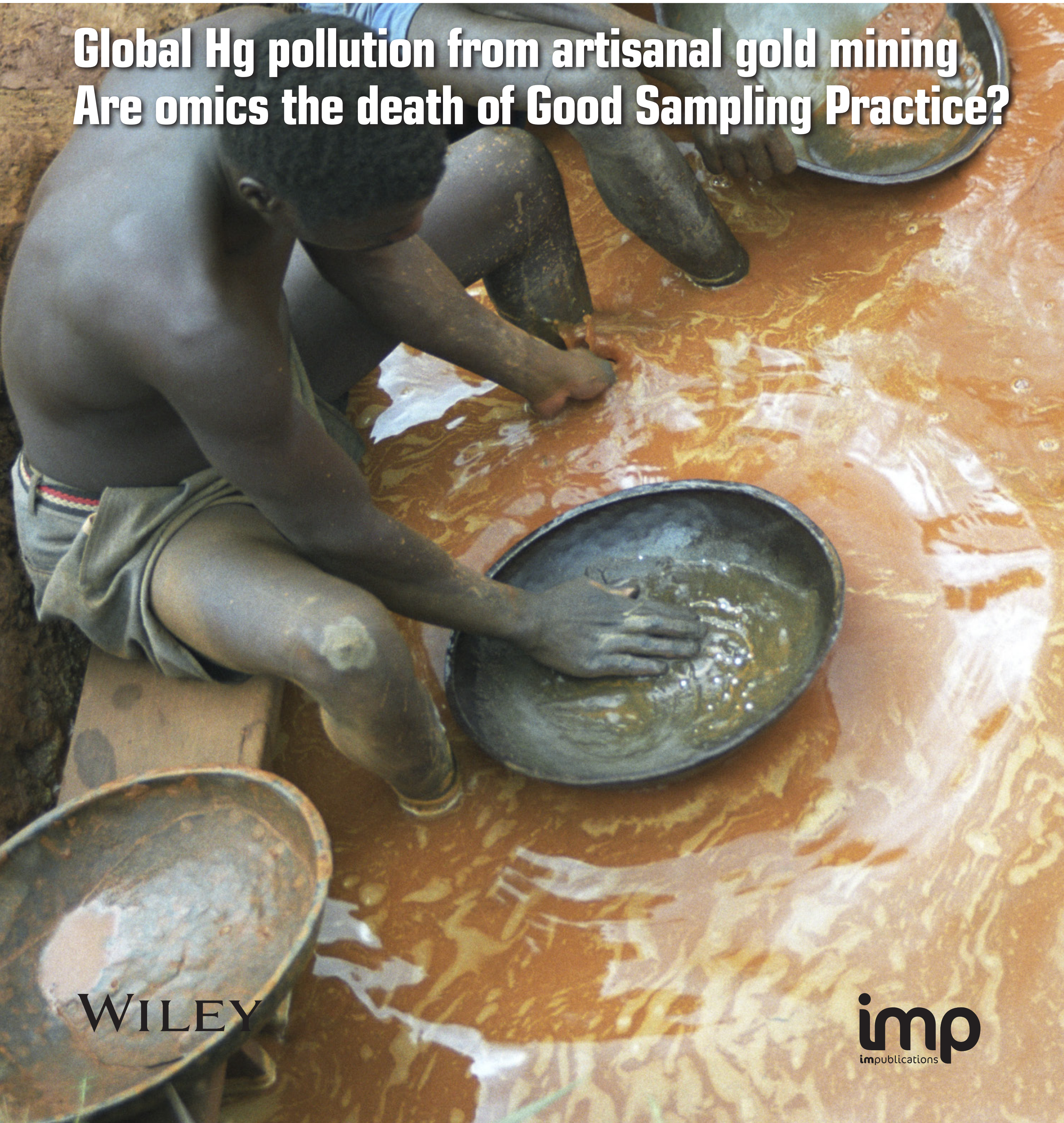
Vol. 31 No. 3 June/July 2019

SPECTROSCOPY europe

Informing European spectroscopists for over 40 years



Global Hg pollution from artisanal gold mining

Are omics the death of Good Sampling Practice?

WILEY

imp
impublications

EDITORIAL

I am sure that all of you are well aware of the multiple threats to the Earth, and its population (human and other), from our activities. Pollution, climate change, deforestation; the list goes on and. When Kim Esbensen (*Spectroscopy Europe* Sampling Column Editor and Editor of *TOS Forum*) sent me an article for preparation for *TOS Forum*, I was horrified by what it reported. I and Kim are keen to share it as widely as possible. The result is an abridged version of the article "in press" in *TOS Forum* (it starts on page 12). The full version is freely available for those who to dig deeper and is referenced in the article.

There are now a huge number of small-scale gold miners who scratch a living (literally) from poor-quality gold deposits. One essential step in the process to produce the end product, pure gold, uses mercury to capture the gold mixed in with rock and other minerals. The quantity of mercury released annually by small-scale gold miners alone is estimated to be 3000 tons—37% of global mercury pollution! Whilst this causes local pollution, much of the mercury ends up being distributed around the world as droplets in "mercury flour". This enters the water supply and hence the food chain of us and other animals. Amongst all the bad news, there is a glint of good news. Chemistry can come to the rescue and can help recover the mercury left behind by the process, and, because gold itself is a by-product, the process could be self-funding.

In the Tony Davies Column, "Are omics the death of Good Sampling Practice?", Tony Davies and Roy Goodacre raise some issues around the reliance just on vast quantities of data collection in omics experiments. As they put it, should we "just keep throwing the mass spectra, nuclear magnetic resonance data sets and our ion mobility fingerprints onto a big pile for the statisticians to fight over?".

We have two reports from meetings. The Sampling Column reports from the 9th World Conference on Sampling and Blending held recently in Beijing and we have a round-up of new mass spectrometry products announced at the annual American Society for Mass Spectrometry conference in Atlanta.

Finally, New Products and the Diary of Future Events wrap up the issue.

Mercury pollution from small-scale gold mining is increasing dramatically, and is a threat to the entire world. A solution to part of the problem is outlined in the article starting on page 12, which also demonstrates the importance of representative sampling and the difficulties in achieving this in the field. Photo: Peter Appel

Publisher
Ian Michael
E-mail: ian@impublications.com

Advertising Sales UK and Ireland
Ian Michael
IM Publications, 6 Charlton Mill, Charlton, Chichester, West Sussex PO18 0HY, United Kingdom. Tel: +44-1243-811334, Fax: +44-1243-811711,
E-mail: ian@impublications.com

Americas
Joe Tomaszewski
John Wiley & Sons Inc.
Tel: +1-908-514-0776
E: jtomaszews@wiley.com

Europe and the Rest of World
Vanessa Winde
Wiley-VCH Verlag GmbH & Co. KGaA, Boschstraße 12, 69469 Weinheim, Germany
Tel: +49 6201 606 721
E-mail: vanessa.winde@wiley.com

Paid subscriptions
Journals Subscriptions Department, John Wiley & Sons, Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, UK.
Tel +44-1243 779777, Fax +44-1243 843232, e-mail: cs-journals@wiley.co.uk

Spectroscopy Europe is a joint publication of John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, UK, and IM Publications LLP, 6 Charlton Mill, Charlton, Chichester, West Sussex PO18 0HY, UK.

Vol. 31 No. 3
June/July 2019

ISSN 0966-0941

CONTENTS

3 Editorial

6 News

12 Reducing global mercury pollution from small-scale artisanal gold mining
Peter W.U. Appel and Kim H. Esbensen

17 Tony Davies Column: Are omics the death of Good Sampling Practice?
Antony N. Davies and Roy Goodacre

20 Sampling Column: Passing a milestone: the successful WCSB9
Lili Jiang and Kim H. Esbensen

24 New Products at ASMS 2019

29 New Products

33 Diary

Spectroscopy Europe is a controlled circulation journal, published seven times a year and available free-of-charge to qualifying individuals in Europe. Others can subscribe at the rate of €152 (Europe), £108 (UK), $208 (ROW, postage included) for the seven issues published in 2016. All paid subscription enquiries should be addressed to: *Spectroscopy Europe*, John Wiley & Sons Ltd, Journals Administration Department, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, UK.

Printed in the UK by Warners Midland

WILEY

impublications

NEWS

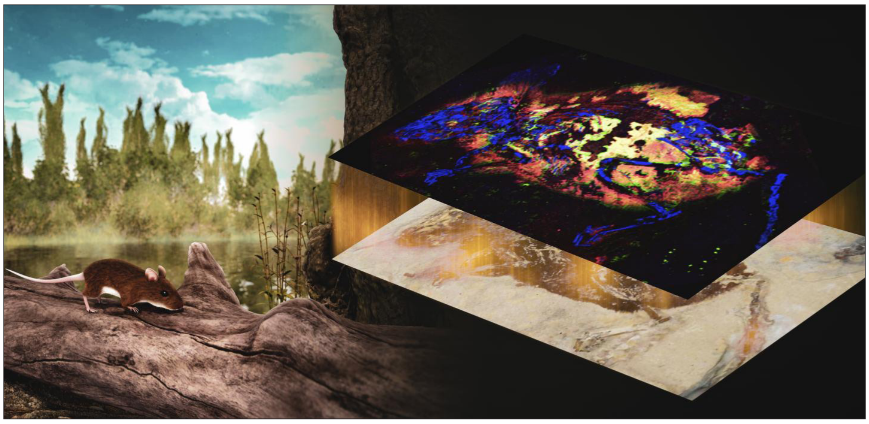
Synchrotron X-ray imaging identifies reddish colouring in an ancient fossil

Researchers have for the first time detected chemical traces of red pigment in an ancient fossil—an exceptionally well-preserved mouse, not unlike today's field mice, that roamed the fields of what is now the German village of Willershausen around 3 million years ago. The study revealed that the extinct creature, affectionately nicknamed "mighty mouse" by the authors, was dressed in brown to reddish fur on its back and sides and had a tiny white tummy. The results were published in *Nature Communications* (doi: 10.1038/s41467-019-10087-2).

The international collaboration, led by researchers at the University of Manchester, used X-ray spectroscopy and multiple imaging techniques to detect the chemical signature of pigments in this long-extinct mouse. X-ray analysis took place at SLAC's Stanford Synchrotron Radiation Lightsource in the USA and the Diamond Light Source in the UK.

"Life on Earth has littered the fossil record with a wealth of information that has only recently been accessible to science", says Phil Manning, who co-led the study. "A suite of new imaging techniques can now be deployed, which permit us to peer deep into the chemical history of a fossil organism and the processes that preserved its tissues. Where once we saw simply minerals, now we gently unpick the 'biochemical ghosts' of long extinct species."

Colour plays a vital role in the selective processes that have steered evolution for hundreds of millions of years. But until recently, techniques used to study fossils were not capable of exploring the pigmentation of ancient animals that is pivotal when reconstructing exactly what they looked like. This paper marks a breakthrough in the ability to resolve fossilised colour pigments in long-gone species by mapping key elements associated with the pigment melanin, the dominant pigment in animals. In the form of eumelanin, the pigment gives a black or dark brown colour, but in the form of pheomelanin, it produces a reddish or yellow colour.



Using synchrotron radiation, researchers were able to untangle the story of key pigments in ancient mouse fossils. The researchers showed that the mouse likely had reddish and brown fur on its back and sides and a white tummy, as shown in Stuart Pond's artist's conception on the left. The bottom image on the right is a photograph of the key fossil examined in this study. Above that is a false colour synchrotron X-ray image of the fossil chemistry. Credit: Gregory Stewart/SLAC National Accelerator Laboratory

Until recently, the researchers had focused on the traces of elements known to be associated with eumelanin, which in previous experiments revealed dark and light patterns in the feathers of the first birds, including *Archaeopteryx*, the famous fossil that first offered a clear link between dinosaurs and birds. In 2016, co-author Nick Edwards, scientist at SLAC, led a study that demonstrated the potential to differentiate between eumelanin and pheomelanin in modern bird feathers. That work provided a chemical benchmark for this most recent paper, which for the first time showed it is possible to detect the elusive red pigment, which is far less stable over geological time, in ancient fossils.

"We had to build up a strong foundation using modern animal tissue before we could apply the technique to these ancient animals", Edwards said. "It was really a tipping point in using chemical signatures to crack the colouring of ancient animals with soft tissue fossils."

"The fossils used in this study preserve amazing structural detail, but our work emphasises that such exceptional preservation may also lead to extraordinary chemical detail that changes our understanding of what is possible to resolve in fossils", said Roy Wogelius, who co-led the study. "Along the way we learned so much more about the chemistry of pigmentation throughout the animal kingdom."

The key to their work was determining that trace metals were incorporated into the fossilised mouse fur in exactly the same way that they bond to pigments in animals with high concentrations of red pigment in their tissue.

NIST infrared frequency comb measures biological signatures

Researchers at the National Institute of Standards and Technology (NIST) and collaborators have demonstrated a compact frequency-comb apparatus that rapidly measures the entire infrared wavelength region and occupies just a few square feet of table space.

Optical frequency combs measure exact frequencies of light. Various comb designs have enabled the development of next-generation atomic clocks and show promise for environmental applications such as detecting methane leaks. Biological applications have been slower to develop, in part because it has been hard to directly generate and measure the relevant infrared light. To showcase biological applications, the NIST team used the new apparatus to measure spectra of NIST's monoclonal antibody reference material, a protein made of more than 20,000 atoms that is used by the biopharmaceutical industry to ensure the quality of treatments.

Agilent TRS100 Raman system

NEWS

Sample preparation technology agreement

Bruker and PreOmics GmbH announced a co-development and co-marketing agreement, which will focus on PreOmics iST sample preparation technology on the timsTOF Pro. The inStageTip (iST) technology removes detergents, polymers, salts, lipids and other contaminants, and has high peptide recovery. New iST protocols enable robust and reproducible sample preparation with a significant time advantage (over 40 h saved) compared to common protocols, and iST is suitable for integration in semi-automated, high-throughput sample prep.

New company for Hiden Analytical

Hiden Analytical have opened a new company, Hiden Analytical Europe GmbH. This is located in Düsseldorf, Germany, and is responsible for sales and service of Hiden Analytical products in Germany and Austria. The new facility includes offices, demonstration equipment, stocks of service spares and communication capabilities for customer support. www.HidenEurope.de

Thermo Fisher Scientific acquires HighChem

Thermo Fisher Scientific has completed the acquisition of HighChem, Ltd, a developer of mass spectrometry software based in Bratislava, Slovakia. HighChem software is used to analyse complex data and identify small molecules in pharmaceutical and metabolomics laboratories. HighChem will be integrated into Thermo Fisher Scientific's chromatography and mass spectrometry business within the Analytical Instruments Segment. Terms of the acquisition were not disclosed.

2D mass spectrometry spin-out secures seed investment

Verdel Instruments Ltd, a spin-out company of the University of Warwick, UK, has developed new two-dimensional mass spectrometry (2DMS) technology and has raised seed investment of over £230,000 from Longwall Ventures and Innovate UK. The company are developing the first benchtop instrument with 2DMS capability. It quickly and efficiently delivers high quality structural analysis and sequencing of every component in a complex mixture at the same time.

"For the first time our frequency combs have simultaneous coverage across the entire infrared molecular fingerprint region", project leader Scott Diddams said. "Other key advantages are speed, resolution and dynamic range in acquiring data."

Mid-infrared light is an especially useful research probe. But, until now, it has been difficult to probe this region due to a lack of broadband or tuneable light sources and efficient detectors such as those available for visible and near infrared light. The new NIST apparatus overcomes these problems. Simple fibre lasers generate light spanning the entire range from 3 µm to 27 µm (frequencies of approximately 10–100 THz). The new system is innovative in detecting the electric fields of the absorbed light using photodiodes operating in the NIR.

"A unique feature is that we detect signals in real time by rapidly sampling the infrared electric field with a near infrared laser", Diddams explained. "This has two advantages: It shifts the detection from the infrared to the near infrared where we can use inexpensive telecommunications photodiodes, and we no longer suffer from the limitations of infrared detectors, which require cryogenic (liquid nitrogen) cooling."

