MARCH 2015 #26

the Analytical Scientist

A Briefcase Full of NMR

Bernhard Blümich – one half of "The Blues Brothers" – tells us how compact NMR evolved and where it's heading.

TRAJAN

Trajan Scientific and Medical

Creating integrated partnerships to enable analysis of the world we live in.

Trajan Scientific and Medical collaborates with academic and industry partners to develop and deliver innovative products.

Our brands are found in analytical laboratories, medical facilities, and research institutions around the world.

Since 1960, **SGE Analytical Science** has grown to encompass a wide range of chromatography consumables.

The **Grale HDS** pathology range has evolved from more than 30 years laboratory supply experience.

We have established a global network of partners, with our headquarters in Australia and significant operations in USA, Europe and Asia.

Join us on an analytical and medical science journey. Together we will enrich the wellbeing of a growing number of communities.

www.trajanscimed.com

Online this Month

Tea with Wolfgang

Rich sits down with Wolfgang Lindner for the fourth instalment of Tea with Rich from ISC2014 in Salzburg, a city very close to Wolfgang's heart. Wolfgang reflects on what it means to bring ISC back to Salzburg and on the importance of bringing people together at conferences; linking industry veterans with young scientists, and bridging applications and theoretical science. He thoroughly believes in the "spirit" of ISC. "Science is about constantly questioning – and you can feel that at ICS." Wolfgang also insists that we must never forget the importance of validation: "If data are not valid then there is no meaning behind them. Most of our colleagues believe in data, so we have the responsibility to deliver the right data!"

Online: tas.txp.to/0215/Wolfgang

Tea with Peter

How does a young scientist get on the 'team'? Peter Schoenmakers offers his advice, while Rich offers tea. In the fifth episode from ISC2014, Peter ponders whether analytical science has become as competitive as professional sports. "You try to get into the team, but you get rejected all the time." With it being more difficult to obtain grants and to make a name for yourself, science is more challenging than ever before – particularly for young scientists. But there is one key difference between getting on a football team and getting into the science 'team' - scientists are willing to help one another to be successful. Peter discusses the importance of collaborating, the analytical issues of the future, and delves into one and a half and three-dimensional chromatography.

Online: tas.txp.to/0215/Peter

Tea with Michael

Michael Lämmerhofer co-chaired the 30th International Symposium on Chromatography with his old professor – Wolfgang Lindner and Wolfgang Buchberger. Michael discusses analytical science's fascinating move into the clinic, from technologies such as the iKnife, which is opening up a new world of yes/no mass spec information for surgeons (for more on that topic, visit: tas.txp.to/0215/precisionmed) to oxidative stress markers – and why they could have a direct clinical application. Michael recently received the Chromatographic Society's Jubilee Award, which he humbly believes also recognizes the people he has worked with. "You get such an award only because you have good coworkers and a good boss or mentor."

Online: tas.txp.to/0215/Michael

THE FUTURE HAS

Flame Blazes a New Trail in Miniature

From Revolution to Reinvention.

With the release of the "World's First Miniature Spectrometer," Ocean Optics helped to make spectroscopy portable, inexpensive and accessible. Researchers, educators and OEM developers have embraced the technology, using our instruments in ways we never imagined. Now, fueled by a passion for innovation and inspired by your feedback, we've reinvented our miniature spectrometer to reflect the challenges of today's most demanding applications.

Ocean Optics

Flame. Forging a New Standard in Miniature Spectrometers.

Flame combines heritage, creativity and insight in a way that gives you the familiar benefits of miniature, modular spectroscopy -- without compromise. This compact, next-generation spectrometer integrates performance-enhancing features and is produced using industry-leading manufacturing techniques. Enjoy the benefits of greater thermal stability and lesser unit-to-unit variability, plus the freedom of interchangeable slits, simpler device connectors and LED status indicators.

www.oceanoptics.com | info@oceanoptics.com | **US** +1 727-733-2447 **EUROPE** +31 26-3190500 **ASIA** +86 21-6295-6600

C Contents

On The Cover

Analytical science's answer to The Blues Brothers

i make the difference

The new driver of i-volution in HPLC analysis

Innovative
- Interactive Communication Mode (ICM)
- Remote monitoring
- Maximum reliability

Intuitive
- Unified graphical user interface
- Quick batch function: Batch creation at your fingertip

Intelligent
- Automation of routine procedures
- Simple transfer of legacy methods

www.shimadzu.eu

New Industry Standard HPLCs

MERCK MILLIPORE

Experience the quintessence

Milli-Q® Integral system
pure and ultrapure water at your fingertips

- Dual POD (point-of-delivery) concept saves space and increases convenience
- Lower running costs and water waste with exclusive Elix® technology
- Millitrack® embedded e-Solutions for optimized laboratory performance and remote access

Experience more www.merckmillipore.com/ultrapure

Merck Millipore is a division of MERCK

Merck Millipore, the M mark, Milli-Q, Elix, Millitrack are registered trademarks of Merck KGaA, Darmstadt, Germany.

Departments

Sitting Down With

the Analytical Scientist

ISSUE 26 - MARCH 2015

Editor - Rich Whitworth
rich.whitworth@texerepublishing.com

Commissioning Editor - Iestyn Armstrong-Smith
iestyn.armstrong@texerepublishing.com

Associate Editor - Stephanie Sutton
stephanie.sutton@texerepublishing.com

Associate Editor - Roisin McGuigan
roisin.mcguigan@texerepublishing.com

Associate Editor - Michael Schubert
michael.schubert@texerepublishing.com

Scientific Director - Frank van Geel
frank.vangeel@texerepublishing.com

Senior Designer - Marc Bird
marc.bird@texerepublishing.com

Junior Designer - Emily Strefford-Johnson
emily.johnson@texerepublishing.com

Chief Executive Officer - Andy Davies
andy.davies@texerepublishing.com

Chief Operating Officer - Tracey Peers
tracey.peers@texerepublishing.com

Publishing Director - Lee Noyes
lee.noyes@texerepublishing.com

Sales Manager - Chris Joinson
chris.joinson@texerepublishing.com

Audience Insight Manager - Tracey Nicholls
tracey.nicholls@texerepublishing.com

Audience Development Assistant - Julie Johnson
julie.johnson@texerepublishing.com

Traffic and Administration Associate - Jody Fryett
jody.fryett@texerepublishing.com

Digital Content Manager - David Roberts
david.roberts@texerepublishing.com

Mac Operator Web/Print - Peter Bartley
peter.bartley@texerepublishing.com

Apprentice, Social Media / Analytics - Stephen Mayers
stephen.mayers@texerepublishing.com

Editorial Advisory Board
Monika Dittmann, *Agilent Technologies, Germany*
Norman Dovichi, *University of Notre Dame, USA*
Gary Hieftje, *Indiana University, USA*
Emily Hilder, *University of Tasmania, Australia*
Ron Heeren, *Maastricht University, The Netherlands*
Tuulia Hyötyläinen, *VTT Technical Research Centre of Finland*
Hans-Gerd Janssen, *Unilever Research and Development, The Netherlands*
Robert Kennedy, *University of Michigan, USA*
Samuel Kounaves, *Tufts University, USA*
Marcus Macht, *AB Sciex, Germany*
Luigi Mondello, *University of Messina, Italy*
Peter Schoenmakers, *University of Amsterdam, The Netherlands*
Robert Shellie, *University of Tasmania, Australia*
Ben Smith, *University of Florida, USA*
Frantisec Svec, *University of California at Berkeley, USA*
Ian Wilson, *Imperial College London, UK*

Published by
Texere Publishing Limited, Booths Hall, Booths Park, Chelford Road, Knutsford, Cheshire, WA16 8GS, UK

General enquiries:
www.texerepublishing.com
info@texerepublishing.com
+44 (0) 1565 752883
sales@texerepublishing.com

Distribution:
The Analytical Scientist is distributed worldwide through 21,000 printed copies to a targeted European mailing list of industry professionals and 58,750 electronic copies, including 27,583 to North/South America, 26,509 to Europe, and 4,658 to the Rest of the World. ISSN 2051-4077

HUMANITY IN SCIENCE AWARD

phenomenex ...breaking with tradition

&

the Analytical Scientist

The winners have been chosen!

Thank you to everyone who submitted entries and nominations for the inaugural Humanity in Science Award. Our winners have been chosen and their inspiring essays were presented at the Humanity in Science Symposia at Pittcon 2015. They also received $25,000 at a Gala Dinner held in New Orleans.

Find out who won at www.humanityinscienceaward.com

Analytical science has been at the heart of many scientific breakthroughs that have helped to improve people's lives worldwide, from delivering safer water to developing new medicines. And yet analytical scientists rarely receive fanfare for their humble but life-changing work. The Humanity in Science Award was launched by Phenomenex and The Analytical Scientist to recognize and reward analytical scientists who are changing lives for the better.

Could you be our winner next year?

Details of the 2016 Humanity in Science Award will be announced soon.

Questioning Our Values

Sometimes it's good to stop and think about what is truly important and whether we need to refocus – or redouble – our efforts.

It gives me great pleasure to have worked briefly with John McLean (Vanderbilt University) well ahead of finally meeting him in person at Pittcon in New Orleans. John is a visionary making big strides in data-driven discovery and he is willing to use any tool at his disposal to solve the challenges that he considers most urgent (1).

Back in the summer of 2014, John said, "Hypothesis-driven research tends to suffer from a subjective bias towards what is being asked and how we are listening for the answers." In other words, our search for the truth can sometimes be clouded by a temptation to focus only on looking for things that we expect or hope to find. And, let's face it, that is not limited to analytical science.

Like John, Jeremy Nicholson (Imperial College London) is also focusing on the (very) big picture (2). Work done by both groups – and a whole host of unsung heroes – will undoubtedly have a huge impact on medicine in the coming decades.

Listening to high-level presentations by such icons is inspirational. And subsequent conversations can border on philosophical. How, I ask, can we (the public) happily support the construction of an Olympic sports doping laboratory in London but find apathy when it comes to jumping over current and future health hurdles? Jeremy's National Phenome Centre was made possible by the adoption of legacy equipment from London 2012. But shouldn't we be equally willing to support research that has the potential to improve everyone's lives? Unfortunately, humankind's naturally shortsighted value system means that we tend to consider issues closer to home to be more important or relevant.

And that leads me to the Humanity in Science Award and a winner's speech that left the audience gasping at the reality of the world in which we live (3). Peter Seeberger and Andreas Seidel-Morgenstern – the winners who received a standing ovation for their great work – highlighted the terrifying fact that 660,000 people die from malaria each year (WHO). Ninety percent of those are children under five. Once we understand that it is a disease of poverty, can we (the public and scientists) do nothing? Analytical science is at the heart of solving problems and most of the solutions have great value to humanity – let's hope humanity reciprocates by facing up to its evident shortcomings.

My personal congratulations to Peter and Andreas – and all of the entrants to the Humanity in Science Award – for making the world a better place.

Rich Whitworth
Editor

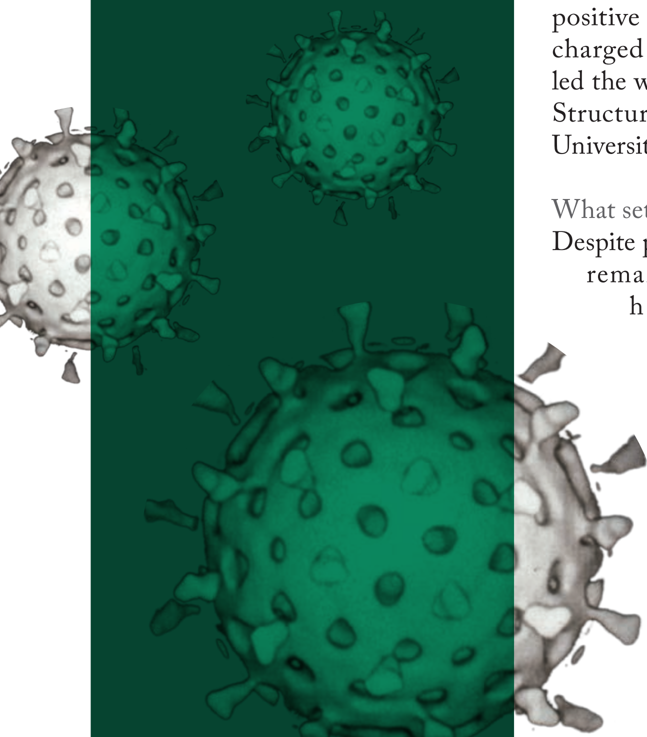
References

1. *Pioneers of Precision Medicine, The Analytical Scientist (http://tas.txp.to/0215/precisionmed)*
2. *Targeting the Untargeted (http://tas.txp.to/0614/target)*
3. *www.humanityinscienceaward.com*

Upfront

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

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



Viral Code Breaker

Spectroscopy lights the path to preventing virus deployment

A research team investigating viruses began their work hoping to find out more about the mechanistic molecular details of RNA viruses, but the results far exceeded their expectations; the group says it has discovered and cracked the 'code' that enables virus assembly (1). Understanding this code means that researchers could potentially prevent virus deployment, offering a new path of drug discovery. Until now, virus assembly – although an impressive feat – was thought to rely on simple electrostatic interactions between positive coat proteins and negatively charged RNA. Peter Stockley, who led the work at the Astbury Centre for Structural Molecular Biology at the University of Leeds tells us more.

What set the project in motion?

Despite progress with vaccines, viruses remain a major threat to human health, as well as causing significant commercial loses to crops and livestock. They are also fascinating molecular machines built for repeated cycles of infection and new virus production. How they achieve these goals is a challenging research problem and we have been fascinated by how at a particular point in the virus lifecycle they spontaneously wrap their genetic material into viral capsids, which are protective transport vehicles to the next host cell. This is the process of virus assembly.

How did the code elude other researchers?

The viral RNA contains two sets of codes. The first, which we have been able to translate for decades, is the genetic code defining the viral protein components. We were able to discover and decode the second by combining experiments with highly specialized bioinformatics analyses carried out by our collaborator Reidun Twarock, professor of mathematical biology at the University of York. This effort in turn was a response to our development of single-molecule fluorescence correlation spectroscopy (smFCS) assays for studying virus assembly.

How was smFCS used?

The smFCS allows us to look in real-time at the hydrodynamic radius of fluorescently dyed molecules in solution. The technique is ideal for virus assembly reactions because the radius changes dramatically as the small coat proteins and larger RNA form a virus particle. The single molecule aspect is also important because it allowed us to work at nanomolar concentrations where we saw features of the assembly mechanism, i.e., the packaging signal mediated assembly – essentially the assembly code hidden previously from view – that are lost at much higher concentrations normally used for such experiments.

It is very satisfying to have realized that there were aspects to viral assembly that were not understood by the existing theories, to have been able to postulate a new idea that explains what we were seeing, and then to do the tests to show that this is in fact the case. Like all the best scientific ideas, we have arrived at the current understanding with more experiments that need to be done, which is great.

What were the main challenges?

This type of analysis for viral assembly reactions is very new and so we had to check constantly that the things we saw happening in smFCS could be interpreted correctly. My colleague Roman Tuma, who is an expert spectroscopist, was instrumental in this. A different kind of challenge was (and in some places still is) the skepticism of colleagues who did (do) not believe that such a mechanism could exist and have remained undetected. The latest results have allowed us to turn a corner with the bulk of the field now realizing that previous ideas were far too simplistic.

Your work will surely have an impact on drug discovery...

