'll openly confess that I never really paid much attention to whether or not there was a practical application. It was just the fun of discovery – but through it, I learnt much about the fundamentals of my field.

What's the most exciting advance of the last 50 years?

That's a very tough question to answer, especially if I consider spectroscopy in general and include the life sciences and molecular spectroscopy. Specifically for atomic spectroscopy, I would say that laser manipulation of atoms and molecules is the most fascinating advance – but there have been many others. I would suggest laser induced breakdown spectroscopy (LIBS) as one of the 'old' analytical methodologies that has been most successfully revisited in recent years. From the ChemCam on Mars to deep ocean studies, what we can learn on both a technical and fundamental level is unbelievable.

What advice would you give to aspiring academics?

First, don't do research if you're not having fun with it. If you're not enjoying your work, then innovation is highly unlikely. Second, be absolutely scrupulous in the data that you present. And third, read the literature; to formulate a novel approach, you must first learn what has been done in the past.

But you're also a big believer in scientific freedom...

Yes. And I have been extremely lucky to be protected from administration for most of my career. In fact, I spent all my time hiding in the lab until very recently, when I moved to the University of Florida. I was lucky enough to receive funding for "exploratory" research. And really, such freedom is the best scenario from an experimental point of view. Going back to the honorary issue, it proves to me (and others) that I used my freedom wisely.

I must also give credit to my wife, who has always let me believe that my work was important. You might say that she supports me, but perhaps it's more like she puts up with me... or that she is able to forgive me! That's a different kind of freedom.

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