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Global Hg pollution from artisanal gold mining
Soil organic matter using vis-NIR spectroscopy
Are omics the death of Good Sampling Practice?

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Soil organic matter can be determined using visible-near infrared spectroscopy and machine learning, providing a green methodology for the analysis. Find out more in the article starting on page 11.

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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 Asia* 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*. 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 our second article, "Determination of soil organic matter using visible-near infrared spectroscopy and machine learning", Felipe Bachion de Santana, Sandro Keiichi Otani, André Marcelo de Souza and Ronei Jesus Poppi describe work they are doing to develop a green methodology to determine soil organic matter. If the World's population is to be fed in the future, improvements to agricultural productivity are required and soil fertility will be key to this. Current methodologies are time-consuming and expensive, but visible-near infrared spectroscopy has the potential to replace them. Sound familiar?

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.

NEWS

Karl Norris: Father of NIR spectroscopy

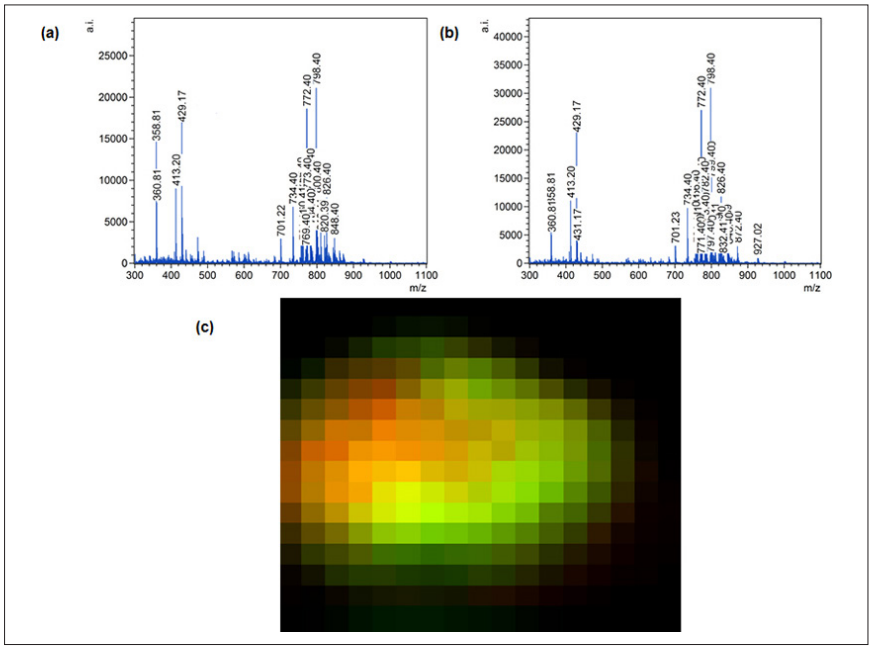
We are sad to announce that Karl Norris passed away peacefully on 17 July 2019 at the age of 98. Karl is rightly known as the "father of near infrared spectroscopy". He invented the technique while working at the USDA Instrumentation Research Laboratory, Beltsville, USA. He had a deep understanding not only of the instrumentation but also of the relation of spectra and chemistry. With his home-coded software, he regularly won the chemometrics "Shootout" at the International Diffuse Reflectance Conference in Chambersburg, PA, until he graciously stood down and let others have a chance!

The whole of the NIR spectroscopy community as well as the billions who benefit from its applications owe so much to Karl.

Karl Norris at Beltsville with the Cary 14 in the background, photographed in 1982.

First MS images recorded using MAIV

The MAIV (matrix-assisted ionisation in vacuum) mass spectrometry technique was developed by Professor Sarah Trimpin and her group in 2012. They observed that as 3-nitrobenzonitrile (3-NBN), a solid-state crystal matrix, sublimed under an intermediate vacuum and at ambient temperature, gas-phase analyte ions were observed. Mass spectra recorded under these conditions contained multiply charged ions and were very similar to those produced by electrospray ionisation. One significant advantage of the MAIV technique is that it generates multiply charged ions from peptides and proteins. This is of interest in tissue imaging and profiling experiments as it facilitates their identification by tandem mass spectrometry.



MAIV-MS lipid profiles (a and b) from a rat brain section. (c) Initial images of a horizontal section of rat brain as a bi-colour overlay of *m/z* 611 and *m/z* 798.4.

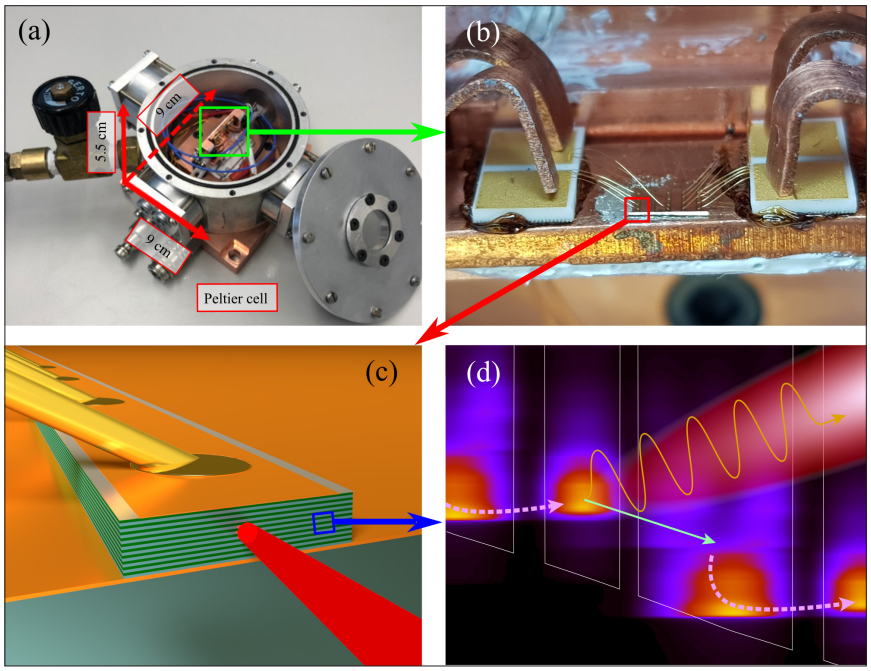
Professor Malcolm Clench and his group at Sheffield Hallam University have recorded the first mass spectrometry images using MAIV mass spectrometry, and the results are published in *JSI—Journal of Spectral Imaging* (doi: 10.1255/jsi.2019.a12). They modified the mass spectrometer's sampling cone and optimised instrumental parameters to enable an area of ~5.3 mm diameter to be sampled. Imaging of a horizontal section of a rat brain recorded lipids' signals at good sensitivity and selected ion signals could be overlaid to produce spatial information.

