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Hyperspectral imaging for recycling

A week in the life of a PhD student

Pittcon 2019 Report

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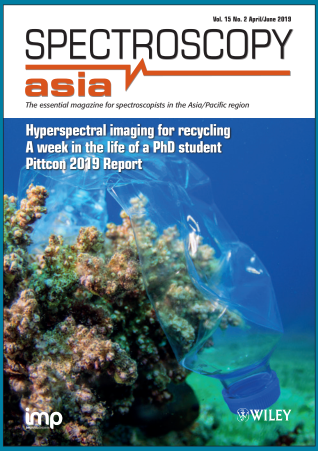

Hyperspectral imaging has many applications in the waste recycling sector, not least in the recycling of plastic. Find out in the article starting on page 6.

Publisher
Ian Michael
(ian@impublications.com)

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

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

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

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EDITORIAL

Last issue I was writing about climate change and hyperspectral imaging, a theme I can continue this issue! Our first article is “Hyperspectral imaging applied to the waste recycling sector” by Giuseppe Bonifazi, Giuseppe Capobianco, Roberta Palmieri and Silvia Serranti from Sapienza University of Rome, Italy. They look at two important areas of recycling of waste materials: concrete and plastics. If aggregates are to be recycled from concrete, the presence of pollutants (plastics, foams, brick etc.) and the degree of removal of cement mortar from the aggregates must be assessed and monitored. NIR hyperspectral imaging with PLS does a good job of both tasks.

Our second article is a bit different. “A week in the life of a PhD student” by Katie Ember of the University of Edinburgh, UK, gives an interesting insight into, well, a week in the life of the author as a fourth-year PhD student. Katie is working on investigating a way of detecting liver damage using spectroscopy, which is “about as interdisciplinary as you can get”! I’m sure all readers will find it interesting and it may be helpful for those you know who may be considering a PhD. We hope to bring you a scientific article on Katie’s work on using handheld Raman spectroscopy to assess the viability of human livers for transplant in a future issue.

In the Tony Davies Column, Tony Davies, Peter Lampen and Robert Lancashire are worried about their metadata, or perhaps the lack of it. With the explosion of data and ways to mine and make use of it, having accurate and appropriate metadata about analytical data sets is vital if they are to be reused efficiently or at all. This is also an area that is being increasingly targeted by regulators, with the US FDA issuing guidance at the end of 2018; others will follow. You have been warned.

We have some other worried columnists in Chris Burgess and John Hammond, who consider “Specifying accuracy and precision criteria for ultraviolet spectrometers”. Some compliance requirements would seem to make impossible demands; Chris and John unravel what’s going on.

I have provided brief details of new products that I found at the Pittcon exhibition. The links at the end of each product section go directly to a page on the manufacturer’s website with more information on the product, saving you some time searching or browsing through menus. Similar links are also available for all New Products.

Ian Michael

NIR Awards

Two awards administered by the International Council for Near Infrared Spectroscopy (ICNIRS) have been announced recently.

2019 Tomas Hirschfeld Award

The winner of the 2019 Tomas Hirschfeld Award is José Manuel Amigo Rubio. José obtained his PhD (Cum Laude) in Chemistry from the Autonomous University of Barcelona, Spain. Since 2007, he has been employed at the Department of Food Science of the University of Copenhagen, Denmark, and also as Guest Professor of the Federal University of Pernambuco, Brazil, since 2017. José's research interests include NIR hyperspectral and multispectral image analysis in different research fields including food production, pharmaceutical research, forensic sciences. Moreover, he is involved in teaching Chemometrics through well-known PhD courses such as the Copenhagen School of Chemometrics. He has authored more than 140 publications (110+ peer-reviewed papers, books, book chapters, proceedings etc.) and given more than 60 conferences and courses at international meetings. José has supervised or is currently supervising several Masters, Post Docs and PhD students and he is an editorial board member of four scientific journals within Chemometrics, chemical imaging and analytical chemistry. In 2014, José received the "Chemometrics and Intelligent Laboratory Systems Award" for his achievements in the field of Chemometrics.

José Amigo

The Tomas Hirschfeld Award is a prestigious award given by the International Council for Near Infrared Spectroscopy (ICNIRS) in recognition of a significant contribution to the science of NIR spectroscopy. It awarded on the basis of excellence in research conducted by a scientist of international standing. This award recognises the many contributions to NIR analysis made by the late Tomas Beno Hirschfeld, who died in 1986 at a relatively young age.

2019 Karl Norris Award

The Karl Norris Award honours the unique contribution of Karl Norris as the internationally recognised founder of NIR spectroscopy in the modern world. In contrast to the Tomas Hirschfeld Award, which is aimed at younger researchers, this award is aimed at researchers in the later stages of their career, with a sustained record of important contributions to NIR spectroscopy.

Graeme Batten

The winner for 2019 is Dr Graeme Batten from Australia. Graeme started his NIR career working for New South Wales (NSW) Agriculture, Yanco, Australia. He and his team were pioneers in developing NIR technology for rice and other cereal grains. He had been working intensively on using NIR on precision agriculture since 2000. As Editor-in-Chief of the *Journal of Near Infrared Spectroscopy* (*JNIRS*) for over 10 years from 2005, Graeme has dedicated body and soul to the continuing success of the journal. His feedback and teaching have helped many scientists around the world to get a successful paper published.

Aquaphotomics shows how plants control their water structure to survive

A small group of plants known as "resurrection plants" can survive months or even years without water. Researchers in Japan and Bulgaria have used NIR spectroscopy and aquaphotomics to monitor the entire processes of drying and subsequent rehydration of one such plant, *Haberlea rhodopensis*. Results were compared to the same processes for its non-resurrection relative. The results showed that during drying, the resurrection plant performs fine restructuring of water in its leaves, preparing itself for the dry period by accumulating water molecular dimers and water molecules with four hydrogen bonds, while drastically diminishing free water molecules. This regulation of water structure is thought to be the mechanism by which the plant preserves its tissues against dehydration-induced damages and allows it to survive in the dry state. The discovery that water structure is important for preservation of the plants during drought stress opens up a new direction for bioengineering and improving the drought tolerance ability of plants. The research was published in *Scientific Reports* (doi: 10.1038/s41598-019-39443-4).

When *Haberlea rhodopensis* was losing water, it kept the number of free water molecules, water dimers, trimers and more hydrogen-bonded water molecules in the same ratios. While the numbers of these molecules diminished, their relationship was kept constant, suggesting orchestrated efforts by the plant to keep the water in a certain state. Such ability was not observed in *Deinostigma eberhardtii*, and the ratios of water species in its leaves randomly fluctuated.

Drastic differences of the water structure in the leaves were observed when both plants were in the completely dried state. In this final phase, *Haberlea rhodopensis* radically diminished free water molecules and accumulated water dimers and water molecules with four hydrogen bonds. *Deinostigma eberhardtii*, in contrast, never showed any such radical transformation of water structure. Up to the very last moment, even in the completely dried state, it still had a lot of free water molecules, but now involved in spoliation and decay processes.

During rehydration, *Haberlea rhodopensis* showed the same orchestrated

Haberlea rhodopensis, a resurrection plant species, was used as a model system to study the underlying mechanisms of extreme desiccation tolerance.

dynamics of reorganisation of water structure, by performing orderly incremental changes of almost all water species.

This research showed for the first time that the structure of water, not its content, is what matters to the survival of the organism. When people think about life, we often associate dynamic features with the processes in living systems. And yet, in this peculiar plant, in the absence of visible signs of ongoing metabolism, achieving a specific water structure was its survival tool.

As a result, the study sheds some light on what may be the most fundamental feature of a living system: it is the structural organisation, rather than the dynamics, that is at its core. And the structure of water is shaped by the numerous substances produced in the cells. These may be sugars, amino acids or other biomolecules, but their final goal is achievement of a certain state of water molecular structure which allows the preservation of tissues and prevention of damage.

This research adds to our growing understanding of the mechanisms by which some organisms achieve their remarkable tolerance to extreme dehydration. It has discovered a target for modification in order to achieve better tolerance to drought in plants, which obviously can be achieved using different strategies (sugars, amino acids, proteins etc.) as long as they exert such influence on water molecular structure that would lead to decrease of free water molecules and increase of hydrogen bonded water. The aquaphotomics NIR spectroscopy method allows direct, non-destructive insight into the living processes and water structure and dynamics in real time and is as a valuable new tool for studying not only the abiotic and biotic stress in plants, but many other phenomena in living systems.

New approach facilitates spectroscopy on individual molecules

An international team led by Professor Jürgen Hauer of the Technical University of Munich (TUM) has succeeded in determining the spectral properties of individual molecules. The researchers acquired the absorption and emission spectra of the investigated molecules over a broad spectral range in a single measurement to accurately determine how the molecules interact with their environment, capturing and releasing energy. Normally, these kinds of measurements are averaged over thousands, even millions, of molecules, sacrificing important detail information. "Previously, emission spectra could be routinely acquired, but absorption measurements on individual molecules were extremely expensive", explains Hauer. "We have now attained the ultimate limit of detectability."

The new method is based on a compact instrument that the Munich chemists developed in collaboration with colleagues at the Politecnico di Milano. The key is that it generates a double laser pulse with a controlled delay in between. The second pulse modulates the emission spectrum in a specific manner, which in turn provides information about the absorption spectrum. This information is then evaluated using a Fourier transformation. Their work is reported in *PNAS* (doi: 10.1073/pnas.1808290116).

Using the method, they hope to now study individual molecules, to understand phenomena such as the energy flow in metal–organic compounds and physical effects in molecules when they come into contact with water and other solvents.

The influence of solvents at the single molecule level is still poorly understood. The chemists also want to display the flow of energy in a time-resolved manner to understand why energy flows faster and more efficiently in certain molecules than in others. "Specifically, we are interested in the transfer of energy in biological systems in which photosynthesis takes place", says Hauer.

The researchers are going to concentrate on the light collection complex LH2 for future applications. "Once we understand the natural light-harvesting complexes, we can start thinking about artificial systems for deployment in photovoltaics", says Hauer. The findings could form the basis for future technologies in photovoltaics. The goal is the development of a novel organic solar cell.