The researchers detected signature vibrations of three bands of amides in the monoclonal antibody reference material. Amide bands in proteins are used to determine the folding, unfolding and aggregating mechanisms. Specific features of the detected bands indicated that the protein has a sheet structure, agreeing with previous studies.

In addition, when combined with novel imaging techniques, the tabletop system could obtain nm-scale images of samples that currently require the use of a much larger synchrotron facility. The work is described in *Science Advances* (doi: 10.1126/sciadv.aaw8794).

Larger semiconductor crystals analysed with an integrating sphere and photoluminescence spectroscopy

Tohoku University researchers have developed a technique using an integrating sphere to measure the electronic and optical properties of large semiconducting crystals. The approach, published in *Applied Physics Express* (doi: 10.7567/1882-0786/ab2165), improves on current photoluminescence spectroscopy techniques and could lead to energy savings for mass producers, and thus consumers, of power devices.

Manufacturers need to be able to detect crystal defects and test their energy conversion efficiency. One way to do this is to measure their internal quantum efficiency, or their ability to generate photons from electrons excited by an electric current or an excitation laser. Currently available methods limit the sample size that can be tested at a time.

Advanced materials scientist Kazunobu Kojima of Tohoku University and colleagues devised a modified approach to photoluminescence spectroscopy that can test larger samples. Standard photoluminescence spectroscopy detects the relative amount of light emitted by a semiconductor crystal when an excitation laser is shone on it. Light energy is lost through these excitation and emission processes, so scientists have been experimenting with photoluminescence spectroscopy that uses an integrating sphere to minimise the loss of photons.

The use of integrating spheres means that the size of the crystal being tested is ultimately limited by the size of the sphere. Kojima and colleagues found they could still test the internal quantum efficiency of a crystal when it was placed directly outside the sphere, allowing larger samples to be used. They conducted their tests on a semiconducting crystal called gallium nitride, which is commonly used in LEDs and is expected to be used in electronic devices because of its superior properties.

"This 'omnidirectional photoluminescence' spectroscopy can be used to evaluate the quality of large-sized crystals or semiconductor wafers, which are essential for the mass production of power devices", says Kojima, adding that this could lead to energy saving and reduce production costs.

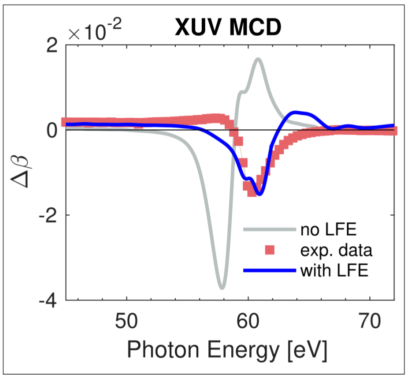
Accurate probing of magnetism with XMCD

The study of the interaction between light and matter is one of the most powerful ways to help physicists to understand the microscopic world. In magnetic materials, a wealth of information can be retrieved by optical spectroscopy where the energy of the individual photons promotes inner shell electrons to higher energies. This is because such an approach allows the magnetic properties to be obtained separately for the different types of atoms in the magnetic material and enables scientists to understand the role and interplay of the different constituents. This experimental technique, called X-ray magnetic circular dichroism (XMCD) spectroscopy, was pioneered in the late 1980s and typically requires a large-scale facility—a synchrotron radiation source or x-ray laser.

To investigate how magnetisation responds to ultrashort laser pulses, the fastest way to deterministically control magnetic materials, smaller-scale laboratory sources have become available in recent years delivering ultrashort pulses in the extreme ultraviolet (XUV) spectral range. XUV photons, being less energetic, excite less strongly bound electrons in the material, posing new challenges for the interpretation of the resulting spectra in terms of the underlying magnetisation in the material.

A team of researchers from the Max Born Institute in Berlin together with researchers from the Max-Planck-Institute for Microstructure Physics in Halle and Uppsala University in Sweden has now provided a detailed analysis of the magneto-optical response for XUV photons. They combined experiments with *ab initio* calculations, and their results have been published in *Physics Review Letters* (doi: 10.1103/PhysRevLett.122.217202). For the prototypical magnetic elements iron, cobalt and nickel, they were able to measure the response of these materials to XUV radiation in detail. The scientists found that the observed signals are not simply proportional to the magnetic moment at the respective element, and that this deviation is reproduced in theory when so-called local field effects are taken into account.

This new insight now allows signals to be quantitatively disentangled from different elements in one material. "As most functional magnetic materials are made up from several elements, this understanding is crucial to study such materials, especially when we are interested in the more complex dynamic response when manipulating them with laser pulses", emphasises Felix Willems, the first author of the study. "Combining experiment and theory, we are now ready to investigate how the dynamic microscopic processes may be utilised to achieve a desired effect, such as switching the magnetisation on a very short time scale. This is of both fundamental and applied interest."



Measured and calculated dichroic absorptive part Δβ of the magneto-optical function of Cobalt. Including local field effects (LFE) and many-body corrections brings the fully *ab initio* theory into very good agreement with experiment.

Tailoring nanolight may improve imaging and spectroscopy accuracy

Spatial resolution of optical microscopy and spectroscopy is determined by how much one can confine light in space, which is usually restricted to about 0.5 µm at the best due to the diffraction limit. However, light can be confined on the nm scale by using metallic nanostructures through excitation of localised surface plasmon resonance (LSPR). Having such "nanolight" at a sharp metallic tip is particularly useful because it can be used in scanning tunnelling luminescence (STL) and scattering-type scanning near-field optical microscopy

NEWS

Verdel's 2DMS technology employs electric pulses to manipulate ions in a linear ion trap before fragmentation to enable parallel acquisition of mass spectra, which operates in combination with UV laser-based fragmentation and a fast mass analyser such as time-of-flight. This data independent analysis technique is claimed to offer better specificity, sensitivity and speed in sample analysis than current techniques in routine use.

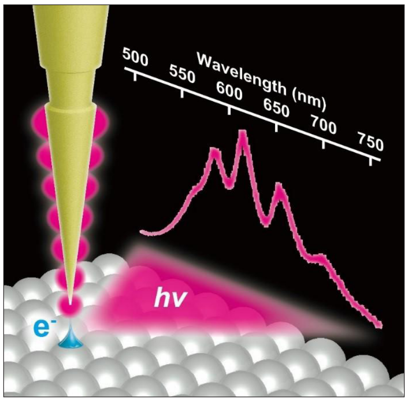
With Verdel's 2DMS technology, only a single 20-minute analysis is required, enabling the analysis of multiple complex samples in one go, with all the data produced in parallel. It will be particularly advantageous for sample types which are water insoluble and pressure sensitive.

Professor Pete O'Connor, Director of Verdel Instruments Ltd and Professor of Analytical Chemistry at the University of Warwick commented: "Two-dimensional mass spectrometry is an incredible tool that allows researchers to get structural information from mixtures of components. We have been working on 2DMS for about eight years using an expensive, high-resolution mass spectrometer and have now solved some key issues to enable its broader uptake as a benchtop instrument."

"We have done analysis of small pharmaceutical and agrichemical molecules, sequenced multiple complex protein or peptides, complex polymer distributions, monoclonal antibodies, proteomics samples and whole proteins, and are currently working to expand the capabilities into environmental testing, petroleum analysis, food-safety and clinical analysis."

"Verdel is developing 2DMS on an inexpensive linear ion trap coupled with a very fast time-of-flight mass spectrometer, greatly expanding the reach of the technique into new markets. We are now looking to work with pharmaceutical companies to analyse samples and test the technology."

(s-SNOM) performing nanoscale imaging and spectroscopy to look at nanomaterials and even single molecules. However, precise manipulation of nanolight in nanoscale junction has remained an outstanding problem. Because the nature of nanolight (LSPR) is determined by the nanoscopic structure of the tip, its manipulation requires a fine processing technique at the nanoscale. In addition, nanolight confined into nanocavities is of key importance due to the strong enhancement effect of an electromagnetic field, which enables ultrasensitive nanoscale imaging and spectroscopy.



Nanolight (localised surface plasmon) is excited in the STM junction by tunnelling electrons (e^-). The emitted light ($h\nu$) shows a modulated spectrum resulting from a Fabry–Pérot interference of the propagating surface plasmon polariton on the shaft. Credit: Takashi Kumagai

A research team at the Fritz-Haber Institute in Berlin, headed by Dr Takashi Kumagai, has demonstrated that manipulation of nanolight spectrum can be attained by shaping accurately plasmonic gold tips with a focused ion beam (FIB) milling technique. As a demonstration, they produced a very sharp tip with a single groove on its shaft as shown in the scanning electron microscope picture. The spectral response of nanolight confined in the nanocavity formed by the grooved tip and an atomically flat silver surface was investigated by using STL; that is the combination of electronic and optical spectroscopies using scanning tunnelling microscopy. The STML spectra with the grooved tips exhibit a characteristic modulation resulting from Fabry–Pérot type interference of surface plasmon polaritons (SPPs) on the tip shaft as the standing wave formation is visualised in the electrodynamic simulation. The spectral modulation can be precisely controlled by the groove position on the shaft. They also demonstrated that the SPP Fabry–Pérot interference can be improved by optimising the overall tip shape.

This work shows the potential of the combination of scanning probe techniques and nano-fabrication of plasmonic tips using FIB in order to study the nature of nanolight and light–matter interactions in nanocavities, which are an important frontier of plasmonics and nanooptics. In addition, the FIB-fabricated plasmonic tips are generally applicable to s-SNOM techniques, thus paving the way for nanoscale imaging and spectroscopy with a high degree of accuracy. Moreover, spectral control of the intense near-field at the apex of plasmonic tips may open up new opportunities for the realisation of coherent laser-triggered electron point sources for low-energy electron microscopy and holography techniques.

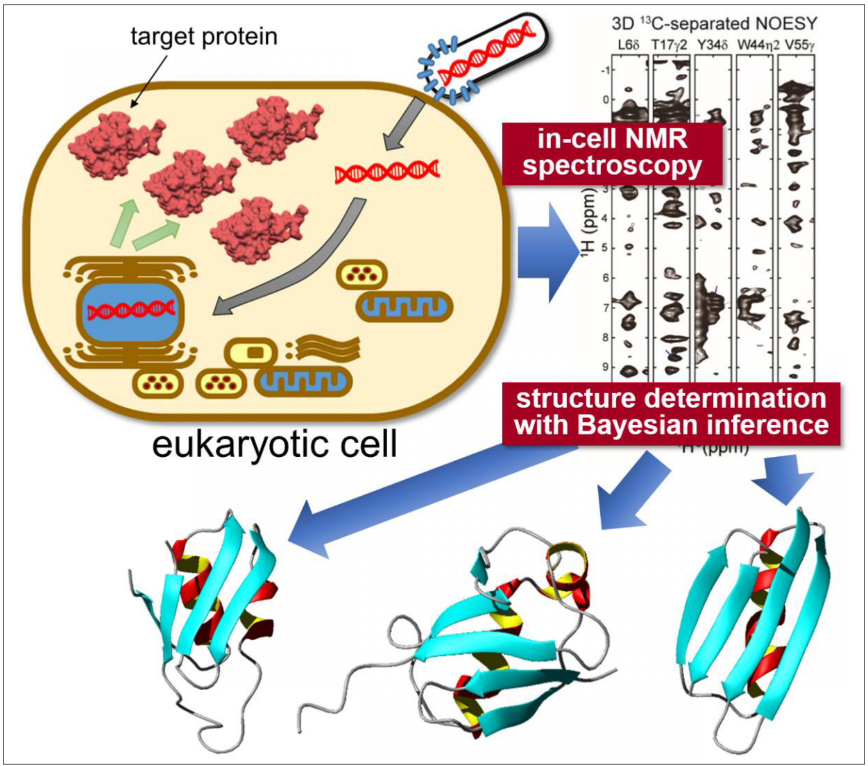
The work is reported in *Nano Letters* (doi: 10.1021/acs.nanolett.9b00558)

In situ measurement of 3D protein structure inside living eukaryotic cells

Researchers from Tokyo Metropolitan University have successfully determined the high-resolution three-dimensional structure of proteins inside living eukaryotic cells. They combined "in-cell" nuclear magnetic resonance (NMR) spectroscopy, a bioreactor system and cutting-edge computational algorithms to determine protein structures in crowded intracellular environments for the first time. The technique promises insight into the intracellular behaviour of disease-causing proteins and novel drug screening applications, allowing *in situ* visualisation of how proteins respond to biochemical stimuli.

Eukaryotic cells are the building blocks of a vast range of organisms, including all fungi, plants and animals. Their internal structure is extremely complex and varied, with an intricate structural hierarchy and a vast range of biomacromolecules distributed around a cytoskeletal network. This has made it difficult to see what each protein inside the cells does in its natural environment, despite the obvious biomedical benefits of knowing, for example, how a particular protein reacts when cells are subjected to chemical stimuli, like pharmaceutical drugs.

To tackle this challenge, a team from Tokyo Metropolitan University led by Assistant Professor Teppei Ikeya and Professor Yutaka Ito applied NMR spectroscopy measurements to specific proteins expressed inside *sf9* cultured insect cells, a strain of cells originally derived from a type of moth larva widely used for protein production. The team's



Target proteins are expressed inside *sf9* cells, then measured using "in-cell" NMR spectroscopy. Unique statistical analysis with the help of Bayesian inference is applied to calculate the accurate 3D structure of the proteins with unprecedented precision. Credit: Tokyo Metropolitan University

NMR work had already succeeded in elucidating high-resolution protein structures inside bacteria (non-eukaryotes). The problem with simply applying the same techniques to proteins in *sf9* cells was the significantly lower concentration of target proteins and short lifetime of cells, making it difficult to collect high quality multi-dimensional NMR spectra for nuclear Overhauser effect spectroscopy (NOESY) which would give precise information about how different atoms are spaced inside individual molecules. Thus, they combined a sparse sampling-based rapid NMR measurement scheme with state-of-the-art computational methods employing statistical techniques like Bayesian inference, methods tailored to elucidate protein structures efficiently based on a limited amount of structural information from in-cell NMR spectra with inherently low-sensitivity. A bioreactor system was also equipped inside the NMR apparatus which kept the cells in a healthy state during the measurements.

With this new data, the team were able to elucidate the 3D structure of three model proteins with unprecedentedly high resolution, with a precision of 0.5 Å for the position of the protein's main chain atoms. In particular, they identified a significantly different conformation in a localised region of one of the proteins compared to its reference structure in dilute solution. The conformational difference between proteins "in cells" and "in test tubes" was presumably caused by non-specific interactions with other molecules inside the cells. It is becoming clear that these interactions contribute to the proteins' biological functions: the ability to locate and quantify structural changes of proteins in an intracellular environment is expected to have a significant impact on biomedical research, making it possible to see how different conditions, e.g. neurodegenerative diseases, affect protein conformations *in situ*, and quantitatively gauge how treatments impact structural anomalies.

They reported their results in *Angewandte Chemie International Edition* (doi: 10.1002/anie.201900840).

Shimadzu's lab4you programme for young scientists

Shimadzu is running the lab4you student programme for young scientists from all over Europe for the fifth year. Young scientists can apply for laboratory bench space for their own research in the modern "Shimadzu Laboratory World" at the European headquarters in Duisburg, Germany. Analytical instrumentation including HPLC/UHPLC, SFC, GC, mass spectrometry, a wide range of spectroscopy equipment (UV, IR, FT-IR, ICP etc.) as well as MALDI-TOF and material testing & inspection equipment is available.

"Over the last four years, we had young scientists from Austria, Poland and Germany working in our lab", stated Björn-Thoralf Erxleben, Manager of the European Innovation Center. "The topics of research were so diverse and interesting that on occasion we accepted two students, rather than just one per year."

"Because of the extensive research environment, providing a unique possibility to work with devices that are best suited to and tailored for their own research, I highly recommend other students to apply for the lab4you student programme", says Dr Carola Schultz, the first lab4you student in 2015. A PhD student at Münster University, Germany at the time, she now works as a Product Specialist for Consumables at Shimadzu Europa GmbH.