Further work is under way to investigate improvements to the sampling area that can be obtained. It remains to be seen whether the selectivity in sampling area obtainable in MAIV mass spectrometry experiments will make it a viable technique for imaging. However, the data acquired so far suggest that there may be a role for MAIV in mass spectrometry imaging.

Terahertz QCL without cryogenic cooling

Terahertz (THz) radiation opens up intriguing prospects for non-invasive imaging and non-destructive quality control, among other applications. But whereas there is no shortage in ideas for potential uses, their implementation is hampered by a lack of practical technologies for generating and detecting THz radiation. Lorenzo Bosco, Martin Franckié and colleagues from the group of Jérôme Faist at the Department of Physics have reported the creation of a THz quantum cascade laser (QCL) that operates at a temperature of 210 K (–63 °C). That is the highest operational temperature achieved so far for this type of device and one where no cryogenic coolants are needed.

QCLs operate according to a fundamentally different concept from other seimiconductor lasers. In short, they are built around repeated stacks of precisely engineered semiconductor structures (see the figure, panel c), which are designed such that suita-



Thermoelectrically cooled THz quantum cascade laser. a) The thermoelectrically cooled laser box with the laser mounted on top of a Peltier element (white square), allowing operation between 195 K and 210.5 K with the laser emitting vertically through the window in the top lid. b) The laser chip as mounted in the laser box, contacted with thin gold wires bonded on top of several laser ridges. c) Schematic of one laser ridge; the horizontal lines show the quantum-well structure formed by layered semiconductors. The ridge (150 µm wide) is sandwiched between thin layers of copper. d) Conduction band edge (white lines) tilted by the applied operation bias, with the electron density resolved in energy shown in colour. The electrical bias drives electrons through the non-radiative transitions indicated by the dashed arrow. This pumps the state in the thin well, which becomes more populated than the state in the wider well indicated by the green arrow, allowing for net stimulated emission of terahertz photons. Credit: ETH Zurich/D-PHYS, Faist group.

ble electronic transitions take place in them (panel d).

Widespread use of QCLs for THz radiation has been hindered by the requirement for cryogenic coolants—typically liquid helium—which adds substantial complexity and cost, and makes devices large and less mobile. Progress towards operation of THz QCLs at higher temperatures got essentially stuck seven years ago, when operation of devices at around 200 K (–73 °C) was achieved.

Writing in *Applied Physics Letters* (doi: 10.1063/1.5110305), the ETH team present a thermoelectrically cooled THz QCL, operating at temperatures of up to 210 K. Moreover, the laser light emitted was strong enough that it could be measured with a room-temperature detector. This means that entire setup worked without cryogenic cooling, further strengthening the potential of the approach for practical applications.

Bosco, Franckié and their co-workers designed their QCL stacks to use the simplest unit structure possible, based on two quantum wells per period (see the figure, panel d). This approach has been known to be a route to higher temperatures of operation, but at the same time this two-well design is also extremely sensitive to the smallest changes in the geometry of the semiconductor structures. Optimising performance relative to one parameter can lead to degradation relative to another. With systematic experimental optimisation not being a viable option, they had to rely on numerical modelling. This is the second area where the group has made substantial progress.

The first demonstration of a THz QCL operating without cryogenic cooling constitutes an important step towards filling the "THz gap", which has long existed between the mature technologies for microwave and infrared radiation.

ARTICLE

Reducing global mercury pollution from small-scale artisanal gold mining

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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.

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.

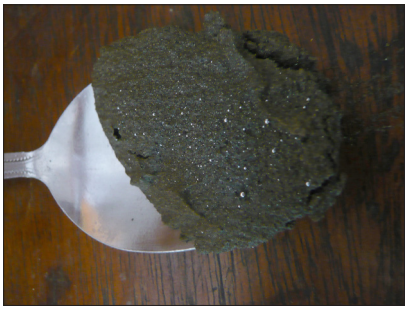

Figure 3. Mercury flour (droplets) in a spoonful of tailings (Philippines). Reproduced from Reference 7 with permission.

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 all droplets, subse-

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.

quent 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 used during the phases of this project was stringently crafted to comply 100% with the demands of the Theory of

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

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]

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.

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 definite information as to whether the tailing gold has been sufficiently crushed to allow complete liberation. While the

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

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]

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Determination of soil organic matter using visible-near infrared spectroscopy and machine learning

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Introduction

United Nations (UN) projections estimate that the world's population will be around 9.6 billion by 2050. Current projections indicate that feeding such a huge population would require dramatically increasing (~70%) overall food production by 2050. To achieve this goal, the agricultural productivity in developing countries such as Brazil would need to increase significantly in order to provide more productive, sustainable and inclusive food systems to fight poverty and hunger in this massive population. One of the most important factors required to accomplish this task is the understanding of soil fertility in order to manage it most effectively.

To achieve this, millions of soil analyses are performed every year around the world to increase crop yields. In Brazil, approximately 4 million soil fertility analyses are performed per year, and soil organic matter (SOM) is one of the main factors that support land management. However, the two main conventional methodologies to determine the SOM (Walkley–Black and dry-combustion) are time-consuming and expensive, and hence are not suitable for use on a large