We have shown that a new mechanistic aspect of virus assembly occurs in viruses that infect bacteria, plants and humans. We believe we understand why it is so widespread: because they give the viruses that work this way a competitive advantage. If we can use small molecules to scramble the code, it would have an anti-viral effect. Thus, we have unlocked novel anti-viral drug targets. However, we will need to do a separate decoding experiment for every type of virus as we cannot immediately identify drugs that might block the common cold.

What next?

The obvious next step is to extend the work to human viruses and begin to examine whether we can isolate anti-viral lead compounds that would provide proof of principle that this could generate clinically useful drugs.

The work emerges out of curiosity driven research, mostly on model viruses that no one in the real world really cares much about… many governments only fund research that has clear, direct relevance, and the essential groundwork here would not have qualified for support. Indeed, reviews of laboratory allocation within my University concluded that in future we were unlikely to be funded, and as a result we had to give up facilities. We were saved because the preliminary smFCS results were clearly unexpected, hinted at a major discovery, and are still providing novel insights into these vital processes.

It just goes to show that progress in science cannot be second-guessed by committees. Unless there is funding and resources for people doing "blue sky" projects, major breakthroughs will be missed.

Reference

1. *N. Patel et al., "Revealing the Density of Encoded Functions in a Viral RNA", PNAS, 112 (7), 2227-2232 (2015).*

Bad Breathalyzer

A start-up company delivers breath analysis technology to an eager consumer market

After being at an after-work cocktail hour with co-workers, Charles Michael Yim suddenly realized that a smartphone bio-sensor attachment that could provide guidance about current blood alcohol concentration (BAC) level (as well as advice on how to get home) would be mighty useful. The idea led to the founding of the company – Breathometer – and the launch of commercial devices that bring breath analysis applications to consumers.

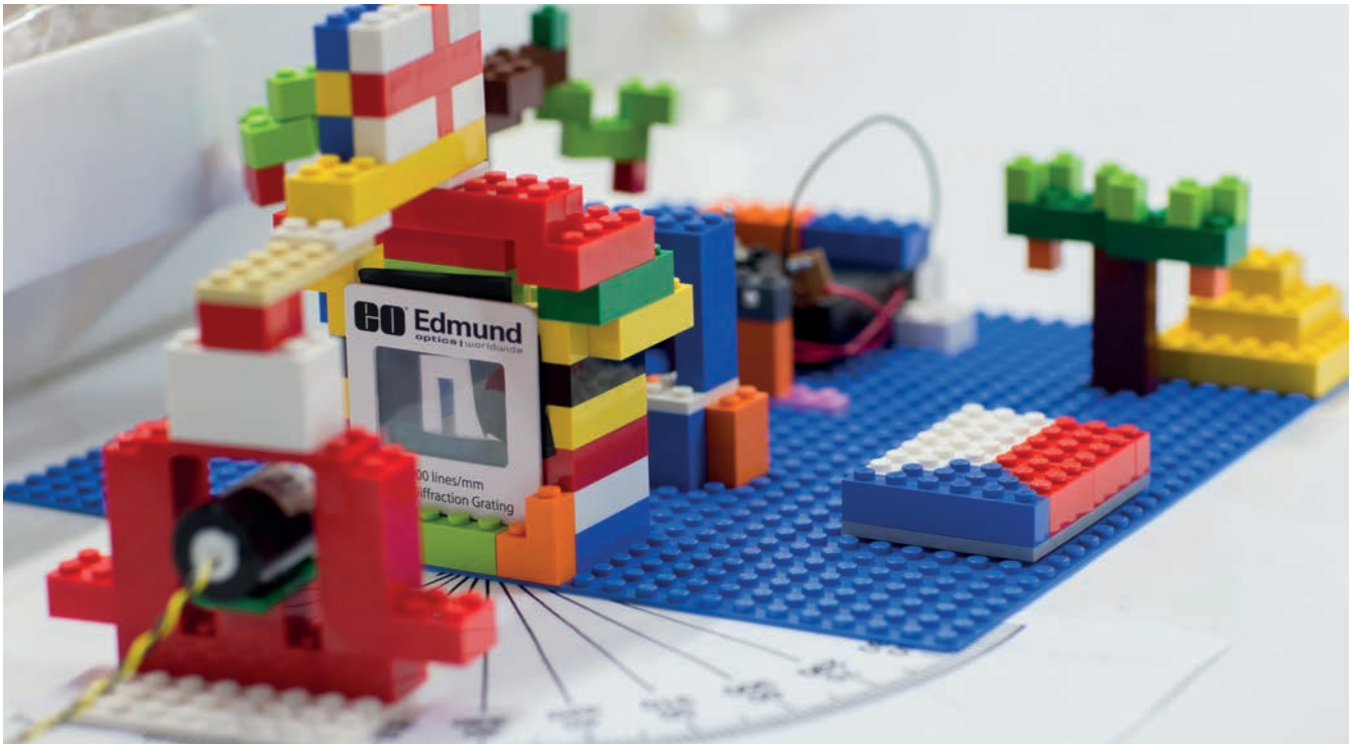
Now, following the launch of two devices for analyzing BAC levels, the company has turned its attention to a new application – a platform that can address "breath quality" and hydration levels. Users will apparently hold the new device to their mouths while an electro-chemical fuel cell sensor detects volatile sulfur compounds (VSCs) at part-per-billion concentrations. The data is sent wirelessly to a smartphone app, which displays the information. If all goes to plan, 'Mint' – the company's third device – will be launched in the summer of 2015.

"Rather than sampling from the lungs (as with our ethanol-detection products) Mint samples air from within the oral cavity. VSCs can be elevated by certain foods and beverages you consume, and may also indicate gum disease and tooth decay. In all cases, elevated VSCs can reduce breath quality. Specifically, the sensor measures hydrogen sulfide, methyl mercapthan and hydrogen disulfide levels," says Yim.

Yim's story once again highlights the commercial potential for simple analytical applications that cater to a technology-obsessed consumer market (myvessyl.com is another slick example). Investors have

sensed a killing: Yim received funding for the breathometer technology via the US reality television series "Shark Tank" which gives entrepreneurs the opportunity to pitch ideas. Notably, all five investors on the show bought into the breath analysis concept back in September 2013.

"Using human breath to detect biomarkers is an exciting opportunity for developers of consumer devices. Driving adoption of breath-based analysis products will be largely based on the type of actionable information that can be presented," says Yim, adding that the company is looking to launch into more application areas in the future. *SS*



Courtesy of Imperial College London

The Lego-lytical Scientist

Plastic spectrometers help students understand instrumental limitations

Have you ever tried to build a spectrometer out of Lego? No? Well, staff of the Department of Chemistry at Imperial College London challenged first-year students to do just that in a fun exercise with a serious problem-solving objective.

"The project started off by wanting first-year undergraduate students to improve measurement techniques in the lab. In order to do this, it is important to understand the limitations of the instrument being used. One way this can be done is by building your own instrument. One of the core objectives of our lab is to remove the 'black box' concept," says Joshua Edel, who led the initiative.

The ubiquitous and flexible nature of Lego made it the ideal platform to support the other essential components: detector, lenses, diffraction grating and light source. A Raspberry Pi computer was used to record the detector signal and the data were analysed using Python. Working in groups, the students were given a basic schematic of a typical spectrometer, but were expected to develop their own solutions as to the optical configuration and data analysis strategy. Solutions varied from functional box-shaped devices to more elaborate creations.

"Outcomes include students understanding the operating principles of a UV-Vis spectrometer, building on python programming ability, improving measurement technique and sample preparation methods, improving problem solving ability, and successfully working in a group," says Edel. "Although the concept of this project was rather simple, behind the scenes it took significant amount of preparation, programming and electronic component development to ensure that everything ran smoothly." In other words, serious commitment – for our full feature on analytical education, see page 38.

Edel is already working on similar activities for second year students, although he says he's likely to replace Lego with the components more typically found in analytical instruments. And in case you're wondering, Edel admits that he was indeed a fan of Lego as a child. "In fact, my kids are playing with the same Lego sets that I had as a child…" *SS*

If you're inspired to build (or force your students to build) an analytical instrument from Lego, we'd love to see a photo on Twitter: #legolytical @tAnaSci

Spectrometry Take Flight

Aerial drones already aid in sample collection. Is in-situ water analysis next?

How do you collect water samples in remote areas with no infrastructure? You fly... Or rather, an unmanned aerial drone does. Such drones – equipped with pumps – are already being used to suck up water samples at various locations for subsequent laboratory analysis. Now, president and founder of PrecisionHawk Ernest Earon says that the company is looking to incorporate an onboard spectrometer for in-situ analysis.

"We have already integrated 15 different plug and play sensors from visual to hyperspectral to Lidar," says Earon, "but technology is now minuturizing and reducing in cost so quickly that it's more about keeping up with new techology rather than whether it is possible… Because it is possible. We just need to learn how to integrate new techologies into existing systems."

The drones weigh around 1.3 kg, are less than one metre from nose to tail, and are able to compute flight paths (automatically adapting for bad weather), survey parameters, take-off and landing paths, as well as other vital information. Once the survey is complete, the on-board computers connect to wireless networks to transfer the high resolution remote sensing data, flight information and diagnostics to remote servers. Sounds futuristic? Actually, they are already being used in a variety of practical applications. Agriculture is a big one, according to Earon."For crop health, we can look for crop stressors in specific spectral bands or use thermal sensors to identify temperature variations caused by crop stress. Access to real-time data allows for a more informed approach."

Assessing water quality has become another popular area for the company, largely driven by industry demands; for example, to evaluate organic material in the water or identify oil spills and pollutants. "The technology was made to cover large areas, very quickly – and in difficult locations," says Earon. "For example, up north, where there is little to no infrastructure, you're going through areas where it is almost impossible to walk… let alone carry sampling equipment. The intention was to serve as a people multiplier, to extend the reach and vision and to touch things we have been previously unable to touch."

And the inclusion of an onboard spectrometer? Earon says that the system will obviously need to be light and high quality, but there is a growing market. "The next step for us is to evaluate which applications would be well suited for an onboard based spectrometer. There are so many potential applications for a technology like this, so we need to understand where the biggest needs are and where the most rapid rollout can be." *SS*

NMR: New Meat Research

Can triglyceride fingerprinting and NMR help find adulterated meat?

No one likes a nasty surprise – especially while eating. Last year, we reported on an LC-MS/MS method for meat speciation testing (tas.txp.to/0215/kosher). Now, a research team from the UK's Institute of Food Research, led by Kate Kemsley, has used nuclear magnetic resonance (NMR) spectroscopy to analyze the chemical composition of fat to distinguish beef from horse. In fact, the work has resulted in the launch of a new instrument from Oxford Instruments. Kemsley tells us more.

How did the project get off the ground?

About three years ago, Oxford Instruments approached me and my group because of our experience in statistical analysis of spectral data. They wanted to work together to develop a benchtop machine for a new class of NMR for industrial applications. Within three months of the project getting up and running, the horse meat scandal in the UK broke out. We reasoned that meat identification would be a very beneficial application.

And what was the result?

We developed a method that looks at the differences in the chemical composition of the fat in meats to determine speciation. We call this triglyceride fingerprinting. The big difference between our method and existing techniques and research-grade NMR is the field strength – we're working at much lower field strengths. It's actually how NMR used to be 40 years ago but today the instrument builder can couple it to modern day electronics and computers. We can collect huge quantities all in one dataset and use modern day computational methods to deal with it. The instrument (Pulsar) is designed to sit on a bench as a low-cost, low-maintenance system, but the underlying spectroscopy by which the data is generated is the same as for high-field NMR.

How does it compare with current detection methods?

The standard methods currently used in the industry now are biological – and it's fair to say they have problems with quantification. Some involve amplification to replicate bits of DNA so you can't say whether you have a trace of contamination or if the sample is 50 percent contaminated. Our method is not intended to look at products retrospectively after the supermarket issues a recall; we envisage it being there right at the start when blocks of frozen meat arrive at the meat processing company. NMR is quantitative in a direct way because it counts the number of protons of a different type that you've got in different positions of a triglyceride molecule; you can directly translate the height or area of your peak to the amount that's present.

My team is an analytical science unit and we have some of the other competing technologies here. We also tried MS for this work (in parallel we're actually developing MS-techniques based on protein fractions rather than triglyceride) but in comparison MS is slow. NMR is so much faster and simpler.

Can it be used for speciation of other types of meat?

We focused on horse and beef, but Oxford Instruments have done work with pork and lamb too. It's safe to say that pork works as well as horse, but lamb is a little trickier. We can also get a spectrum from processed meats. We've used the technique for rapid labelling information on whole foods, such sausages, to get saturated and polyunsaturated fat content. But we couldn't do species identification on a product that quite legitimately had, say, sunflower oil in it since this would interfere with the triglyceride profile.

How sensitive is the test?

It's difficult to say, but we're definitely not working in the contamination area. We only look at the fat constituent of meat so we'd have a much lower limit of detection if you had say steak mince adulterated with a really fatty piece of pork.

What were the major challenges?

The production protocol is simple but there are some steps that really help improve your result, such a filtering step. Low fat samples are the main challenge, such as very lean steak, and the spectra can be a bit noisy if you only collect for five minutes. We've done a lot with computational excluding routines to try and improve the data post collection so that we don't have to collect for an hour; our aim is to keep the process quick. Speed is something we can compete on and if you need two to three hours then you might as well use DNA-based or MS methods.

What's next?

Meat isn't the only area we've looked at and I think the triglyceride fingerprinting technique would also be good for looking at edible oils. In fact, we have a project in the pipeline that is in the final stages of approval at the moment where we would work as a partner to have NMR trialled for authenticating olive oil.

Reference

1. *W. Jakes et al., "Authentication of Beef Versus Horse Meat Using 60 MHz 1H NMR Spectroscopy", Food Chem. DOI: 10.1016/j.foodchem.2014.11.110 (2015).*

TOSOH

YOUR SPECIALIST IN SEPARATION

DISCOVER NEW SOLUTIONS FOR LIQUID CHROMATOGRAPHY

- NEW SEC COLUMNS FOR ANTIBODY SEPARATION
- HILIC, RPC, IEC, HIC & SEC BIOPOLYMER ANALYSIS
- ADVANCED GPC/SEC SOLUTIONS FOR POLYMER ANALYSIS
- HIGH CAPACITY PROTEIN A, IEC, HIC & MIXED-MODE MEDIA

MEET OUR SPECIALISTS THE HPLC 2015, JUNE 21-25 IN GENF, SWITZERLAND, TO FIND OUT MORE ABOUT OUR SOLUTIONS FOR SEC/GPC, HPLC, UHPLC AND DOWNSTREAM PROCESSING OR VISIT OUR WEBSITE WWW.TOSOHBIOSCIENCE.DE

TOSOH BIOSCIENCE

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

Ruining Science by Writing it Up

How to maximize your chances of success when preparing manuscripts for publication.

By Thomas Annesley, deputy editor, Clinical Chemistry, and author of the book "Designing and Writing Scientific Research Papers".

"How could the editor not see that my paper was appropriate for the journal?"

"How could two expert reviewers both be so stupid?"

"It's a wonder that good science is ever appreciated..."

Ever had any of these thoughts? If so, consider that the quality of the science is generally not the problem. The failure often lies in the presentation. Even cutting-edge science becomes a dull-edged manuscript if not written well.