ARTICLE

Hyperspectral imaging applied to the waste recycling sector

Giuseppe Bonifazi, Giuseppe Capobianco, Roberta Palmieri and Silvia Serranti*
Department of Chemical Engineering, Materials & Environment (DICMA), Sapienza University of Rome,
Via Eudossiana 18, 00184, Rome, Italy. E-mail: silvia.serranti@uniroma1.it

Introduction

The need to develop and deploy increasingly effective, fast and robust sensing techniques capable of detecting, characterising and sorting solid waste products and materials represents one of the most challenging aspects in the industrial recycling sector. Most waste is of low value, so innovative technologies must be cost-effective and, at the same time, achieve high performance in terms of materials identification, both for sorting and quality control in recycling plants, so as to end up with high-quality secondary raw materials that are competitive in the market with the corresponding primary raw materials. In this perspective, the use of hyperspectral imaging (HSI) technology to carry out products/materials characterisation, through fast and reliable handling/processing, is becoming more and more important. In this article, some HSI-based applications in the waste recycling sector, originally developed by the authors, are presented and discussed. All the procedures have been designed, implemented and set up with the aim of providing sensing/inspection tools able to perform non-invasive, contactless and real-time analyses at both laboratory and/or industrial scale.

Hyperspectral imaging

Hyperspectral imaging is an innovative technique that combines the properties of digital imaging with those of spectroscopy.[1] Using this approach, it is possible to detect the spectral signature of each pixel of the acquired image in different wavelength regions (visible, near infrared, short-wave infrared etc.) according to the characteristics of the selected sensing device. A hyperspectral image can thus be considered as a three-dimensional dataset with two spatial dimensions and one spectral dimension, the so-called "*hypercube*". HSI can be considered one of the best and most powerful non-destructive technologies for accurate and detailed information extraction from the acquired images, with a high level of flexibility.

The large amount of spectral information collected by HSI from the sample surfaces must be processed in order to extract the information of interest. Furthermore, as a preliminary step in any inspection or quality control logic development, hyperspectral libraries of reference spectra, to be utilised for unknown sample recognition, must be built. To reach the previously mentioned goals, algorithms and procedures for spectral data pre-processing, exploration and classification are usually implemented through chemometric strategies. Different pre-preprocessing algorithms can be applied to hyperspectral data, finalised to linearise relationships among variables and remove external sources of variation that are not of particular interest for the analysis. Principal Component Analysis (PCA) is applied for exploratory purposes, providing an overview of the complex multivariate data.[2] PCA decomposes spectral data into several principal components (PCs), linear combinations of the original data, embedding the spectral variations of each collected spectral data set. The first few PCs, resulting from PCA, are used to analyse the common features among samples: in fact, samples characterised by similar spectral signatures tend to aggregate in the score plot as a cluster.

Finally, the recognition of different products and/or materials is obtained utilising classification methods, such as Partial Least-Squares Discriminant Analysis (PLS-DA). PLS-DA is a supervised classification technique requiring prior knowledge of the data and allowing the classification of samples into predefined groups.[3] In order to do that, starting from reference samples, a discriminant function is built and then this is later applied to classify samples belonging to an unknown set. Once the model is built, it can be applied to validation images. An interesting and powerful classification method is hierarchical modelling. Adopting this kind of classification logic,[4] objects are divided into subsets and then they are split again into further subsets, until each of them contains only a single object. During each step, objects that are different from the others are selected, isolated and compared through successive PLS-DA classification models.

Applications to the solid waste recycling sector

The utilisation of expensive and/or sophisticated devices is not appropriate in the waste recycling sector for several reasons. These are mainly technical (e.g. particles of different size, shape, composition, physical status), environmental (e.g. harsh conditions) and economic (e.g. low values of recovered materials or products). Therefore, efficient, but low-cost, technologies for the characterisation, sorting and quality control of the waste and recycled products are needed. A solution is represented by the application of procedures based on the utilisation of HSI devices. These procedures are growing rapidly in the waste management sector for materials coming from different sources, i.e. Construction and Demolition Waste (CDW), Waste from Electric and Electronic Equipment (WEEE), Municipal Solid Waste (MSW) and End-of-Life Vehicles (ELV). Below, two different case studies related to the solid waste recycling sector are reported; the first one deals with end-of-life concrete and the second one with mixed plastic waste.

HSI sensing devices

Two different HSI-based sensing architectures have been utilised, both located at the Raw Materials Laboratory of the Department of Chemical Engineering, Materials & Environment (Sapienza - University of Rome).

The first HSI device works in the NIR range (1000-1700 nm) and consists of a Spectral Camera NIR (SPECIM Ltd, Finland) using an ImSpector™ N17E with a spectral sampling/pixel of 2.6 nm, coupled with a TE-cooled InGaAs photodiode array sensor (320 × 240 pixels) and a pixel resolution of 12 bits. The device is fully controlled by a PC unit. Objects/materials to be investigated are laid on a moving conveyor belt (width = 26 cm and length = 160 cm) with adjustable speed (variable between 0 mm s^{-1} and 50 mm s^{-1}). Spectra acquisition can be carried out continuously or at specific time intervals. The lighting source uses a diffused light cylinder architecture, optimised for the NIR (i.e. hosting cylinder aluminium internal coated), embedding five halogen lamps.

The second HSI device works in the SWIR range (1000–2500 nm) and is made up of a SISUChema XL™ Chemical Imaging Workstation (Specim, Finland), with an ImSpector™ N25E imaging spectrograph, having a spectral sampling/pixel of 6.3 nm [active pixel 320 (spatial) × 240 (spectral) pixels], coupled with a MCT camera with pixel resolution of 14 bits. The device is controlled by a PC unit equipped with the ChemaDAQ™ data acquisition software (Specim, Finland). Objects/materials to investigate are placed into a moving sample tray/s.

In both cases the acquired hyperspectral images were processed using the PLS_Toolbox (Eigenvector Research, Inc.) running inside Matlab® (The Mathworks, Inc.).

End-of-life concrete

The possibility to utilise efficient and reliable sensing technologies able to perform detection/control actions, in order to assess concrete physical–chemical characteristics before demolition and during the recycling process of the different constituents, represents a key issue for the demolition waste sector.[5–7] Particular attention has been devoted in recent years to the recycling of concrete aggregates, contributing to reducing non-renewable natural resources exploitation. Characterisation of the aggregates during each step of the end-of-life concrete recycling process is important in order to obtain a final product able to satisfy market and regulatory requirements, with technical properties comparable with those of primary raw materials. In more detail, in order to recycle aggregates from concrete, two important aspects that can affect quality must be taken into account: 1) the presence of materials considered as pollutants (i.e. plastic, foam, brick, wood, gypsum) with respect to the aggregates[5] and 2) the degree of removal of mortar paste from the surface of recycled concrete aggregates.[6]

HSI was successfully used to recognise and identify the pollutants in a recycled aggregates stream as well as to evaluate the degree of removal of mortar paste from aggregates' surfaces. For contaminant detection, the investigated materials are characterised by different spectral signatures in the NIR range (1000–1700 nm) (Figure 1a). PCA shows the variance differences between the analysed classes of the materials. In fact, as shown in the score plot (Figure 1b), it is possible to observe the presence of six different clusters, based on the grouping of pixels according to their spectral similarity, corresponding to the different materials. After exploring the data by PCA, PLS-DA was applied as the classification method (Figure 1c). The six-

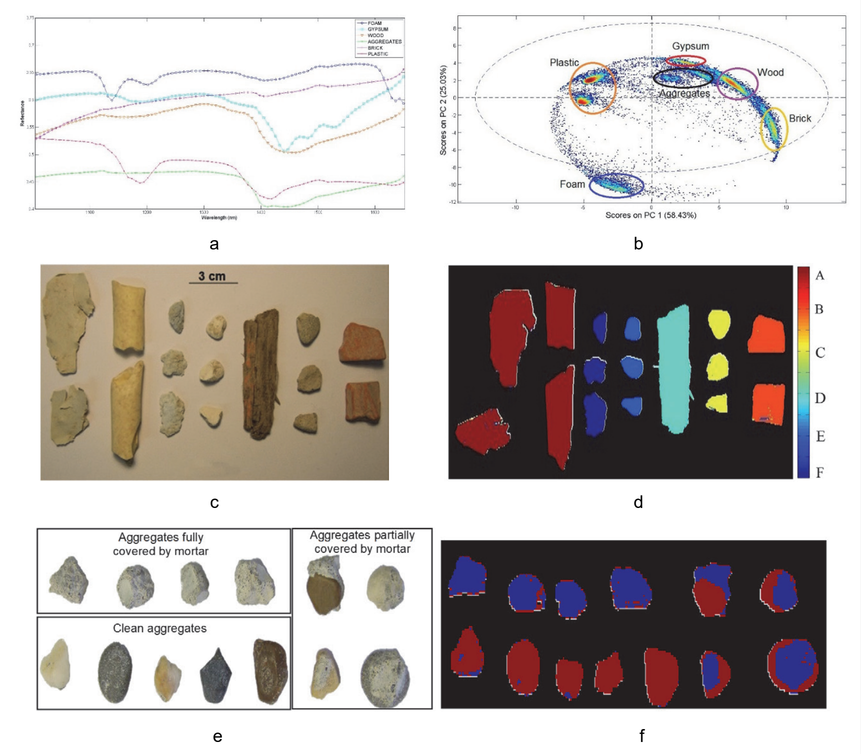

Figure 1. a: Average reflectance spectra of the different materials identified inside the EOL concrete waste stream; b: PCA score plot; c: source digital image; and d: corresponding classified hyperspectral image. Plastic (A), brick (B), concrete aggregates (C), wood (D), gypsum (E) and foam (F); e: source digital image of recycled concrete aggregates; f: corresponding classified hyperspectral image (red: clean aggregate surface; blue: mortar).

Table 1. Sensitivity and specificity values for the six-classes PLS-DA built for the different concrete contaminants.