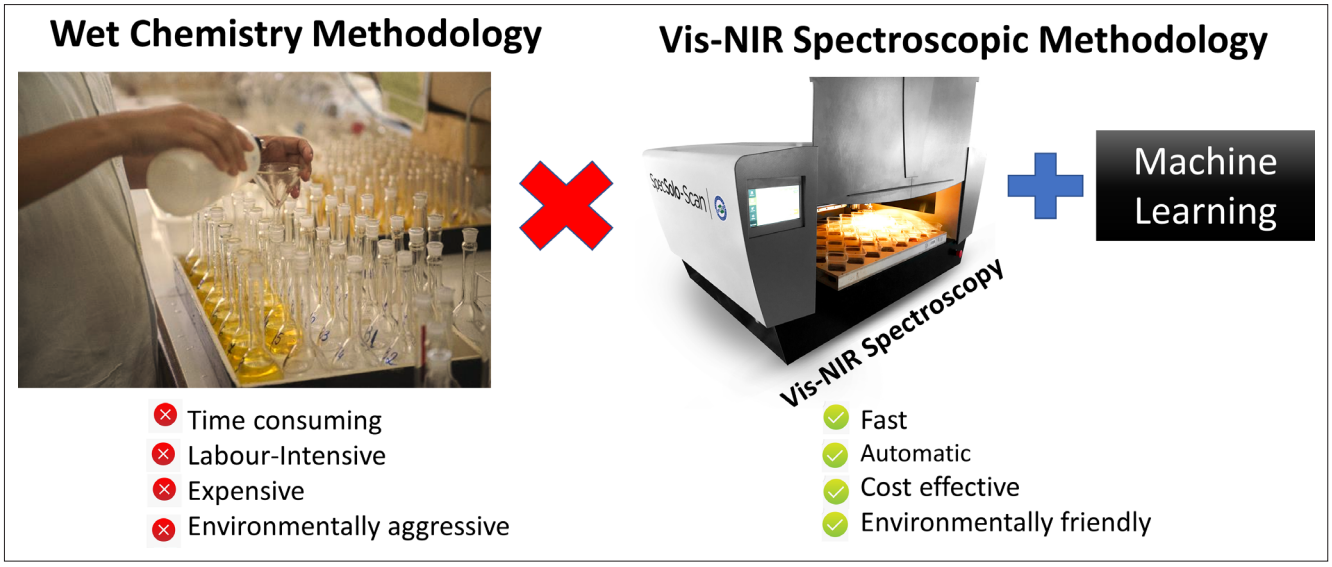

Figure 1. Comparison between the wet and vis-NIR spectroscopic methodology for SOM analysis.

scale. Also, the Walkley–Black method is damaging to the environment, generating residues that require treatment, and, therefore, is not suitable for sustainable agricultural practices.[1]

As an alternative to the traditional methods, visible-near infrared (vis-NIR) spectroscopy can provide fast, low-cost and accurate results for SOM analyses in an environmentally friendly way. Also, the methodology is non-destructive and does not require additional sample preparation. A comparison between the two methodologies is illustrated in Figure 1.

However, vis-NIR spectra are composed of wide and superimposed bands and thus the application of this type of spectroscopy in SOM determinations requires the development of multivariate regression models capable of correlating these bands with the SOM reference values. Also, the soil matrices are very heterogeneous, complex and require a tremendous number of samples to create robust vis-NIR calibration models. Due to these problems, machine learning methods with high generalisation power have been employed in the development of the models. Among the machine learning methods that are suitable, we highlight the support vector machine (SVM).[2]

Support vector machine

Support vector machine is a kernel-based machine learning method proposed by Vladimir N. Vapnik, which uses implicit mapping of the input matrix (vis-NIR spectra) into a high-dimensional feature space defined by a specific kernel function; in this case the radial basis function (RBF):[2]

$$K\left(x_i, x_j\right) = exp\left(-\gamma \left\| x_i - x_j \right\|^2\right),\ \gamma > 0 \quad (1)$$

In the feature space, a linear hyperplane is built with the maximal margin between the support vectors of each class, and this hyperplane is set up to solve the initial separation problem. The SVM can also be extended to regression problems by adding and subtracting a positive k number in the y_i reference value, creating a positive $(y_i + k)$ and negative class $(y_i - k)$. In this situation, the optimal separation hyperplane will pass by the original values of y_i, because the best separation will be $y_i + 0$. As in linear regression models, the y prediction value can be estimated using a linear regression function:

$$y = w \cdot K(x) + b \quad (2)$$

where w and b are the slope and offset of the regression line. The optimal w and b are obtained by minimising Equations 3 and 4.

$$\text{Minimise: } \frac{1}{2}\|w\| + C\sum_{i=1}^{n}\left(\xi_i + \xi_i^*\right) \quad (3)$$

$$\text{Subject to: } \begin{Bmatrix} y_i - w.K\left(x_i\right) - b \le \varepsilon + \xi_i \\ w.K\left(x_i\right) + b - y_i \le \varepsilon + \xi_i \\ \xi_i, \xi_i^* \ge 0 \end{Bmatrix} \quad (4)$$

where ε is the sensitive parameter which represents the tolerated error and C is the cost parameter, which controls the influence of each individual support vector. The slack variables ξ_i and ξ_i^* are introduced to account for samples that do not lie in the ε-sensitive zone.[3]

During this process the combination of two parameters must be optimised, the cost parameter (C) already described and the RBF kernel parameter (γ). γ is the regularisation parameter of the RBF function, which controls the width of this function. In order to reduce the time required to find this optimum combination, Bayesian optimisation can be used. The Bayesian optimisation algorithm attempts to minimise the root mean square error of cross validation (RMSECV) in a specific domain for each parameter; in this case [10^{-3} to 10^{3}] for C and γ. The algorithm selects the combination of C and γ points that provides the greatest potential improvement of RMSECV.[4] SVM modelling and Bayesian optimisation were implemented in Matlab R2016b with the Statistics and Machine Learning Toolbox 11.0.[4]

Materials and methods

In order to obtain a spectral library that represents the major producing regions of Brazil, 42,471 soil samples from several regions of Brazil were collected. The SOM reference analyses were based on the Walkley–Black method. These analyses were performed in collaboration with the IBRA Laboratory, Brazil, that holds a certification of proficiency from the Brazilian Agricultural Research Corporation (Embrapa Soils) and is accredited to ISO/IEC 17025:2005.

Before the vis-NIR spectra acquisition, the samples were oven dried at 40 °C for 48 hours, a rubber mallet was used to break the soil clusters and the granule size was controlled by a sieve (Ø<2 mm). The spectra were obtained using a vis-NIR spectrometer customised for this determination, called SpecSoil-Scan (Speclab Holding S.A., Campinas - SP, Brazil). This instrument can analyse 40 soil samples per batch and the spectral range is 432–2448 nm, with a spectral resolution of 3.3 nm.

A principal component analysis (PCA) model was applied to the spectral data set to find outliers. Samples with high values of Hotelling T^2 and residuals in spectral data (Q-statistics) at a significance level of 5 % were considered outliers. The Hotelling T^2 is related to leverage, which measures the distance of the sample from the centre of the data and Q residuals represent the unmodelled vis-NIR spectra.[5]

Representative samples were selected for development and validation of the models, resulting in 28,314 samples for the calibration set and 14,157 for the validation set.