Interested students can apply in the English language by submitting a short abstract of their research via www.shimadzu.eu/lab4you by 31 October 2019. The successful applicant will be selected by an expert jury at Shimadzu Europa GmbH. Laboratory space will be available for the duration of the research project. Requirements for participation are an undergraduate degree in science, an interesting topic of research and experience in the chosen technology. This applies to master students, doctoral students and post-docs from all scientific disciplines that require instrument-based analytics or material testing equipment.

Shimadzu offers a selection of promotional material for universities that can be forwarded to potential participants. Contact: Uta Steeger (us@shimadzu.eu).

ARTICLE

Reducing global mercury pollution from small-scale artisanal gold mining

Peter W.U. Appel[a] and Kim H. Esbensen[b]
[a]Senior research scientist, www.Appelglobal.org. E-mail: appelglobal@gmail.com
[b]Consultant, independent researcher, Dr (h.c.), www.kheconsult.com. E-mail: khe.consult@gmail.com

Introduction

Mercury pollution is rapidly becoming a very serious problem for life on Planet Earth.[1] Through organisations such as the United Nations Environment Programme (UNEP), the World community has become acutely aware of the dramatic increase of global mercury pollution. The treaty designed to protect human health and nature, the "Minamata Convention", has been signed by the majority of world countries. Signatory countries are obliged to start initiatives to reduce and, preferably, even stop mercury use. Small-scale gold mining accounts for 37% of global mercury pollution. Millions of poor people have to resort to this type of mining as the only way of sustaining their families.[2] A large part of the mercury used in the final step of gold extraction ends up as mm-sized droplets in dumps (tailings) from which mercury slowly evaporates to the atmosphere. These droplets make up what is referred to as "mercury flour", which is a major contributor to global mercury pollution. The flour also contains large amounts of gold—and herein lies an opportunity. This article describes a road map to clean up mercury from tailings with both environmental and economic benefits. The gold in the mercury flour, when recovered, will cover most, if not all of the cleaning-up costs and may even provide a handsome profit. Possible ways of safe long-time storage of the recovered mercury are also outlined.

Small-scale gold mining

Global mercury pollution affects millions of poor people in Southeast Asia, Africa, Central and South America who, in order to provide a livelihood, resort to gold mining using primitive equipment and low-tech approaches. The final step in the gold extraction process relies on mercury to capture the numerous small gold grains in pulverised hard rock or river sediments. Carried out for hundreds of years, this type of local gold mining has in the past caused only relatively minor mercury pollution, and usually only local. However, the dramatic population increase during the last century has caused a massive increase of this pollution. While we cannot easily provide immediate alternative sources of income for millions of small-scale gold miners, we *can* influence the prevalent way of thinking about how to extract gold in an equally efficient, mercury-free approach and, furthermore, simultaneously be able to show an avenue to clean up the hundreds of thousands of heavily polluted mining dumps that litter Planet Earth.

Gold occurs in mineralised hard rock as µm- to mm-sized grains, either as pure grains, but more often enclosed in other minerals, and as free gold in river sediments. Small-scale gold mining is carried out from pits, shafts or tunnels. The ore is crushed and further milled down to mm-sized powder in order to liberate the gold grains from their host minerals. The next step is to concentrate the heavy minerals, among these, gold. The gravitational methods used vary greatly from simple to complex. The former, such as panning, are the most common, but more complex methods generally result in higher yields. The outcome is a mineral concentrate comprising a variety of heavy minerals including gold. The next step is to separate gold from the other heavy minerals. This is more often than not done by adding mercury to the concentrate (Figure 1). Mercury has the capacity to amalgamate elements such as gold, silver and copper into an alloy. The key next step is to burn off the amalgam so that mercury evaporates and gold is left behind (Figure 2). This simple process does not require much investment in equipment, but is extremely toxic. The waste tailings are simply dumped. This procedure is used by millions of artisanal miners.

Besides the very serious atmospheric mercury pollution, from the point of view of the extraction technology itself, there is also a serious disadvantage in the form of the mercury flour, a product of the mixing.

Mercury flour

During milling and hand mixing, part of the mercury is transformed into mm-sized droplets referred to as "mercury flour" (Figure 3). This can float on water because the individual droplets are very small. Many of the droplets may float close together but they never coalesce, neither do they coalesce when dispersed in milled gold ore. Mercury flour disperses into the environment and so is lost to the miners. The remaining flour is scattered in the tailings and is, likewise, unattainable to the miners.

Mercury flour is one of the main contributors to a rapid growing global

Figure 1. Hand-mixing mercury with milled gold ore (Tanzania). Reproduced from Reference 7 with permission.

Figure 2. Gold has been concentrated and smelted to a small bead. Reproduced from Reference 7 with permission.

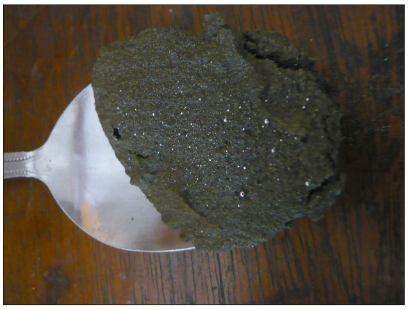


Figure 3. Mercury flour (droplets) in a spoonful of tailings (Philippines). Reproduced from Reference 7 with permission.

mercury pollution crisis. It constitutes one of the most severe threats to the environment and to the health of us all on Planet Earth. Mercury flour in the tailings gradually evaporates. Through wind, the vapour is actually incrementally spread all over Planet Earth. Rain brings the atmospheric mercury to the surface of the Earth where it enters the drainage system. In the rivers and in the soil metallic mercury is changed into methylated mercury, which enters the food chain. The mercury is thus not only a health risk in the countries where it originates, but it very quickly creates a global problem.

Mercury flour also contains large amounts of gold, which, if realised, has such a high value that this could provide quite a substantial lift to the miners' livelihood. Reaping this gold amounts to a win–win achievement, but the awareness of this option is not widely known.

Capturing mercury flour

At first sight, it would seem an insurmountable task to recover the immense number of very fine droplets scattered throughout all the innumerable local artisanal tailings from small-scale gold mining, on several continents. There is a way, however …. The first attempt at this was carried out in 1894 by the Australian Government during the major gold rush in Western Australia.[3] The Australians termed the new facilities "State Batteries", but they apparently soon went out of use. The next attempt was in 2011 where a research group supported by the Benguet Federation of small-scale miners in the Philippines, the Sumitomo Foundation (Japan) and the Geological Survey of Denmark and Greenland (Denmark) improved the working processes inherent in the State Batteries.[4] The resultant facility is now known under the name "Peter Plates", a name coined by the Benguet Federation of small-scale gold miners.

"Peter Plates"

"Peter Plates" consist of a number of copper plates stacked at an inclined angle, one plate on top of the next in a continuous flow train (Figure 4). Before use, the plates are thoroughly cleaned with nitric acid, after which they are treated with metallic mercury, which forms a thin coating of copper amalgam. Tailings with mercury flour are slowly flushed down the plates. On contact with the copper amalgam, the flour sticks to the plate and is so captured. If the first plate does not retain

ARTICLE

Figure 4. Prototype of "Peter Plates" in action (Philippines). Tailing slurry from the tub is passed over the plates in succession. Reproduced from Reference 7 with permission.

Figure 5. Mercury Recovery Plant (MRP) being loaded with tailings (Nicaragua). Reproduced from Reference 7 with permission.

all droplets, subsequent plates come into play in a classic cascade process. When the plates are at capacity, the amalgam is scraped off and the process can easily be repeated.

After processing, the amalgam is heated and the vapour captured in a cold trap. Testing carried out in the Philippines in 2010 and 2011 proved that this method can extract up to 60% mercury from tailings.[4] Although this is promising by itself, reflecting a capacity of about 100 kg tailings processed per hour, when considering the millions of tons of polluted dumps that today wait to be cleaned, a long-term viable solution still would appear far away.

Thus, the efficiency of "Peter Plates" to capture mercury is promising, but their capacity is currently not at a level to make a significant quantitative contribution to the clean-up that is needed in order to reduce the many tons of tailings in existence already.

In 2013, the Californian company Oro Industries invented a Mercury Recovery Plant (MRP; Figure 5). It is a large mobile machine on wheels, towable by truck and thus suitable for reaching tailing dumps spread across large geographical areas. It processes heavy mineral concentrates through a series of cyclones with the concentrate from each cyclone directed on to the next. The concentrates from the two first cyclones are directed into a centrifuge, and the concentrate here from is finally directed into the last cyclone. One MRP unit has a capacity of 15–20 tons per hour. Based on this, each plant produces a concentrate in the order of 10–20 kg heavy minerals per hour, including mercury and gold. The combination of MRP and Peter Plates increases efficiency significantly; the latter hooked on the MRP outlet extracts mercury flour and gold from the heavy mineral concentrate as shown in Figure 6.

The capacity of the *combined* MRP and Peter Plates can extract auriferous mercury from 20 tons per hour, 24/7.[5] A rough estimate of the total tonnage of current tailings produced per day will require in the order of 5000 processing plants to travel Africa, South and Central America and Southeast Asia to just to keep up with the daily production! It will thus require *many more* processing stations if the target is to clean the tailings produced previously. However, the thrust of the present communication is that the necessary dual-purpose technology **is** now at hand, and that the clean-up rate can in fact be tackled—technologically it is simply a matter of scaling-by-numbers of the combined MRP–Peter Plates units.

Sampling—a critical success factor

In order to benchmark the combined MRP–Peter Plates process, it is essential to get a reliable assessment of the overall mercury and gold content *before* processing. The specific sampling issues involved are far from standard. How does one obtain a reliable figure for mercury and gold content in a typical, say, 10-ton tailings stock, in which both elements are very irregularly distributed? In fact, the average tailing concentration is at the ultimate low end of trace levels for both elements. Due to the resulting extreme heterogeneity, there are fewer more challenging sampling scenarios, when almost all levels of sampling technology and equipment are absent. "Barefoot sampling" was what was needed,[6] but with the exact same stringent objective—obtaining a reliable estimate of the concentration levels.

Under such difficult field conditions, the best way to achieve this sampling goal is by so-called incremental composite sampling, a technique developed at research institutes and private companies over many years. The specific approach

Figure 6. Mercury Recovery Plant (MRP) hooked up with Peter Plates (Nicaragua). Reproduced from Reference 7 with permission.

used during the phases of this project was stringently crafted to comply 100% with the demands of the Theory of Sampling (TOS). In initial tests, the critical primary sampling procedure comprised ~2000 increments (each ~100 g) from each test tailing (ranging from 4 ton to 21 ton in weight), which, when aggregated, resulted in primary composite samples of the order of 200 kg (Figures 7 and 8). After these documented representative samples were collected, they were subsequently further mass-reduced both in the field (Nicaragua) as well as in the laboratory (GEUS, Denmark), in order to arrive at reasonably sized aliquots for analysis for mercury and gold, which was subsequently carried out in a commercial laboratory. The full "from-lot-to-aliquot" sampling pathway is described in full detail by Esbensen and Appel.[6]

Fate of recovered mercury

When the combined MRP–Peter Plates system goes into production across three continents, the amount of mercury recovered will reach many tons per year. This raises the important question about the destiny of this mercury. Fortunately, there are several research groups currently working on this problem, which is not only relevant to gold mine tailings but also to cleaning up other sites with large mercury spills. Two of these are:

i) Nomura Kohsan Co. of Japan (www.nkcl.jp) which has constructed a solidification system which provides safe, long-term storage of mercury. The company has expressed interest in constructing a portable processing plant that can follow the MRP–Peter Plates activities.
ii) Batrec Group in Switzerland (www.batrec.ch) has to date solidified more than 600 tons of metallic mercury into the naturally occurring cinnabar (HgS). The cinnabar is stored in German salt mines.

Conclusions

Initial studies have shown that the combination of MRP–Peter Plates is able to recover substantial amounts of mercury from the numerous tailings from small-scale gold mining that litter Southeast Asia, Africa, Central and South America. It is clear that local adjustments will be needed in order to be able to characterise local tailing compositions more comprehensibly to be able to compensate for differences in mineral composition of the tailings from one area to the next, especially regarding the degree of liberation of the most prominent amounts of gold. It would be highly advantageous to be able to use fast "barefoot" mineralogical assessment methods to assess gold particle liberation, i.e. allowing artisanal miners

Figure 7. Halfway through the intensive task of moving a complete original lot one shovel at the time, taking great care to extract an increment from each, as detailed in Figure 8. Reproduced from Reference 6 with permission.

ARTICLE

Figure 8. Incremental composite sampling from each shovel used to transport the original lot, see Figure 7. Reproduced from Reference 6 with permission.

definite information as to whether the tailing gold has been sufficiently crushed to allow complete liberation. While the gold liberation issue has been the target of an enormous R&D effort in the gold mining industry for numerous decades, an easy approach has not yet emerged. Should not the gold mining industry be able to divert just a minute fraction of its revenues to this low-tech challenge, and thereby help millions of starkly impoverished artisanal mining communities in addition to contributing towards the Minamata convention goals? It will also likely be important to observe and compensate appropriately for the characteristics of local climatic conditions regarding whether the climate is humid or dry.

The major remaining scientific and technological question concerns *why* some tailings are more amenable to mercury extraction than others? First generation mineralogical investigations have not provided a clear answer,[4] but to date it has not yet been possible to carry out more comprehensive studies due to lack of appropriate funding. The specific comminution/crushing/milling approach further developed, and attendant problem-dependent processing times, will likely also play an important role in increasing the degree of recovery. However, today we finally have complete knowledge on how to design, plan and implement **the** sufficient-and-necessary feasibility study that will put produce numerical answers to all queries described above. The world cannot wait any longer…

Acknowledgements

The first author is grateful for economic support from the Danish Ministry of Environment and Food. The initial steps in the 2011 testing of "Peter Plates" were undertaken during employment at the Geological Survey of Denmark and Greenland, with support from the Benguet Federation of Small-scale gold miners, Philippines and the Sumitomo Foundation, Japan. A major part of the work was carried out with Elplatek A/S, the Department of Metallurgy, Danish Technical University and the Geological Institute, University of Copenhagen. Oro Industries, California, participated in all testing of the MRP. Encinal, a Nicaraguan company (www.recursos-encinal.com) graciously allowed two visits to their Northern Nicaragua site where an MRP was located, while another a Nicaraguan company, Ensome (www.ensomeinfo.com) also offered generous logistic support. The second author worked in the capacity of research professor at GEUS when parts of this study was carried out before 2015. GEUS' management is thanked for allowing at least *some* R&D endeavours to be targeted on decidedly non-profit areas.

This article is an abridged version of one to appear later in the year in *TOS Forum*,[7] and is reproduced here, with permission, to help raise awareness of the dangers of mercury from small-scale mining activities and the role representative sampling can play in their mitigation. An earlier article detailing the sampling, sub-sampling and analytical intricacies was also published in *TOS Forum*.[6]

References

1. AMAP/UNEP, Technical Background Report for the Global Mercury Assessment 2013. Arctic Monitoring and Assessment Programme, Oslo, Norway / UNEP Chemicals Branch, Geneva, Switzerland (2013).
2. L.J. Esdaile and J.M. Chalker, "The mercury problem in artisanal and small-scale gold mining", *Chem. Eur. J.* **24,** 6905–6916 (2018). https://doi.org/10.1002/chem.201704840
3. State Batteries: https://en.wikipedia.org/wiki/State_Batteries_in_Western_Australia
4. P.W.U. Appel, L.D. Na-Oy, Y. Hatsukawa, T. Osawa, J. Kystol and L.L. Sørensen, Cleaning Mercury Polluted Mine Tailings in the Philippines. Danmarks og Grønlands Geologiske Undersøgelse Rapport 2011/127, 39 pp. (2011).
5. P.W.U. Appel, Final Report Concerning MUDP Projects Reduction of Global Mercury Pollution Phase I 2014-2015 (mst-144-00929) and Phase II (mst-141-01164). June 2017. 2018
6. K.H. Esbensen and P.W.U. Appel, "Barefoot sampling in San Juan de Limay, Nicaragua: remediation of mercury pollution from small scale gold mining tailings", *TOS Forum* **7,** 30–37 (2017). https://doi.org/10.1255/tosf.98
7. P.W.U. Appel and K.H. Esbensen, "Reducing global mercury pollution with simultaneous gold recovery from small-scale mining tailings", *TOS Forum* **9,** in press (2019). https://doi.org/10.1255/tosf.108

Are omics the death of Good Sampling Practice?