Class	Sensitivity		Specificity	
	Calibration	Cross validation	Calibration	Cross validation
Aggregates	0.993	0.995	0.004	0.062
Brick	0.997	1.000	0.996	0.996
Gypsum	0.984	1.000	0.999	0.999
Plastic	1.000	1.000	1.000	1.000
Wood	0.982	0.983	0.994	0.825
Foam	1.000	1.000	1.000	1.000

class model gives a good classification, as shown in Figure 1d. Furthermore, it was also possible to correctly identify the mortar attached to the aggregate surface, as shown in Figures 1e–1f. In fact, using a two-class PLS-DA model (i.e. mortar and aggregate classes), it was possible to identify clean aggregates, aggregates totally covered by mortar paste and aggregates partially-covered by mortar paste. The sensitivity and the specificity values of the model built for contaminants are reported in Table 1. Sensitivity measures the actual positive values identified as such, whereas specificity measures the negative values correctly identified. A perfect prediction model is characterised by values of sensitivity and specificity equal to 1.

Mixed plastic waste

Nowadays, there is an urgent need to recycle increasing amounts of plastic waste, and to improve the recycling strategies currently adopted in this field in order to identify and sort the different types of plastics into single polymer streams, especially with reference to those most difficult to be separated by commonly used technologies. In order to produce high-quality plastic products for the market in secondary raw materials, it is in fact necessary to obtain mono-polymer streams characterised by very low levels of contamination from other polymers.[8] Efforts must be made to achieve a high quality standard for plastic recycling, both in terms of products fed to recycling plants and the final recovered product characteristics. The possibility of using HSI to implement analytical logics able to sort different polymers and/or to provide an accurate quality certification of products, can contribute to achieve this goal. Based on the experience developed by the Authors in hyperspectral imaging for the recognition of different plastic waste coming from different sources,[8–14] a flexible hierarchical classification model based on PLS-DA has been developed and implemented to classify many classes of polymers at the same time. In more detail, HSI in the short-wave infrared range (1000–2500 nm) was applied to identify eight different classes of polymers, representing the most used ones in many different applications and products (packaging, construction, electronic appliances, vehicles etc.): HDPE, LDPE, PA, PET, POM, PP, PS and PVC. In Figure 2a, the average reflectance spectra of the analysed plastics are reported, showing different characteristics useful for their further recognition. After exploring polymer spectral differences by PCA (Figure 2b), a hierarchical PLS-DA model was built, allowing the identification of the eight different polymer classes (Figures 2c and 2d). The proposed methodology, based on hierarchical classification, is very powerful and fast, allowing the eight different polymers to be identified in a single step.

The sensitivity and specificity values obtained for the built model are presented in Table 2. The values are very good, ranging from 0.953 to 1.000 for both parameters. The proposed HSI approach has many advantages, being fast, non-destructive and accurate, with-

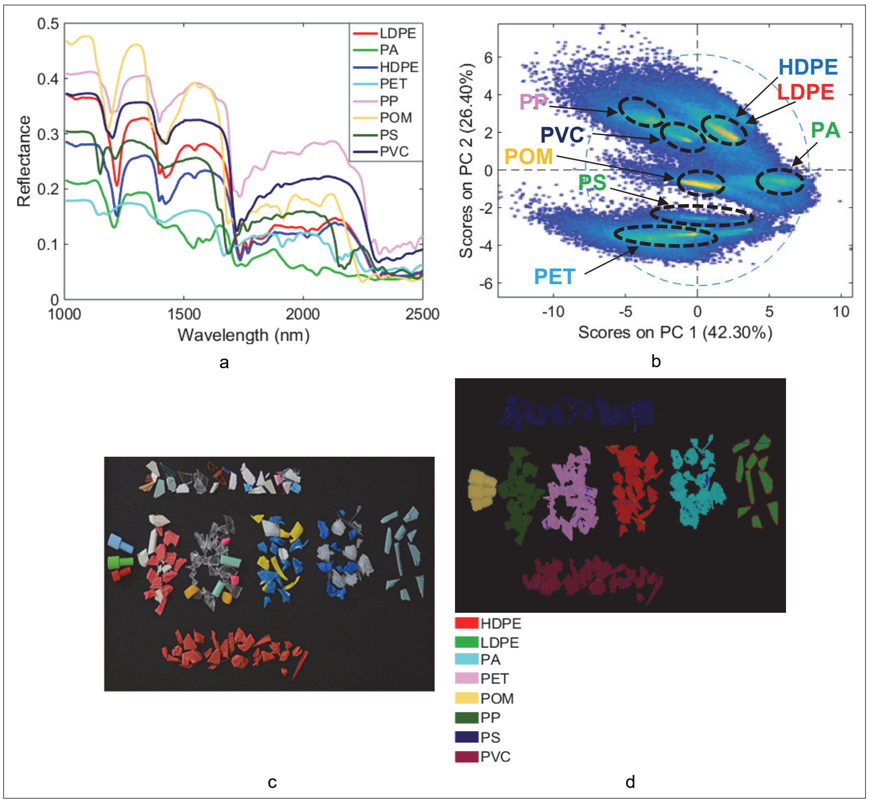

Figure 2. a: Average reflectance spectra of the different classes of polymer waste samples; b: PCA score plot; c: source digital image of different plastic flakes; d: corresponding classified hyperspectral image.

Table 2. Sensitivity and specificity for the eight-class hierarchical PLS-DA built for the different plastic samples.

Class	Sensitivity		Specificity	
	Calibration	Cross validation	Calibration	Cross validation
LDPE	0.993	0.993	0.998	0.998
PA	1.000	1.000	0.953	0.953
HDPE	0.998	0.998	0.993	0.993
PET	0.999	0.999	0.998	0.998
PP	0.992	0.992	1.000	1.000
POM	0.953	0.953	1.000	1.000
PS	0.998	0.998	0.999	0.999
PVC	1.000	1.000	1.000	0.992

out any need to perform specific sample preparation.

Conclusions

HSI can be profitably applied in the waste recycling sector to develop innovative analytical procedures (laboratory scale) and sorting or quality control strategies (industrial scale) specifically targetted to solve classification/identification problems related to the detection of different materials and related characteristics, unwanted contaminants etc., sometimes difficult to “qualify” and “quantify” through conventional strategies. The use of HSI and the development of procedures for extraction of useful information based on chemometric strategies were successfully applied to two different complex waste streams, i.e. end-of-life concrete and mixed plastic waste. The characteristics of the devices and the potential offered by chemometric tools, allow such an approach to be used to set-up innovative, flexible, reliable and low-cost detection/control devices and strategies that can be easily integrated, both at laboratory and industrial level, as well as inside existing consolidated analytical path and/or processing plant layouts.

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ARTICLE

A week in the life of a PhD student

Katie Ember
University of Edinburgh and University of Strathclyde. E-mail: K.J.I.Ember@ed.ac.uk

Monday

On the walk to Haymarket station, I avoid the stares of curious commuters. I try not to be envious of their tiny handbags or compact briefcases. I attempt to maintain a steady course and a nonchalant look. Because at 8 o'clock in the morning, it's hard to remain inconspicuous whilst wheeling a large yellow Pelican case through the streets of Edinburgh.

Pelican cases were originally designed for military and law enforcement use. They are durable, waterproof and typically used to transport "sensitive equipment", e.g. cameras or guns, but my cargo is significantly nerdier: a 785 nm portable Raman spectrometer. After some trials at the University of Edinburgh, I'm now returning the device to its home at the University of Strathclyde in Glasgow.

I drag the case through the barriers, heave it from platform to train and spend the rest of the journey reading papers whilst remaining acutely aware of how much room the spectrometer is taking up in the luggage rack.

I'm halfway through the final year of my PhD in Optical Medical Imaging, and collaboration between universities and departments has been a large part of my project. The aim of my research is to develop a way of detecting liver damage using spectroscopy and it's about as interdisciplinary as you can get. To achieve this, I've been working with physicists, chemists, biologists and transplant surgeons in both the cities of Edinburgh and Glasgow. It involves a lot of travel, but it's been a great way to learn about a whole host of different subjects and there's very rarely a dull day.

Fifty-eight minutes after the train pulls out of Haymarket, I arrive at Strathclyde's Technology and Innovation centre—affectionately called the TIC. For such an unpleasant acronym, it's a gorgeous building. From a bird's eye view it is triangular, and its seven stories are home to state-of-the-art labs carrying out some of Scotland's most innovative research, ranging from renewable energy to photonics.

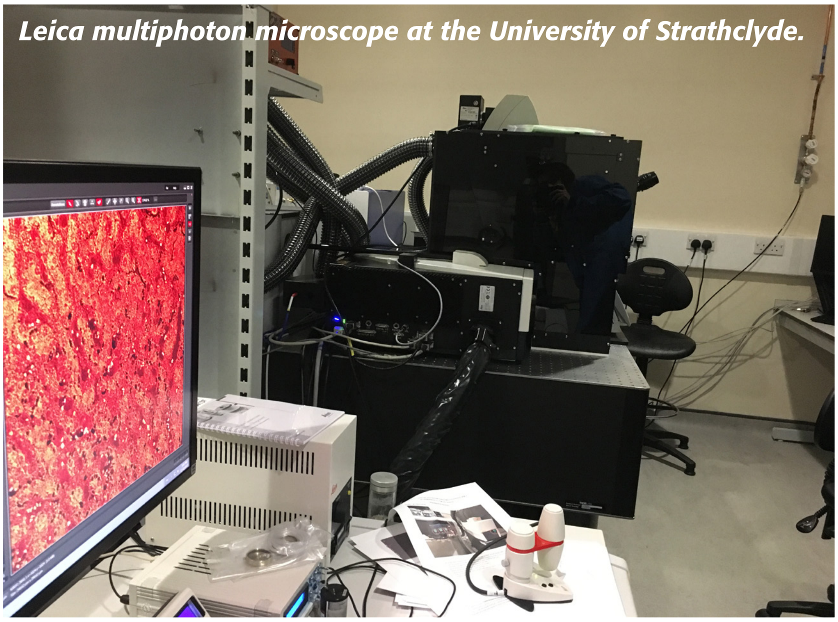
My supervisor here is Karen Faulds, Professor of Pure and Applied Chemistry at the Centre for Nanotechnology. Professsor Faulds' work focuses on the biological applications of Raman spectroscopy, a technique which uses the inelastic scattering of laser light to yield molecular information about samples.