Results and discussion

The original vis-NIR spectra of all soil samples are shown in Figure 2a, where the mean spectrum is represented by the black line. The NIR spectra contains useful information related to the SOM, due to absorptions in the C–C, C=C, C–H, C–N, N–H and O–H chemical bands. In the visible region, information on the SOM can be determined from absorption bands due to chromophores and darkness of the soil.[6]

To reduce baseline variation and spectral noise, the vis-NIR spectra were preprocessed by Savitzky–Golay smoothing and first derivative, with a window size of 11 points.[7] The preprocessed spectra are shown in Figure 2b, where the major variations in the absorption bands at 400–600, 1100, 1400, 1800–

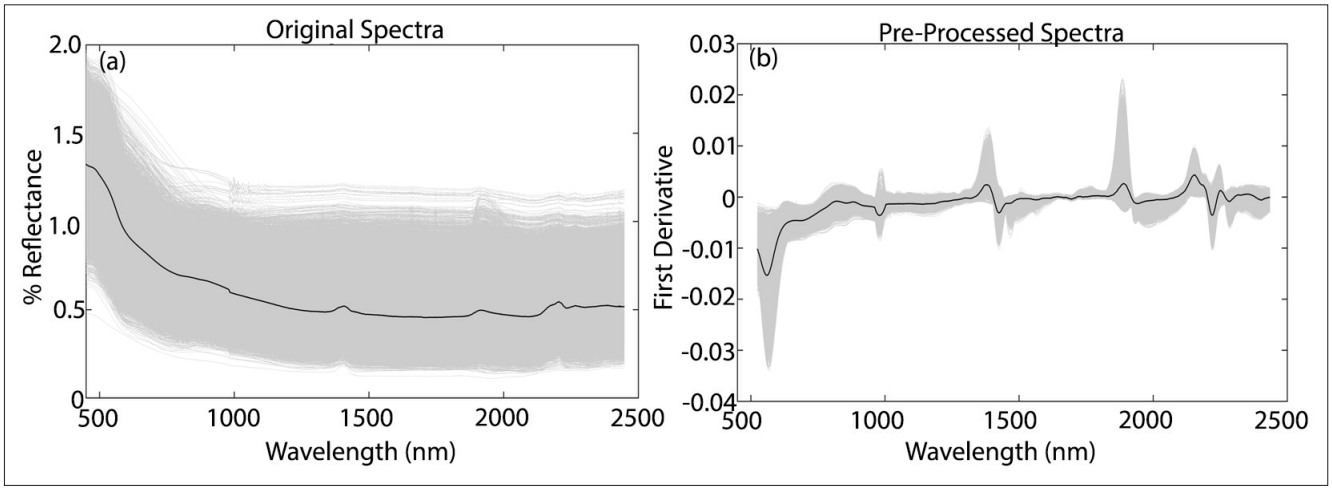

Figure 2. Original vis-NIR soil spectra (a) and preprocessed spectra (b).

2000 and 2200–2400 nm are highlighted, common to most soil samples.[6]

The three main absorptions bands are in the region of 500–650 nm, 1400 nm and 1900 nm. The absorptions at 500–650 nm can be associated with minerals that contain iron and the band at 1400 nm and 1900 nm can be associated with the OH group. The absorption band at 1100–1150 nm can be associated to aromatics and C–H stretch, and at 2200–2500 nm they are mainly due to vibrations involving metal–OH.[6]

The SVM model was built using the calibration samples and the choice of the optimal combination of C and γ values was performed as described above. To avoid overfitting in the regression model, the validation set was considered a set of unknown samples and these samples had no influence on the choice of C and γ parameters of the SVM model.

The scatter plots showing the reference versus predicted values by the SVM model are shown in Figure 3. Due to the high number of samples a colour bar containing the recurrence of the predicted values for each reference value was inserted in this plot. The SOM reference content in both sets were distributed along the range evaluated. The R^2_{cal}, R^2_{val}, RMSEC and RMSEP were close indicating the concordance between the calibration and validation sets. In other words, the SVM regression model adequately modelled the huge diversity of soils of the spectral library without overfitting the model.

Analysing the recurrence of the predicted values in Figure 3, it is possible to conclude that most of the samples were predicted with SOM values close to the reference ones. Only a few samples (dark blue) had the predicted values far from the reference values.

This fact can also be observed in Figure 4, which shows the histograms of the prediction errors in calibration

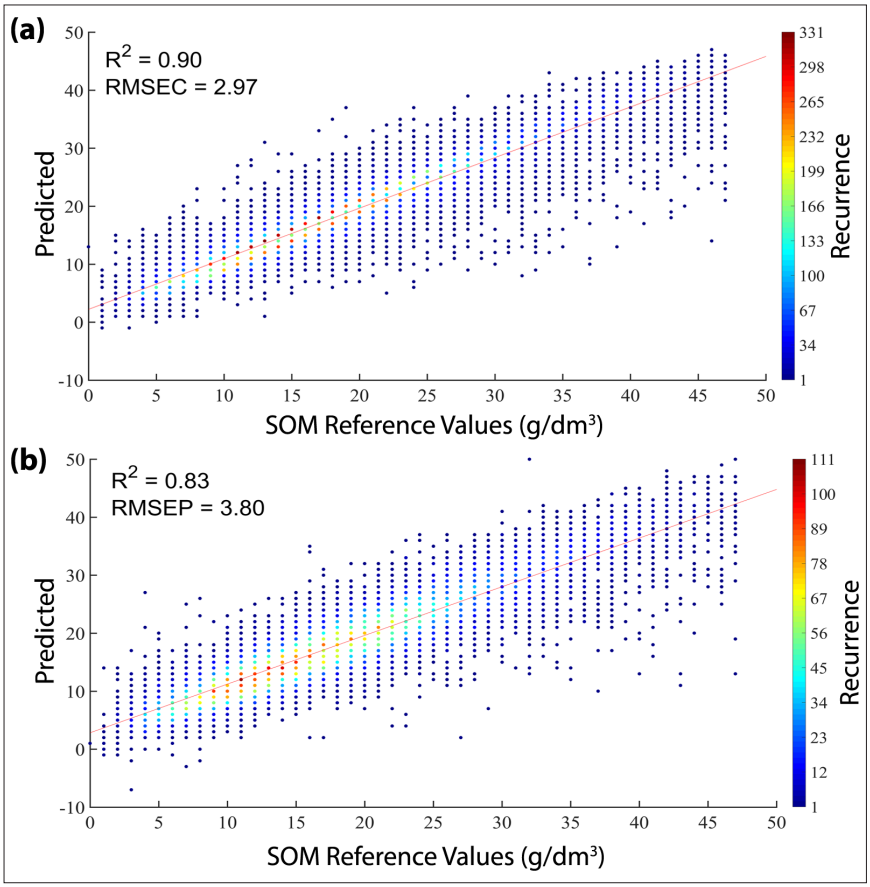

Figure 3. Plot of reference versus predicted values by SVM model in calibration (a) and validation (b) sets.