A well-written manuscript tells a story that is concise, clear, and written with the reader in mind. It is a story in which you give the proper amount of information, presented clearly and logically, so that the reader can appreciate the argument you have built in favor of your work by the time they come to the end.

Although the editor and peer reviewers are the first to see your manuscript, they are readers as well and you cannot assume that they are going to "get it" simply because they work in the same field as you. The onus is on you to make your case by using a story that weaves together the hypothesis or question, the methods used to test the hypothesis or answer the question, the answer you obtained, and why the answer provides new and valuable information.

A manuscript becomes easier to write if you, the author, consider what readers (including, editors and peer reviewers) need to know to appreciate your work:

- What was the general topic of the study?
- Why was the topic important to begin with?
- What was the knowledge gap that needed to be filled?
- What was your hypothesis, question or goal?
- What experiments and methods did you use to seek an answer to your question?
- What specifically did you measure?
- What did you observe?
- What did your results show?
- What answer did you obtain?
- What do your results mean?
- What are the strengths and limitations of your study?
- How do your results contribute to the field of study – what's in it for the reader?

Once you understand what information the reader needs to know, you then need to organize your manuscript to have the greatest clarity for the reader. I intentionally used the phrase "weaves together" earlier because the best manuscripts (and the stories they tell) link all of the sections of a manuscript together in a logical fashion. You want readers to see how your experiments derived from your hypothesis or question; how your results derived from your experiments; how your answer derived from your results; and how your discussion derived from your answer.

Just as important, the various sections of the manuscript (Introduction, Methods, Results and Discussion) must be consistent with one another. For example, every hypothesis/question posed must have an answer somewhere in the manuscript. Experiments performed must have corresponding results presented in the manuscript, and vice versa. Your discussion must reflect your results, and vice versa. In other words, the reader should be able to go back to any section of the manuscript and understand how it fits into the story being told. The reader should never wonder "why is this here"?

The literature is vast and no one can keep up with it all. We all have limited time and make value judgments often based more on the quality of the story told than on the quality of the science. If an author cannot convince me in the introduction that the topic is important and that the hypothesis/question is worth pursuing, then the quality of the science becomes irrelevant. And, if the author cannot convince me in the discussion that the results have answered an important question and thus added value to the field, then once again the science may be lost forever.

> *"Even cutting-edge science becomes a dull-edged manuscript if not written well."*

I am not advocating that you write tales or embellish your ideas and results. What I am saying is that a good story enhances good science. A poor story ruins good science. If you put the proper effort into organizing a manuscript, you can present your science in the best light. Don't ruin your science by writing it up.

What's in the Surprise Gift Box?

Structure elucidation of small organic molecules requires a concerted analysis using several techniques.

By Lothar Brecker, associate professor and deputy head of the Institute of Organic Chemistry, University of Vienna, Austria.

Modern spectroscopic methods have a great importance in many areas of molecular sciences. Apart from structure determination they are used to analyze dynamic phenomena and interactions between molecules. In particular, NMR spectroscopy and mass spectrometry are key techniques in these analyses, perhaps because of their wide range of analytical applications. However, to gain a reliable description of structures and processes on a molecular level, data from different spectroscopic and spectrometric techniques have to be combined for interpretation.

Getting a sample of an unknown organic compound for structural analysis is like receiving a present in a gift box. The receiver of the gift is likely to be inquisitive, shaking the gift box lightly. Next, he or she might make

MARKES international

VOCs in air?
Talk to the experts in sampling and analysis

Markes International leads the world in analytical thermal desorption (TD) and associated air sampling technologies.

Why buy from us?

- Best analytical performance.
- Versatile and reliable – full compliance with key standards e.g. EPA Methods TO15/17 and 325.
- Money-saving and high-throughput – operates cyrogen-free for up to 100 tubes or 27 canisters.
- Expert support.

For further information visit www.markes.com

enquiries@markes.com

A company of the SCHAUENBURG International Group some estimations about its content before unwrapping the present. A spectroscopist, however, does not really have the chance to unwrap the object in the gift box. Rather, a given spectroscopic method can be used to take a look inside the box. The analytical process at work here can be described as making a little hole into one side of the box and looking into it with a magnifying glass. The view into the hole provides a single two-dimensional image of the three-dimensional object within. Notably, it only allows a view from one spatial direction. An interpretation of the view can be made by the spectroscopist, resulting in a conclusion about the structure of the wrapped object.

Let's assume the first spectroscopist, Nicolas M. Resonance, sees a ring-like object when he looks through his little hole in the gift box. In the interpretation, he will use all of his knowledge and experience about three-dimensional structures of circular looking objects. This will likely lead him to the conclusion that there is almost certainly a ball inside the box. The second spectroscopist, Mary Spectrometry, makes a second hole in the box from another spatial direction. She has a completely different view of the object and sees a rectangle. The rectangle does not have a perfect shape – its two shorter sides are slightly curved. But in her opinion, this effect can be explained by inaccuracies in the measurements. She therefore concludes that there is certainly a cuboid in the box.

Presumably, M. Spectrometry and N. M. Resonance will strongly disagree about the shape of the object in the gift box. They turn to Ian Red, also a spectroscopist, to make another hole in the box from a third spatial direction. His impression is rather similar to those of M. Spectrometry. He also sees a rectangle with two slightly curved sides and also draws the conclusion that there is a cuboid in this box.

At this point, two of the three spectroscopists agree about the structure of the object, which is hidden in the gift box. They write a joint publication, not considering or mentioning the results of N. M. Resonance. The presented results and conclusions appear to be consistent, and are hence accepted for publication and quoted in future papers. However, the conclusion about the structure has a slight blemish: it is completely wrong!

Considering all results of the three analyses, including the slightly curved sides of the rectangles would lead to an entirely different and somehow surprising conclusion about the object's structure. A cylinder explains all three two-dimensional views, which have been gained from the different spectroscopic methods. Therefore, a joint publication from N. M. R., M. S. and I. R., probably together with some other spectroscopists, presents a well-founded and reliable argument about the cylindrical structure in the gift box.

The moral of the story? Sometimes even two techniques are not enough to find the right answer; it makes much more sense to combine all the results from several different analytical methods – especially when there is any doubt.

Of course, though such an approach sounds logical and simple in theory, there are often many factors that block the way to finding the correct solution. And sometimes communication between researchers isn't always as good as it should be. But if we spectroscopists work well together, there are very few difficulties we cannot overcome.

Moving Lab Safety Higher Up the Agenda

The death of a University of California staff research assistant back in 2008 put safety concerns on the agenda. Where are we now?

By Kimberly Moser, instructional laboratory manager, Department of Chemistry and Biochemistry, University of Oklahoma, USA.

Typically the halls of education within our 'ivory towers' are filled with tradition, so making changes can be difficult and slow. Everything from curriculum to regulations and compliance for things like laboratory safety can be affected.

Bluntly put, academicians dislike being told what to do – and this is exactly what compliance and regulations try to accomplish. Many academic environs continue to be "buried in the lab bench" despite all the publicity surrounding accidents. In my opinion, a single motivated person can make a difference when it comes to opening a discourse on safety in the laboratory and starting positive change on behalf of students, graduates, faculty and staff. However, they need to think about how the topic is approached and be mindful that culture change can be a slow continual process over several years, particularly as the population is so fluid. Therefore, it is the long-term employees that must form the core around which culture change evolves.

I am witness to this type of environ and the unique situations involved with making changes to any part of the program. For me, it all comes down to the students; without them there is no university. When I started 11 years ago, safety was lax. Accidents happened frequently and no one had accountability despite liability being firmly ensconced on the university. Now, the media, courts, families and regulatory agencies like to associate names and faces with liability when incidents occur. In my own area – I am that person.

Having a responsible party overseeing laboratory safety is key to developing a safety culture. The person needs to be able to take the lead and develop material for the laboratories based on the audience. In the case of undergraduate teaching laboratories, for example, such material needs to be easy to understand and presented in a non-threatening, every day manner. Yes, there are rules and regulations to be followed, but having participatory activities that explain why these rules are in place helps everyone understand the importance of being compliant.

I also think that the integration of first-hand experiences is important, so that both students and colleagues do not perceive you as preaching or self-righteous. I have worked in laboratory environments since I was sixteen and I have accumulated spectacular, true-life tales of near misses, disasters and miraculous outcomes, many of which actually happened to me. I use these experiences with a few props or pictures to further demonstrate what can go right and what can go wrong. In addition, I believe in what I am presenting, because an audience will not tolerate fakery for the purpose of being right. Above all, I try to make my discussion interesting and if possible interactive.

Laboratory safety consistency can be maintained by having active, dedicated individuals involved – and over time the safety culture will change as rules and regulations are integrated into everyday tasks, such as laboratory prep ("Please put on your protective equipment before getting out the glassware!"). If you are the responsible person, be responsive and willing to answer questions, but above all do not hide behind the regulations. When people realize you genuinely care about them, they will have a greater understanding and patience of things you ask them to do.

39th International Symposium on Capillary Chromatography & 12th GCxGC Symposium

May 17 - 21, 2015 Ft. Worth, Texas

www.rivaintexas.com

The International Symposium on Capillary Chromatography (ISCC) is the premier meeting for pressure and electrodriven microcolumn separations and related techniques. GCxGC brings together world leaders in the application of comprehensive multidimensional gas chromatography. Together, these meetings provide a rich forum for fundamentals and applications of widely used analytical techniques. Visit our website for more information about short courses, speakers, student travel grants, and a complete list of awards.

Plenary lectures by:

George Whitesides (Harvard University) &

Sandy Dasgupta (The University of Texas at Arlington)

Registration and online abstract submission is now being accepted!

www.isccgcxgc2015.com

What Do You Want 'Now'?

Safer than radioactive labelling, fluorescence detection offers workflow streamlining and quicker results.

By Andrew Dix, staff scientist, Thermo Fisher Scientific, Eugene, Oregon, USA.

We live in a world of 'now'. How many times have we heard "I need these results ASAP", or dreaded, "I can't even start my all-day experiment until I run another experiment to standardize my samples", turning your 10-hour day into a 15-hour tour-de-force?

It's not always been this way. We scientists are stereotypically meticulous, detail-oriented, and borderline obsessive about our work. We appreciate that good results take time. While this remains true, with the rise of technology, the availability of information, and the ever-increasing pressure for results, we scientists can no longer afford to labor as we once did.

'Now' isn't simply a millennial mantra. Businesses have been thriving on 'now' for years. In the world of analysis, instruments and protocols are being geared toward simplifying and streamlining, with a focus on minimization and faster throughput without compromising the integrity of the results. While businesses may use this approach to leverage new products, the end result for the bench scientists is that they can get their work done quicker. For example, if we don't spend several hours making buffer from scratch and pH balancing it and instead buy it in "just add water" packets, then we can get to our real experiments quicker. And if we no longer have to filter our samples several times before running them through the newly optimized flow cytometer, then we can get our results quicker. These workflow changes are already happening, and as bench scientists, this means that we can do the same amount of work in a fraction of the time.

Many workflows require standardization, either to previous samples or to established values. For these experiments, which are in fact most analytical experiments, this is a repetitive, time consuming, and often monotonous task taking up valuable time before one can get on to the real questions. We should be able to streamline this workflow and allow scientists to get to the good stuff more quickly. In a time when my dog can have a Bluetooth collar or my car can have its own Internet connection, this doesn't seem to be asking too much.

Personally, I spend most of my time working with fluorescence-based quantitation. Most labs have left (or are leaving) radioactivity-based assays in favor of this more eco- and user-friendly class of reagents. Indeed, it appears fluorescent reagents can be used to measure almost anything these days from DNA to heavy metals and from enzymatic activity to cell viability. Also, most half maximal effective concentration (EC50) assays and flow cytometry analyses are built on florescence. But in the age of 'now', why am I still preparing a 10-point standard curve for my single unknown sample every time I run an experiment? With instruments and reagents both evolving, why can't the workflow?

When the Qubit Fluorometer was introduced a few years ago it changed the landscape of fluorescence-based detection. Its programs are equipped with a pre-optimized standard curve allowing the tablet-sized benchtop instrument to report on the concentration of your analyte with a mere five to 15 minutes worth of prep-time. The user only has to prepare their unknowns and transfer the pre-made standards. Currently, the instrument primarily works for DNA, RNA and protein quantification. There are also online resources to enable the user to quantify cholesterol and glucose. Using the customizable MyQubit interface, I have helped to expand this from the molecular biology realm to peroxide, sucrose, galactose, glutamic acid, and green fluorescent protein (GFP). While these assays aren't as streamlined as those currently existing (yet), any user can build a new detection application and expand on this list. This is fluorescence-based quantitation in the age of 'now'.

"If my dog can have a Bluetooth collar or my car can have an Internet connection, a streamlined work flow doesn't seem too much to ask."

As an R&D scientist working in cell biology, I have an opportunity to help streamline the analytical experience for others. There are thousands of fluorescent reagents out there capable of detecting thousands of analytes. We are working to tap into this vast wealth of possibilities and help other scientists analyze their samples – any sample – with more efficiency so that they can get on with their real experiments quicker and with confidence. Good results will always take time, but in the age of 'now', I don't think increased efficiency is asking too much. So... what do you want 'now'?

- High-performance NMR system for every chemistry lab
- Perfect for Chemistry Education, Synthesis Confirmation and Reaction Monitoring
- ^{1}H, ^{13}C, ^{19}F & ^{31}P options plus advanced 2D NMR experiments for research
- Spinsolve is quick and easy to use with low purchase & running costs…and no cryogens

Contact Magritek now for a quotation & demonstration
sales@magritek.com

USA +1 (855) 667 6835
Germany +49 (241) 70525 6000
NZ +64 (4) 920 7671

Visit the web and learn more
www.magritek.com/spinsolve

magritek
www.magritek.com

A Briefcase Full of NMR

One half of The Blues Brothers – Bernhard Blümich, a leading expert in compact nuclear magnetic resonance (NMR) spectroscopy – shares the story behind the innovative technology that is enabling scientists to perform spectroscopic analyses in minutes instead of hours or even days.

By Iestyn Armstrong-Smith

In the late 1940s and early 1950s, NMR spectroscopy opened up a new world of knowledge (1). Today's impressive high-field instruments use powerful, helium-cooled superconducting magnets to provide unprecedented resolution – in other words, they are expensive and large, which restricts their use to specialized facilities with plenty of floor space. It took a brainstorming session and a simple question about simplicity to spur development in a different direction – downsizing.

Call them portable, benchtop or compact, these smaller devices are cheaper, they are robust and they can be moved from bench to bench. And, though they are clearly not a replacement for the larger scale systems required for investigation of complex molecules, portability has made NMR spectroscopy more accessible to a wider range of scientific investigators.

Indeed, the greater availability of benchtop, transportable instruments is opening up new opportunities for biochemistry and organic chemistry, quality control and chemical reaction monitoring, where smaller molecules are the target. And recent advances in miniaturizing magnet and radio frequency (RF) spectrometer electronics point the way to truly portable NMR spectroscopy (2).

"Compared with high-field NMR, the benefit of benchtop NMR is the speed that you get results. It takes just a few minutes, including sample preparation," says Bernhard Blümich, a professor and chair of macromolecular chemistry at RWTH Aachen University, Germany, and one of the leading experts in the field.