There are a number of variations on the theme of Raman spectroscopy and Professor Faulds' group are making use of a number of them. For example, surface-enhanced Raman spectroscopy (SERS) employs metal nanoparticles (or other metal surfaces) to enhance the otherwise weak Raman signal.

These particles and surfaces can be functionalised with molecules that bind to specific cells or react to particular environmental conditions, telling us about organ health. It is not a technique I've been using, but Faulds' group have used SERS to detect multiple types of pathogenic bacteria.[1,2]

After catching up briefly with some of the other students at the TIC, I place the spectrometer carefully back on its lab bench and switch on the Leica multiphoton microscope. A scientist probably shouldn't have favourite instruments as they all have their advantages and limitations, but it's hard not to love the multiphoton.

If someone said "imagine a fancy microscope designed by Batman", that's what the Leica looks like—a huge, gleam-



Leica multiphoton microscope at the University of Strathclyde.

ing, jet-black exterior housing a glimmering assortment of filters, mirrors and lenses. The software, however, seems to have been developed by the world's biggest fan of rainbows and, in all honesty, it's a welcome addition to the dark microscopy room.

A major advantage of the Leica is that it possesses multiple excitation sources, lending it CARS, SRS and fluorescence imaging capabilities. Stimulated Raman spectroscopy (SRS) and coherent anti-Stokes Raman spectroscopy (CARS) both make use of two lasers: a pump beam and a Stokes beam. By tuning these lasers to specific frequencies, you can enhance the signal at the Raman shift of interest. Although this limits the spectral information acquired, it is possible to gain high-quality, high-resolution images of your target peak in an extremely short time.

For example, you can label a molecule of interest with an alkyne tag. As alkynes have a Raman signal in the middle of the "cell silent" region, the distribution of the tagged molecule can be rapidly imaged.

After a day at the microscope, I take the train back to Haymarket carrying nothing but my small backpack and a USB full of images.

Tuesday

Thesis-writing day. My alarm goes off at 6:30 am: I'm much more productive in the mornings. Besides, it's exam season and the library becomes packed with undergrads as the day goes on—so packed sometimes the only available desk space is in the downstairs cafe. My tiny purple laptop is on its last legs and the Edinburgh Uni library has hundreds of desktop computers, complete with software necessary to reference, create graphs and do statistical analysis. It's not surprising that it's so popular.

I've been writing my results into a paper and processing data as I go, which has been incredibly helpful. Paper writing has also ensured that I've been using multiple methods throughout my PhD to confirm my findings. Although Raman spectra are informative, no single experimental technique is sufficient to categorically prove something, especially within the field of biological sciences. For this reason, I've been using well-characterised techniques such as NMR spectroscopy and histological staining in parallel with Raman to support my findings.

Edinburgh Glossary

Haymarket Station: Train station towards the West end of Edinburgh, lesser known than the more central Waverley Bridge station

The Meadows: central park in Edinburgh, beloved by runners, barbeque-ers and people doing strange acrobatic sports

The Royal Infirmary: one of Edinburgh's multiple hospitals; relatively new and in the southern outskirts

King's Buildings: the science campus of the University of Edinburgh

George Square: the University's Central campus. A mix of Edwardian houses and brutalist concrete surrounding gardens open to students in the summer

NMR spectroscopy uses a magnetic field and radio-frequency electromagnetic radiation to induce energetic transitions in a sample. The peaks are sharper than those obtained with Raman or IR spectroscopy, so you can resolve individual molecules more easily. However, NMR requires samples in the form of biofluids or a biopsy which limits its application to the clinic. Nevertheless, I've used NMR to measure changes in the metabolic profile of damaged livers versus control livers and these are the spectra I've been focussing on today.

By 11:15 am, my eyes can't take any more NMR spectra and I'm craving caffeine, so I leave my desk and walk to one of the tiny coffee boxes in George Square. It looks a bit like a TARDIS (it is in fact an old police box) and they make excellent Americanos.

Back to the library, to an email saying that lab meeting is still going ahead. Lab meeting. Cool. I had absolutely not forgotten about that. My chemistry supervisor, Dr Colin Campbell, is currently on sabbatical in Colorado where he is developing ways of culturing and imaging cells in 3D, and we have lab meetings via Skype.

The rest of the team meet in Room 232 in the School of Chemistry and it's a good chance to catch up with other members of the group. Many of us work in different departments, so it can be easy to forget that there are others who have faced similar problems at another point in their PhD. We have all benefitted from advice after presenting our work at these meetings.

Other students in Dr Campbell's group have been using SERS in a similar way to

MacEwan Hall near George Square at sunset.

Spring in the Meadows near the George Square library.

researchers at Strathclyde, but functioning the nanoparticles with redox-sensitive molecules. As the redox state of the environment changes, so do the Raman spectra of the molecules attached to the metal nanoparticles. Therefore, the Raman spectra can be used as a readout for the redox state within 3D cell cultures or even tumour models.[3]

After the meeting, I go straight to the University gym. The building is only a few years old and is kitted out with cardio rooms, free weights, fixed weights, basketball and squash courts, and a climbing wall. I aim to exercise at least five times per week; whether that's at the gym, playing football or running around the Meadows. It allows me to switch off completely from PhD life; much as I love science, it's good to separate work and home.

Wednesday

The number 24 bus winds its way through what feels like the whole of Edinburgh, but finally we arrive at the Royal Infirmary. This morning, I have a meeting with Mr Gabriel Oniscu, a transplant surgeon I'm working with at the Royal. One of the reasons we're developing a way of detecting liver damage using spectroscopy is to see if we can assess the health of donated livers.

Liver transplants take around six to eight hours and they're remarkable to observe. The entire team—composed of nurses, surgeons and anaesthetists—remain alert and focused throughout the process, each carrying out their own critical role with utmost care. However, the one point where the transplant team use subjectivity is during assessment of the donated liver. The operating surgeon mostly achieves this by visually inspecting the liver and checking it isn't fatty or visibly injured. Being able to detect damage at a molecular level in real time would be invaluable.

A handheld Raman spectrometer used in our tests.

Unfortunately, introducing a laser-based device into the well-oiled transplant process will be far from simple. Mr Oniscu and transplant theatre sister Ms Fiona Hunt have been vital sources of practical, clinically-relevant information. Any spectroscopic solution must be able to take into account surgical lights, motion and variations in biochemistry from patient to patient. The device needs to give molecular information without requiring a surgeon to analyse raw spectral data. And it has to be able to do so rapidly.

After Mr Oniscu and I have talked through my most recent results, I join another PhD student who is having liver samples graded by a pathologist and has invited me along. To assess the samples, the pathologist is using a microscope with multiple eyepieces, so I and the other student can see exactly what he's talking about. We're learning a lot.

"These white spots are vacuoles, it's sort of a mark for reversible cell damage… And here, you have necrosis, it's only in a small area though." Necrosis is a type of cell death that transplant surgeons want to avoid. The liver has a remarkable capacity to regenerate, but serious levels of necrosis can result in scarring, loss of function and cancer.

After our mini pathology tutorial, we grab a coffee from the hospital cafe, before heading back to the office to try to make sense of the new results.

Thursday

"Let's try lower acquisition time, higher laser power; just to see what happens."

This morning, I'm teaching a new PhD student how to use the Renishaw InVia Raman spectrometer. It's been more time-consuming than we had anticipated, especially as her samples are organoids (tiny spheres of cells) and we're not sure what data to expect. With the Renishaw, there are so many parameters you can change: laser power, acquisition time, streamline or point acquisition, lens, map size… and there are two lasers—532 nm and 785 nm excitation.

Moreover, there are unique challenges to face when using biological samples.

Renishaw InVia at the Edinburgh Bioquarter.

Sometimes you'll be using frozen sections, other time cells growing in a monolayer, sometimes biofluids such as serum. Each sample will have different optical properties and hence the experimental set-up must be adjusted accordingly. It is also important to make sure that the surrounding medium isn't giving a strong Raman signal that would drown out the signal of the molecules you are trying to detect.

And then there is the problem of laser intensity. When I first started using liver tissue, I set the spectrometer to run a mapping experiment for 8 hours. The idea was to take tens of thousands of spectra from a tiny rectangle within the tissue. I returned the next morning to find a perfect 500 µm by 700 µm oblong had been vaporised from my sample.

After we've determined the optimal parameters for the experiment, I take the bus to the Business School at George Square. I know what you're thinking—where does studying Business fit into detecting liver damage? It's a good question: I am a member of OPTIMA, the Centre for Doctoral Training in Optical Medical Imaging. Many scientists lack the skills to take their ideas from bench to business, so this four-year programme has been specifically designed to help PhD students gain training in entrepreneurship as well as interdisciplinary science.

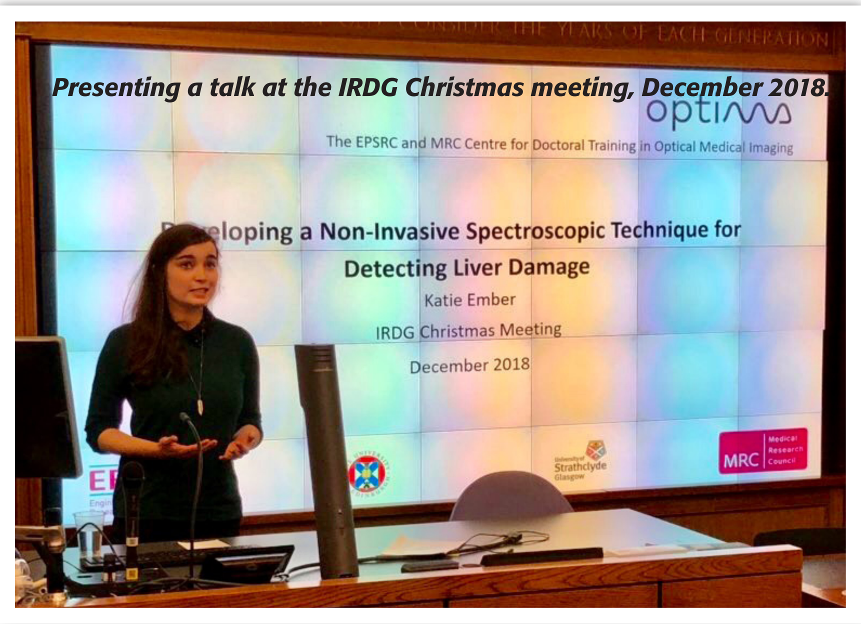
In this module, our group has been learning about the steps required to take an implant from Phase I trials right the way through to market. We've learned about intellectual property, ethics and finance—it's been a fascinating course and I wish all biomedical scientists were able to gain an insight into these processes.