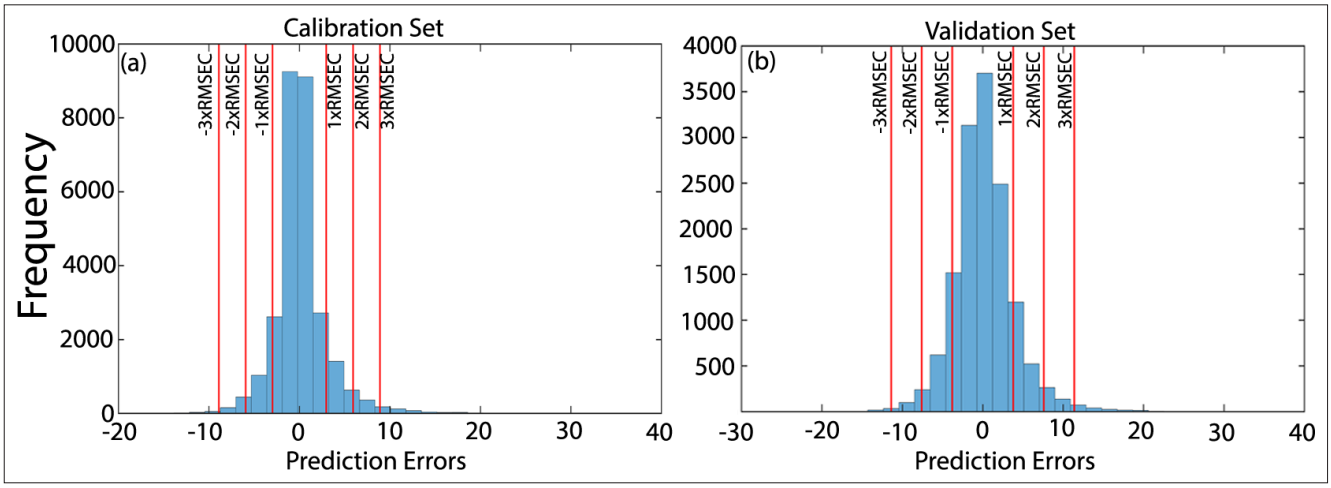

Figure 4. Histograms of the prediction errors in calibration (a) and validation (b) sets.

and validation sets. The histograms show that most of the samples were predicted with residues of up to 2 × RMSE in both sets, while few samples were predicted with higher residues.

Conclusions

The support vector machine algorithm was successful in dealing with an extensive and complex soil spectral library to determine SOM content. Brazil's soils are very diverse and heterogeneous with regards to chemical composition and soil organic matter content. The robustness presented by the proposed methodology involving vis-NIR spectra and machine learning has created high expectations for the possibility of mitigating/eliminating the use of heavy metal reagents in soil fertility analysis. Also, the methodology has potential to be used as a replacement for the traditional method in the future. Knowledge of soil fertility, supported by a green analytical methodology, could pave the way for increasing sustainable agricultural productivity.

Acknowledgements

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TONY DAVIES COLUMN

Are omics the death of Good Sampling Practice?

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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

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underpowered.[5] At the beginning of this year, Wu and co-authors published a "selective" review on integrating data 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

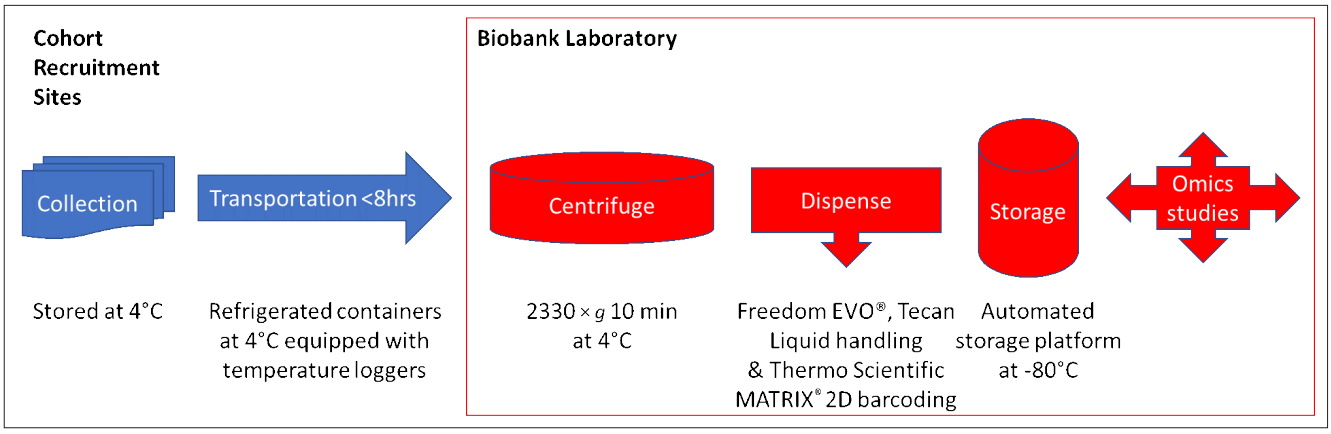

Figure 1. The TMM cohort sample collection and storage protocol.

place on the not unreasonable 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.

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SAMPLING COLUMN

Passing a milestone: the successful WCSB9

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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.