"Traditionally, with high-field NMR spectroscopy the user prepares a sample, puts it into a sample tube, sends it to the NMR lab (usually down in the basement of the building) where it goes into a sample changer. The sample eventually gets measured. And, if they're good results, they'll appear on the intranet so that the chemist can check whether the reaction went the right way. All of that typically takes half a day, sometimes a full day," says Blümich, who points out that he has an advisory and commercial interest in Magritek, a company that specializes in cryogen-free, compact NMR and magnetic resonance imaging (MRI) systems.

On a mission from God?

Let's go back to 1993 and a brainstorming session between "The Blues Brothers" – as Blümich and his friend Peter Blümler were known (Blümler is currently a senior scientist in the Institute of Physics, at Johannes Gutenberg University in Mainz, Germany).

"Peter is extremely creative and out of our brainstorming came the question: 'Why can't we simplify NMR?' The manufacturers at that time were all building instruments using superconducting magnets, aiming for higher and higher field strengths and they were complicated – they still are. We started to consider the simplest way to get an NMR signal. Admittedly, we hadn't given much thought to applications at that stage. Peter drew a design and that led to the development of a small sensor now known as the NMR-Mouse," says Blümich. Mouse stands for "mobile universal surface explorer."

A few years later, after that initial mind-melding session, Blümich moved to the university in Aachen and hired Blümler to work in his lab.

"The Blues Brothers were back together and our first project was to actually build the NMR-MOUSE. We got our first signals from that initial instrument in 1995. The sensor uses what is generically called stray-field NMR and we used it to test various materials. We looked at the signals and investigated their differences – and we also looked at increasing sensitivity so that we could measure faster. In the early days, it could take 20 minutes to get a signal, which was impractical but fine for our investigations. It kept our students enthusiastic and curious, because it was a fun thing to do," says Blümich.

Funding the compact revolution

The German Research Society funded Blümich's group investigation into single unilateral imaging – or single-sided MRI – which gave them some financial security, although he now views the technique as obsolete.

"Single-sided MRI as far as I am now concerned is a dead end. It's interesting scientifically, but from a practical point of view it is useless. We then received funding through a European Community Project on Cultural Heritage award, where the NMR-MOUSE again came into play for investigating works of art, which was published in Scientific American (3)," he says.

Because of the funding, the group was able to improve the technique, plus Blümich reports that he was fortunate in having some very good students who were able to optimize the sensor's stray field shape. Blümich started up a small company to manufacture the NMR-MOUSE, to meet demand for the device. Much has been done to reduce the size of the sensor, which is now available in sizes of less than 2 cm^3 – and they are likely to be even smaller in the future…"We kept looking forward and our next step was to build a permanent magnet suitable for spectroscopy. It had been done before, but the magnets were huge. Varian, for example, had produced a beautiful machine, but it was cubic meter in size, so it was more floortop than benchtop… Our aim was to build a much smaller device, which we thought would be feasible if we could get the magnet right," says Blümich.

"We needed to know whether we could build a small magnet with a homogeneous field. Now, many will say that you can't have a homogeneous stray field field outside of the magnet, but that's not completely true or, in practical terms, relevant. What you really need is sufficient homogeneity to achieve good chemical analysis. It doesn't have to be a completely homogeneous field; it just needs to be good enough."

Sheer magnetism

Federico Casanova and Juan Perlo, two of Blümich's post-doctoral researchers, built a small magnet that measured no larger than a C-size torch battery and could be used with a 5 mm sample tube (4). The magnet had a field strength of 27 MHz proton NMR frequency, which could be adjusted using shims, meaning that such a permanent magnet could be used to perform spectroscopy.

"Magnets aren't expensive and are readily available from many sources in China; however, the big issue is quality control. Every magnet with supposedly the same specifications will vary in geometry and size. Also, the granular structure of the sintered material used to manufacture the magnet will vary, which affects the direction and magnitude of magnetization. And that affects homogeneity," says Blümich.

Apparently, the best way to build a magnet to overcome these problems is to use the design proposed by Klaus Halbach back in 1980 (5). Blümich adds, "The best homogeneity for a magnet is 10^{-4} and we need this to be 10^{-8} for spectroscopy – which means the magnetic field across your sample tube should not vary more than 10^{-8} of your total magnetic field. As scientists we deal with numbers such as 10^{-23} and so on. But, 10-8 is like building a 100 km long x 1 mm thick road or having the ability to spot a truck on the moon. So that's the type of precision we want. Of course, you can do this with big superconducting magnets – but Federico and Juan achieved it with a battery-sized permanent magnet based on Halbach's design."

Success breeds success

Casanova and Perlo's magnetic prowess led to the formation of a new business called Magritek, which Blümich set up with the late Sir Paul Callaghan. He developed the electronics in New Zealand, while the group in Aachen continued to develop the magnet.

Today, desktop spectroscopy is not better than high-field spectroscopy in terms of resolution, chemical shift and dispersion, but it does offer features that the latter lacks, Blümich says. "You can take a benchtop instrument and put it inside a fume cupboard to observe a hazardous reaction as it happens. You can't do that with a high-field machine down in the basement of a building – the lack of convenience, the fact that you'd hold everyone else up and the expense of replacing the spectrometer if something goes wrong, make it impractical.

"So, the beauty of these small devices is the ability to do reaction monitoring in situ – and that saves a lot of time and effort when performing product, quality or reaction control during synthesis. It takes only 10 minutes from sample preparation to obtaining the results to do – the spectrum takes only one minute to develop. That has to be interesting for both academics and scientists working in industrial labs."

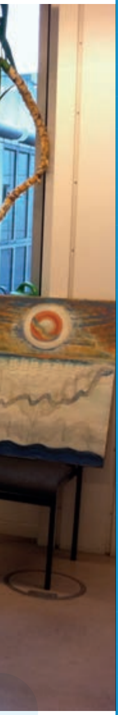
Blümich says the sensitivity of compact instruments is constantly improving and he says achieving homogeneity is the key to this. "Some say that sensitivity is proportional to field strength, but I believe homogeneity is more important. Think again about the truck on the moon – I may be able to see the whole, but how much of it can I see in detail? With improved homogeneity, comes better discrimination of the molecules or chemical groups of interest.

"And chemists don't really care about your spectrums or if there are some effects going to different fields; he or she just wants to know how many scans will it take to measure the substance and how long it will take to do the experiment and whether all the necessary information will be available. That comes with homogeneity."

Finding The Holy Grail

Carbon-13 was discovered in 1945 (6) and ^{13}C spectroscopy was still seen as miraculous when Blümich began his PhD in 1977. Today, it's just a commonplace feature of modern high-field machines. Now, it is also possible to perform it with a benchtop device.

"We've been able to measure ^{13}C spectra with the Magritek, which is unusual; we're also able to produce two-dimensional NMR spectra. Ultimately, what the chemist needs out of a workhorse benchtop machine is the ability to get more than one-dimensional proton spectra. So, they will do a simple analysis, then run a ^{13}C spectrum – and if they want even more they do a



Clockwise from top left:
Wasif Zia analyzing Beltacchi forgeries at the state bureau of criminal investigations in Berlin in 2011; The Blues Brothers: Peter Blümler (left) and Bernhard Blümich (right); NMR spectroscopy – on the bench; even babies like the NMR-MOUSE…; Federico Casanova measures a Rembrandt painting at Walraf-Richartz Museum in Cologne in 2010; first measurement outside with the NMR-MOUSE in 1995 with Gunnar Eidmann testing a tire from Blümich's car; Bernhard Blümich, Federico Casanova and Juan Perlo measuring "Ötzi the Iceman" at the Archeological Museum in Bozen in 2006.

Magnets to Market

Andrew Coy, CEO of Magritek, shares his vision of the future.

What is Magritek's contribution to the field of benchtop NMR?

In the last two years, we introduced a high-performance benchtop NMR spectroscopy system called Spinsolve. It has been very well received in terms of design, performance and capability. Indeed, our industry is going through a very exciting time; we are not the only company selling these instruments, and many people now recognize the benefits that benchtop and portable NMR systems bring.

What does the benchtop market look like today?

Process chemists and chemical engineers are using our technology to monitor reactions in real time using continuous flow NMR operation. These customers come from a range of industries from pharmaceutical to petrochemical to polymers. We also supply our machines to universities and contract research organizations for research and education applications. Some of the new and emerging sectors are in the food industry using NMR spectroscopy to detect adulteration from a quality control perspective.

One of the most recent and compelling benchtop NMR stories is that of Lee Cronin's group at the University of Glasgow. He took the concept of self-optimized flow systems with in-line analytical monitoring and extended it so that multinuclear and 2D NMR can be performed in the fume hood (1).

What direction is compact NMR moving?

As the field develops, we think NMR will become a far more common analytical measurement technique. Instead of centralized facilities there will be NMR available in the lab next to all the other techniques. You no longer need to be an NMR expert to operate the instrument; in fact, we envisage many applications where the customer does not need to see a spectrum and just gets a result that is useful and valuable. I believe we will see NMR being deployed in a range of environments and applications where people previously considered it impossible.

Where will we be in 10 years?

Over the next five to 10 years, we expect to see benchtop NMR spectrometers appearing in a large percentage of chemistry labs alongside other analytical instruments. We'll also see new designs that are more robust so that they can be placed in production environments for process control applications, although we expect it will take longer to develop these markets.

NMR spectroscopy is one of the most useful and information rich spectroscopy techniques available to a chemist today. However, the traditional cost, size and fragility of the instruments has meant they are only available in centralized facilities and access is tightly controlled and managed. We think benchtop NMR will enable more people to benefit from the technique, and in turn, funding for research and development in NMR is likely to increase as the value and utility of the technique increases.

Reference

1. L. Cronin et al, Chem. Sci., 2015, DOI: 10.1039/c4sc03075c

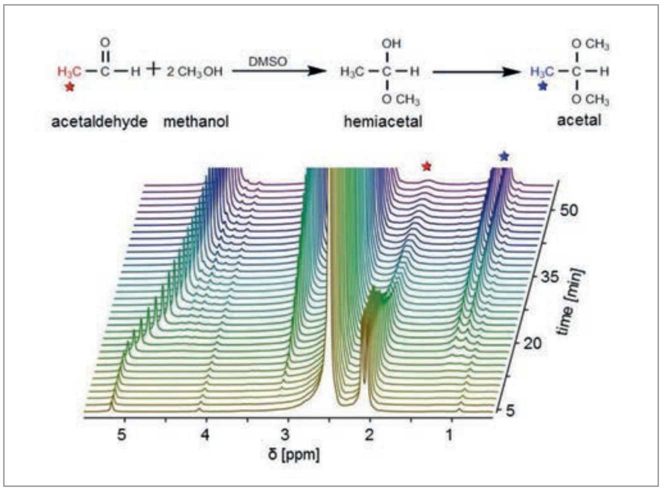


Figure 1. Acetylization spectrum obtained from benchtop NMR spectrometer.

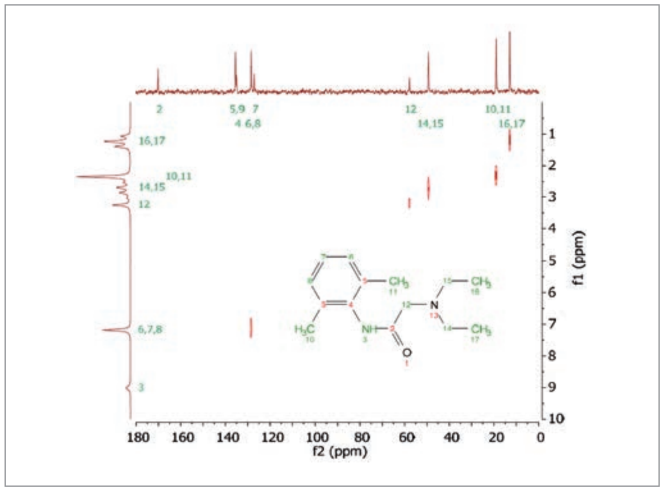


Figure 2. HETCOR spectrum of 1 M lidocaine in CDCl3 obtained from benchtop NMR spectrometer.

2D or even a DEPT spectrum, which will edit the ^{13}C spectrum into the different chemical groups," says Blümich. "Eventually, small desktop spectrometers will cover more and more of the ground that high-field machines are used for today. However, the very high-sensitivity of high-field machines will be maintained as they are needed for large molecule work, such as protein structure determination. But, science is full of surprises, so who really knows what we shall see in the future; three years ago no one would have believed that ^{13}C 2D spectroscopy would be possible on a benchtop machine."

Looking to the future

Blümich sees a very clear path for future developments worldwide, with smaller magnets enabling the manufacture of even smaller and more powerful spectrometers. "I'm relatively cautious with my predictions, but I am intrigued by Google[x] Life Sciences. Two NMR specialists – Vik Bajaj and Vasiliki (Vicky) Demas – are leading the team. Vicky in fact did part of her PhD in my group and researched portable magnetic resonance (MR) and ultra-low field MR imaging (MRI) in the laboratories of Alexander Pines, Jeffrey Reimer, and Robert Maxwell, with research applications in chemistry, materials, and biology.

"Vicky also worked at T2 Biosystems, a company that manufactures benchtop spectrometers for analysing human fluid samples using functionalized nanoparticles to identify disease markers. She also had the idea of an NMR tricorder."

The tricorder idea was investigated further by Blümich's group, with a student being assigned a feasibility study to design what it would look like as an end-user device for personalized medicine.

Blümich explains, "It would need to be as small as possible, capable of accepting human fluid samples and using lab-on-a-chip chemical analysis. It would feed it into a miniaturized NMR machine about the size of a smartphone, which would house the magnet and all the software. The phone transmits the data over the internet to do the chemometrics analysis and comparison against various databases before sending the information back to the user. It would tell you important information about your nutritional needs, exercise plan, whether you ought to see a doctor, and so on.

"We grew up with fever thermometers and in the age of smartphones these will be replaced by smart analytical devices, which will likely include a magnetic resonance analyzer together with other detectors. NMR has outstanding spectroscopic specificity, and by enhancing the sensitivity using functionalized nanoparticles, you can look at blood and other opaque samples, which other types of spectroscopy cannot do.

"We also need to consider the miniaturization of NMR electronics by Donhee Ham's group (7). The ability to produce a 2-cm^2 chip, including RF amplifiers enables the electronics to disappear into the magnet. Therefore, the dominant size determining component of a compact spectrometer is the magnet – and we are working hard on making that smaller as well!"

References

1. *Purcell group, Harvard University; Bloch group, Stanford University. Edward Mills Purcell and Felix Bloch shared the 1952 Nobel Prize in Physics for their discoveries.*
2. *R. Whitworth, "NMR Seeds of the Future", The Analytical Scientist, September 23, (2014). https://theanalyticalscientist.com/issues/0914/nmr-seeds-of-the-future/*
3. *B. Blümich, "The Incredible Shrinking Scanner: MRI-like Machine Becomes Portable", [Preview] A portable version of a room-size nuclear magnetic resonance machine can probe the chemistry and structure of objects ranging from mummies to tires, Scientific American, Oct 3, (2008).*
4. *E. Danieli et al., "Small Magnets for Portable NMR Spectrometers", Angew. Chem. Int. Ed., 49: 4133–4135 (2010). DOI: 10.1002/anie.201000221*
5. *K. Halbach, "Design of Permanent Multipole Magnets with Oriented Rare Earth Cobalt Material", Nuclear Instruments and Methods 169 (1): 1–10 (1980). DOI:10.1016/0029-554X(80)90094-4. ISSN 0029-554X.*
6. *W.F. Libby, "Atmospheric Helium Three and Radiocarbon from Cosmic Radiation", Physics Review 69: 671–672 (1946). Bibcode:1946PhRv...69..671L. DOI:10.1103/PhysRev.69.671.2.*
7. *D. Ha et al, "Scalable NMR Spectroscopy with Semiconductor Chips", PNAS 111 (33) 11955-11960 (2014). DOI: 10.1073/pnas.140201511*

Giants Go Pico

Mark Dixon, NMR product manager in Molecular Spectroscopy at Thermo Fisher Scientific, sheds light on how the NMR market may evolve.