Friday

Friday morning is the Forbes group lab meeting, based at the Centre for Regenerative Medicine (CRM). Professor Stuart Forbes is my clinical supervisor and a consultant hepatologist at the Royal Infirmary. His lab at the CRM specialises in liver regeneration—a complex and fascinating process. Given time, human livers are able to regain structure and function even after large sections are damaged or removed; and the Forbes group aim to discover the cellular mechanisms behind this process.[4]

The other lab members mostly use light microscopy, biochemical and proteomic techniques, but they've been endlessly patient in teaching me how to process tissue samples and interpret the data in terms of the biological state of the liver. The diversity of the knowledge and skills in the lab is astounding and they've given me access to cell lines, mouse models, rat models, patient biopsies and discarded livers. Cell lines are easier to obtain and less biologically complex than whole organs. However, they are not a true reflection of the state within living organisms so it is useful to be able to carry out experiments on tissue samples too.

After the meeting, I spend the afternoon working on a conference presentation from the Campbell office at the School of Chemistry. Every few months,



Presenting a talk at the IRDG Christmas meeting, December 2018.

I try to present at a conference or do some form of public engagement: the impact of research is limited if you don't communicate it with a wider audience. Fortunately, my supervisors are all very encouraging of science communication and I've had the chance to present in London, Barcelona and Canada to audiences ranging from school children to surgeons.

Once the PowerPoint is in good shape, it's time to head to *The Southern*—a pub patronised by PhDs and postdocs alike. It's the weekend and our conversations turn to upcoming holidays, sports and our life plans for next year. Failed experiments and PhD problems are forgotten.

Concluding thoughts

A PhD isn't for everyone and, before starting, it is worth researching the project, the lab culture and the city you're going to call home. Postgraduate degrees can be psychological and emotional rollercoasters: I've had moments where NMR tubes have shattered, where experiments have run on for seventeen hours and my entire first year's work has been filed under "optimisation". But these have been insignificant setbacks in three incredible years.

Katie Ember is in the fourth and final year of a PhD in Optical Medical Imaging at Edinburgh University and is developing a way of sensing liver damage using spectroscopy. Follow her on Twitter at @KatieEmber for over-enthusiastic tweets about scientific breakthroughs and the natural world.

I've been free to learn countless new research techniques, develop communication skills and explore multiple areas of science. All things considered; I wouldn't change the last few years for anything.

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Are you taking your Metadata seriously?

Antony N. Davies,[a,b] **Peter Lampen**[c] **and Robert Lancashire**[d]
[a]Expert Capability Group – Measurement and Analytical Science, Nouryon, Deventer, the Netherlands
[b]SERC, Sustainable Environment Research Centre, Faculty of Computing, Engineering and Science, University of South Wales, UK
[c]Leibniz-Institut für Analytische Wissenschaften – ISAS, Dortmund, Germany
[d]The Department of Chemistry, The University of the West Indies, Mona, Kgn 7, Jamaica

As spectroscopists we tend to focus on spectra. Nothing new there then, but maybe we need to be paying more attention to the information surrounding our measurements which define the context and relevance of the data and in many cases the fundamental ability to display the spectra correctly. I must admit to having somewhat neglected the creation and fate of metadata in all the data handling and migration work we have carried out over the years. It was occasionally funny to see certain spectrometer manufacturers using the ##OWNER= field in JCAMP-DX files to claim they owned the spectra we were creating and to be honest we pretty much ignored this when helping the vendors to get the actual data migrations compliant to the standards. However, there are increasing demands on scientists to upload accompanying data with their peer-reviewed papers, companies to make better use of the big data and machine learning tools are becoming ever more accessible. This means it is the metadata which gives meaning to the measured spectra and it is the metadata which will probably outlive the original creator of the spectra and almost certainly the organisations within which the data were created. In a world where digital rights management is ever more important, do you really want to leave the ownership of your data in the hands of your instrument vendor?

Why are metadata so important?

Last year we reported from the IUPAC/CODATA workshop in Amsterdam "Supporting FAIR Exchange of Chemical Data through Standards Development".[1] This was followed up by IUPAC formally endorsing the Manifesto of the Chemistry GO FAIR Implementation Network (ChIN) on 28 January 2019. This chemistry network is part of a larger global science network that supports the FAIR guiding principles for scientific data management and stewardship.

In the original report last year, we mention that the follow-up would include a Project Group 2: focussing on metadata for data publication and the items that could be considered important to FAIRify the data. A workshop was held titled Fair Publishing Guidelines for Spectral Data and Chemical Structures on 29–30 March 2019 during the American Chemical Society National Meeting & Exposition in Orlando, Florida which threw up some interesting challenges for IUPAC and the future data standards work. The original JCAMP-DX formats were never designed to transport all the metadata from an instrumental measurement to a vendor-neutral file format. The JCAMP-DX CORE fields were just those essential to correctly reading and interpreting the data and which were accepted by all the vendors working on the development of the various standards. There are also many potential labels defined in the standards which were not essential, but their use was not controlled by us. We know of at least one vendor who developed a JCAMP-DX export software which made extensive use of the $$ prefixed private labels to export all their instrumental parameters to their JCAMP-DX files. This allowed the vendor to completely re-create the data set on another software system. As they were un-documented to the outside world could not be used by anyone except the vendor.

From my regulatory compliance experience any records created in a regulated environment fall under some record retention policy or other, so discussing whether to store individual bits of the record—the metadata—as if it had a life all on its own seemed utterly pointless. Indeed, the original FDA 21CFR part 11 guidelines created all sorts of questions about the use of the JCAMP-DX standard file format in this scenario as it did not require the storage of all the original metadata (see below for the new Guidance which makes it much easier to accept JCAMP-DX files in this environment).

As the discussions continued since last year, it has become clear that increasing demands on scientists publishing research to upload their "raw data" to some open public repository or other has caused issues when the only metadata available were linked to the publication rather than the data itself. This is fine if your scope is simply limited to locating data in the repository from the perspective of the specific publication they are cited in, but what if you would like to find all the ^{13}C-NMR spectra measured with instruments with 500 MHz field strengths or better using deuterated chloroform as the solvent?

Metadata are critical to the correct functioning of our data systems!

My overly cited quote from Sherlock Holmes that "It is a capital mistake to theorise before one has data” from *A Study in Scarlet* has unfortunately turned on me and should now probably read “It is a capital mistake to theorise before one has data, and the associated domain-specific metadata to ensure that the data are Findable, Accessible, Interoperable and Reusable”.[1,3,4]

What do we need to consider here? I have recently talked to a system owner with a widely deployed Chromatography Data System (CDS) from one of the top international vendors. Even though the CDS was professionally deployed, maintained and continually updated to the latest release versions, the highly professional outsourced data storage provider had, without reference back to their customer, decided at some point into their contract not to back up the metadata tables in the database. I think you all know what is coming, yes… I will not spell it out as it is too painful but the inevitable did happen…. Major lesson learned (hopefully) to test your disaster recovery position REGULARLY! All the data could be restored but none of the metadata. Fortunately, as far as I know this system did not fall under any sort or regulatory compliance position. And to think of all the times I have jealously praised the chromatographers for having better and more reliable tools at their disposal than us poor spectroscopists!

Metadata is often described as information about data. The loss of metadata goes to show that metadata is critical for the operation of our scientific society in the short to medium term but in the longer term the metadata may well need to evolve as the context changes to remain relevant. In the short term, being able to identify five chromatograms, six NMR spectra and a couple of infrared spectra as being measured as part of a specific analytical question is essential to generating and validating results. In the longer term, these data sets may become part of a much greater set of essential evidence in proving a new drug is safe to use. After an audit the same data sets and the way they were processed could be called upon forming the basis of proving compliance to good laboratory practises for an organisation. In this way the “information about the data” and the way it is used can evolve.

The original Dublin Core

So, let us go back a little in history and look at one of the early initiatives to standardise on specific metadata fields to create some order out of the chaos of retrieving information from diverse sources and location in the internet age. Figure 1 shows an early attempt to start to define metadata than could be applied to any digital or physical object such as videos, pictures, web pages, books, DVDs, artworks or even spectra, known as the Dublin Core.[4] Unfortunately for our Irish readers, the Core was named after the original invitational Metadata workshop called by The Online Computer Library Center (OCLC) and the National Center for Supercomputing Applications (NCSA) on 1–3 March 1995, in Dublin, Ohio, USA, to address the issue of the search and retrieval of data from the internet. The attendees were librarians, archivists, humanities scholars and geographers according to the report from the meeting, along with with IT standardisation experts. This original work was expanded and adopted by various bodies and is now also an ISO standard ISO 15836-1:2017, which establishes 15 core metadata elements for cross-domain resource description, the Dublin Core metadata element set—Part 2: DCMI Properties and Classes is awaiting approval before publication as ISO/DIS 15836-2 due in 2019.

This would lend itself to our spectroscopic data storage system and if necessary we could use the original “Form”, now “Format”, element to indicate the record was a particular IUPAC JCAMP-DX spectroscopy data file, but there is little in here to help or future researcher locate records which meet the search question identified above.