Antony N. Davies[a,b] and Roy Goodacre[c]
[a]Expert Capability Group – Measurement and Analytical Science, Nouryon, Deventer, the Netherlands
[b]SERC, Sustainable Environment Research Centre, Faculty of Computing Engineering and Science, University of South Wales, UK. 0000-0002-3119-4202
[c]Department of Biochemistry, Institute of Integrative Biology, University of Liverpool, UK.
E-mail: roy.goodacre@liverpool.ac.uk, 0000-0003-2230-645X

During the recent Royal Society of Chemistry, Faraday discussion meeting in Edinburgh on Challenges in Analysis of Complex Natural Mixtures I found myself wondering if the power that our modern spectrometers bring to the study of highly complex systems can sometimes overwhelm our natural scepticism around poor sampling practices.[1] Some targeted questions put by Roy Goodacre in this direction to several speakers seemed to indicate I was not alone in my concerns, so I thought it might be worth looking at the temptations and some good practices in this area.

My spectrometer has identified 30,000 separate chemical entities so why do I need eight replicate samples?

As regular readers know, this column never aims to be deliberately provocative (!) but as our analytical spectroscopic and spectrometric toolbox gets stronger and stronger, there is always going to be a temptation to revel in the glory of the latest high-resolution enhancement for its own sake and to forget, just for a moment, why we are carrying out the experiments in the first place. In the world of omics experiments it is even more important to be sure that the results we are churning out by the Petabyte are robust and fit-for-purpose. If we leave aside the cost of the instrumentation, the societal costs of sloppy-omics as more data becomes openly available for other scientists to use, could lead to false conclusions being drawn and resources being diverted down apparently promising dead-ends. We are reminded by George Poste in his editorial "Bring on the Biomarkers" in 2011[2] that, at that time, of the 150,000 clinical biomarkers described in the literature a mere 100 were routinely used in the clinic.

Omics experiments in themselves present an enormous issue for classical statisticians just by their huge dimensionality. Conventional wisdom has it that the greater the dimensionality of your problem, the greater the number of unique un-related samples you need if you wish to analyse the problem successfully. But where the promises of the omics approach are being sung the loudest is also the area where it is always notoriously difficult to recruit large sample populations.

In the health care environment, omics is believed to be one of the key analytical spectroscopic advances which will form the backbone of personalised medicine. However, inconsistent ethics committees, medical practitioner patient notes and a simple lack of enough patients taking part in trials who are the same sex, age, weight (or BMI), ethnic origin, diet, alcohol intake, fitness regime, medical history etc. and who are, for example, at the same stage of say a non-small cell carcinoma, could well hinder this approach well into the future. Let us not even start discussing the need for healthy controls with the same characteristics or even wander into the analytical minefield of comparing results from continuous monitoring against grab sampling with different storage strategies taken by different projects. Let us not forget that in most case-control studies the cases (those with some form of disease) are usually already on medication (or self medicating), so this strong confounding factor also needs to be considered.

There is an enormous gap between delivering theoretical correlations with the hope of finding causation from studies of cell cultures in Petri dishes to catching the developing lung cancer in a fit, football-playing 45 year-old engineer before he starts coughing blood into his handkerchief.

So is it really appropriate in such an environment to ignore all our Good Sampling Practice that was drummed into us at university (hopefully) and just go all out for as much data as we can get and (ethics committees willing) just keep throwing the mass spectra, nuclear magnetic resonance (NMR) data sets and our ion mobility fingerprints onto a big pile for the statisticians to fight over? Several years ago Raji Balasubramanian and co-workers compared some classification algorithms used in omics spectroscopic technologies driven by the high-dimensionality of the data.[3] Lauren McIntyre looked last year at the lack of samples compared to the complexity of metabolites/genes and the lack of acknowledgement of over-fitting in the literature proposing a slightly different two-stage approach to the data analysis challenge.[4] Drupad Trivedi and colleagues recently surveyed the metabolomics literature and found that the vast majority of studies were unfortunately underpowered.[5] At the beginning of this year, Wu and co-authors published a "selective" review on integrating data

TONY DAVIES COLUMN

from different types of omics experiments who want to add another level of complexity to their lives![6] Thus an absolutely essential components of any study that generates megavariate data is the need to reduce false discovery.[7]

If so, then how on earth do we continue to convince the governmental funding bodies that it is wise to pour money into these areas of research in the long term? Those in the medical spectroscopy field who passionately believe in this approach, will need to answer the question every three to five years about how many lives did your last project save? (As those approaching the next UK Research Excellence Framework will have to think about…). Maybe the best approach is to keep all these issues in mind when designing your experiments in the first place as the next story shows.

Studying the aftereffects of a natural disaster by omics

Tohoku Medical Megabank (TMM) Project was created to operate prospective cohort studies in Japan for regions where the population were impacted by the Great East Japan Earthquake on 11 March 2011.[8] The project has at its heart the desire to support personalised medical support for the earthquake-damaged regions in the future. A good deal of thought went into this multi-omics study going right back to the sampling procedures. Two cohort studies are discussed—one an adult study and a second birth and three generations study with over 150,000 participants being recruited from 2013 to 2017. Molecular profiling of each participant is important to catch genetic and environmental factors. The analytical centre at the biobank carries out standard non-targeted mass spectrometry (MS) and NMR analyses making the data available to the scientific community.

The authors discussed the difficulty in carrying out sample collection during omics cohort studies—where although the genome will not alter, target metabolites may well be unstable and will be influenced by many factors which must be captured at the time of sampling. Indeed, they make the nice statement that the quality of the omics data largely depends on the quality of the collected samples. They studied which type of blood collection procedure was best for omics studies, deciding that it was best to collect EDTA plasma, as proteins and metabolites can be unstable during serum clotting. To remain consistent with other laboratories, however, they decided to continue to collect both serum and plasma samples. Figure 1 shows the sample collection and transportation plan from the cohort recruitment sites to the biobank.

The TMM central laboratory protocols for proteome and metabolome analysis

For proteome analysis, the TMM team carried out LC-MS/MS measurements in triplicate of the plasma samples after they had been denatured, reduced and alkylated followed by digestion and de-salting. Unfortunately, these studies take over an hour per sample, which clearly was going to cause problems with a project of this size.

For the metabolome analysis they adopted a non-targeted approach using NMR and both positive- and negative-ion mode LC-MS.

Metabolites were extracted from the plasma samples into a sodium phosphate buffer for the NMR studies on a 600 MHz instrument collecting standard 1D NOESY and CMPG spectra successfully identifying and quantifying 37 metabolites. For the MS analyses, an automated sample preparation robot was used which could process around 100 samples per hour, detecting over 1000 peaks and identifying 250 metabolites. For positive-ion mode analyses, the team used an UHPLC QTOF/MS system with electrospray ionisation and a C18 column (Acquity HSS T3; Waters) was used for LC separation. For negative-ion mode, a NANOSPACE SI II HPLC (Shiseido, Tokyo) and a Q Exactive Orbitrap system was deployed using a HILIC column for separation (ZIC pHILIC; Sequant, Darmstadt). The MS measurements could be run at four per hour.

Sample quality control in metabolome analysis

Not satisfied with the level of sampling standardisation and analysis described above, the team also put protocols in place on the not unreasonable

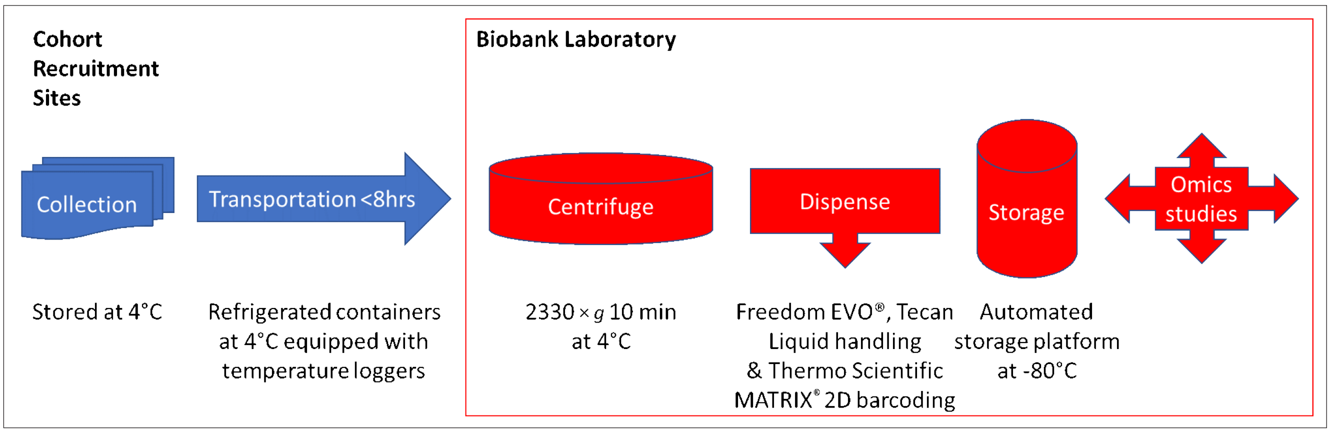


Figure 1. The TMM cohort sample collection and storage protocol.

assumption that there would be some sample handling errors dealing with such a large study. Samples were excluded as outliers if the NMR data on certain control metabolites were outside the ranges expected. For example, the blood glucose values needed to be no lower than 70 % of that measured by an original blood test carried out at the recruitment site and the lactose levels could not exceed more than 2× standard deviation of the cohort average. Samples were also excluded if they breached some aspect of the protocol, such as accidental storage for longer periods before entering the biobank.

Finally, the quality controlled data are being made available at the jMorp Japanese Multi Omics Reference Panel at https://jmorp.megabank.tohoku.ac.jp/201905/ and 8 May saw jMorp release 201905 of the 5KJPNv2 Genotype Frequency dataset from 3500 individuals. The metabolites database release (ToMMo Metabolome 2018 20180827) currently contains distributions of metabolite concentrations identified by NMR, and distributions of peak intensities of metabolites characterised by LC-MS detected in samples from an initial 10,719 volunteers (only 3012 for LC-MS so far).

For those interested in how to use quality controls in metabolomics the reader is directed to an article in *Metabolomics* that won this year's prize for the most downloads—a testament that many researchers are aware that quality assurance and quality control is a very important aspect of any large-scale omics studies.[9]

Conclusions

So, for what the TMM project authors claim to be one of the biggest planned multi-omics longitudinal studies currently underway, it is clear that those with responsibility for the planning and execution of the project are certainly of the opinion that sampling really is critical to the quality of the whole omics project. Time will tell if they have taken enough precautions as the data sets increase in size and the analytical scientists start to use the resource to support the deployment of personalised medicine to these regions.

References

1. http://www.rsc.org/events/detail/29574/challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion (accessed 10 June 2019).
2. G. Poste, "Bring on the biomarkers", *Nature* **469,** 156–157 (2011). https://doi.org/10.1038/469156a
3. Y. Guo, A. Graber, R.N. McBurney and R. Balasubramanian, "Sample size and statistical power considerations in high-dimensionality data settings: a comparative study of classification algorithms", *BMC Bioinformatics* **11,** 447 (2010). https://doi.org/10.1186/1471-2105-11-447
4. A. Kirpich, E.A. Ainsworth, J.M. Wedow, J.R.B. Newman, G. Michailidis and L.M. McIntyre, "Variable selection in omics data: A practical evaluation of small sample sizes", *PLoS ONE* **13(6),** e0197910 (2018). https://doi.org/10.1371/journal.pone.0197910
5. D.K. Trivedi, K.A. Hollywood and R. Goodacre, "Metabolomics for the masses: the future of metabolomics in a personalized world", *Eur. J. Mol. Clin. Med.* **3,** 294–305 (2017). https://doi.org/10.1016/j.nhtm.2017.06.001
6. C. Wu, F. Zhou, J. Ren, X. Li, Y. Jiang and S. Ma, "A selective review of multi-level omics data integration using variable selection", *High Throughput* **8(1),** 4 (2019). https://doi.org/10.3390/ht8010004
7. D.I. Broadhurst and D.B. Kell, "Statistical strategies for avoiding false discoveries in metabolomics and related experiments", *Metabolomics* **2,** 171–196 (2006). https://doi.org/10.1007/s11306-006-0037-z
8. S. Koshiba, I. Motoike, D. Saigusa, J. Inoue, M. Shirota, Y. Katoh, F. Katsuoka, I. Danjoh, A. Hozawa, S. Kuriyama, N. Minegishi, M. Nagasaki, T. Takai-Igarashi, S. Ogishima, N. Fuse, S. Kure, G. Tamiya, O. Tanabe, J. Yasuda, K. Kinoshita and M. Yamamoto, "Omics research project on prospective cohort studies from the Tohoku Medical Megabank Project", *Genes Cells* **23(6),** 406–417 (2018). https://doi.org/10.1111/gtc.12588
9. D. Broadhurst, R. Goodacre, S.N. Reinke, J. Kuligowski, I.D. Wilson, M. Lewis and W.B. Dunn, "Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies", *Metabolomics* **14,** 72 (2018). https://doi.org/10.1007/s11306-018-1367-3

Passing a milestone: the successful WCSB9

Lili Jiang[a] and Kim H. Esbensen[b]

[a]BGRIMM MTC, Marketing Department, Daxing District, Beijing, 102628 China, www.analysis-bgrimm.com, E-mail: jianglili@bgrimm.com

[b]Consultant, independent researcher, Dr (h.c.), www.kheconsult.com. E-mail: khe.consult@gmail.com

On 7–9 May 2019, 555 delegates from 23 counties gathered in Beijing for the 9th World Conference on Sampling and Blending (WCSB9), the latest in the successful conference series which commenced in Denmark in 2003 (WCSB1), followed by Australia in 2005 (WCSB2), Brazil in 2007 (WCSB3), South Africa in 2009 (WCSB4), Chile in 2011 (WCSB5), Peru in 2013 (WCSB6), France in 2015 (WCSB7) and Australia in 2017 (WCSB8). WCSB9 took place in the Beijing International Conference Center and had the highest attendance of any preceding conference, the highest number of accepted papers in the Proceedings and the highest number of exhibitors as well. This event marks a welcome culmination of the first 20 years of organised activities for the International Pierre Gy Sampling Association.

Readers can find *links* to the Conference presentations (in *.pdf versions by kind permission from almost all authors), Conference Proceedings (Open Access and directly downloadable) and a large collection of photos from the conference at the end of this report. The next (WCSB10) conference will take place in Kristiansand, Norway in 2021.

Host and organisation

WCSB9 was hosted by BGRIMM Technology Group and jointly organised by BGRIMM MTC Technology Co., Ltd. and Unismart Events Ltd, with support from China Mining Association, China Association for Instrumental Analysis and The Chinese Society for Metals. WCSB9 had five sponsors: platinum sponsor Nanjing Yinmao Lead-zinc Mining Co. Ltd, silver sponsors FLSmidth, Yosion Laboratory Technologies Co. Ltd (Name Tags), Jiangxi Naipu Mining Machinery and New Materials Co. Ltd (Note Pads) and Agilent Technologies Inc. (Drinks for Gala Dinner).

WCSB9 aimed to discuss, in depth, cutting-edge academic and technological research results and commercial developments in the fields of sampling and blending, to share the latest technical knowledge, practical experience and technological progress, and to foster a communication and exchange platform for regulatory and authentication bodies, end users, relevant service enterprises, and educational and scientific research institutions.

The conference gathered the world's top sampling experts, scholars and delegates from well-known enterprises from all over the world covering mining, metallurgy, cement, food, pharmacy, agriculture, environmental protection and process industry in general. WCSB9 attracted 555 delegates from 23 countries; this was the highest ever in WCSB history. There is a good reason for this veritable quantum leap in relation to all preceding conferences—in one word: China.