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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

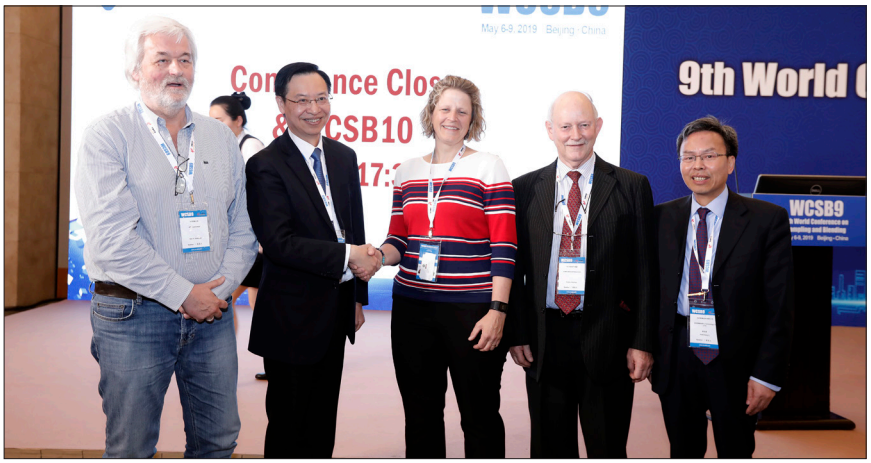
A sight to enjoy: with 555 participants, WCSB9 surpassed all previous conferences, which had boasted 137–235 attendees. The number of oral presentations, Proceedings papers and exhibitors were consequently also record-breaking—to everybody's delight.

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.spectroscopyasia.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.

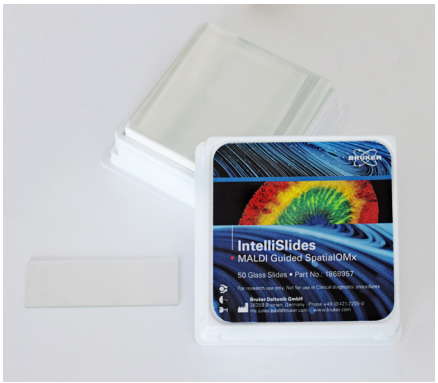
Accompanying the launch of the LC/MSD iQ is a new release of Agilent's MassHunter WalkUp Software for open-access drug discovery and chemistry labs, developed side-by-side with medicinal chemists. This new version has a touch-screen enabled interface and preconfigured analyses and reports that further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

Agilent Technologies

http://link.spectroscopyasia.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.



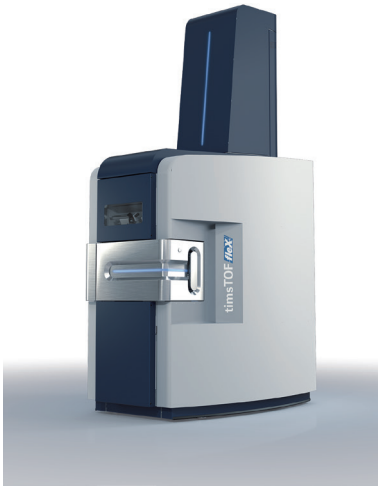
Bruker

http://link.spectroscopyasia.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



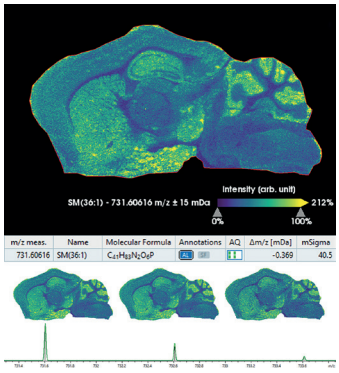
proteins, low-level cancer antigen peptides, lipids, glycans, metabolites or xenobiotics, which cannot be observed by traditional staining or labelling techniques. MALDI-guided SpatialOMx allows for specific targeting of cell sub-populations for subsequent ESI-TIMS/PASEF-based dda or dia 4D proteomics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

Bruker

http://link.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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,

PRODUCTS AT ASMS 2019

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.

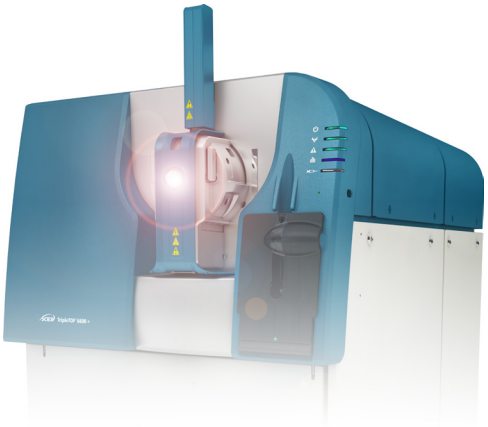
AEMS technology has been conceived by the Open Innovation Project, a collaboration between SCIEX and the US Department of Energy's Oak Ridge National Laboratory. Led by SCIEX Principal Research Scientist, Tom Covey, the Open Innovation Project developed the OPI, a key part of AEMS technology.

SCIEX

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

2D chromatography-mass spectrometry software

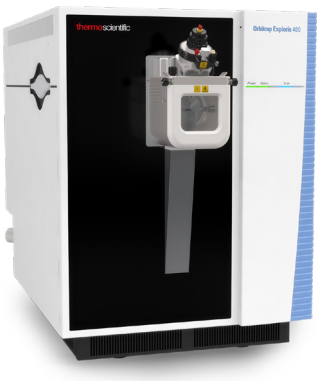
AnalyzerPro XD is a vendor-neutral, two-dimensional data processing solution for all chromatographic-mass spectrometry data. Although 2D chromatography greatly increases the effective resolution and peak capacity of the separation, chromatographic deconvolution still has an important part to play in 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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.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.spectroscopyasia.com/31-069

NEW PRODUCTS

ATOMIC

SPECTROLAB S OES analyser

SPECTRO Analytical Instruments has introduced the SPECTROLAB S high-performance arc/spark optical emission spectrometry (OES) analyser for the analysis of metal in process control and research applications. The instrument includes SPECTRO's proprietary CMOS+T technology. Its high speed enables it to analyse low alloy steel, for example, in less than 20 s. Calibration is easy and cost-efficient, needing only a single-sample, 5-minute standardisation. In most cases, iCAL 2.0 diagnostics ensure stable performance from then on—regardless of most shifts in ambient temperature or pressure. New elements or matrices can be added via a simple software update, eliminating the need for hardware modifications. The SPECTROLAB S's sealed, no-purge optical system maximises light transmission stability, even in the far UV. Its software utilises online drift correction and iCAL 2.0 temperature compensation for reproducible readings, even over successive shifts or maintenance intervals.