Where are we now?

NMR spectroscopy has been out of reach for so many scientists due to the large cost of entry and subsequent cost of ownership. Previously, to satisfy their need for the unique information that NMR spectra provide, companies and institutions that could not afford to own or run one for themselves have had to use core or external facilities at great monetary and time cost. The affordability and convenience of a benchtop NMR spectrometer makes great sense, and the vast majority of analyses using NMR can be achieved using sub-100 MHz instrumentation. Currently, the organic chemistry education market appears to be the battleground. Various industrial applications are coming to light: food safety, polymers, petrochemicals, and illicit drug analysis, to name a few, but the vast majority of sales today are primarily being made in educational institutions ranging from two-year colleges to four-year degree universities.

Where are we going?

The benchtop NMR field is probably going to split into two distinct markets over time: i) undergraduate teaching and simple industrial applications, in which today's technology more or less already covers the scope of the needs; and ii) research instrumentation that complements the high-field NMR market. In the latter market, some significant engineering challenges must be overcome before the quality and speed of data collection is up to a standard where a research chemist would use a benchtop NMR instrument for everyday use, only relying on their centralized high-field NMR facility for specialized work.

Where will we be in 10 years?

The next five to ten years will probably see one or more of the smaller players disappear, either by acquisition or for financial reasons; street prices will inevitably come down over time, which may challenge any small business that has high costs or limited reach.

Another component that may drive the uptake of benchtop NMR is any dramatic rise in liquid helium prices due to a predicted drop in supply, which will have a severe effect on the remaining high-field NMR vendors who rely on liquid helium to keep their magnets superconducting. Capabilities of the benchtop instruments themselves should approach those of the current crop of budget-class high-field instruments, but at lower magnetic field strengths.

A new field for portable NMR is likely going to be in process analytical technology. On-line or at-line usage of benchtop NMR in a pilot plant, for example, should be a valuable addition to chemical engineers who currently only use NMR in special situations for troubleshooting. The potential for benchtop NMR in more biochemical or biological applications has not been widely tested or proven yet, but one can see where unique structural information present in NMR spectra would also be of great benefit in those areas.

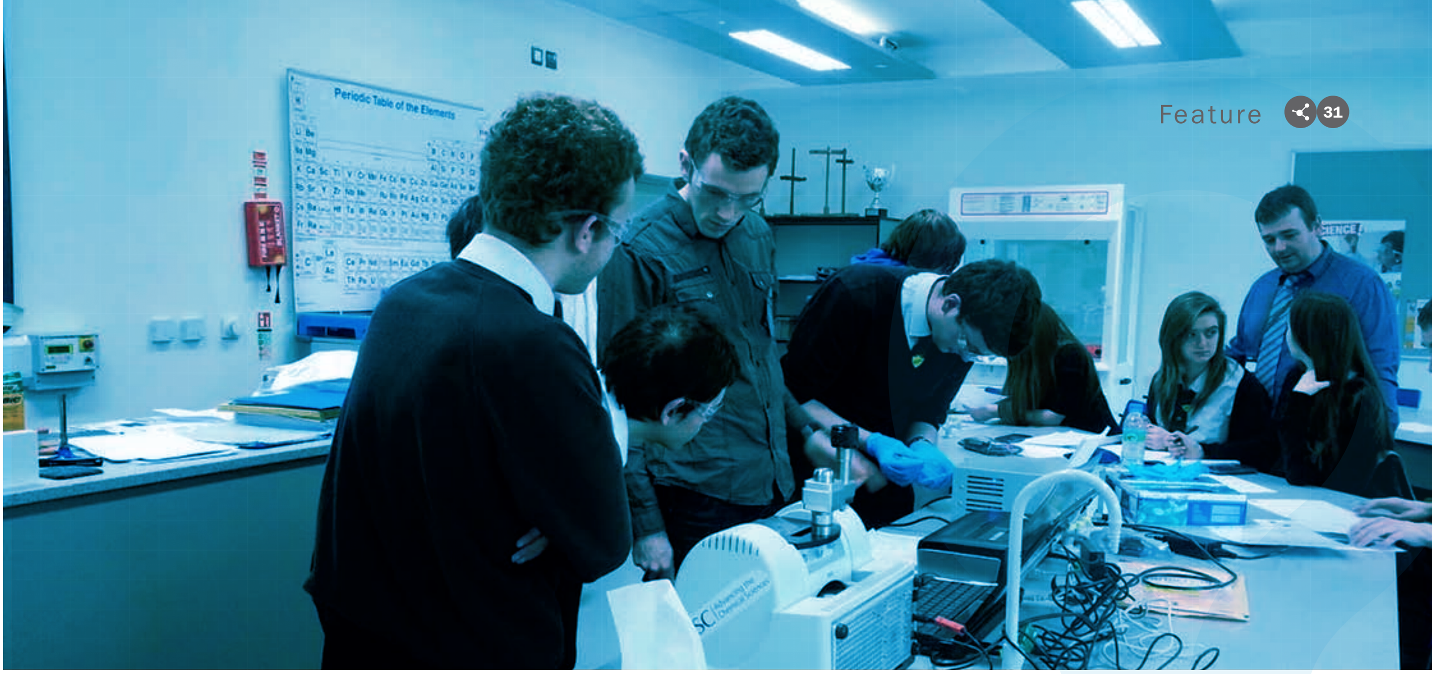
Spin Snapshot

Tyler England, mechanical engineer at SpinCore Technologies Inc., puts compact NMR in a nutshell.

Market We sell portable NMR devices (the iSpin series). The iSpin-NMR is a complete system console for NMR with spectrometer frequencies from 0 to 100 MHz. The NMR marketplace is growing – we are seeing steadily increasing sales.

Applications Applications are diverse: process control, explosives detection, porous media, solid-state and solution-state NMR for characterization, high-resolution solid-state NMR under MAS (magic angle spinning), wellbore NMR, multi-spectral sensing on autonomous vehicles, medical imaging, quantum computing, optically detected NMR, solid-state physics experiments, nanomagnetism and spintronics – and many others. All of our customers are doing interesting work with NMR. Many of them work with healthcare or academic research applications.

Future Applications for NMR are already widespread – as the technology improves, there is no telling where it can ultimately end up.



Never too Young to Learn

More than 15,000 UK school students have been given the opportunity to learn about spectroscopy through hands-on experience thanks to The Royal Society of Chemistry's Spectroscopy in a Suitcase (SIAS) scheme.

By Claire Doyle, Spectroscopy in a Suitcase UK and Ireland Coordinator, Student Recruitment and Outreach, The Royal Society of Chemistry, London, UK.

When the SIAS scheme started in 2008, the standard kit included a portable IR spectrometer and a UV-Vis spectrometer. Now, we've introduced portable NMR spectrometers into the mix. As well as covering the principles of spectroscopic techniques, our activities primarily use real-life contexts to demonstrate the applications of various techniques.

Modern analytical techniques are a core part of post-16 learning, but high costs of instrumentation and lack of technical support means that most schools do not have access to spectroscopic equipment. SIAS provides access to both the instrumentation and the analytical support through undergraduates and postgraduates at SIAS Host Universities, which not only aids understanding for school students but also provides a glimpse into the kind of practical work that may be included in a university degree.

The feedback received from both students and teachers taking part in this programme indicated clearly that the most valuable improvement would be the introduction of practical hands-on NMR experience. Thanks to funding from the Welsh Government through a National Science Academy grant, we were able to pilot the use of portable NMR spectrometers in 2013 – we now have nine Thermo Scientific picoSpin NMR spectrometers based at SIAS Host Universities across the UK. Students can compare IR with NMR spectroscopy for a range of chemicals, which supports theoretical knowledge and offers students a unique perspective that is currently often only available to PhD students.

NMR spectroscopy is the method of choice for many organic chemists because of its versatility in determining molecular structure, measuring reaction kinetics, monitoring reaction progress and controlling product purity. Students learn that the technique provides a wealth of information on chemical and structural aspects of molecules. We also describe its many applications in process control, whereby the quality of a chemical product, such as petroleum, biodiesel or food and drinks, can be followed by NMR. In situ monitoring and testing of process applications is also possible, as NMR is a non-invasive, non-destructive technique.

Benchtop NMR spectrometers are cryogen-free and our SIAS instruments have a temperature-controlled permanent magnet. They are portable (making them ideal to transport to schools), easy to operate, and affordable. Moreover, they can be set up and ready for use in an acceptable time: approximately one hour for the magnet to warm up, 15 minutes to shim, and only a few minutes for sample acquisition.

The development of benchtop NMR spectrometers has really improved access to this technique for research, undergraduate teaching and most excitingly, in schools. More recent developments in this field seem to be focusing on making this technology even smaller and more portable, whilst increasing resolution to reveal chemical information not available using smaller magnetic fields – that's exciting to hear.

Feedback from schools has suggested that a portable mass spectrometer would be beneficial for students. The technology already exists, we just need the funding to expand into this area!

If you would like to more about SIAS, visit: tas.txp.to/0315/SIAS


UTAS

The Cream of Chromatography

We started with a simple question: who's leading the way in chromatography? Here, we present our findings from a publication and citation analysis of international institutions represented in The Analytical Scientist's 2013 Power List.

By Xiaoying Geng, Fuling Li, and Qi Wang

Chromatography is a powerful tool that plays a very important role in both research and economic development. But – as with other sciences – comparing and ranking institutions and their academic achievements can be tricky. In 2013, The Analytical Scientist compiled The Power List, which featured "the top 100 most influential analytical scientists" (1), including 37 chromatographers from 31 institutions. Statistical analysis of chromatography-related literature in the Web of Science allowed us to compare the number of SCI papers, the number of citations, and the number of highly cited papers of those 31 institutions.

Why?

Investment in science research and development has greatly increased as the Chinese economy has developed. Unsurprisingly, the government is very anxious to assess the impact of such support – and academic societies are also becoming increasingly interested in how they match up to international academic standards.

For us at the Dalian Institute of Chemical Physics, chromatography is a major research field and we have a large team focused on chromatography-centered analytical chemistry. We too became interested in learning how our institute was performing in the world of chromatography. Clearly, there is no standard for making such assessments – opinions can differ and any number of indices can be used, such as paper number, citation number, patents, awards, foundations, achievement revenue, and so on. In the beginning, we tried to use a method based on total publication numbers from the Web of Science. Unfortunately, certain well-respected and famous US universities were excluded based on metrics alone.

How?

How else could we judge impact? Well, the Analytical Scientist's Power List offered a new angle of approach. There were 37 chromatographers on the list, representing 31 institutions and 15 countries (among them, 15 from the US, five from China, three from Germany, two from Australia, two from Belgium, and one each from Canada, Finland, Hungary, Britain, Italy, Singapore, Japan and the Netherlands).

Generally speaking, the institutions represented on the Power List are at the top of their game, so we reasoned that if we wanted to learn more about our own institute's standing, a comparison should be made with "Power" institutions. Fortunately, three scientists from our own institute were included on the list, so that made any comparisons even more compelling.

Using the 31 Power List institutions as a starting point, we conducted a statistical analysis of chromatography-related papers in the Web of Science up until September 2014. Next, we compared the quantity and quality of papers published by these institutions to evaluate their development and international academic status in view of paper output.

The findings

Research by country

We used Topic=*chromatogr* to search for chromatography-related papers from "Science Citation Index Expanded." If "chromatogr" was included in the title, key words or abstract then the paper was included. As shown in Figure 1, from 2009 to 2013 the number of chromatography-related SCI papers from China has been significantly increasing year on year. Indeed, since 2011, the number of papers from Chinese scientists has been

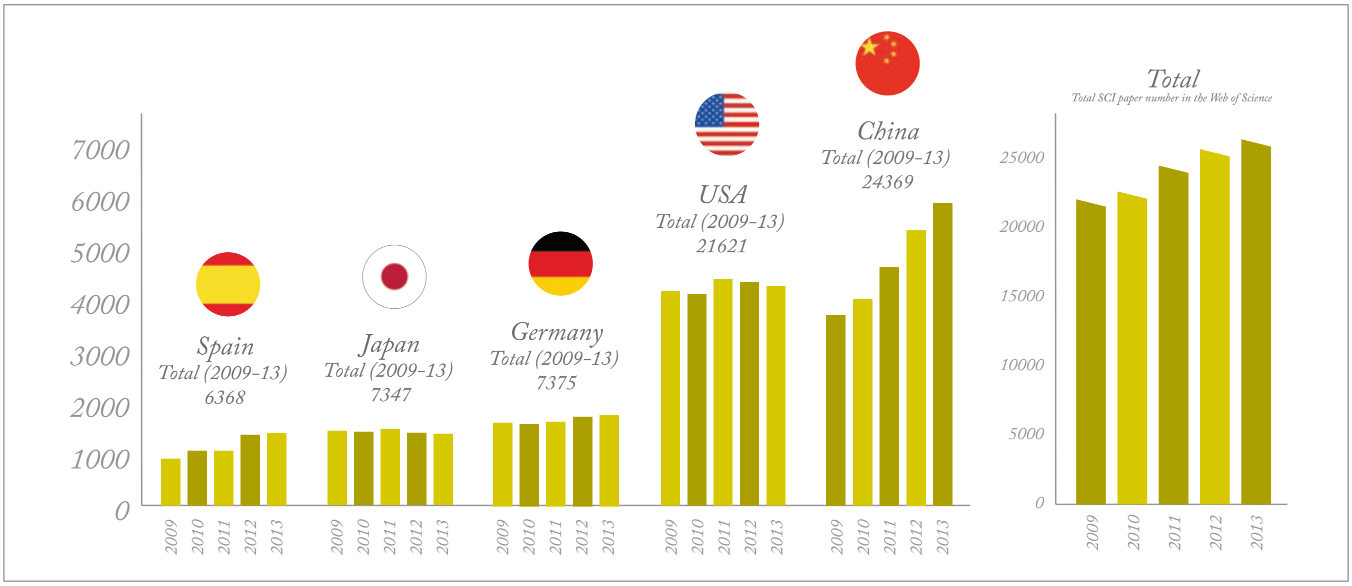


Figure 1. World's Top Five countries in chromatography-related paper quantity published 2009 to 2013.

greater than any other country; the US, Germany, Japan and Spain ranked from second to fifth respectively over the last five years. The data show that China has been focusing significantly on chromatography research and applications in recent years.

In particular, the main fields of interest are in new separation/analytical methods and techniques, new columns and enrichment materials, new equipment and applications of chromatography in environmental analysis and life science. China's rise to the number one producer of chromatographic research could be attributed to the technique's relative immaturity in the country compared with more developed nations whose research outputs are being maintained at a more steady state. Similar conclusions were previously reported in another literature analysis (2).

Research from "Power" Institutions

The 37 scientists in The Power List 2013 come from 31 institutions. However, the number of SCI papers published by AMT corp. were few, so we based our analysis on the remaining 30 institutions.