China has become the world's largest importer of oil, agricultural products, mineral products and other bulk commodities. Moreover, China is now the largest trading partner of dozens of countries, as well as a major producer and consumer of non-ferrous metals, steel, gold and cement in the world. As an important world economy and a major goods manufacturer, China has realised a critical need for proper sampling and blending technologies to assist in global trade, product quality control and environmental protection. As well as carrying on the well-established scientific objectives of the WCSB series, the 9th edition thus also had a national aim, to contribute to promoting the upgrading and further development of China's own sampling competence and technologies. The organisers spared no efforts in order to facilitate a constructive synergy between all these goals—and their success was resounding. Congratulations are in order!

WCSB9 organising committee and volunteers. Centre (from left) Mr Li, Mr Han long, Mr Roy Xu (see text and WCSB9 website for full descriptions and affiliations of all the organisational and scientific committees, including Unismart Events).

Conference programme

Two pre-conference workshops complemented the main technical programme and exhibitions. The first, *Sampling Theory, Sampling Practices and Their Economic Impact*, was presented by Dr Dominique François-Bongarçon and Dr Francis F. Pitard. The second, *Sampling for Industrial Process & Product Manufacturing, Processing, Monitoring and Quality Control—TOS applications in commodity industries: pharma, food, feed, agriculture, environmental monitoring*, was given by Dr Kim H. Esbensen.

Eight keynote presentations were made by international sampling experts who shared their knowledge and views on various aspects of sampling and blending over the three-day conference. Dr Francis Pitard: *Minimising Extreme Empiricism to Preserve the Logical Structure of the Theory of Sampling*; Professor Pentti Minkkinen: *Sampling Close to the Aliquot Stage—Theoretical Modifications and Consequences*; Dr Dominique François-Bongarçon: *The Liberation Factor—Are We at the End of the Journey?*; Dr Li Huachang: *Development of Online Sampling, Blending and Analytical Technology in China*; Dr Ralph Holmes: *Best Practice in Sampling Iron Ore Shipments*; Dr Ana Chieregati: *The Advances in Drill Hole Sampling*; Dr Kim H. Esbensen: *Theory of sampling (TOS)—What's Next?*; and Charles Ramsey: *Theory of Sampling Applied to Food Safety and Environmental Protection*.

After scientific review of a large number of submitted abstracts, the review team of international and Chinese experts accepted 100 papers for the WCSB Proceedings: 57 papers from China and 43 papers from Australia, Brazil, Canada, Denmark, Finland, France, Germany, Norway, South Africa, Sweden and the United States. Reviewing criteria were two-fold: i) scientific value, presentation quality and/or innovation; ii) showcasing the current state and level of sampling and blending in China in theory and practice.

Pierre Gy Sampling Gold Medal

At the official conference dinner, Dr Geoffrey Lyman was awarded the Pierre Gy Sampling Gold Medal to honour his outstanding contributions in the teaching and application of the Theory of Sampling. Dr Lyman is the Principal of Materials Sampling & Consulting Pty Ltd in Brisbane, Australia. He has carried out consultancies in particulate sampling for over 32 years for clients in Australia and overseas. He has worked in the areas of precious metals (Au and PGMs), diamonds, coal, iron ore, sulphides and spent auto catalysts, and grain and meat. For some years, he consulted for Anglo Platinum in South Africa, working on sampling and metallurgical accounting. The work also involved QA/QC within laboratories and general advice on and mathematical solutions to special statistical problems. He has also worked with the Canadian Grain Commission on the sampling of grain for mycotoxins and other types of contamination and has been involved in sampling/geostatistical simulation for diamond exploration with DeBeers.

CSTM Material Sampling and Blending Technical Committee

In order to promote the exchange and advancement of sampling science and related technologies and industries in China, as well as to participate more in international sampling science and technology communication, China's first sampling-related academic organisation, the "CSTM Material Sampling and Blending Technical Committee", was formally established at the official conference dinner. Affiliated to the China Materials and Testing Standards Committee, it will function as an academic and non-profit social organisation, the main functions of which will be in establishment of appropriate new standards, revision and promotion of sampling technology and equipment, while also working to prepare for future WCSB events in China, all in order to promote increased interaction and international exchanges regarding sampling and related fields in China and abroad. The members of the First CSTM Material Sampling and Blending Technical Committee include:

Chinese consultants: Academician Wang Haizhou (China Iron & Steel Research Institute Group), Academician Sun Chuanyao (BGRIMM Technology Group) and Professor Han Long (General Manager of BGRIMM Technology Group).

Foreign consultants: Dr Ralph Holmes [President of the International Pierre Gy Sampling Association (IPGSA) Council], Dr Kim H. Esbensen (member of the IPGSA Council, Treasurer and Editor of *TOS Forum*) and Dr Francis Pitard (member of the IPGSA Advisory Group).

Dr Li Huachang (General Manager of BGRIMM MTC Technology Co., Ltd) will hold the post as Director of the committee and Mr Bao Lei (Deputy General Manager of NCS Testing Technology Co., Ltd) will act as Deputy Director. The secretariat is located in BGRIMM MTC Technology Co., Ltd,

The Pierre Gy Sampling Gold Medal committee awarding the WCSB9 (2019) Medal to Dr Geoff Lyman.

and 21 other members have been formally enrolled in the First Technical Committee as well.

Special Panel of differences and practices between China and other countries

Today, China is the world's largest importer and consumer of bulk commodities. The total value of China's foreign trade in 2018 is US$4.62 trillion. China has a huge demand for proper sampling and blending knowledge and expertise. In the trading of bulk commodities between China and other countries, there are often differences regarding the understanding of proper sampling and blending. To throw light on this issue, the organisers invited representatives and guests from all parties and stakeholders involved to discuss the differences between China and other countries regarding sampling and blending theories and practices for bulk commodity trading. The special panel was hosted by Han Long (chairman of the WCSB9 organising committee), who was joined by six guests: Mr Oscar Dominguez (BHP Group Limited), Mr Aldwin Vogel (Bureau Veritas), Dr Li Huachang (BGRIMM MTC Technology Co., Ltd), Dr Ana Carolina Chieregati (São Paulo State University), Reinaldo Dantas Novaes (FLSmidth) and Mr Gao Zhengbao (Shandong Humon Smelting Co., Ltd). This special panel was an innovation to the World Conference on Sampling and Blending. The invited guests voiced their opinions and had in-depth exchanges with participating delegates, and also advised all delegates to make full use of the platform of the 9th World Conference on Sampling and Blending to exchanges ideas on aspects of theory, academic study, technology, equipment and application practice, and enhance mutual understanding, so as to make positive contributions to reducing trade frictions and achieving win–win outcomes.

Exhibition

The associated exhibition attracted 43 exhibitors, including 29 Chinese exhibitors and 14 foreign exhibitors, which can all be found on the conference website: http://www.wcsb9.com (starting from 2015, by decree from the Council of the IPGSA, conference websites must be kept open and active indefinitely). Coffee breaks and presentation stands for 11 conference posters were all held in the exhibition area, maximising opportunities for networking.

Closing speech by Han Long, chairman of WCSB9 organising committee

Dear Dr Ralph Holmes, Ladies and Gentlemen!

With the joint efforts of all the participants, 9th World Conference on Sampling and Blending has successfully completed its agenda. On behalf of the 9th WCSB Organising Committee and BGRIMM Technology Group, I would like to extend my warm congratulations to the successful holding of this conference, and congratulations to all the awards winners, you really deserve it, and your great achievement and performance really add glory to this event.

By the time of conference closing, I would like to summarise a few highlights of 9th WCSB.

The biggest highlight is the conference attendance. 555 registered delegates, 100 papers, 12 sessions, 50 oral presentations. All these numbers are record high in WCSB history.

Another highlight is the Chinese factors in the conference. You have seen the majority delegates and authors are from China. Yes, normally local participants should be involved more, the point is, 4 years ago, in 7th WCSB, there is only one Chinese delegate, Dr Li Huachang, and 2 years ago, in 8th WCSB, there are only three Chinese delegates, Dr Li, Roy Xu and Ms Tang. Obviously it is a milestone for WCSB, it means the event popularity in China has increased dramatically from now on. More important is the establishment of China's first academic organisation for sampling—the CSTM Material Sampling and Blending Technical Committee, which paves the way for Chinese professionals in sampling field to connect with the international sampling community.

The third highlight I would like to mention is that, we follow all the traditions of previous WCSB, we also initiate something new, such as special Panel on Wednesday, focus on the "Differences between China and Other Countries in Sampling and Blending Theories and Practices for Bulk Commodity Trading", aiming to enhance the understanding among parties involved in commodity trading sampling.

In summary, I would say, the conference has achieved great success, hopefully all the delegates and participants have got what they expect by intensive exchanges, discussion, demonstration and communication.

The success of the conference is the result of the active efforts and strong support of all parties involved. First of all, I would like to express my sincere gratitude to IPGSA Council, it was your wise decision two years ago in Perth, that brings WCSB to China for the first time. In particular, I want to thank Dr Ralph Holmes for his great contributions to 9th WCSB, as the president of IPGSA and the senior advisor for 9th WCSB, he made tremendous efforts from time to time in the entire process of conference preparation. Thank you Ralph!

My gratitude also goes to the other experts involved, Academician Wang Haizhou, Sun Chuanyao, Dr Kim H. Esbensen and Dr Francis Pitard for their remarkable contribution to the conference and establishment of CSTM Material Sampling and Blending Technical Committee. My appreciation also goes to all the keynote speakers, oral presenters, all the authors who delivered high quality papers, representing world class academic level in sampling and blending field. I would also like to thank all the sponsors and supporting institutions, without our contribution, the conference wouldn't be possible. Thanks to all the delegates, exhibitors, medias, volunteers, your participation is also critical for conference success. Special thanks to BGRIMM MTC, and Unismart Events Limited, the organiser of the conference, who have been working hard for two years, numerous work have been done and finally led to the success of the conference, Thank you Mr Li, Mr Xu and your team. Well done and good job!

Last but not the least, I wish all of you enjoy your stay over the conference in Beijing, I wish you a safe journey back to home, and I wish WCSB a bright future. And I am looking forward to seeing you at the next WCSB in Norway.

Thank you!

Mid-conference tour

During a mid-conference break, attendees had the opportunity, amongst others, to tour the BGRIMM R&D Centre in the south of Beijing, visiting no less than 14 laboratories located there. BGRIMM expressed its sincere interest in future collaborations at all levels in science and technology, as

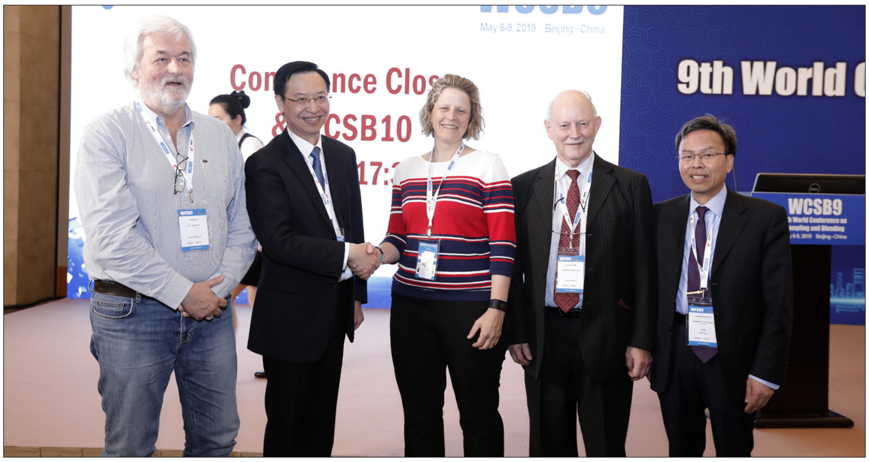
A sight to enjoy: with 555 participants, WCSB9 surpassed all previous conferences, which had boasted 137–235 attendees. The number of oral presentations, Proceedings papers and exhibitors were consequently also record-breaking—to everybody's delight.

well as regarding potential joint industrial and commercial endeavours.

Scientific and social: the final verdict

A complete overview of the scientific and technological achievements associated with WCSB9 can be found via the links in the Further reading section and through the conference website (http://www.wcsb9.com). There one will find an abundance of up-to-date information as to the state of the Theory of Sampling (TOS) and its applications, as well as many perspectives attesting to the intended Chinese goals behind taking on hosting and organising the conference. The WCSB9 Proceedings forms a comprehensive platform to gauge the various levels of current sampling knowledge, competence and technologies available in China and in the 22 other countries represented. There is much interesting work to do in order to reach full TOS-compliance in many different industry sectors and application fields. This task will not necessarily be easy, nor will it be a small one—but this common journey ahead has been made immensely easier by way of the event of WCSB9. The authors strongly recommended that you consult the readily available *complete* record of the conference activities, only a couple of clicks away.

It is safe to say that our Chinese colleagues met all expectations with flying colours. The International Pierre Gy Sampling Association (IPGSA) expresses its highest praise and **Thank You** to the hosting organisation, BGRIMM Technology Group and to the Organising Committee, authors, paper reviewers, session chairpersons and all sponsors and exhibitors who made it possible to entertain this vastly augmented format for a WCSB. The professional conference hosting and catering company, Unismart Events, played an essential role in making the entire five-day event flow effortlessly and smoothly, for which a similarly very big **XieXie** is in order.



Hand over from WCSB9 conference chairman Dr Han Long to WCSB10 Conference Chairperson Mrs Elke Thisted. At opposite ends, the chairmen of two scientific committees (right: Dr Li, WCSB9, left: Dr Kim H. Esbensen, WCSB10)—presided over by IPGSA President Dr Ralph Holmes.

WCSB10

At the last session on the concluding conference working day, the long-awaited announcement was made of the venue and hosting responsibilities for WCSB10 in 2021. The city of Kristiansand, Norway will be the venue, and WCSB10 will be hosted and organised under the leadership of the Eyde Industrial Cluster.

Head of the organising committee will be Elke Thisted, Glencore "Nikkelverk", with Kim H. Esbensen as head of the scientific committee and Editor for the conference Proceedings, which will be published by IMP Open (who published the Proceedings of WCSB7). It is obvious that WCSB10 will in no way even try to match the quantitative achievements of WCSB9, which will likely never be surpassed in the next 20 years. WCSB10 will instead focus on establishing a forward-looking generic framework for WCSBs that is scale-invariant w.r.t to the scientific objectives, but also designed to allow future organisation committees full licence to make their own local, regional and national imprints, as was so prominent in Beijing!

Further reading

General website for WCSB9: www.wcsb9.com

BGRIMM Technology Group: english.bgrimm.com

BGRIMM MTC Technology Co, Ltd: www.analysis-bgrimm.com

Website for UNISMART Events: www.bj-unismart.com/En/index.asp

Eyde Industrial Cluster: www.eydecluster.com/en/

Proceedings of WCSB7: impopen.com/wcsb7

PRODUCTS AT ASMS 2019

908 Devices broadens the ZipChip platform

908 Devices announced several advancements to their ZipChip® product line. Two consumable enhancements dubbed BOOST and SHIFT improve sensitivity and enable native protein analysis on a broader range of Thermo Fisher Scientific mass spectrometers. BOOST gives researchers 20× greater sensitivity when performing native intact protein analysis, revealing detail that was previously unresolvable. SHIFT brings native analysis to mass spectrometers with limited high-mass sensitivity. This now allows biopharmaceutical scientists to run native capillary electrophoresis-mass spectrometry assays on their existing, non-extended-mass range instrumentation without a hardware upgrade.

The company also announced compatibility of their ZipChip platform with a wider range of high-resolution accurate mass instrument manufacturers. Compatibility now expands to a broader set of SCIEX mass spectrometers to include SCIEX TOF instruments in addition to Triple Quad and QTRAP® series systems. 908 Devices and Bruker have also entered into a collaboration agreement to integrate ZipChip onto Bruker mass spectrometers. This collaboration is specifically aligned to bring fast and simple ZipChip CE separations to the Bruker line of TOF instruments including the timsTOF Pro and MaXis systems for the characterisation of Critical Quality Attributes in the biotherapeutics area.