SPECTRO Analytical Instruments

http://link.spectroscopyasia.com/31-089

IMAGING

New look for Lumetta fixed grating spectrograph

HORIBA Scientific has announced a new look for its Lumetta fixed grating spectrograph. The new design houses an F/2 spectrograph with a large area sensor. It is designed to gather light from most fibres and high angle scattering phenomena. As an imaging spectrograph, it also enables advanced techniques such as multitrack spectroscopy and fast hyperspectral imaging. With multitrack spectroscopy, multiple independent spectroscopy channels can be measured with Lumetta, either improving sample measurement throughput for similar measurements on different samples, or simultaneous measurement of different but complementary spectra such as photoluminescence and absorbance from the same sample. A scientific grade I CCD deep cooled to –50 °C, together with low noise 16-bit electronics, produces a signal-to-noise ratio of 1200 : 1 and its deep cooling allows signal integration for hours. Lumetta also offers a flexible signal input interface, accommodating free-space as well as FC, SMA and ferrule fibre interfaces. Spectral resolution can be controlled from a selection of interchangeable slits.

HORIBA Scientific

http://link.spectroscopyasia.com/31-093

MASS SPECTROMETRY

New mass spectrometers for clinical diagnostic laboratories

Thermo Fisher Scientific has expanded its range of mass spectrometers for clinical diagnostic laboratories with the addition of two systems now listed as Class I medical devices with the United States Food and Drug Administration (US FDA): the Thermo Scientific TSQ Altis MD Series and the Thermo Scientific Quantis MD Series. The analytical solutions are designed to provide confidence in laboratory developed tests (LDTs) through a complete suite of LDT-enabled software with a laboratory information system (LIS) option. In addition, the enhanced product portfolio is designed to increase throughput of clinical diagnostic assays for the detection of small to large molecules within complex biological matrices. The TSQ Altis MD Series and TSQ Quantis MD Series mass spectrometers offer similar throughput for the analysis of human samples, but differ by sensitivity. The MD portfolio uses Thermo Scientific TraceFinder LDT 1.0 Software. Included as standard, the software provides a workflow-oriented approach to high-throughput quantitation,

NEW PRODUCTS

including an administrator console for managing user-based permissions, data repositories and auditing capabilities. In addition, an optional middleware solution is available to provide bidirectional communication between TraceFinder LDT Software and the LIS.

Thermo Fisher Scientific

http://link.spectroscopyasia.com/31-095

Waters introduces new tandem quad mass spectrometer

Waters has added to its tandem quadrupole mass spectrometry portfolio with the introduction of the Xevo TQ-S cronos. This is a new, tandem quadrupole mass spectrometer designed for routine quantitation of large numbers of small-molecule organic compounds over a wide concentration range. It is suited to meet regulatory requirements for pesticide residue analysis, the monitoring for contaminants in processed foods, identifying drugs of abuse and performing impurity profiling of pharmaceuticals.The Xevo TQ-S cronos comes with many of the features of the Xevo product line, including the StepWave™ ion guide for long-lasting sensitivity and performance, tool-free probe maintenance and ionisation source cleaning, a choice of ionisation sources including UniSpray™ for analysing a broader range of compounds with greater ionisation efficiency, automated start up and system optimisation provided by IntelliStart™, simplified method development and transfer with Quanpedia™ and streamlined data review and processing with TargetLynx™ XS Software.

Waters

http://link.spectroscopyasia.com/31-094

RAMAN

New Raman microscope from Edinburgh Instruments

The RM5 is a compact and fully automated Raman microscope, suitable for analytical and research purposes. It is truly confocal, with variable slit and multiple position adjustable pinhole for higher image definition, better fluorescence rejection and application optimisation. It can accommodate up to three computer-controlled lasers and has a five-position grating turret enabling spectral resolution of 1.4 cm^{-1} (FWHM) and optimisation over the full spectral range of 50–4000 cm^{-1}. Up to two integrated detectors can be added, including high efficiency CCD, EMCCD and InGaAs arrays.

The microscope is driven by Ramacle software which controls all RM5 functions. The software provides control, visualisation, data acquisition, analysis and presentation of the RM5 whether it is used for generating Raman spectra or with advanced upgrades such as Raman mapping. Ramacle enables sample visualisation, live signal monitoring and parameter optimisation before every measurement. The instrument status and signal are displayed and constantly updated during measurements.

Edinburgh Instruments

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X-RAY

ED-XRF spectrometer for fuel and lube oil analysis

SPECTRO Analytical Instruments' SPECTROCUBE Petrochem ED-XRF benchtop spectrometer is designed for the analysis of fuel and lube oil. The SPECTROCUBE Petrochem is designed to meet all relevant refining and petrochemical analysis standards. Its sulfur content testing of fuel oils complies with test methods including ISO 13032, ASTM D7220, ASTM D4294, ISO 20847, and ISO 8754. It enables a precise analysis of lube oil per ASTM D7751. SPECTROCUBE Petrochem enables a smooth workflow, even for minimally trained users: samples are analysed in three steps, with the intuitive software presenting the relevant information on a single screen. The instrument has a high-resolution silicon drift detector and is optimised for testing of element concentrations in the range from sodium to uranium. Its lube oil method, for instance, covers 24 elements.

SPECTRO Analytical Instruments

http://link.spectroscopyasia.com/31-090

Conferences

2019

3–5 September, Salvador, Brazil. **6th Brazillian 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?WebsiteKey=2e25ab5a-1f6d-4d78-a498-19b9763d11b4.

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.

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

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

15–19 September, Cartagena, Colombia. **SETAC Latin America 13th Biennial Meeting.** setac@setac.org, https://sla2019.setac.org/.

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

16–18 September, Melbourne, Australia. **International Conference on Materials Science and Engineering 2019.** Rakshith Kumar, rakshith.kumar@materialsoceania.com, https://www.materialsconferenceaustralia.com/.

17–20 September, Santa Rosa, Argentina. **10th Argentinean Congress in Analytical Chemistry.** https://www.facebook.com/caqa2019/.

22–25 September, Phoenix, Arizona, 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.

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.

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

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

24–26 September, Sao Paulo, Brazil. **6th Analitica Latin American Congress.** analitica@nm-brasil.com.br, https://www.analiticanet.com.br/pt/perfil-do-evento.

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.

29 September–3 October, Portland, United States. **2019 Materials Science and Technology Conference (MS&T19).** metsoc@cim.org, http://www.matscitech.org/.

6–11 October, Mendoza, Argentina. **15th Rio Symposium on Atomic Spectrometry.** secretary@15riosymposium.com, https://www.15riosymposium.com/.