Table 1 shows that Ghent University, the University of Helsinki, the University of Washington, the University of Tennessee and the University of Michigan are the top five in terms of total papers produced. When looking at the last five years, our Dalian Institute of Chemical Physics moves up to second place (from sixth), pushing the University of Michigan out of the top five. We attribute this increase to proper research policies and growing financial support from both the institute and the Chinese government.

Citation power and quality

The number of SCI papers is an important parameter to evaluate the academic level of the Power Institutions, but we feel that much more attention should be paid to "quality". In literature metrology, citations are a very important indicator of the quality of a given paper and it can be argued that the higher the citation number, the stronger the academic influence of that paper. For example, the average citation number per paper of all chromatography-related SCI papers is 6.5. If the average citation number of an institution is higher than 6.5, we speculate that the institution lies somewhere between average and advanced in chromatography research. We performed a comparative analysis of paper quality in two ways: (i) the citation time per paper and (ii) the number of highly cited papers.

As shown in Figure 2, several institutions have a citation number per paper (total years) over 30, including the University of Washington, the University of Waterloo, the University of North Carolina at Chapel Hill, Indiana University Bloomington, the Lawrence Berkeley National Laboratory, the Kyoto Institute of Technology, the University of Michigan, and the University of the West of England. We suggest that these institutions are traditionally powerful in chromatography. In the last five years, the Lawrence Berkeley National Laboratory's citation number per paper has enabled it to climb up to first place, followed by the University of Michigan. The citation numbers per paper (total) of the three Chinese institutions are not very high; however, in 2009–2013, citations for the Dalian Institute of Chemical Physics' papers increased rapidly, raising the ranking from 27th to 9th.

Highly cited papers are determined as those ranked in the top 5 percent by citations in the chromatography-related field and year of publication. First, the minimum citation number of the top 5 percent of papers is acquired (42 for 2009; 34 for 2010; 24 for 2011; 15 for 2012; 6 for 2013). If the citation number of the paper is higher than the minimum number of the top 5 percent of papers in the published year, the paper is considered a highly cited paper.

From 2009 to 2013, the absolute number of highly cited papers published by the Dalian Institute of Chemical Physics is 60 overall, placing it first (see Figure 2). The University of Tennessee and University of Michigan come second and third, respectively.

Representing highly cited papers as a percentage of all papers published by each institution offers another snapshot of quality. The University of the West of England, the Lawrence Berkeley National Laboratory, and the University of Michigan take the top three spots in this analysis.

What does it all mean?

Many metrics can help characterize the international influence of an institution – publications, patent licensing, funding support, famous scientists, scientific achievement transformations are all credible approaches. But we feel that the analysis of academic papers is a concise and robust indicator of scientific research capacity – especially in terms of basic scientific research. In recent years, the number of papers published by Chinese scientists in chromatography-related fields has been increasing, putting China in the top spot in terms of quantity. Indeed, many leading Chinese scientists and institutions have been working hard on chromatographic research in the last five years – and some remarkable progress has been made, especially when it comes to new chromatographic material, sample preparation technology, metabolomics and proteomics research.

However, our analysis also shows that there is plenty of room for improvement in the quality – or influence – of Chinese papers. We believe that Chinese chromatographers should pay attention not only to the broader chromatography research frontier, but also to producing original and creative work.

Overall, chromatography research will continue to see increasingly complex systems, demanding higher resolution, higher precision, higher selectivity, higher sensitivity and higher throughput. And it is in those challenges that we are all united!

Xiaoying Geng, Fuling Li, and Qi Wang work at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China.

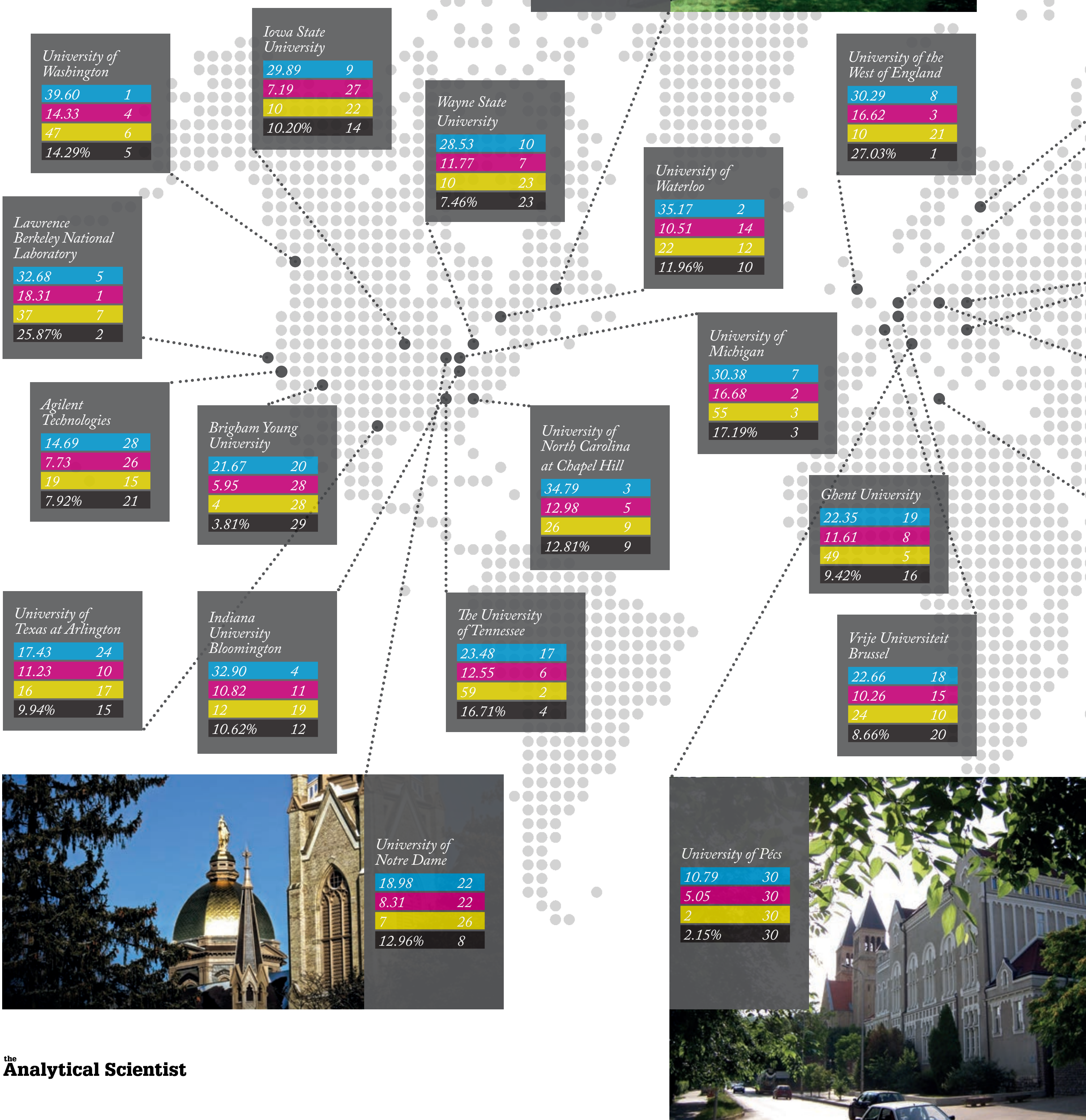
References

1. *The Power List 2013, The Analytical Scientist, 9, 23–37 (2013). (https://theanalyticalscientist.com/the-power-list-2013/)*
2. *X. Zhang et al., "Recent Advances of Chromatographic Research in China", Chinese J. Chromatogr., 30 (3), 222–231 (2012).*

Institution Name	Total papers	2009–2013 papers
Ghent University	2239	520
University of Helsinki	1969	395
University of Washington	1804	329
The University of Tennessee	1670	353
University of Michigan	1533	320
Dalian Institute of Chemical Physics, CAS	1453	504
National University of Singapore	1396	379
University of Tubingen	1335	165
University of Vienna	1293	253
Iowa State University	1208	134
University of North Carolina at Chapel Hill	1202	203
Vrije Universiteit Brussel	1147	277
University of Amsterdam	1115	205
University of Waterloo	783	184
Wayne State University	697	98
University of Tasmania	668	210
Indiana University Bloomington	610	113
Northeastern University	586	104
Institute of Chemistry, CAS	545	183
University of Messina	536	171
Brigham Young University	520	105
Agilent Technologies	498	240
Lawrence Berkeley National Laboratory	419	143
University of Pardubice	364	135
Kyoto Institute of Technology	363	46
University of Texas at Arlington	278	161
University of Pécs	269	93
Research Center for Eco-Environmental Science, CAS	219	103
University of Notre Dame	208	54
University of the West of England	126	37

Table 1. Comparison of chromatography-related paper numbers published in all years and in the last five years by "Power Institutions".

Figure 2. Comparison of citations per paper published in all years, and in the last five years; and highly cited papers (Top 5 percent papers) published in the last five years (2009-2013).



University of Helsinki

28.04	11
10.17	16
31	8
7.85%	22

University of Amsterdam

26.51	13
10.58	13
21	13
10.24%	13

University of Vienna

24.62	16
9.91	19
23	11
9.09%	18

Dalian Institute of Chemical Physics, CAS

14.84	27
11.24	9
60	1
11.90%	11

University of Pardubice

18.66	23
10.15	17
10	24
7.41%	24

Research Center for Eco-Environmental Science, CAS

15.71	26
5.32	29
6	27
5.83%	27

University of Tuebingen

25.84	14
8.18	23
11	20
6.67%	25

Institute of Chemistry, CAS

12.59	29
8.85	21
17	16
9.29%	17

University of Messina

17.38	25
7.87	25
8	25
4.68%	28

National University of Singapore

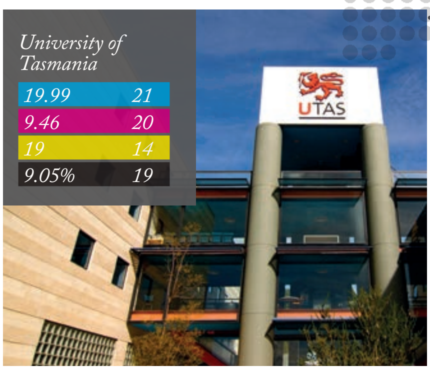
25.21	15
10.82	12
50	4
13.19%	7

Kyoto Institute of Technology

30.44	6
8.02	24
3	29
6.52%	26

University of Tasmania

19.99	21
9.46	20
19	14
9.05%	19



KEY

Total citations per paper / Rank

2009–2013 citations per paper / Rank

Number of Top 5% papers / Rank

Top 5% paper as percentage of all papers / Rank

CMC Workshop 2015

April 13-15

Hyatt Regency Bethesda
Bethesda, MD

Tabletop Exhibiting
Opportunity Available

DIA DEVELOP INNOVATE ADVANCE

aaps®

Interactive Workshop Focused on Current Chemistry, Manufacturing, and Controls (CMC) Challenges

Register at
DIAGlobal.org/CMC

We Don’t Need No Education?

Teachers of the analytical sciences have a hard job. Lesson preparation time is limited – and, if the teacher's own educational background is lacking, he or she could struggle to deliver what students really need. So, what is the answer? Here, I offer my opinions, while two initiatives – COAST and SALSA – really shake things up.

By Frank van Geel

The way in which today's students work and learn is continually changing. They have access to new educational tools and the Internet is always at hand if they want to look up something quickly. And, let's face facts, not all professors are good presenters, so listening to lectures can be a drag. Have you ever visited a lecture theater recently? If you have, you probably noticed that half of the students are busy with their smart phones, another quarter of them are pretending they are not asleep at the back, and those on the front rows are trying their best to please the professor by practicing their smiles. Only a few are really listening and trying to understand.

Is it a big problem?

I think it is. For example, it is clear that analytical science is a 'multiplier' in R&D. "If analytical science is zero, the outcome is zero," as Oscar van den Brink, managing director of COAST, noted recently. Today, therefore, the need for analytical knowledge and understanding both in industry and in academia is substantial. And this need crosses all areas: industry and academia, life sciences, pharma, petrochem... if these organizations fail to achieve good analytical results, their work comes to an abrupt end.

Slowly but surely the importance of analytical science is growing; however, some maintain it should grow faster. Fortunately, the need for it is strong, especially in the life science 'omics' areas – proteomics, metabolomics, and even foodomics – and also in imaging and clinical pathology cooperations. Analytical scientists are getting involved in numerous multidisciplinary projects; they can no longer afford to live their scientific life in their own silo.

Analytical scientists are by nature service oriented; they like to solve problems and they love to help others. It is a great attitude to have, but the downside is that they have failed to position themselves among the decision makers. And in universities they have often failed to position themselves within the academic groups that receive the bulk of funding. Additionally in industry, large service labs are taking over chemical analysis because they are fast and cost effective. They do what their customers ask of them and that is to deliver results, quickly and at low cost. For routine analyses this is fine, but I don't think they can always be relied upon to solve newer or tougher problems.

Meeting the educational challenge

Clearly, we need to focus on those students who are attracted to analytical sciences. They are the people who are fascinated by the immeasurable possibilities that analytical tools can bring them and also have the drive to find the answers to the many questions from society. We cannot spend our precious time on the backbenchers; we must focus on those students who occupy the front seats of the lecture hall and are keen to learn. We must attract their attention with interesting science and involve them in our world and work, making clear what we can do as analytical scientists. I think part-time professors who come into the universities play an important part in captivating the attention of the students as they can bring new perspectives. Finally, we need to step away from dull learning materials. Our goal must be to involve students instead.

"Flipping the classroom is the natural way to study for students these days."

Can new educational tools help?

Teachers have little time to prepare for their classes, plus they have to deal with a lot of unenthusiastic students. They need a solution that will give them more quality time with their students. In my view, lectures cannot be classed as 'quality time'. Students should be able to find the learning materials they need using their computers or tablets. There is an abundance of technological tools that facilitate electronic learning, but it isn't enough simply to give students access to materials – the material must be embedded in a stucture.

Flipping the classroom gives students access to lecture-style materials for study in their own time. It means that time with the teacher can be used to deepen their knowledge, ask questions, and solve problems. Involvement is strong and learning efficiency is high. This, in my opinion, is the way to go. The front row students thrive, and the unenthusiastic are tempted into engaging or lost (some were probably lost already). Flipping the classroom is the natural way to study for students these days. And it is the most efficient way – guidance is all that's needed.

There's an old Chinese proverb that goes something like this: "Tell me: I'll forget, show me: I may remember; involve me: I will understand." That's the true essence of learning. For analytical sciences this means that education will change immensely over the coming years. Educators will focus on getting their students more involved and we already see it happening in a number of initiatives in the world, for example, in large collaborative projects, such as COAST (see page 41) and SALSA (see page 42).

And so, the time is right for change. Students are telling us that they want to be involved, we have the right tools, and it is the direction in which general education is heading at an accelerated rate. It will go faster than you think, maybe faster than many would wish! After all, it takes real educational pioneers with great determination to go through all the trouble of preparing online classes in advance. Fortunately, we have such pioneers in all areas of analytical sciences, in industry, in universities and colleges.

Are we getting there?

Indeed, times are changing and it's exciting to be an educator; I see that with my involvement with Chromedia, which is pioneering education for analytical scientists. We started eight years ago by offering a web-based, interactive platform where experts put their expertise online; now it has grown to be a trusted source for many, including schools, universities, and industry.