908 Devices

http://link.spectroscopyeurope.com/31-083

Agilent introduces LC/MS system for chromatographers

Agilent Technologies has introduced the InfinityLab LC/MSD iQ System that incorporates "designed-in" smart features, software and hardware developed specifically for chemists and chromatographers. The instrument incorporates intelligent instrument health monitoring; embedded sensors gather and display data allowing a quick assessment of the system's readiness, status and configuration. The instrument incorporates features such as a system suitability check that uses a test mixture designed to permit an overall assessment of the whole LC/MS system before the collection of data. An early maintenance feedback feature allows lab managers to plan routine maintenance on the lab's schedule resulting in a focus on overall productivity. The InfinityLab LC/MSD iQ system is designed to sit beneath a stack of Agilent's InfinityLab HPLC instruments. It is designed to be serviced without dismantling the stack.

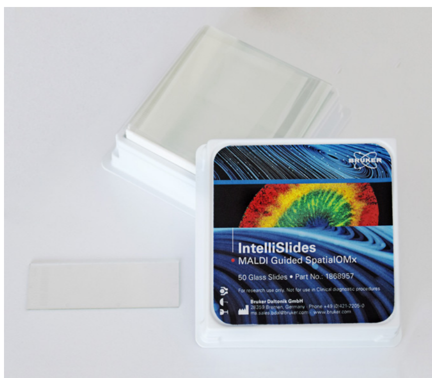
Accompanying the launch of the LC/MSD iQ is a new release of Agilent's MassHunter WalkUp Software for open-access drug discovery and chemistry labs, developed side-by-side with medicinal chemists. This new version has a touch-screen enabled interface and preconfigured analyses and reports that further streamlines simple sample submission and requires virtually no training to use.

Agilent Technologies

http://link.spectroscopyeurope.com/31-079

IntelliSlide automated sample loading for MS imaging

Bruker is also launching IntelliSlides™ specifically designed to automate timsTOF fleX workflows. The IntelliSlides come pre-inscribed with software-readable "teach marks" on the conductive surface to indicate where to place the tissue sample, a bar code and tracking number. IntelliSlides automation removes sources of inefficiency from sample loading, as they are inherently correctly labelled, oriented properly and MALDI image registration occurs at the touch of a button.



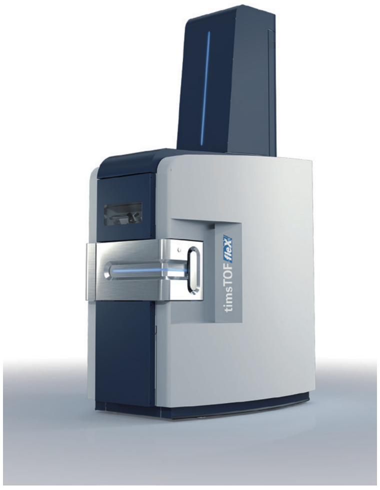
Bruker

http://link.spectroscopyeurope.com/31-072

PRODUCTS AT ASMS 2019

New MS imaging capabilities

Bruker introduced the timsTOF fleX™ mass spectrometer, which includes a software-switchable MALDI source adapted to the ESI timsTOF Pro™platform. This new, combined ESI/MALDI capability enables spatially-resolved omics (SpatialOMx™) on a single instrument. The timsTOF fleX comes with Bruker's proprietary 10 kHz SmartBeamTM 3D laser with true pixel fidelity for rapid, label-free MALDI imaging at high-spatial resolution, while preserving the 4D proteomics and phenomics sensitivity of the timsTOF Pro in ESI mode. With this SpatialOMx approach, researchers gain insights into spatial molecular distributions in tissues from MALDI imaging, to guide 4D omics molecular expression studies, e.g. on



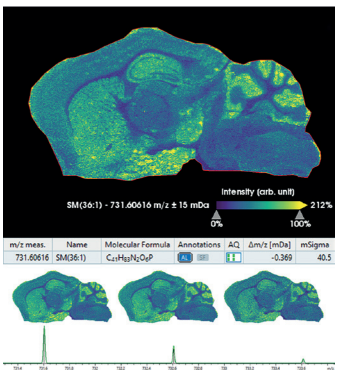
proteins, low-level cancer antigen peptides, lipids, glycans, metabolites or xenobiotics, which cannot be observed by traditional staining or labelling techniques. MALDI-guided SpatialOMx allows for specific targeting of cell sub-populations for subsequent ESI-TIMS/PASEF-based dda or dia 4D proteomics or 4D lipidomics/metabolomics.

Bruker

‣ http://link.spectroscopyeurope.com/31-071

MALDI imaging software

Bruker has introduced SCiLS Lab 2020 MALDI imaging software, which is now integrated with MetaboScape5.0 for automated annotations of lipids and metabolites in tissue molecular images in spatialOMx. This automatically matches ions measured on tissue to molecular information in metabolomics and lipidomics workflows, highlighting biologically relevant pathway information using MALDI imaging. The new integrated imaging and metabolomics workflow also supports data from



Bruker's scimaX™ MRMS platform, as well as from the new timsTOF fleX. MetaboScape's T-ReX 2D algorithm performs feature extraction, de-isotoping and ion deconvolution on MALDI imaging datasets. Within MetaboScape, molecular features are annotated based on accurate mass and isotopic fidelity using SmartFormula™ and molecular information, e.g. from public databases such as HMDB and LipidMaps. MetaboScape now also offers the unique ability to increase ID scoring confidence by integrating accurate TIMS collision cross-sections (CCS) from timsTOF analyses. Identifications flow back to SCiLS Lab for fully annotated molecular images.

Bruker

‣ http://link.spectroscopyeurope.com/31-073

Novel ultra-high sensitivity 4D lipidomics workflow

Bruker has announced advances to ultra-high sensitivity 4D lipidomics workflows on the timsTOF Pro and timsTOF fleX platforms using LC-TIMS-MS/MS. Optimisation of PASEF 4D lipidomics methods now enables the number of identified lipids in single-shot analysis to be almost doubled, whilst obtaining attomole sensitivity. This innovative workflow uses nanoLC-TIMS-PASEF to quantify approximately 500 lipids with very high quantitative accuracy and reproducibility from just a few thousand cells, in addition to building a library of more than 1000 accurate CCS values from human plasma, mouse liver and human cancer cells.

Bruker

OMEGATOF fully integrated benchtop instrument for high-mass MALDI

CovalX has partnered with Shimadzu Scientific Instruments to offer the OMEGATOF, an integrated MALDI solution for ultra-high-mass detection, with a focus on the detection of large molecules including biotherapeutics, protein complexes, aggregates and antibody-antigen interactions in a benchtop footprint at an affordable price. The OMEGATOF combines the Shimadzu 8020 linear MALDI TOF mass spectrometer with the latest CovalX high-mass detection system capabilities. This new instrument has been designed with benchtop portability and quiet operation without compromising on sensitivity. This linear MALDI-TOF mass spectrometer combines easy transport and installation with the ability to detect macromolecules and complexes up to 1500 kDa. The OMEGATOF allows rapid sample introduction with a solid state 200 Hz laser and the FlexiMass™ series of microscope slide-format sample targets.

CovalX

‣ http://link.spectroscopyeurope.com/31-084

PRODUCTS AT ASMS 2019

Genedata Expressionist 13.0

Genedata have released Genedata Expressionist 13.0. A new, flexible, user-definable approach to peptide mapping and sequence variant analysis (SVA) reduces false-positive annotations while maximising sensitivity, enabling best-in-class molecule characterisation—important for next-generation Multi-Attribute Method (MAM) implementations. Advanced iterative review and commenting capabilities together with insightful visualisers that streamline the curation of peptide mapping results. Further, curated results can now be easily incorporated as custom libraries and leveraged in downstream MAM monitoring processes, aiding automated quantification of Critical Quality Attributes (CQAs). Increased configurability allowing customised reporting and preventing time-consuming report reformatting. A unique integrated report approval process with signing functionalities is useful for MAM deployment in regulated environments.

Genedata

‣ http://link.spectroscopyeurope.com/31-085

IonSense DART mass spectrometers can now use nitrogen

IonSense has announced that its Direct Analysis in Real Time (DART) mass spectrometry systems can now utilise nitrogen gas and avoid the need for a helium supply. IonSense worked with Peak Scientific to validate Peak's NG-3000A nitrogen generator for use throughout the IonSense product line. The NG-3000A system can deliver a supply of ultra-high purity nitrogen from ambient air for DART operation in both laboratory and mobile lab facilities.

The ionisation efficiency of excited nitrogen is high enough that almost all but the very smallest organic compounds can be easily ionised. Further, fragmentation is often reduced due to the lower energy of nitrogen metastables.

IonSense

‣ http://link.spectroscopyeurope.com/31-067

MS Bench system with integrated gas supply

Peak Scientific has introduced the new MS Bench system. Developed exclusively for SCIEX, Peak's MS Bench SCI product line provides a modular workstation with integrated gas generation and a sound-dampening vacuum pump enclosure. MS Bench SCI is designed specifically for use with the current and latest mass spectrometers from SCIEX (excluding IVD medical device instruments). Two variants of the MS SCI Bench are available, both identical in form factor, aesthetics and work surface. MS Bench (G) SCI features a self-contained gas generator, providing a source of both nitrogen (Curtain Gas™) and clean, dry oil-free air for source and exhaust gas at flows and pressures configured to meet SCIEX instrument requirements. This is the first time that Peak's validated and compliant Genius "plug & play" (no external compressed air source required) generator technology has been fully integrated into an LC-MS workbench.

The other variant, the MS Bench SCI, comes without the gas generator and provides a noise-abated compartment below the bench. It is suitable for housing up to two MS roughing pumps. Both MS Bench variants are on height-adjustable laboratory-grade castor wheels for easy mobility and seamless integration with surrounding lab work surfaces.

Peak Scientific

‣ http://link.spectroscopyeurope.com/31-082

SCIEX Triple Quad 5500+ LC-MS/MS system—QTRAP®

SCIEX has launched the SCIEX Triple Quad™ 5500+ LC-MS/MS System—QTRAP® Ready, coupling triple quadrupole and QTRAP® functionality in a single system. The QTRAP® functionality can be implemented at any time by simply activating a field upgradable

licence. Increased Polarity Switching Time provides increased efficiency of positive- and negative-ion analysis in the same acquisition (with 5 ms in MRM and Scheduled MRM™) analysing more analytes in a single run without compromising data quality. There is Linear Dynamic Range of up to six orders. QTRAP® functionality: 12,000 Da s^{-1} enables rapid qualitative confirmation of analytes in parallel with MRM quantitative data.

SCIEX

‣ http://link.spectroscopyeurope.com/31-076

SCIEX debuts breakthrough Acoustic Ejection Mass Spectrometry technology

SCIEX has introduced Acoustic Ejection Mass Spectrometry (AEMS) technology. AEMS incorporates the Open Port Interface (OPI) and Acoustic Droplet Ejection (ADE) and is being introduced by SCIEX ahead of commercialisation. SCIEX intends to bring the technology to market as Echo MS. In early testing, AEMS technology has shown the potential to reduce screening times from 115 days to 4 days for 1 million compounds. AEMS technology can also enable: up to 50× faster sample analysis; accelerated speed of analysis, capable of up to three samples per second; low CVs of quantification (5–8 %), leading to high reproducibility regardless of the matrix; and sample analysis direct from the plate—no LC required, eliminating carry over and errors.

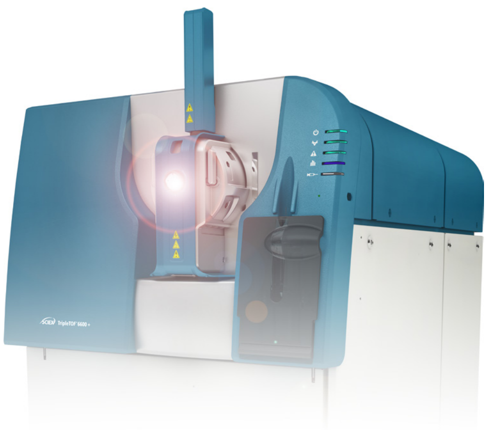
AEMS technology has been conceived by the Open Innovation Project, a collaboration between SCIEX and the US Department of Energy's Oak Ridge National Laboratory. Led by SCIEX Principal Research Scientist, Tom Covey, the Open Innovation Project developed the OPI, a key part of AEMS technology.

SCIEX

http://link.spectroscopyeurope.com/31-078

TripleTOF® 6600+ LC-MS/MS system

SCIEX has launched the TripleTOF® 6600+ LC-MS/MS System, and introduced Scanning SWATH® Acquisition alongside high-performance data processing with OneOmics™ in SCIEX Cloud. The TripleTOF® 6600+ LC-MS/MS system is built for large-scale



quantification and flexible use. The key features of the TripleTOF® 6600+ include: OptiFlow® Turbo V Source: a single source for all low-flow applications, with flow rates of 100 nL min^{-1} to 200 µL min^{-1}. Up to 100 Hz MS/MS scan speeds. Analyst® TF Software 1.8 has a scheduled ionisation and target TIC function, giving the user temporal control over the number of ions entering the system, eliminating the acquisition of unwanted data and maximising system uptime.

Alongside the TripleTOF® 6600+, SCIEX introduces the innovation of Scanning SWATH® Acquisition, to be hosted on the system. Scanning SWATH creates a digital data record of all detectable analytes from a sample, capturing more detail about potential markers than its predecessor. Utilising a sliding Q1 window scanned across the mass range, Scanning SWATH produces four-dimensional data where the correlation between fragment and precursor provide better confidence.

SCIEX also introduced a new generation of OneOmics™, now integrated into SCIEX Cloud. Customers can integrate their data into a cloud-based environment to translate big data generated from proteomics, metabolomics and genomics approaches into biological results.

SCIEX

http://link.spectroscopyeurope.com/31-077

2D chromatography-mass spectrometry software

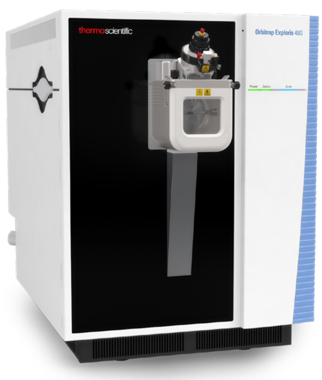
AnalyzerPro XD is a vendor-neutral, two-dimensional data processing solution for all chromatographic-mass spectrometry data. Although 2D chromatography greatly increases the effective resolution and peak capacity of the separation, chromatographic deconvolution still has an important part to play in being able to effectively separate closely eluting components. Current software, which tends to deal with the data on a pixel-level, such as imaging software, no longer meets the requirements of being able to extend chemometric analysis to peak-level data. Applicable to both 2DGC-MS and 2DLC-MS, the software supports all the major manufacturers' data formats. Analyzer Pro XD brings the same targeted, untargeted and quantitative data processing, statistical analysis and visualisation to both 1D and 2D data.

SpectralWorks

http://link.spectroscopyeurope.com/31-087

New benchtop mass spectrometer

Thermo Fisher Scientific have introduced a new compact, benchtop mass spectrometer, the Thermo Scientific Orbitrap Exploris 480 mass spectrometer that provides enhanced quantitative performance across label-free and tandem mass tag (TMT) experiments, as well as access to new Thermo Scientific SureQuant methods for ultra-sensitive targeted protein assays. This combination allows researchers to conduct rapid, multiplexed analysis of proteins within complex biological matrices.



The instrument has a smaller footprint than previous generations, as well as new features to extend uptime and improve serviceability for researchers in high-throughput laboratory environments. Expanded protein coverage is available through enhancements to instrument design and use of the Thermo Scientific FAIMS Pro interface to enhance precursor ion selectivity. Management of this interface is fully incorporated into control software for easy integration.

PRODUCTS AT ASMS 2019

The Orbitrap Exploris 480 mass spectrometer can easily be integrated into a laboratory's routine workflows with the Thermo Scientific Almanac web-based application, which allows users to view instrument operation and data acquisition in real time and receive notifications on the status of runs. This offers scientists the convenience of improved visibility to the utilisation of their laboratory systems, no matter how busy they are or where they are.