9–10 October, Coventry, United Kingdom. **Photonex Europe 2019.** Laurence Dereereux, ld@xmarkmedia.com, https://photonex.org/.

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.

17–19 October, Rome, Italy. **Frontiers in Materials Science & Engineering THEME: Synergy to Rehabilitate the Innovations in Material Science.** info@frontiersmeetings.com, https://frontiersmeetings.com/conferences/materialsscience/.

3–7 November, Toronto, Canada. **SETAC North America 40th Annual Meeting.** https://toronto.setac.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/.

1–6 December, Boston, United States. **Materials Research Society 2019 Fall Meeting (MRS 2019).** https://www.mrs.org/fall2019.

9–13 December, San Francisco, United States. **2019 American Geophysical Union (AGU) Fall Meeting.** meeting-info@agu.org, https://meetings.agu.org/upcoming-meetings/.

2020

12–18 January, Tucson, Arizona, 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://

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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.

26–29 April, Oviedo, Spain. **The 5th International Glow Discharge Spectroscopy Symposium.** Peter Robinson, pete@masscare.co.uk, https://www.ew-gds.com/.

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

24–28 May, Chiba, Japan. **Japan Geoscience Union (JpGU) Meeting 2020.** http://www.jpgu.org/en/articles/20171208meetingplan.html.

24–28 May, Winnipeg, Canada. **103rd Canadian Chemistry Conference.** http://www.ccce2019.ca/.

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.** https://www.asms.org/conferences/annual-conference/future-annual-conferences.

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

21–26 June, Honolulu, Hawali, 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.

5–8 July, Skagen, Denmark. **International Association for Spectral Imaging (ASIM) 2020.** 2020@iasim.net, https://2020.iasim.net/.

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/.

6–10 September, Singapore, Singapore. **SETAC 8th World Congress.** setac@setac.org, https://singapore.setac.org/.

9–17 September, Reno, NV, United States. **47th Annual Conference of Federation of Analytical Chemistry and Spectroscopy Societies (SciX2020).** scix@scixconference.org, https://www.scixconference.org/index.php/scix-home/future-conferences.

13–16 September, Orlando, United States. **134th AOAC International Annual Meeting & Exposition.** meetings@aoac.org, http://www.aoac.org.

20–25 September, Kyoto, Japan. **11th International Conference on Laser-Induced Breakdown Spectroscopy (LIBS2020).** Yoshihiro Deguchi, ydeguchi@tokushima-u.ac.jp, http://www.fm.ehcc.kyoto-u.ac.jp/Sakkalab/member/sakka/LIBS2020/index.htm.

20–26 September, Aachen, Germany. **17th International Symposium of Trace Elements in Man and Animals (TEMA17).** Prof. Dr. Lothar Rink, immunologie@ukaachen.de, https://www.ukaachen.de/kliniken-institute/institut-fuer-immunologie/institut.html.

4–8 October, Pittsburgh, United States. **2020 Materials Science and Technology Conference (MS&T20).** metsoc@cim.org, http://www.matsc-itech.org/.

25–28 October, Montreal, Canada. **2020 GSA Annual Meeting.** http://www.geosociety.org/.

15–20 December, Honolulu, Hawaii, United States. **The International Chemical Congress of Pacific Basin Societies 2020.** https://pacifichem.org/.

2021

15–21 February, Houston, United States. **2021 AAFS 73rd Annual Scientific Meeting.** https://www.aafs.org/home-page/meetings/future-past-aafs-meetings/.

6–10 June, Philadelphia, PA, United States. **69th ASMS Conference.** https://www.asms.org/conferences/annual-conference/future-annual-conferences.

Exhibitions

2019

25–27 September, Bangkok, Thailand. **Thailand Lab International 2019.** http://www.thailandlab.com.

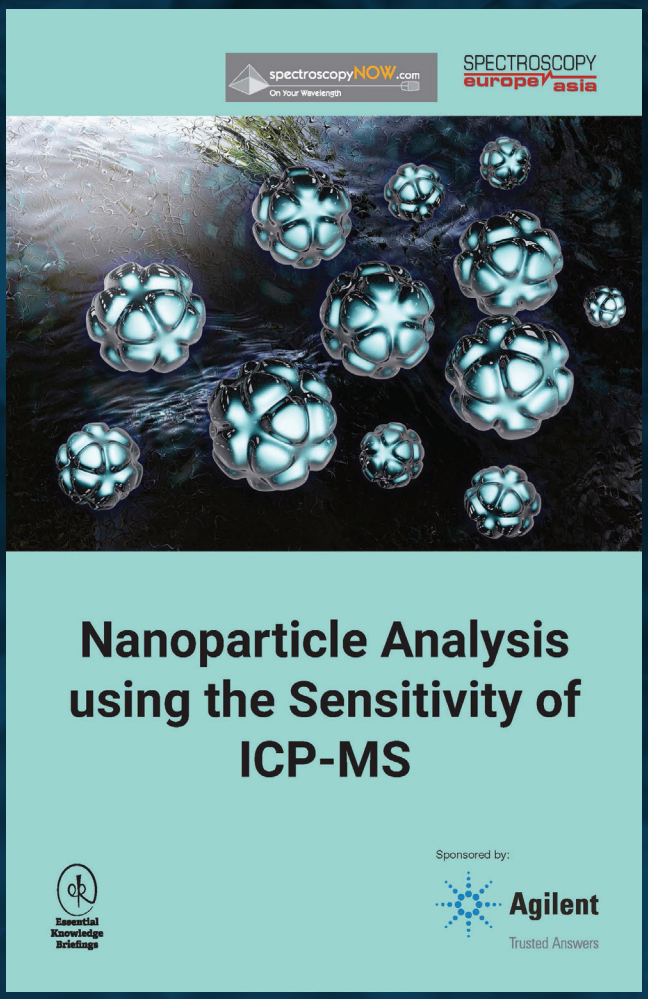
15–17 October, Kuala Lumpur, Malaysia. **LabAsia 2019.** enquiry@ecmi.com.my, http://www.lab-asia.com.

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

2020

1–5 March, Chicago, United States. **Pittcon 2020-Conference on Analytical Chemistry and Applied Spectroscopy.** pittconinfo@pittcon.org, https://pittcon.org/.

16–18 March, Dubai, United Arab Emirates. **ARABLAB 2020.** info@arablab.com, https://www.arablab.com/.



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