Teachers approach Chromedia for help, industry collaborates with us to prepare their employee training materials, and initiatives such as COAST ask us to host educational material online. In addition, pioneering teachers who are flipping their classrooms to improve educational quality are working with Chromedia in preparing their lessons for online delivery, using David Harvey's free online book Analytical Chemistry 2.0 as textual support for their video presentations. The first release will ensure that their students get the basics of analytical chemistry, and the second will be a course in instrumental analysis. Soon, the entire analytical chemistry curriculum will be online; teachers will be able to selecting the appropriate material from the site and students will be more involved in the learning process.

In any case: please don't "leave them kids alone."

Frank van Geel is the Scientific Director of The Analytical Scientist and the founder of Chromedia, an innovative web-based interactive educational and training resource for analytical science (www.chromedia.org).

Molding a New Type of Student

By Peter Schoenmakers

In 2008, COAST (which stands for Comprehensive Analytical Science and Technology) was formed to address three major concerns in analytical science: i) a decline in highly innovative fundamental analytical research, ii) limited access to rare, high-end analytical instrumentation, and iii) a lack of high-quality researchers and analysts at PhD, MSc and BSc (HBO) levels.

Indeed, the need of industry for competent and knowledgeable analytical scientists was a major catalyst for COAST. Experts from the field were expressing grave concerns about the quality of students graduating from chemistry programs in general and analytical chemistry in particular. I picked up on this need and made a case for full-time students, believing that it is more useful to have them filling autosampler trays than supermarket shelves. And so, we decided to broaden the scope and raise the level of education of analytical science students by organizing extra courses and greatly increasing their interaction with industry. In COAST's educational programs, students are exposed to the industrial environment during their training and experts from industry contribute actively to their education. Also, through their links with COAST, teachers can easily keep their knowledge of recent developments and practice up-to-date. Furthermore, the initiative is helping to retain top-quality people in analytical-science jobs by offering challenging options for continued education and public-private collaborations.

The entire program is carried out and funded by industry, research laboratories and academic groups that participate in COAST. The initiative is staffed by the equivalent of two full-time employees, supported by many part-time teachers who engage in COAST for one or more days each year. We have about 60 (vocational) BSc students and 10 MSc students enrolled in the program. Notably many of the students are from all over the world – so it has clearly become an international initiative.

Students of the future

Times are definitely changing. Students are always connected to the Internet. They have to know less, because they can look up or ask for an answer to just about anything and they can access solutions very quickly. However, they now have to understand more about what they are looking for or how to frame their questions, and to make sense of all the information. Students and graduates are changing more quickly than prospective employers and teachers would like. After all, many employers will have received their education in a different era – perhaps even several decades ago, while academia tends to be extremely conservative by default, especially with regards to education.

Although I've been an academic for more than 10 years, I still lean a little towards industry. It does not really matter whether this is right or wrong, but let's remember that most students will eventually work in industry. If the employers' perception is that the students are not good enough, then there is a problem.

I believe that through COAST we have achieved a major breakthrough that has taken us out of the downward spiral by creating a new type of full-time student. They receive extra teaching and extra tasks, and they perform projects within their academic programs together with industry. In return they receive grants. Our industry partners are now starting to reap the first benefits of the program. In other words, we are starting to deliver graduates to the market.

I firmly believe that COAST stands out because of the involvement of industry. All the companies and (research) institutes that contribute to the program are working closely together with academics towards common goals. Yes, it is frustrating occasionally, but much more often than not it is stimulating and satisfying as we work towards closing the gap between the academic and industrial worlds. Students are confronted with the outside world much earlier in their program and they must work with several different companies, so that they get a much better idea of what the practical application of analytical science is all about.

Jumping hurdles, gaining ground

I have to say that the one of the biggest hurdles to running a complex academic program is minimizing bureaucracy. Education generally has to contend with enormous bureaucratic overheads (at least in the Netherlands). Thankfully, we are an industry-sponsored program and industry demands an efficient, lean-and-mean organization. It's a tough hurdle to jump, but it forces us to create a more sustainable program. We are also overcoming the psychological hurdle of academics not accepting criticism from outside. However, those working on the program clearly see the value of direct feedback from our partners.

I am pleased to say the program is largely in place, although I admit we do need to improve the mechanisms for promoting and implementing life-long learning. Dozens of teachers from industry and academia have made it possible and we are working towards a sustainable model to compensate teachers in kind, with free courses for their students or coworkers. Sustainability is a key requirement for the program as is satisfying the needs of our industry partners through increasing the numbers of available students, especially those at MSc level and above, as well as international students.

All of us engaged in COAST believe that more analytical scientists can benefit from the program and our graduates will be the proof of the pudding. We have a few XQ (Xtra Qualified) graduates now and their number will grow by the end of the year – five years from now I would like to see them play an important role in the community and in sustaining the current program. Some students are beginning work in industry; while some will study for a while longer (from BSc to MSc, from MSc to PhD).

Eventually, we hope that (almost) all of our students will be employed in the broad field of analytical chemistry and that we will gradually meet the need for better analytical scientists in general.

Peter Schoenmakers is education director of COAST, editor of the Journal of Chromatography A, and professor of Analytical Chemistry/Forensic Science at the University of Amsterdam, the Netherlands.

Hot Analytical Thinking

By Janina Kneipp and Katharina Schulten

Analytical sciences are at the core of many fundamental and applied scientific problems and innovations. Did you know that one out of every two chemists working in industry is working in analytical sciences? Nevertheless, there remains a lot of fragmentation throughout the relevant disciplines.

In the late summer of 2009, the three analytical chemistry representatives for Humboldt Universität (Janina Kneipp, Ulrich Panne and Michael Linscheid) had the idea of increasing graduate education. We developed the idea further and found that we needed help from our colleagues from chemistry, physics and other disciplines, and we also involved a lot of people especially from the Berlin-Brandenburg area. It took us about three years from the first internal pre-proposal to kick-off the SALSA project, and along the way we lost and gained supporters while refining our concept.

SALSA (the Graduate School of Analytical Sciences Adlershof) was established at Humboldt-Universität zu Berlin, Germany, in 2012. SALSA receives funding for the next five years from the German government (through the German Research Foundation (DFG) within the framework of the German Excellence Initiative), and offers a structured, three-year period of multidisciplinary research combined with an integrated curriculum in analytical sciences. Essentially, SALSA is focused on achieving a fundamental renaissance of analytical sciences that will simultaneously transform the field itself into a coherent discipline at the interface of chemistry, biology and physics.

We intend SALSA to be the place in Germany for analytical science education and also to be an important part of the European analytical science world. We aim to educate young natural scientists so that they are capable of thinking outside the box, and able to identify problems in their respective discipline. We take a multidisciplinary research approach that incorporates three themes which we – and others – consider important in guiding modern analytical sciences:

- Limits & Scales
- Sensitivity & Selectivity
- Make & Measure

Innovating education

We also need people who can help with developing a new way of teaching, since one of our main objectives is to establish an intensive case-based learning program. The first funding phase of the program (due to finish in 2017) will lay the foundation for a new master's program in analytical sciences. It is our desire that people working in scientific fields should practice analytical thinking. Therefore, we involve universities and other academic institutions, as well as industry to ensure the implementation of analytical thinking in all walks of science and technology. For example, we set up application labs where graduate students can meet with potential future employers or where they have the opportunity to try out new technologies in their individual research projects.

We have 45 faculty members located at 10 research partners mostly in the Berlin-Brandenburg area. Many of those are non-university institutions; for example, the BAM Federal Institute of Materials Research and Testing or the Helmholtz-Center Berlin. Currently, 48 doctoral fellows are pursuing projects within SALSA. By the end of our first funding period in 2017, we will have at least 60 dedicated doctoral fellows finishing projects within our research framework. Importantly, we also work internationally through our partners at ETH Zurich in Switzerland and the University of Oviedo in Spain, and we have fellows from more than 20 nations.

Pushing the limits

Graduate PhD-level students are the main driving force in academic research in German and international educational systems. Similarly, many of them will pursue careers in industry and in this way they will spread the news to the outside world.

Interestingly, we find that most graduate students applying for our doctoral program do not want to limit themselves to one specific type of research; many of them will seek employment outside academia, so they want to exchange information and experiences with peers who are living through the same problems and successes. We think it is safe to say that before the introduction of SALSA, a structured program that emphasizes and develops the problem-solving abilities in a case-based curriculum with opportunities for multidisciplinary and cultural exchange did not even exist. Why? That's a good question.

> *"We often find graduate chemistry and biology students in chemistry using methods without thinking about the specifics of their respective problem."*

Students usually encounter analytical chemistry early in their career, which either encourages them to become analytical chemists or means that they see it simply as a collection of methods that may or may not be useful. We often find graduate chemistry and biology students – and experienced researchers – using methods without thinking about the specifics of their respective problem. Therefore, the students should learn problem-oriented thinking, along with an acquisition of knowledge in instrumentation, the physical basis, and data analysis.

Towards sustainability

To drive progress in analytical science, we need sustainable input from those who are actually involved in research work in other disciplines. It was clear from the beginning that we must use a multidisciplinary approach both in research and in teaching.

For example, we have colleagues from inorganic chemistry who identify problems that they cannot solve with their own tools talking with people in physics who suggest other instrumentation that might help. The perception of analytical sciences has to change – not in analytical chemistry itself – but in all other walks of chemistry, biology, physics, and so on.

The highest hurdle to SALSA is funding, especially as the German Excellence Initiative is one of the most competitive environments in Europe. SALSA was originally underfinanced in the region of ~30 percent in third-party funding, compared to the amount required by our project plan. As for the project itself, the international, cultural and scientific diversity within the school is enriching, but it can pose certain challenges. Some of our doctoral fellows can take the term 'student' very literally and expect step-by-step guidance from their supervisors. This appears to be common in certain scientific environments and cultures, whereas we feel that getting a doctoral degree traditionally implies very independent thinking and a working process where naturally a lot of responsibility is shifted to the doctoral researcher.

All doctoral researchers are co-supervised by two SALSA principal investigators, often from very different disciplines. Though such a strategy has a tremendous pay off, it can pose organizational challenges to the doctoral candidates at times.

Currently in Germany, most doctoral students in the sciences are individualists, and graduate education means lab work. However, in SALSA, we provide a curricular framework and a social environment. If you compare SALSA to other graduate schools or similar structured doctoral programs, we probably stand out because we don't have any particular research focus! We focus on analytical problems that can be found virtually everywhere in science – and everybody willing to think about their research from a problem perspective is welcome.

Success breeds success

SALSA currently has 48 doctoral fellows working on co-supervised research projects and we have established several unique teaching and learning formats. For example, we host bi-weekly sessions that are prepared by the more advanced doctoral fellows, which involve group work on analytical problems, explanations of approaches and methods, and short lectures from experts on specific aspects of the topic. Working in groups and switching to the role of 'teachers' for other fellows is proving beneficial to anyone who wants to learn.

SALSA fellows are inquisitive and manage to work at the intersection of different disciplines; one of our fellows with an MSc in Chemical and Biological Engineering is now working in a physics group at Helmholtz-Center Berlin. Although she had the opportunity to choose from different projects – and her other options included a project that fitted exactly with her research experience to date – she chose a project in a completely new area. Now, she is collaborating with people from biology and physics and researching interactions of nanoparticles and cells. Openness to new fields is a big part of our vision.

In 2014, we took our group work approach even further during our KOSMOS Summer University on "Limits and Scales in Analytical Sciences". Ten groups of fellows worked for several months to get acquainted with the scientific research of our Summer University guests. Each day began with a challenge session, where the groups presented the research of the guests along with their own research and interviewed the guests about their topic. The challenge session prepared everyone really well for the afternoon plenary talks by the same guests – and made the question and answer sessions much livelier than usual!

We engage in a joint class with ETH Zurich, using video lectures, and we've been very successful in establishing an infrastructure for research and teaching within our university. It includes two Application Labs, one for mass spectrometry, the other for photonics. On the faculty side of things, we have hired several renowned guest researchers and visiting fellows, also with the help of Einstein Foundation Berlin and Humboldt Universität. And we have created a new professorship for nanoanalytics – we are close to appointing a renowned researcher for the position.

SALSA is on a long journey and we've only just got started. But having made a start, we can now see which of our former goals remain realistic and those that may need more time and work. Five years from now, we will have successfully extended our idea of a concise graduate education in analytical sciences across the whole scale, from masters to PhD, and we'll have made use of those structures that we have been establishing so far. We also expect to have additional supporters from our own as well as other institutions.

Janina Kneipp is a co-founder and co-speaker of SALSA and a professor of Physical Chemistry at Humboldt Universität, Berlin, and Katharina Schultens is managing director of SALSA.


4 - 6 May 2015 | Radisson Blu Scandinavia Hotel, Copenhagen, Denmark
CMC STRATEGY FORUM
ADVANCING BIOPHARMACEUTICAL DEVELOPMENT
EUROPE 2015
SCAN to browse CASSS for forum updates at casss.org
For program updates, hotel and registration information, as well as sponsoring opportunities, please visit the Forum Website frequently at www.casss.org.
CASSS™
AN INTERNATIONAL SEPARATION SCIENCE SOCIETY
www.casss.org

Business

Economic drivers
Emerging trends
Business strategies

The Challenge of China

As the world's most populous country and the second largest global economy, the potential for growth is significant. But how does an analytical services company break into China?

By Fadia AlKhalil

Much has been made of the advantages of doing business in China in recent years. Unlike western markets, it is far less mature – the pharma sector is growing at double-digit rates, for example. In fact, it is already the world's second largest pharmaceutical market, and the IMS Institute for Healthcare Informatics predicts the annual spend may reach $185 billion by 2018 in its report, 'Global Outlook for Medicines through 2018', published in November 2014.

Per capita spending may be low, but the huge population bumps up the total, and this per capita spending is predicted to grow by more than 70 percent in the next five years; even then, it will still be just 9 percent of the level in the US. Little wonder then that western pharma companies see China as a huge opportunity.

Alongside this burgeoning market for pharma products is a growing outsourcing market, thanks to western pharma companies' eagerness to outsource the more routine pharma research operations to Chinese companies, from chemical synthesis to biological screening, with the aim of saving money. Although it is not the cheap option it once was, there is still a heavy reliance on outsourcing research to China. The authorities' requirement that any medicines licensed in China must have undergone Chinese trials has also encouraged western companies to carryout clinical studies there. And let's not forget that the large, untreated population can offer a huge pool of potential trial subjects.

The tide is turning

Growth has now started in the other direction, as well. China has a well-established manufacturing industry but Chinese companies in the pharma sector are increasingly outsourcing to the western companies, who have set up operations within China.

Even with the flood of returnees – young scientists trained in western universities and pharma companies heading back to China (often to care for ageing parents) – there is still an enormous need for the experience, knowledge and skill-set offered by western experts. I have visited many small-to-mid sized Chinese pharma companies and found that while they have money and enthusiasm, they are often very short on technology and know-how.

Yes, many large Chinese pharma companies have already collaborated with partner companies in the west to secure the expertise they are missing or hired the talent they need to run their operations from overseas. Indeed, most of the large western pharma companies have entered the Chinese market via some form of joint venture with a big local rival; brand names are everything and while some of the Chinese companies have managed to develop their own brands fairly successfully, the additional cachet of big western brands is perceived as extremely advantageous to their prospects. However, their smaller counterparts frequently have not entered into such arrangements. I think if it is properly packaged, marketed and targeted, an annual growth rate of 10 percent, if not 15 percent, should be easily achievable for companies looking to work with smaller Chinese companies. As well as technology and knowledge, western partners can offer quality improvement and organization, with more streamlined business processes and expertise in GLP and GMP procedures. Western partners can also act as a conduit to help Chinese companies to expand globally by using their knowledge of markets and regulatory demands.