Thermo Fisher Scientific

▸ http://link.spectroscopyeurope.com/31-074

New mass spectrometer with intelligent data acquisition strategies

The new Thermo Scientific Orbitrap Eclipse Tribrid mass spectrometer features advancements that improve system sensitivity over previous generations and expand its ability to characterise and quantify complex biomolecules and biological systems. These enhancements are suitable not only for native omics and translational research, but also for the structural and biopharmaceutical analysis of intact proteins and their complexes. The real-time capabilities of the Orbitrap Eclipse Tribrid use data acquisition strategies to enhance experimental efficiency and ultimately accelerate tandem mass tagging (TMT) for multiplexed quantitative analysis of proteomes. Peptide spectra are searched in real-time against a study-specific database.

Those that match then proceed for further analysis, significantly increasing the speed of analysis and accuracy of results. In addition, the new system extends structural analysis up to *m/z* 8000, which enables the isolation and selective dissociation of protein complexes into their individual components, as well as revealing further insights about their exact structure.

Thermo Fisher Scientific

▸ http://link.spectroscopyeurope.com/31-075

Waters introduces cyclic ion mobility to new mass spectrometer

Waters has introduced the Select Series Cyclic IMS, which integrates cyclic ion mobility (cIM) technology into a research-grade time-of-flight mass spectrometer. The Select Series Cyclic IMS replaces the traditional linear ion mobility region with a compact cyclic ion guide. Ions traverse around the ion guide and with

every pass, greater ion mobility resolution is achieved. The cyclic device provides scalable, high-resolution ion mobility separations and introduces the unique ability to perform ion mobility/ion mobility and IMS^n experiments, extending the benefits of routine ion mobility.

Waters

▸ http://link.spectroscopyeurope.com/31-068

Enhancements to Waters' SYNAPT XS

Waters' SYNAPT™ XS is a new flexible, high-resolution mass spectrometer for R&D labs focused on discovery applications. It provides high-levels of flexibility through inlets and acquisition modes. New technology building blocks provide increased

sensitivity for challenging compounds, while improving levels of analytical robustness at superior mass resolution than previous models. In addition, complementary modes of operation increase analytical peak capacity providing "clean and clear" fragmentation data.

Waters

▸ http://link.spectroscopyeurope.com/31-069

NEW PRODUCTS

ATOMIC

Hitachi High-Tech Analytical Science launches new Vulcan+ LIBS range

Hitachi High-Tech Analytical Science Corporation has launched a new line of handheld laser-induced breakdown spectroscopy (LIBS) analysers, the Vulcan+. The range sees updates to the existing Smart and Expert models, whilst a new Optimum+ model is added to the product line. The new Vulcan Optimum+ model has been optimised for analysing aluminium alloys. It features a new spectrometer, enabling the measurement of lithium in aluminium alloys and also capable of measuring boron–aluminium alloys. Boron and lithium are both elements that cannot be measured with any handheld X-ray Fluorescence analyser.

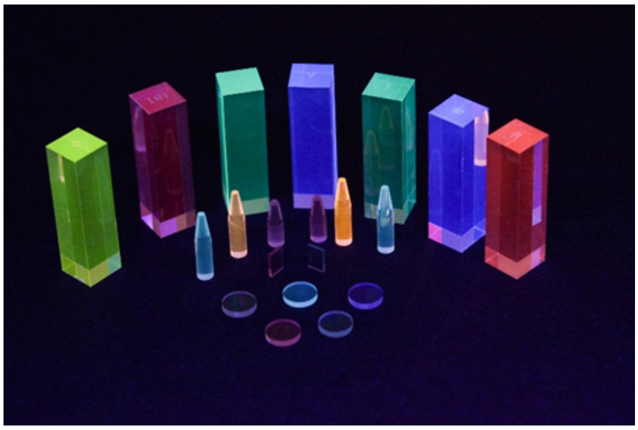
The calibrations for the updated Vulcan Smart+ and Expert+ models have been revised and extended based on feedback from customers. New elements have been added and performance optimised. The Vulcan+ range continues to have advanced reporting direct from the instrument as well as the ExTOPE Connect mobile phone app and cloud connectivity for data transfer and storage.

Hitachi High-Tech Analytical Science

http://link.spectroscopyeurope.com/31-063

FLUORESCENCE

Traceable fluorescence references



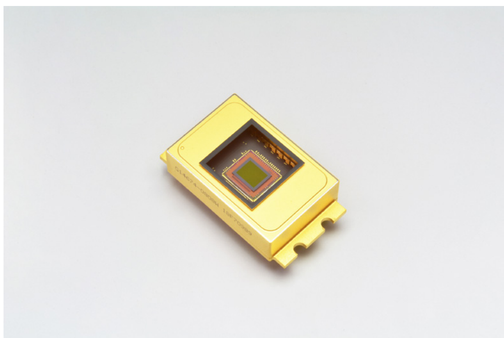
A new series of five polymer block fluorescence references from Starna Scientific can be supplied with certified spectral scans for spectral correction that are traceable to NIST Standard Reference Materials. In some cases, they can be traceably certified for calibrated intensity as well. Designed for the routine performance qualification of fluorescence spectrophotometers and fluorimeters, they can be used in both continuous- and flash-source instruments and a wide spectral range allows the user to select a reference material with broadly similar spectral properties to those of the analyte. They are available in a variety of physical formats, suitable for use in conventional spectrofluorometers or for specialist applications such as microscopy or PCR.

Starna

http://link.spectroscopyeurope.com/31-086

IMAGING

InGaAs area image sensor for hyperspectral cameras



Hamamatsu Photonics has developed an InGaAs area image sensor for hyperspectral cameras capable of detecting short-wavelength-infrared light up to 2.55 µm: the longest wavelength detectable by this type of area image sensor. Hamamatsu have used compound opto-semiconductor manufacturing technology to produce the new G14674-0808W area image sensor made of indium gallium arsenide (InGaAs). If used in hyperspectral cameras for plastic recycling, it will increase the recycling rate plastics containing flame-retardant resin can be separated from other plastics.

Hamamatsu

http://link.spectroscopyeurope.com/31-081

NEW PRODUCTS

INFRARED

Diamond ATR accessory

Pike Technologies have introduced the IRIS diamond ATR accessory. The backbone of the IRIS is its optics: powered mirrors have been designed and processed using diamond-turning technology. All mirrors are gold-coated for maximum reflectivity. The small monolithic diamond, less than 2 mm diameter, provides access to the full mid-IR spectral range. The diamond plate's PTFE gasket seals between the diamond and the plate allowing the IRIS to be used for the analysis of strong organic solvents and caustic samples due to the inertness of PTFE. An optional Ge ATR crystal is available for high refractive index samples as are additional flow-through attachment and liquids retainer sampling tools.

Pike Technologies

▸ http://link.spectroscopyeurope.com/31-066

MASS SPEC

Automated protein sample preparation for MS

PreOmics has launched PreON, their first automation system, which has been built to provide reproducible, robust and sensitive sample preparation of samples for mass spectrometry-based protein analysis. It automates the use of the company's iST and iST-NHS kits. Every step of the PreON workflow is also traceable for use in regulated laboratory environments. The PreON can process 4–12 samples in less than 3 hours and has an onboard heated shaker that can run at 10–2000 rpm with a heating range up to 70 °C. Other automated features include a swing-out centrifuge (max. 12,000 g), pipetting over the 10–200 µL range and cartridge gripper. PreON is a bench top device (H 81 cm, W 65 cm, D 62 cm, Weight 71.5 kg.

PreOmics

▸ http://link.spectroscopyeurope.com/31-065

NIR

NIR MEMS spectrometer

AP Technologies are distributing OtO Photonics' new RedSparrow series of MEMS-based grating-collimator NIR spectrometers. RedSparrow is compact (40 × 40 × 18 mm^3, <30 cm^3) including the removable external control board, and with its rigid metal package and optical bench provides excellent thermal, humidity and shock/vibration stability performance. It has a 128-pixel InGaAs linear sensor and is initially offered with a 50 µm slit offering high sensitivity with FWHM resolution of 8–13 nm over the 950–1700 nm operating range. Communication is via OtO's optional control board featuring high speed (480 Mbps) USB2.0 or six user-programmable digital I/Os. There is also an 8-pin extension port and 4-pin UART port.

AP Technologies

▸ http://link.spectroscopyeurope.com/31-061

NEW PRODUCTS

DA 6200 NIR analyser for meat and olive processors

PerkinElmer has launched the DA 6200™ near infrared (NIR) analyser from its Perten group, which will help meat and olive processors to conduct quality and process control more accurately, easily and quickly. The DA 6200 uses diode array NIR transmission spectroscopy, which enables the analyser to provide accurate test results of fat, moisture and protein levels in a sample, as well as collagen, salt and ash, in 30 seconds. This accuracy and speed also translate to very large, inhomogeneous samples.

Its compact size and battery power option make the DA 6200 analyser fully portable, and it has a built-in touchpad screen. It comes with customised meat and olive product calibrations designed to work across a range of product types, eliminating the need for onsite collaboration development.

PerkinElmer

▸ http://link.spectroscopyeurope.com/31-070

SOFTWARE

New version of SIMCA

Sartorius Stedim Data Analytics has introduced the new SIMCA® 16 software for multivariate data analytics. SIMCA 16 software has enhanced functionality which will save time for expert users, as well as newcomers. Usability improvements provide novices with an intuitive introduction to SIMCA and existing users with superior plot interactivity and quick raw data visualisation capabilities. The software's updated graphical interface with context-based ribbons and panes means scientists will spend less time looking for functions and the new ribbons will be especially useful for those working with batch data. The new data analytics software also includes a wizard that adapts to users' modelling objectives (rather than focusing on which algorithm to use) and guides them through set-up, making the initial steps of creating each model easier. Additionally, its advanced data merging functionality saves time by eliminating the need to manually combine and align data in Excel.

To make pattern data in models easier to interpret and use, SIMCA 16 comes with score space exploration and multivariate solver tools, which help turn models into real-life factor combinations. In just one click, the score space exploration tool allows users to convert scatter plots into real factor settings to, for example, detect which sample is missing in a stack of observations. With the multivariate solver tool, scientists can determine optimum factor settings for desired process outputs such as Critical Quality Attributes and can also lock model parameters to a specific batch of raw material to find the process parameters for achieving consistent product quality and operational efficiency. Both tools make trouble shooting process data and performing deviation analysis simpler tasks.

To increase application and functional flexibility, SIMCA 16 includes MOCA, a novel tool for analysing more than two blocks of data and new Python plugin capability. MOCA provides a quick overview of an entire system, delivering information for continuing analysis, and is helpful for scientists such as systems biologists wanting to compare data from one system that has been obtained using different "omics" and other techniques. The Python plugin functionality in SIMCA 16 provides greater workflow flexibility by enabling users to create a file reader plugin which can read files like any other file format as they are being imported.

The use of SIMCA is recognised by the EMA and US FDA for Real-Time Release testing and the SIMCA 16 software have been developed and extensively tested and validated for use in a highly-regulated environment.

Sartorius Stedim Data Analytics

▸ http://link.spectroscopyeurope.com/31-060

NEW PRODUCTS

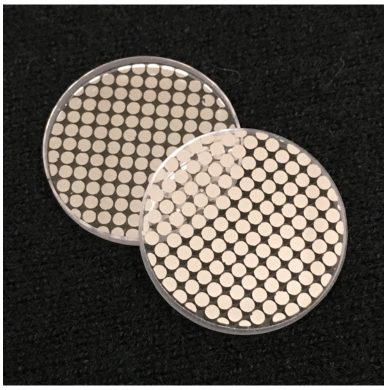
VIS/NIR

New polka-dot beamsplitters from Teledyne Acton Optics

Teledyne Acton Optics has introduced a series of new polka-dot beamsplitters for broadband sources such as xenon, deuterium and tungsten halogen. Using a patented UV coating process, these can now be supplied for use down to 120 nm, depending on the coating and substrate selected. Standard UV-NIR broadband polka-dot beamsplitters for 190–2500 nm are also available. These new polka-dot beamsplitters can be ordered with custom spectral ranges spanning 120–8000 nm. In addition to standard UV fused-silica substrates, Teledyne Acton Optics offers polka-dot beamsplitters that utilise calcium fluoride, magnesium fluoride and sapphire substrates. Custom beamsplitter ratios (stock ratio 50/50) are also available upon request.

Teledyne Acton Optics

‣ http://link.spectroscopyeurope.com/31-064



PocketHawk compact 330–1050 nm spectrometer

OtO Photonics' PocketHawk series of crossed-cavity Czerny–Turner spectrometers operating from 330 nm to 1050 nm come in a package of just 65 × 65 × 25.2 mm^3 (<107 cm^3), including the external control board. They utilise a high-sensitivity, 3000-pixel CCD sensor with a choice of slit sizes from 10 µm to 200 µm giving FWHM resolution in the range of 2.2–12 nm over the spectral range of 330–1050 nm. A choice of two 500 grooves/mm gratings blazed at 330 nm (VNIR6) and 770 nm (VNIR6A) allows users to specify the optimum sensitivity grating to suit their application. Communication with PH-Series spectrometers is via high speed (480 Mbps) USB2.0 or six user-programmable digital I/Os.

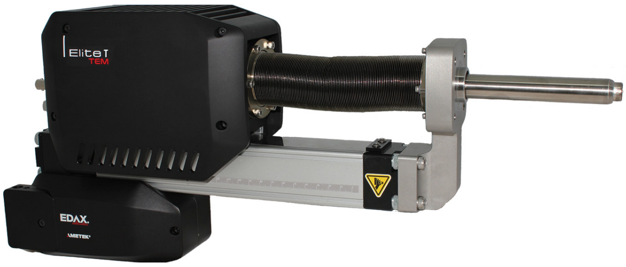
AP Technologies

‣ http://link.spectroscopyeurope.com/31-062

X-RAY

EDAX adds a new detector to the Elite T EDS

AMETEK EDAX has added a new 160 mm^2 detector to its Elite T Energy Dispersive Spectroscopy (EDS) system for transmission electron microscopes. The Elite T EDS System utilises fast Silicon Drift Detectors, now with 70 mm^2 and 160 mm^2 options and integrated electronics. The geometric design of the Elite T EDS System provides an optimised solid angle that increases the count rates for the best performance with optimal results. The Elite T EDS System includes window-less detectors that are designed specifically not to require the typical protective window in front of the module. This design improves the light element sensitivity of the detector, enhancing the mapping speed and light element detection in low concentrations. It also allows flexibility for placement of the sensor to ensure the maximum exposure to the signal.



AMETEK EDAX

‣ http://link.spectroscopyeurope.com/31-080

Conferences 2019

17 July, Manchester, United Kingdom. **Environmental and Food Analysis Special Interest Group (EFASIG) 2019.** David Megson, d.megson@mmu.ac.uk, https://www.bmss.org.uk/bmss-environmental-food-analysis-sig-meeting-2019/.

28 July–2 August, Yokohama, Japan. **International Geoscience and Remote Sensing Symposium (IGARSS 2019).** https://igarss2019.org/.

5–9 August, Lombard, IL, United States. **68th Annual Denver X-ray Conference (DXC 2019).** http://www.dxcicdd.com.

5–9 August, Ephesus, Kusadasi, Aydin, Turkey. **4th International Turkish Congress on Molecular Spectroscopy (TURCMOS 2019).** Pinar Tekbas Çam, info@leoncongress.com, http://turcmos.com/.

18–23 August, Barcelona, Spain. **Goldschmidt 2019.** https://goldschmidt.info/2019/.

25–30 August, Berlin, Germany. **21st International Society of Magnetic Resonance (ISMAR) Conference joint with EUROMAR 2019.** https://www.weizmann.ac.il/ISMAR/.

25–30 August, Berlin, Germany. **EUROISMAR 2019.** euroismar2019@fmp-berlin.de, https://conference.euroismar2019.org/event/1/.