As this discussion continues it is well worth noting a few key observations from the original workshop which we should not lose sight of…

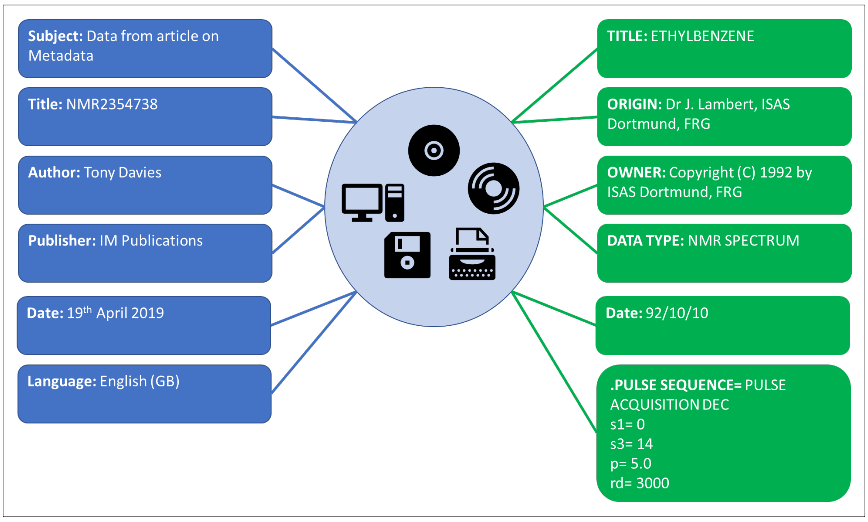
> “…*indexes are most useful in small collections within a given domain. As the scope of their coverage expands, indexes succumb to problems of large retrieval sets and problems of cross disciplinary semantic drift*…”

Or in layman’s terms, what might be stored under the label PULSE SEQUENCE from an NMR spectrum or FID would cause a medical practitioner quite a headache. So, clearly a need exists to separate the technical metadata, which effectively points you towards a specific record on a particular system and will clearly change over time, from the business metadata which gives meaning to the record within a particular discipline or environment. This brings us back to the current question of how to meet the demands of Open Access storage of scientific data in a way which fulfils the FAIR requirements. Fortunately, there is a clear route to managing what the original Dublin Core authors described as the *problems of cross disciplinary semantic drift*.

1. **Subject:** The topic addressed by the work
2. **Title:** The name of the object
3. **Author:** The person(s) primarily responsible for the intellectual content of the object
4. **Publisher:** The agent or agency responsible for making the object available
5. **OtherAgent:** The person(s), such as editors and transcribers, who have made other significant intellectual contributions to the work
6. **Date:** The date of publication
7. **ObjectType:** The genre of the object, such as novel, poem, or dictionary
8. **Form:** The physical manifestation of the object, such as Postscript file or Windows executable file
9. **Identifier:** String or number used to uniquely identify the object
10. **Relation:** Relationship to other objects
11. **Source:** Objects, either print or electronic, from which this object is derived, if applicable
12. **Language:** Language of the intellectual content
13. **Coverage:** The spatial locations and temporal durations characteristic of the object

Figure 1. The original 13 Dublin Core Metadata Element Set.

Under the REUSABLE part of the FAIR principles is **R1.3. (Meta)data meet domain-relevant community standards**. So as a specific data record may be relevant and shared across different "communities" it becomes essential that the metadata which makes a specific data record relevant to that community is clearly separated from what could be an identical metadata term standardised by a different community. Both sets of metadata items can be equally relevant at the time they are generated and have different lifetimes depending on usage (Figure 2).



Subject: Data from article on Metadata

Title: NMR2354738

Author: Tony Davies

Publisher: IM Publications

Date: 19th April 2019

Language: English (GB)

TITLE: ETHYLBENZENE

ORIGIN: Dr J. Lambert, ISAS Dortmund, FRG

OWNER: Copyright (C) 1992 by ISAS Dortmund, FRG

DATA TYPE: NMR SPECTRUM

Date: 92/10/10

.PULSE SEQUENCE= PULSE ACQUISITION DEC
s1= 0
s3= 14
p= 5.0
rd= 3000

Figure 2. All relevant metadata about the same record but show clear conflicts if the domain relevance of the specific metadata item is not retained.

The GoFair initiative has a nice section explaining what "R1.3. (Meta)data meet domain-relevant community standards" means in practice, which opens the way to integrate our well-established spectroscopic data standards into this environment:

> *"It is easier to reuse data sets if they are similar: same type of data, data organised in a standardised way, well-established and sustainable file formats, documentation (metadata) following a common template and using common vocabulary. If community standards or best practices for data archiving and sharing exist, they should be followed. For instance, many communities have minimal information standards (e.g., MIAME, MIAPE). FAIR data should at least meet those standards."*

Metadata in regulatory compliance

And this is where this debate gets a lot more serious and is not just some sort of fancy theoretical exercise. As many of you may have read, the Food and Drug Administration has been cracking down on data integrity in the pharmaceutical industry. So much so that they decided to issue a new guidance note in December 2018 in the form of a Question and Answer session to support corporate data compliance in companies. This guidance note helps users understand some of the key underlying regulatory requirement laid out in the so-called predicate rules… in this case those that make up current good manufacturing practice (CGMP) for drugs, as required in 21 CFR parts 210, 211 and 212.[5] In case anyone thought that the retention of metadata was not a key component of an overarching data integrity policy the guidance is very clear:

> *"What is 'metadata'?*
>
> *Metadata is the contextual information required to understand data. A data value is by itself meaningless without additional information about the data. Metadata is often described as data about data. Metadata is structured information that describes, explains, or otherwise makes it easier to retrieve, use, or manage data. For example, the number '23' is meaningless without metadata, such as an indication of the unit 'mg'. Among other things, metadata for a particular piece of data could include a date/time stamp documenting when the data were acquired, a user ID of the person who conducted the test or analysis that generated the data, the instrument ID used to acquire the data, material status data, the material identification number, and audit trails.*
>
> *Data should be maintained throughout the record's retention period with all associated metadata required to reconstruct the CGMP activity (e.g., §§ 211.188 and 211.194). The relationships between data and their metadata should be preserved in a secure and traceable manner."*

Of course, none of this is new, but the increased focus on data integrity is now shining a bright spotlight on industry practises and the software solutions we have in place to generate, process, archive and restore our data.

There are two other pieces of guidance in the document which I want to reproduce before we end this article as food for thought…

> *"9. Can electronic copies be used as accurate reproductions of paper or electronic records?*
>
> *Yes. Electronic copies can be used as true copies of paper or electronic records, provided the copies preserve the content and meaning of the original record,* ***which includes all metadata*** *required to reconstruct the CGMP activity and the static or dynamic nature of the original records."*

And in question 10 the equivalency of paper and electronic records is discussed, for printouts from pH meters and balances this might satisfy the record retention requirements however,

> *"10. Is it acceptable to retain paper printouts or static records instead of original electronic records from stand-alone computerized laboratory instruments, such as an FT-IR instrument?*

continued on page 21

Specifying accuracy and precision criteria for ultraviolet spectrometers

Chris Burgess[a] **and John P. Hammond**[b]
[a]Burgess Analytical Consultancy Limited, 'Rose Rae', The Lendings, Startforth, Barnard Castle, Co. Durham, DL12 9AB, UK
[b]Starna Scientific Ltd, 52–54 Fowler Road, Hainault Business Park, Hainault, Essex, IG6 3UT, UK

The performance specification of "fitness for purpose" for ultraviolet (UV) spectrometers used in regulated environments, applying documented control, e.g. pharmacopoeial monographs or internationally recognised control standards, includes the need to specify requirements for absorbance accuracy and precision. This would seem a relatively easy task, but there are a variety of ways of specifying the acceptance criteria and hence Decision Rules. These include absolute values, percentage limits, ranges of values and, for precision, standard and relative standard deviations.

The wording specifying these performance requirements should be scientifically sound, clear and unambiguous. Unfortunately, however, given the global nature of international standards, this is not always readily achievable.

Let us consider the easier one of accuracy. This is usually determined by comparative replicate measurements of a certified reference material (CRM). A typical statement of requirement might be:

The absorbance accuracy can be determined from the mean value of six replicate measurements of absorbance of a CRM. The absorbance accuracy of the mean must be ±0.005 from the certified value (for absorbance values below 1.0A) or ±0.005 multiplied by A (for absorbance values above 1.0A) and that the range of individual values must not exceed ±0.010 from the certified value (for absorbance values below 1.0A) or ±0.010 multiplied by A (for absorbance values above 1.0A).

With precision, we have two options; one based upon a standard deviation and the other on a range. Typical statements might be:

The absorbance precision can be determined from the standard deviation of six replicate measurements. This standard deviation must not exceed 0.5% or 0.5% multiplied by A for absorbance values above 1.0A.

or

The absorbance precision can be determined by the range of deviations from the mean of six replicate measurements. This range must not exceed ±0.005 absorbance units (for absorbance values below 1.0A) or ±0.005 multiplied by A (for absorbance values above 1.0A).

Therefore, we can imagine a specification for absorbance accuracy and precision with four possible acceptance criteria Decision Rules (Table 1).

So, will the selection of some of these criteria make a difference to the decision regarding the "fitness for purpose" of an instrument? The answer is it depends!

Assume that we have a certified reference standard with a certified absorbance value at a specified wavelength of 1.000 and we make six measurements on four different instruments. The results are shown in Table 2.

- Instrument 1 is both sufficiently accurate and precise for all four criteria, so is unambiguously "fit for purpose".
- Instrument 2 meets three of the four criteria but fails on the range (Decision Rule 3).
- Instrument 3 meets three of the four criteria but fails on the mean (Decision Rule 1).
- Instrument 4 fails all four criteria so is unambiguously not "fit for purpose".

From a practical point of view, a choice has to be made to select either Decision Rule 2 or Decision Rule 3. Looking at instrument 2, the standard deviation is comfortably below 0.50% but the range is outside the acceptance criteria. Contrast this with Instrument 1, for which the range is only 0.001 lower at the upper acceptance limit.

Table 1. Decision Rule types.

Decision Rule number	Criteria	Acceptance limits
#1	Mean absorbance	±0.005A from the certified standard
#2	SD of individual absorbances	Not greater than 0.5%
#3	Range of individual absorbances	±0.010A
#4	Range of individual deviations from observed mean absorbance	±0.010A

Table 2. Results from six measurements on four different instruments of a CRM.