Analytical opening?

There is another area ripe for partnerships between western and Chinese companies in the pharma sector: analytical services. Outsourced analytical services is still a fairly young market and, therefore, offers plenty of potential for growth. SGS established its Life Science Services operations in the Chinese market in 2006 at a time when there was huge demand in the country for testing, a lack of fundamental knowledge and, crucially, an absence of that all-important international accreditation which allows a business to create products that will be acceptable for export to international markets. In 2006, SGS began its Life Science Services operations with a small team of 10 employees in response to a request from a global client. By mid 2014, the laboratory space had increased to 1,500 square meters with 75 employees. Recently, SGS announced additional investments to increase the laboratory to 2,000 square meters, also increasing its capabilities to include extractables–leachables packaging testing, inductively coupled plasma mass spectrometry (ICP-MS) to address upcoming USP<233> Elemental Impurities guidelines, a dissolution lab for generic drug stability studies, and a highly active compound (HAC) testing laboratory to meet growing market demand.

As the Chinese start to develop this know-how, acquire the skills and develop potential, they will surely start to become more protective of their own companies. Though they were sadly lacking before, the money and market are now there, and their knowledge and expertise are growing, why allow foreign companies to compete? And another notable factor that must be taken into account is that as Chinese exports stagnate or even decline, companies are starting to put a much greater focus on serving their own domestic market. After all, a population of 1.4 billion generates a lot of consumers! The upshot? Well, I would say that unless a US or European company providing analytical services already has a foothold in the Chinese market, they will find it increasingly hard to enter. In other words, the clock is ticking...

However, despite the steadily growing challenges, China still offers great potential to western companies in terms of analytical services. In many cases, Chinese companies remain behind the bar when it comes to implementing and complying with international standards, such as ICH and GMP, because they simply cannot keep up with the growing demand. As they struggle to become a major force in overseas markets as well as at home, they need western companies to help them bridge the quality gap. Even at home, as the wealth per capita increases, consumers are ever more likely to want products that offer them quality rather than just simply being cheap. And quality is what the west has experience in providing.

One country – five markets

The tactic of providing a one-stop shop service to customers across the whole of China is very unlikely to succeed. Quite simply, China is far too big a country, with far too many people. My advice would be to treat China as four or five distinct markets, based on its different regions and dialects, including Mandarin, Wu, Yue (Cantonese), Min and Jinyu. The one-stop shop approach would mean having to find a way to satisfy the unique conditions of all five of these separate market segments, which would be complicated (and therefore costly) and doomed to fail.

Of course, there are local Chinese suppliers who meet some of the needs of local pharma companies. There is an

Six Tips for Success in China

1. Hire locals with international knowledge
2. Train globally (especially in terms of quality/compliance)
3. Follow both local and global regulations closely
4. Understand the local and national culture
5. Offer capabilities based on your clients' needs within each region
6. Focus on global clients' needs and grow your capabilities accordingly

abundance of local laboratories who offer contract analytical support. That said, adherence to those all-important GLP and GMP standards remains somewhat questionable. Many analytical service providers in China – both local and western companies with Chinese operations – aim to service western companies from their operations within China. And herein lies the big opportunity: working with the pharma companies whose needs are still under-served.

When it comes to keeping the Chinese regulators happy, it has to be said that they appreciate companies working with western partners, because they are more likely to adhere to international quality standards. However, they still expect those partners to respect and meet all relevant local regulations. Therefore, to be successful, it is vital that companies fully cooperate with the Chinese regulators and demonstrate that Chinese criteria are being fully satisfied. For SGS, having a laboratory in Shanghai means that we have local accreditation, and our scientists and quality experts have a good understanding of the local regulations. Importantly, this lab is part of the global SGS Life Science Services network, and therefore automatically works under our global quality standards, ensuring high quality and compliance with western regulations, as well.

Chinese requirements

In recent years, the Chinese FDA has revised its guidance, and it now tracks very closely to the guidance set by the US FDA. This converging approach is also reflected in other documents. For example, the Chinese Pharmacopeia strives to harmonize with the existing guidelines set by the US and Japanese pharmacopeias.

Even though the Chinese FDA is now trying to streamline its processes, many overlaps in authority, requirements and agency oversight exist within the Chinese government. It is therefore very important to identify the correct regulatory agency prior to moving forward in business to ensure compliance with local and global regulatory agencies. The real area where western quality testing labs can make their money is in final testing of products for export. The importing country will have different testing requirements to those for the Chinese domestic market. And in many cases the requirements will be more stringent than those for internal use. The west does not fully trust the quality of testing work carried out by the Chinese regulatory agencies, so a western company in China with international accreditation for its laboratories can charge a premium to Chinese pharma companies wanting to export goods.

Chinese consumers often have a deep mistrust of their own regulatory agencies too, and this boosts the demand for outsourced testing of products for consumption at home. The most recent restructuring of the Chinese FDA has provided consumers with the ability to have an input into the formulation of food standards, the selection of risk assessments, the reporting of crimes, and even criminal punishment; we should never underestimate consumers' knowledge and awareness – after all, they drive the future success of any product.

> *"The Chinese FDA has revised its guidance, and it now tracks very closely to the US FDA."*

The most important piece of advice I can give to any company looking to set up as a service provider in China is to remember the essential point that it really is not a single market. Western companies tend to cut China up into homogeneous regions, but I would actually consider it as five different countries, each with their own unique culture, people, resources and business environment. Making generalizations that what's right in Shanghai is also right in Chengdu or Hainan is guaranteed to hinder your growth – or even lead to failure.

SGS's success in China is rooted in an understanding of the importance of China in the global market as well as the local market, local culture, hiring qualified local people and offer a continuing training from our global quality and compliance.

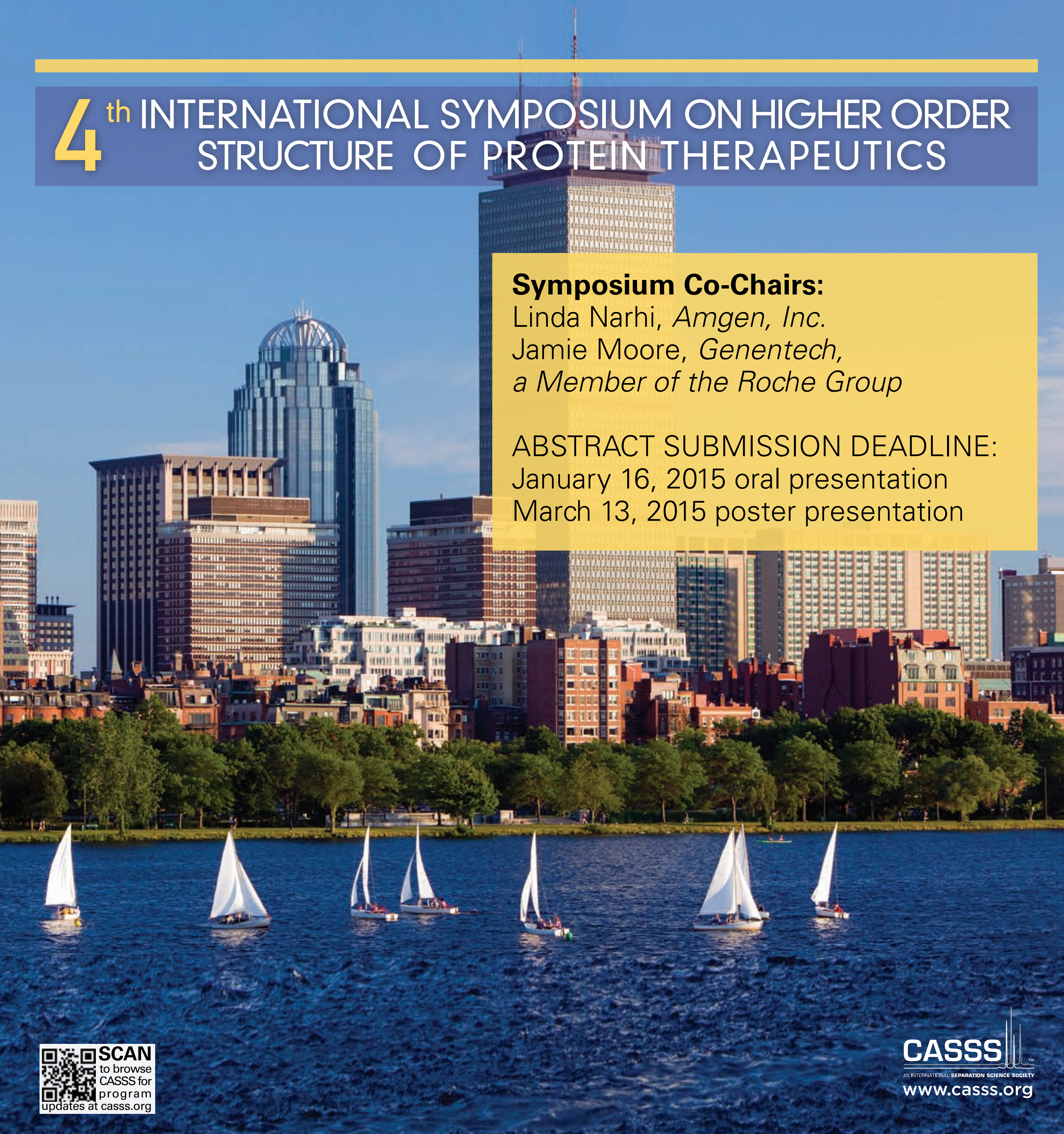
Fadia AlKhalil is vice president of Global Alliance & Partnership, SGS Life Science Services, Fairfield, New Jersey, US.

HOS2015

BECAUSE STRUCTURE MATTERS

April 13-15, 2015

Courtyard Boston Downtown
Boston, MA



4th INTERNATIONAL SYMPOSIUM ON HIGHER ORDER STRUCTURE OF PROTEIN THERAPEUTICS

Symposium Co-Chairs:
Linda Narhi, *Amgen, Inc.*
Jamie Moore, *Genentech, a Member of the Roche Group*

ABSTRACT SUBMISSION DEADLINE:
January 16, 2015 oral presentation
March 13, 2015 poster presentation

SCAN to browse CASSS for program updates at casss.org

CASSS
AN INTERNATIONAL SEPARATION SCIENCE SOCIETY
www.casss.org

Five Star Separation Science

Sitting Down With... Guowang Xu, Director of the Metabonomics Research Center and Deputy Director of the Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China.

Why analytical chemistry?

When I was in middle school, I was told that analytical chemistry is "the eye of chemistry – it can be used in everywhere". So when I passed the national examination for university, I chose it as my specialty.

And separation science in particular?

Actually, that was very accidental. One day, I was filling out my masters entrance examination form, when Zhiqing Qi, my organic chemistry teacher, asked me who I had chosen as my supervisor. I told him about the petroleum chemist in Beijing I had selected. Qi quickly asked, "Is he famous?" I replied that I didn't know but was basing my decision on the probability of being accepted; two students from our university had passed the exam in the last two years. Qi then offered me some excellent advice: "If you want to become a great scientist, you must become the student of a great scientist." And it's true – very often, the scientists who achieve greatness do so by following in the footsteps of giants. Influenced by Qi, I selected Peichang Lu, a member of the Chinese Academy of Sciences (CAS) and a real pioneer of chromatography in China. I passed my entrance examination, joined the CAS Dalian Institute of Chemical Physics in 1984 and obtained my masters degree and doctorate. And I've specialized in chromatography ever since.

Qi and Lu were clearly influential – any other mentors?

Many people have influenced my career, but in particular I'd like to call out professors Yukui Zhang and Shengli Yang – their combined wisdom certainly helped me advance through my scientific career.

How has your research changed over time?

The aim of our research tends to revolve around important scientific questions that face our country's continued growth. But as China's economy has developed, my research focuses have moved from pure chromatography method development and into metabolomics – a very hot field both in China and around the world. We are no longer satisfied with chasing other countries – we want to move with the times and take the most prominent position in certain aspects.

And you consider chromatography to be key in metabolomics?

Metabolomics is playing an increasingly important role in life science – and its success will greatly rely on chromatography-MS. Plenty of great challenges remain, in terms of peak capacity, sensitivity and peak identification. And that makes it a fantastic field for any analyst with a background in chromatography – you can really prove just how valuable your expertise is. My group has been involved in metabolomics since the late 1990s – and we've established several joint laboratories and translational medicine centers with the hospitals in Dalian, Harbin and Shanghai.

What about international collaborations?

In 1995, I got a Max-Planck Institute fellowship and then worked in the University Hospital Tübingen in Germany for two years. When I returned to China, I continued to collaborate with my colleagues in Tübingen – in fact, even today we're still working on projects together. Additionally, the late Karl-Siegfried Boos and I coordinated the Sino-German Cooperation Research Group for Separation and Analysis of Complex Samples. And more recently, I helped to establish the Sino-Dutch Centre for Personalized and Preventive Medicine with Leiden University, the Netherlands Genomics Initiative and TNO.

How does research in China compare to research elsewhere?

That is not a simple question! There are both similarities and differences between Chinese and Western research. China's increasingly global economy tends to mean that the drive and direction of research are similar. However, China is a developing country with a set of specific or even unique questions that must be answered.

What big issues need to be addressed by analytical science?

Analytical science must always strive to provide methods and techniques that offer increased sensitivity, selectivity, accuracy and throughput. Take just one example – body fluids – in a given sample you can find 10,000 compounds with different sizes, polarities and concentrations; but so far, no single analytical tool can collect all information. That's likely to be a challenge for some time into the future.

And the main challenges for separation science specifically?

Peak capacity is a big issue in separation science. Multi-dimensional chromatography helps, and we've seen great successes in GCxGC. Now, we must work on improving LCxLC methods to offer comparable increases in practical peak capacity.

What drives you towards success?

Firstly – and simply – the nature of my profession; we must work hard to satisfy the country and the institute's requirements. Secondly, I want to be one of the world's leading scientists in my field. The constantly shifting landscape of science always keeps me moving forward in both of these aspects.

And your aspirations for the future?

I hope we are lucky enough to define real metabolic biomarkers for the early diagnosis of disease using our well-developed metabolomics platform. Successfully negotiating the translational journey from discovery to clinical application is the ultimate dream of my scientific career.

Perfect fit!

Example: MPS Dual Head WorkStation with Centrifuge, Filtration, and Vortex (^{m}VORX) options

Example: ALEX-GC-MS/MS-System for QuEChERS, Metabolomics ….

Modular solutions that work!

Whatever your sample preparation requirements, we help bring the pieces together for the perfect solution to meet your GC/MS and LC/MS needs:

- ✔ Standards & Dilution Series
- ✔ SPE, Online SPE and Filtration
- ✔ Automated GC Liner Exchange (ALEX)
- ✔ Dynamic Headspace (DHS), HS & SPME
- ✔ SBSE, Thermal Desorption & PYRO
- ✔ Intelligent PrepAhead productivity
- ✔ Application support at your service

What can we do for you?

GET GERSTELIZED!

CERTIFIED QM-SYSTEM ISO 9001 ISO 9001:2008 CERTIFICATE NO. 0086 D

Agilent Technologies
Premier Solution Partner

GERSTEL

www.gerstel.com