29–30 August, London, United Kingdom. **Structural Mass Spectrometry of Membrane Proteins.** https://www.eventsforce.net/biochemsoc/frontend/reg/thome.csp?pageID=27337&eventID=62&traceRedir=2.

1–5 September, Istanbul, Turkey. **Euroanalysis XX.** Alen Demirel, alen.demirel@brosgroup.net, http://euroanalysis2019.com/.

3–5 September, Manchester, United Kingdom. **40th British Mass Spectrometry Society Annual Meeting 2019 (BMSS40).** bmssadmin@btinternet.com, https://www.bmss.org.uk/bmss-annual-meeting-2019/.

3–5 September, Salvador, Brazil. **6th Brazilian Meeting on Chemical Speciation.** espeqbrasil2019@ufba.br, http://www.espeqbrasil2019.ufba.br/.

8–11 September, Denver, United States. **133rd AOAC International Annual Meeting and Exposition.** meetings@aoac.org, https://www.aoac.org/aoac_prod_imis/AOAC_Member/MtgsCF/19AM/AM_Main.aspx.

8–13 September, Maui, Hawaii, United States. **15th International Conference on Laser Ablation (COLA 2019).** Vassila Zorba, vzorba@lbl.gov, https://cola2017.sciencesconf.org/resource/page/id/11.

8–13 September, Brno, Czech Republic. **10th Euro–Mediterranean Symposium Laser-Induced Breakdown Spectroscopy (EMSLIBS 2019).** Jozef Kaiser, info@emslibs.org, https://emslibs.com/.

11–13 September, Brescia, Italy. **VISPEC Conference on Emerging Trends in Vibrational Spectroscopy.** http://vispec2019.unibs.it/.

11–12 September, Amsterdam, Netherlands. **4th Annual European Forum on Nanoscale IR Spectroscopy.** yan.liu@bruker.com, https://www.bruker.com/events/2019/efns.html?campaign=SPEC.

15–20 September, Gold Coast, Australia. **NIR-2019.** nir2019@yrd.com.au, http://www.nir2019.com/.

22–25 September, Ioannina, Epirus, Greece. **11th International Conference on Instrumental Methods of Analysis (IMA-2019).** Maria Ochsenuhn-Petropoulu, ima2019@chemistry.uoc.gr, http://www.conferre.gr/congress/ima2019.

22–25 September, Phoenix, AZ, United States. **2019 Geological Society of America (GSA) Annual Meeting.** meetings@geosociety.org, http://www.geosociety.org/GSA/Events/Annual_Meeting/GSA/Events/2019info.aspx.

23–26 September, Freiberg, Germany. **Colloquium Analytical Atomic Spectroscopy (CANAS 2019).** canas@chemie.tu-freiberg.de, https://tu-freiberg.de/canas.

23–25 September, Ulm, Germany. **16th Confocal Raman Imaging Symposium.** https://www.raman-symposium.com/.

24–25 September, Graz, Austria. **International SAXS Symposium 2019.** https://www.anton-paar.com/tu-graz/saxs-excites/.

24–26 September, Amsterdam, Netherlands. **10th Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing (WHISPERS).** http://www.ieee-whispers.com.

13–18 October, Palm Springs, United States. **SciX 2019 Conference (formerly FACSS): Annual National Meeting of Society for Applied Spectroscopy (SAS)/The 46th Annual North American Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies.** scix@scixconference.org, http://www.scixconference.org.

5–8 November, Prague, Czech Republic. **9th International Symposium on Recent Advances in Food Analysis (RAFA 2019).** jana.hajslova@vscht.cz, http://www.rafa2019.eu/.

22–23 November, Leipzig, Germany. **7th Workshop on Field-Flow Fractionation-Mass Spectrometry (FFF-MS).** Dr Björn Meermann, nanoanalytics@univie.ac.at, https://www.ufz.de/index.php?en=46025.

SPECTROSCOPY europe READER SERVICE

Use this page to register for a free subscription to *Spectroscopy Europe* You can also register online at the address below.

Online version at http://www.spectroscopyeurope.com/register

Your Details

Title (Professor/Dr etc.):	City:
First Name:	State/Region:
Last Name:	Postal Code:
Job Title:	Country:
Organisation Name:	E-mail:
Address:	

☐ Please send me/continue to send me a free copy of *Spectroscopy Europe*. Signed: ______________________

Field of Work:
(please tick ALL that apply)

- ☐ Agriculture
- ☐ Analytical Chemistry
- ☐ Biotechnology
- ☐ Chemicals
- ☐ Electronics/Semiconductors
- ☐ Energy and Fuels
- ☐ Environmental
- ☐ Food
- ☐ Genomics and other -omics
- ☐ Instrumentation
- ☐ Life Science
- ☐ Materials Science
- ☐ Medical Sciences
- ☐ Metals and Minerals
- ☐ Nanotechnology
- ☐ Pharmaceuticals
- ☐ Polymers and Peptides
- ☐ Security and Forensics
- ☐ Water

Techniques:
(please tick ALL that apply)

- ☐ Atomic Absorption
- ☐ Atomic Emission
- ☐ Chemometrics
- ☐ Computers/Automation
- ☐ ICP/MS
- ☐ Infrared
- ☐ Laser Spectroscopy
- ☐ Luminescence/Fluorescence
- ☐ Mass Spectrometry
- ☐ Microscopy and Imaging
- ☐ MRI
- ☐ Near Infrared
- ☐ NMR, ESR, EPR
- ☐ Photonics and Optics
- ☐ Raman
- ☐ Separation Science
- ☐ Surface Analysis
- ☐ UV/Vis
- ☐ X-Ray Diffraction
- ☐ X-Ray Spectrometry
- ☐ None

Area of employment:
(please tick ONE only)

- ☐ Industry
- ☐ Independent Lab
- ☐ University/Institute
- ☐ Hospital
- ☐ Government
- ☐ Research Inst/Foundation
- ☐ Other______________________

Job function: *(please tick ONE only)*

- ☐ Analyst
- ☐ Quality Control/Assurance
- Research Scientist
- ☐ Lab Manager
- ☐ University Professor
- ☐ Engineering/Design
- ☐ Manufacturing/Processing
- ☐ Teaching
- ☐ Marketing/Sales
- ☐ Other______________________

Do you recommend, specify or authorise the purchase of spectroscopic instrumentation or services: ☐ Yes ☐ No

Your Personal Data (we will never pass your personal details to any third party)

John Wiley & Sons Ltd and IM Publications LLP will use the information you have provided to fulfil your request. Tick the options to let us know how you would like to be kept informed about the latest developments in spectroscopy:

Digital options

☐ Tick to receive e-mail from *Spectroscopy Europe* about new content, products and services

☐ Tick to receive e-mail with information from carefully selected spectroscopy companies (your details are never disclosed)

Postal options

☐ Tick to receive mailings with information from carefully selected spectroscopy companies (your details are never disclosed)

☐ Tick to receive mailings from John Wiley & Sons and IM Publications

Now fax this page to +44-1243-811711, or return by mail to: *Spectroscopy Europe*, 6 Charlton Mill, Charlton, Chichester, West Sussex PO18 0HY, UK.

DIARY

2020

12–18 January, Tucson, AZ, United States. **2020 Winter Conference on Plasma Spectrochemistry.** Ramon Barnes, wc2020@chem.umass.edu, http://icpinformation.org.

29–31 January, Ghent, Belgium. **16th International Symposium on Hyphenated Techniques in Chromatography and Separation Technology.** https://kuleuvencongres.be/htc16/.

16–21 February, San Diego, United States. **2020 Ocean Sciences Meeting (OSM).** meetinginfo@agu.org, https://www2.agu.org/ocean-sciences-meeting/.

17–22 February, Anaheim, California, United States. **2020 American Academy of Forensic Sciences (AAFS) 72nd Annual Scientific Meeting.** https://www.aafs.org/home-page/meetings/future-past-aafs-meetings/.

23–27 February, San Diego, United States. **The Minerals, Metals & Materials Society (TMS) 2020 150th Annual Meeting.** mtgserv@tms.org, https://www.tms.org/tms2020.

22–26 March, Philadelphia, United States. **259th American Chemical Society National Meeting.** natimtgs@asc.org, https://www.acs.org/content/acs/en/about/governance/committees/cwd/meetings.html.

4–7 April, San Diego, United States. **Experimental Biology 2020.** eb@faseb.org, https://experimentalbiology.org.

3–8 May, Vienna, Austria. **2020 European Geosciences Union (EGU) General Assembly.** secretariat@egu.eu, https://www.egu2020.eu/.

24–28 May, Chiba City, Japan. **Japan Geoscience Union Meeting 2020.** http://www.jpgu.org/.

24–26 May, Rome, Italy. **8th CMA4CH Meeting, Measurements, Diagnostics, Statistics in Environment and Cultural Heritage fields.** infocma4ch@uniroma1.it, http://www.cma4ch.org.

31 May–4 June, Houston, Texas, United States. **68th ASMS Conference on Mass Spectrometry.** https://www.asms.org/conferences/annual-conference/future-annual-conferences.

4–5 June, Münster, Germany. **2nd Workshop on Laser Bioimaging Mass Spectrometry.** Michael Sperling, ms@speciation.net, https://bit.ly/2VbCvoH.

7–10 June, Loen, Norway. **10th Nordic Conference on Plasma Spectrochemistry.** Yngvar Thomassen, yngvar.thmassen@stami.no, http://nordicplasma.com/.

21–26 June, Honolulu, Hawaii, United States. **2020 Goldschmidt Conference.** helpdesk@goldschmidt.info, https://goldschmidt.info/2020/.

24–26 June, Warsaw, Poland. **European Symposium on Atomic Spectrometry 2020.** Ewa Bulska, esas2020@uw.edu.pl, http://www.esas2020.uw.edu.pl/.

28 June–4 July, Gangwon, South Korea. **AOGS 17th Annual Meeting.** info@asiaoceania.org, http://www.asiaoceania.org/society/public.asp?view=up_coming.

25–31 July, Chambersburg, United States. **International Diffuse Reflectance Conference (IDRC) 2020.** info@cnirs.org, http://www.cnirs.org/.

23–28 August, Boston, MA, United States. **XXIX International Conference on Magnetic Resonance in Biological Systems (ICMRBSXXIX).** John Markley, jmarkley@wisc.edu, http://www.icmrbs.org/.

Courses

2019

28 July–3 August, Brixen, Italy. **FEBS 2019 Advanced Course / 13th European Summer School on Advanced Proteomics.** Shabaz Mohammed, shabaz.mohammed@chem.ox.ac.uk, https://advancedproteomics2019.febsevents.org/.

5 September, Tongham, United Kingdom. **Training: Hyperspectral Imaging–Innovative Inspection in Machine Vision.** info@stemmer-imaging.co.uk, https://tinyurl.com/y3jo28vq.

9–13 September, Brescia, Italy. **VISPEC International Summer School on Vibrational Spectroscopy.** Prof. Ivano Alessandri, ivano.alessandri@unibs.it, http://vispec-school2019.unibs.it.

13–20 September, Dresden, Germany. **5th International Summer School Spectroelectrochemistry.** https://www.ifw-dresden.de/news-events/scientific-events/summer-school-spectroelectrochemistry/.

15–20 September, Sitges (Barcelona), Spain. **4th International Mass Spectrometry School (IMSS).** imss2019@activacongresos.com, https://4th-imss-2019.es/.

30 September–4 October, Philadelphia, United States. **Interpretation of Infrared and Raman Spectra.** James A. de Haseth, dehaseth@ircourses.org, https://www.ircourses.org/.

Exhibitions

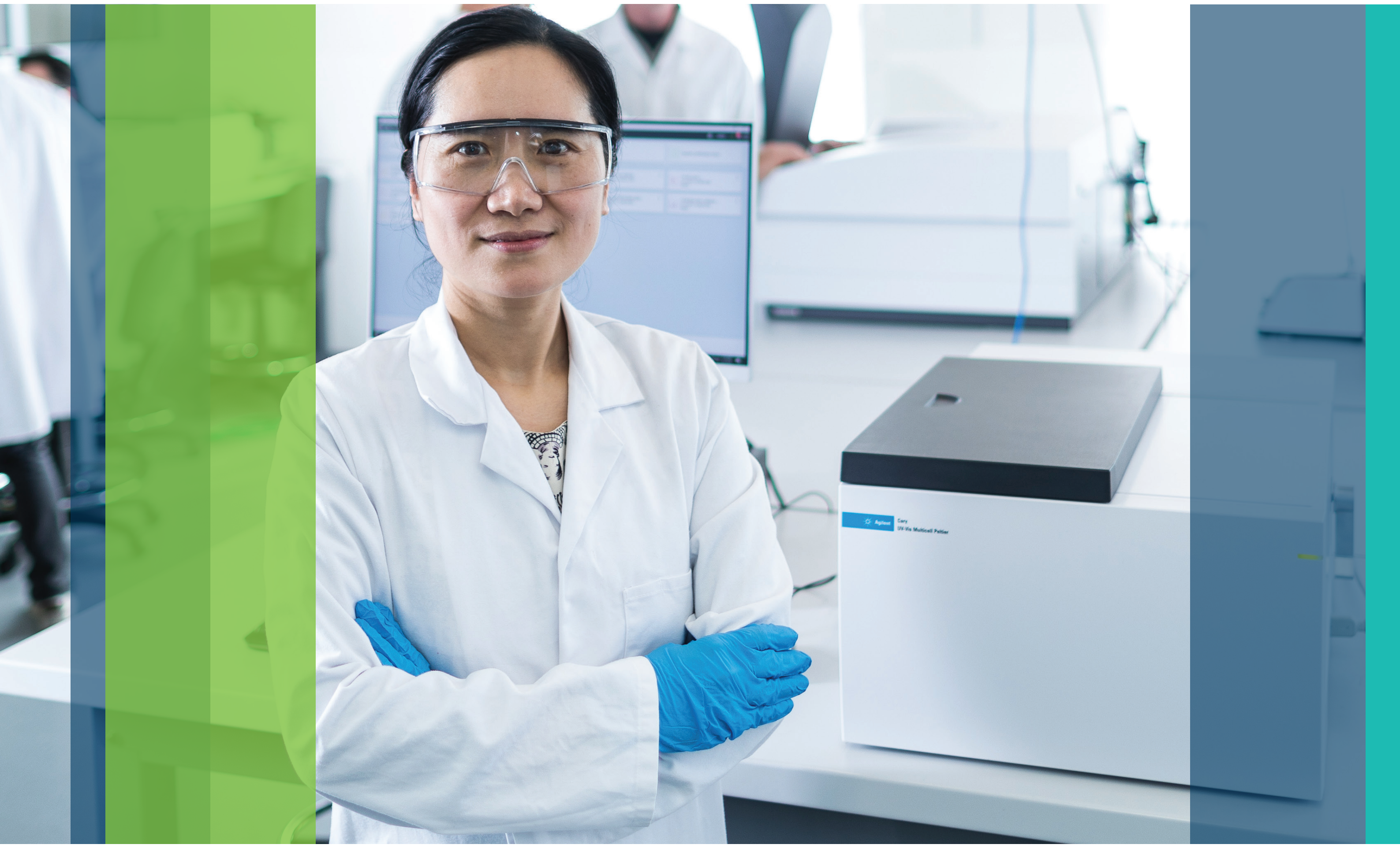
2019

24–26 September, Amsterdam, Netherlands. **Spectro Expo 2019.** http://www.spectroexpo.com.

18–20 November, Princeton, NJ, United States. **Eastern Analytical Symposium (EAS) and Exhibition.** askEAS@eas.org, http://www.eas.org/.

Agilent

Trusted Answers



Multiply Your UV-Vis Experimental Possibilities

The new Agilent Cary 3500 UV-Vis spectrophotometer will transform your laboratory. Designed with you in mind, it will streamline your experimental design and amplify confidence in your results.

The Cary 3500 UV-Vis will change the way you:

- Monitor enzymatic reactions at temperature
- Calibrate and determine sample concentration
- Perform temperature ramping experiments
- Quantify nucleotides and proteins

Find out more at: www.agilent.com/chem/cary3500uv-vis