Observed absorbances				
#	Instrument 1	Instrument 2	Instrument 3	Instrument 4
1	1.005	1.010	1.008	1.007
2	0.995	0.999	0.999	**0.989**
3	0.997	1.002	1.008	0.992
4	1.003	1.008	1.007	0.999
5	1.001	1.006	1.007	**0.988**
6	0.999	1.004	1.004	**0.986**
Mean	1.000	1.005	**1.006**	**0.994**
SD	0.37%	0.40%	0.35%	**0.80%**
Range	0.010	**0.011**	0.009	**0.021**
Deviations from mean absorbance				
#	Instrument 1	Instrument 2	Instrument 3	Instrument 4
1	–0.005	–0.005	–0.003	**–0.014**
2	0.005	0.006	0.006	0.004
3	0.003	0.003	–0.003	0.001
4	–0.003	–0.003	–0.002	–0.005
5	–0.001	–0.001	–0.002	0.005
6	0.001	0.001	0.001	0.007

Whilst it is easier to rely on a data range, the standard deviation Decision Rule is more forgiving, although it requires a calculation. If Instrument 2's values were 1.010, 0.996, 1.004, 1.008, 1.006, 1.004 giving a range of 0.014, the standard deviation is still only 0.48%.

In the above example, whilst there is clearly a discussion around which of the Decision Rules to choose, however, the acceptance criteria clearly allow a "fit for purpose" decision to be made, and therefore these acceptance criteria, whilst they may be described as challenging, do fulfil the role for which they were intended, i.e. they establish effective control of a system.

This analysis of a simple set of measurements shows that various Decision Rules can be applied, even in this simple scenario.

If one now considers absorbance accuracy data as a set of measurement results from a CRM, with the intention of using this data "as evidence of control" in the qualification of an instrument system, the analysis takes on another level of sophistication with respect to the ISO-based Decision Rule(s).[1]

These rules give a prescription for the acceptance or rejection of a product based on the measurement result, its uncertainty and the specification limit or limits, taking into account the metrological uncertainty. This includes an acceptable level of the probability of making a wrong decision.[2]

Based on these Decision Rules, an "acceptance zone" and a "rejection zone" are determined, such that if the measurement result lies in the acceptance zone the system is declared compliant and if in the rejection zone it is declared non-compliant.

Figure 1 shows typical scenarios arising when measurement results from a CRM are used to assess compliance with an upper specification limit, as defined above. The vertical lines show the expanded uncertainty ±U on each result and the associated curve indicates the inferred probability density function for the value of the measurand (measured value of the CRM on the spectrophotometer under test), showing that

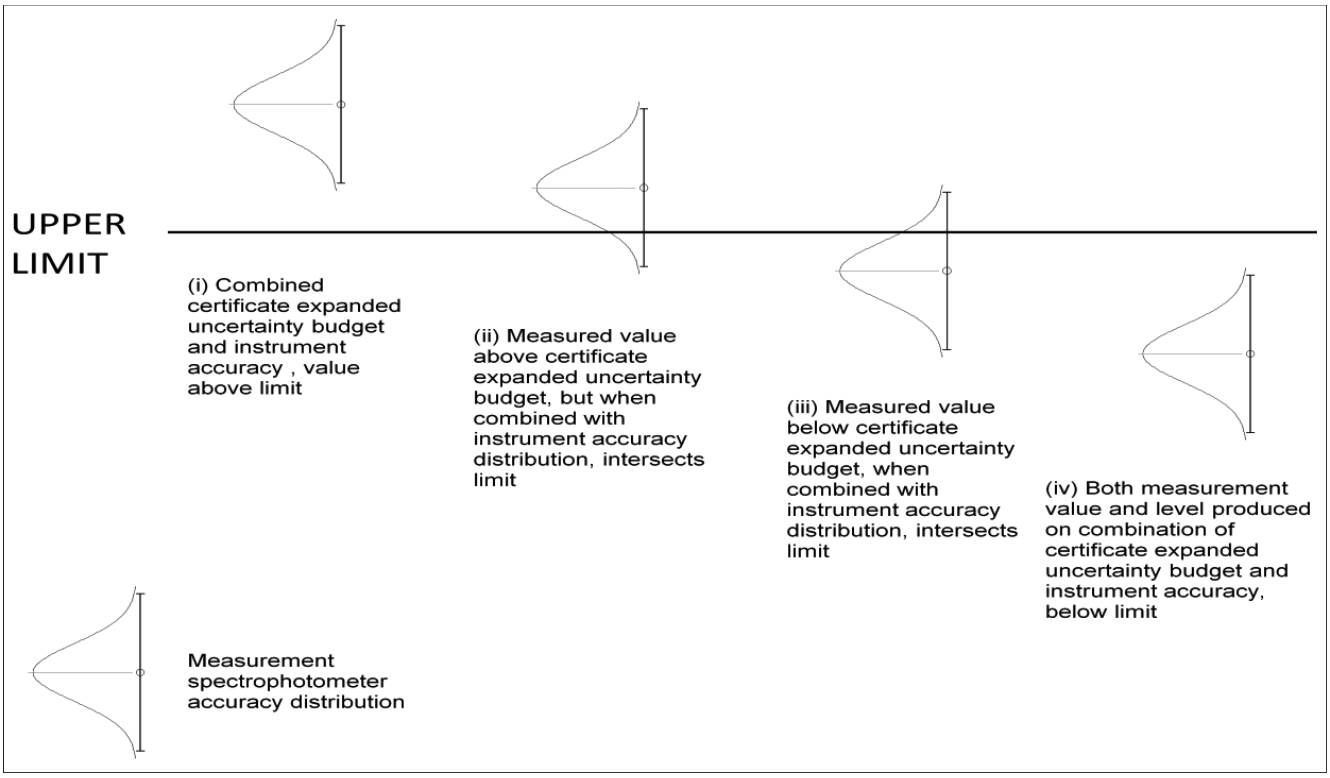


Figure 1. Assessment of Compliance with Upper Limit (CRM certified value + measurement spectrometer accuracy).2

Table 3. Calculated absolute absorbance (A) limits.

Measured absorbance (A)	0.5 % tolerance (A)
0.2000	0.0010
0.3000	0.0015
0.4000	0.0020
0.5000	0.0025
0.6000	0.0030
0.7000	0.0035
0.8000	0.0040

there is a larger probability of the value of the measurand lying near the centre of the expanded uncertainty interval than near the ends.

Cases i) and iv) are reasonably clear; the measurement results and their uncertainties provide good evidence that the value of the measurand is well above or well below the limit, respectively. In the case of (ii), there is a probability that the value of the measurand is above the limit, but the limit is nonetheless within the expanded uncertainty interval. Similarly, in case (iii), the distribution intersects the limit, and there is an increased probability that the value of the measurand is within the specification limit.

In a previous article,[3] the authors discussed "Is your Spectrometer in Calibration" and described the use and applicability of the above Decision Rule based on the simple linear addition of the Expanded Uncertainty Budget of the CRM to the accuracy specification of the spectrometer "under test".

Now consider the following accuracy statement, and the analysis thereof, using this generally accepted Decision Rule.

In the absorbance range encompassing 0.2 to 0.8, the photometric accuracy shall not differ by more than ±0.5 % of samples whose absorbance has been established by a standardising laboratory.[4]

Whilst the use of "0.5 %" may at first glance seem "similar" to the above discussed accuracy example, however, closer examination reveals the following.

Within the stated 0.2–0.8 A range, if you calculate the 0.5 % tolerance then you produce the results shown in Table 3.

Given the above requirement, in absorbance terms, let us consider various scenarios, and the associated possible Decision Rules.

Scenario #1

Criteria: In absolute absorbance values the above statement now becomes:

In the absorbance range encompassing 0.2 to 0.8, the photometric accuracy of a reference material established by a standardising laboratory shall certify a value in this range with a tolerance of ±0.001 A at the 0.2 A level, and ±0.004 A at 0.8 A.

There are photometric accuracy materials that have certified expanded uncertainty budgets, i.e. NIST primary standard reference materials (SRMs) and secondary CRMs from ISO/IEC 17025 certified organisations which lie within this range. But, with respective budgets of 0.0023 A and 0.0027 A, even these high-quality CRMs cannot meet the lower end of the range requirement below these values.

Scenario #2

In the absorbance range encompassing 0.2 to 0.8, the photometric accuracy shall not differ by more than ±0.5% of samples whose absorbance has been established by a standardising laboratory.

Criteria: This statement relates to a system "under test" and not just specifically referring to the limits associated with the reference material.

Now the required levels cannot be achieved, as already stated, by use of the uncertainty budget associated with the CRM, or by the specification of a good quality laboratory UV/vis spectrometer even when considered individually. Apply the Decision Rule where they also have to be combined in a linear manner and clearly you have a problem.

For example:

A double-beam, double-monochromator has a typical specification of ±0.0015A.

A single monochromator instrument typically has a specification of ±0.003 to 0.005A.

The "best measurement" capability of NIST in the above range was produced by their certification of SRM 930e, at ±0.0023A.[5]

So, adding these values together we get 0.0038 A "at best", and typically 0.0053A to 0.0073A.

Clearly, in both above scenarios, compliance with the requirement cannot be achieved with the Decision Rules stated, so the question must be:

"…what Decision Rule is expected to be applied and, given the above discussion, how is it expected that an accuracy of ±0.001 A at the 0.2A be achieved?"

In addition, which UV spectrometer are you going to use to achieve such measurement performance when the requirement is better than the best measurement capability of national laboratories?

References

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3. C. Burgess and J.P. Hammond, "Is your spectrometer in compliance", *Spectrosc. Europe* **28(2),** 16-17 (2016). https://www.spectroscopyeurope.com/quality/your-spectrometer-calibration
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5. Certification for SRM 930e, *Neutral Density Glass Filters*. National Institute of Standards and Technology (NIST), USA. https://www-s.nist.gov/srmors/certificates/archives/930e.pdf

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continued from page 17

> *… However, electronic records from certain types of laboratory instruments—whether stand-alone or networked—are dynamic, and a printout or a static record does not preserve the dynamic record format that is part of the complete original record. For example, the spectral file created by FT-IR (Fourier transform infrared) spectroscopy is dynamic and can be reprocessed. However, a static record or printout is fixed and would not satisfy CGMP requirements to retain original records or true copies [§ 211.180(d)]. Also, if the full spectrum is not displayed in the printout, contaminants may be excluded.*"

But please go and read the full guidance for all this information to be put into context.

Conclusions

Well for me this whole experience has been a bit of an eye opener. The challenges of getting the data exchange between vendors through a vendor-neutral standardised human-readable format has always been around the data content section and carrying enough metadata through the migrations to ensure the data could be correctly read and interpreted in a second data system (meeting the new FDA guidance explanation of electronic copies needing to preserve the content and meaning of the original record, which includes all metadata required to reconstruct the CGMP activity). So, our new challenge for 2019—to be discussed at the IUPAC 100-year celebrations at the 50th IUPAC General Assembly taking place from 5 to 12 July 2019, in Paris, France—will be to decide what improvements we need to make, together with the instrument vendors, to meet these new metadata challenges. Any volunteers out there?

References

1. L. McEwen, D. Martinsen, R. Lancashire, P. Lampen and A.N. Davies, "Are your spectroscopic data FAIR?", *Spectrosc. Europe* **30(4),** 21–24 (2018). https://www.spectroscopyeurope.com/td-column/are-your-spectroscopic-data-fair
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4. http://www.dublincore.org/specifications/dublin-core
5. *Data Integrity and Compliance with Drug CGMP, Questions and Answers Guidance for Industry* (December 2018). https://www.fda.gov/downloads/drugs/guidances/ucm495891.pdf

CONSUMABLES

High-purity acids for ICP-OES

Thermo Fisher Scientific has introduced a range of high-purity acids for digestion for ICP-OES analysis. The new range includes nitric acid, hydrochloric acid and sulfuric acid, which are all packed in PVC-coated glass with colour-coded caps.

Thermo Fisher Scientific

http://link.spectroscopyasia.com/31-022

Disposable glass liners for microwave digestion

CEM has introduced disposable glass liners for use with their MARSXpress Plus vessels in MARS 6 microwave digestion systems equipped with iWave temperature measurement sensors. The liners eliminate the need for vessel washing and reduce the risk of cross-contamination.

CEM Corporation

http://link.spectroscopyasia.com/31-043

IMAGING

EMCCD camera

Raptor Photonics' Hawk 252 is a 1.3 megapixel, EMCCD camera with spectral range of 180–1100 nm. Pixel size is 8 × 8 µm, dimensions 45 × 50 × 75 mm and weight 230 g.

Raptor Photonics

http://link.spectroscopyasia.com/31-038

INFRARED

QA/QC FT-IR

Thermo Fisher Scientific's new Summit FT-IR spectrometer replaces the iS5 and is intended for QA/QC labs and teaching labs. It incorporates the same LightDrive Optical Engine technology used in more advanced Thermo Scientific instruments, and also benefits from extended warranties on critical optical components. OMNIC Paradigm software helps manage multiple users and sample types, and there is a new, visual-based workflow editor. As well as a touchscreen interface, the Summit also has a multi-coloured LED LightBar that provides visual feedback on instrument status and sample pass/fail results.

Thermo Fisher Scientific

http://link.spectroscopyasia.com/31-023

Milk analyser

Bruker's MIRA IR milk analyser provides quality control of raw milk and liquid milk products, analysing parameters such as fat, protein, total solids and lactose. A high-pressure homogeniser ensures evenly homogenised samples, and, optionally, the MIRA can determine the freezing point.

Bruker

http://link.spectroscopyasia.com/31-018

Milk homogenisation analyser

The GLOBULYSER from Bruker is a stand-alone analyser for the determination of the mean fat globule size in milk and liquid milk products as well as in dissolved milk powders. It measures the intensity of transmitted and forward-scattered light interacting with fat globules present in the sample cell. The forward scattering directly depends on the size of the fat globules. The software will compare the measured values with the values of clean water and calculates the difference to determine the mean size of the fat globules.

Bruker

http://link.spectroscopyasia.com/31-019

Grazing angle FT-IR microscope

Czitek's Film SurveyIR is a grazing angle FT-IR microscope for thin film (<1 µm) characterisation. It uses the external output beam of a FT-IR spectrometer with optics that direct the beam to the sample at 60–85° from normal. At these angles, there is increased sensitivity to thin films on surfaces. Automated aperture masks isolate microscopic areas for measurement and a megapixel camera provides sample observation and documentation.

Czitek

http://link.spectroscopyasia.com/31-029

Gas leak detection system

ABB have introduced the Ability mobile gas leak detection system. It is based on ABB's laser, off-axis ICOS analyser for methane and ethane. This is mounted in a vehicle along with a GPS sensor, a sonic anemometer and proprietary leak detection software that provides real-time geospatial maps of multiple gas concentrations. Data can be reported at driving speeds up to 55 mph.

ABB Analytical

▸ http://link.spectroscopyasia.com/31-030

Custom gas sensors

MIRPHAB is an EU-funded (Horizon 2020) consortium aiming to produce a fabrication platform with open access for fast mid-IR device prototyping. A range of building blocks can be assembled into a custom gas sensor. Lasers can be ICLS or QCLs, there can be SOI, SiGe/Si or Ge/SiGe waveguide technologies and detectors can be specified from Type-II In/As/GaSb superlattice (T2SL), InAsSb QCD and photoacoustic cells.

MIRPHAB

▸ http://link.spectroscopyasia.com/31-050

MAGNETIC RESONANCE

TD-NMR for pharma

Bruker's minispec Form Check is a time-domain NMR spectrometer to monitor phase purity and quantify physical API forms including amorphisation. It uses ^{1}H or ^{19}F relaxometry data as fingerprints for expected components in solid mixtures, instead of the need for calibration, sample prep and expertise.

Bruker

▸ http://link.spectroscopyasia.com/31-017

Honey-Profiler 2.0

This is a new method for the Bruker NMR FoodScreener that improves the detection of sugar syrups and expands the range of geographical and botanical honey origins that can be verified, including manuka honey, which is frequently subject to fraud. The database now covers over 18,000 honey samples, 50 geographical origins and 100 botanical varieties. Automated analysis of authenticity and quality can be performed in 25 minutes.

Bruker

▸ http://link.spectroscopyasia.com/31-020

Autosampler

Magritek have introduced a 20-position autosampler for their Spinsolve benchtop NMR spectrometers. The autosampler can be easily added to the spectrometer, is fully controlled by the Spinsolve software and provides easy configuration of all protocols for sample analysis. New samples can be added or removed during a running queue and a preset series of experiments can be loaded from a previously saved list.

Magritek

▸ http://link.spectroscopyasia.com/31-028

MASS SPECTROMETRY

GC-MS/MS

Jeol's new JMS-TQ4000GC is a GC-triple quadrupole mass spectrometer with high-speed SRM switching of 1000 channels/s. It is designed with a short collision cell that provides ion accumulation with reduced noise level, rapid pulsed ion ejection without crosstalk and high-speed GC measurement for routine analysis. The short collision cell accumulates ions and ejects them in rapid pulses. The noise level of the signal is reduced by synchronising the timing between pulsed ion ejection and signal acquisition, making high sensitivity analysis possible. In addition to the standard electron ionisation source, chemical ionisation and photoionisation sources are supported. It is also possible to perform analyses with two types of direct insertion probes.

Jeol

▸ http://link.spectroscopyasia.com/31-026

Enhanced qualitative analysis software

Jeol has developed new software, msFineAnalysis, to enhance qualitative analysis of compounds using high-resolution GC-MS. It integrates information from multiple ionisation techniques with database search, exact mass and isotope data. The produced report compares spectral matches from a NIST or NIST-formatted MS database search with elemental compositional information from soft-ionisation data analysis. For unknown components, the program determines the elemental composition for the intact molecule by using the soft ionisation data. Elemental compositions are reported for fragment ions in the EI data. If both GC/EI data and the corresponding GC/soft ionisation method data are available, all five qualitative analysis processes are automatically performed on the peaks of the chromatogram.

Jeol

▸ http://link.spectroscopyasia.com/31-027

Point-of-need bioprocessing

Microsaic's MiD ProteinID has been designed for real-time protein characterisation at the point-of-need. It is a small footprint mass spectrometer and the mass range has been increased to 50–3200 *m*/*z* to meet the requirements of biopharma. The instrument has "plug and play" consumables, integrated software designed for rapid setup and

data analysis. A remote operating software module allows integration with third-party equipment. Maintenance costs are low with a completely tool-free front end, as are operating costs due to reduced power and N_2 consumption.

Microsaic

- http://link.spectroscopyasia.com/31-042

MISCELLANEOUS

Pellet press

The semi-automatic 25 t SpectroPress from Chemplex is designed for production of pellets for FT-IR or XRF analysis requiring intermediate pelletising forces. It is in a compact, benchtop design and the target force can be programmed and there is simple two-button (up and down) operation.

Chemplex Industries

- http://link.spectroscopyasia.com/31-041

Multipoint sampler for gas analysis

Gasera introduced the Multipoint Sampler designed to enable multi-channel monitoring with any Gasera One analyser, increasing the number of sample inlets up to 12. Functions are controlled from the Gasera One, providing easy programming of the sequence and duration of sample intake.

Gasera

- http://link.spectroscopyasia.com/31-046

Fibre-optic spectrometers

Wilson Analytical have introduced a range of portable spectrometers offering fluorescence, absorption, reflectance and transmission measurements on liquid and solid samples, covering the range from deep UV to near IR. All are based on optically stabilised LED light sources, and make use of Ocean Optic spectrometer engines.

Wilson Analytical

- http://link.spectroscopyasia.com/31-051

On-line chiral reaction monitoring

BrightSpec have introduced the Discovery MRR Diastereomer/Enantiomer analyser for chiral and diastereomer process monitoring. It uses molecular rotational resonance (MRR) spectroscopy, which does not require offline sample preparation, chromatography or chemometrics. The instrument uses a Fabry–Perot cavity for enhanced sensitivity in targeted monitoring. Sample introduction is directly from a continuous synthesis manufacturing process, without prior sample preconditioning, drying or separation. It provides diastereomer and enantiomer quantification in 18 min cycle times and uses argon or neon as carrier gas.

BrightSpec

- http://link.spectroscopyasia.com/31-054

NIR

Handheld NIR

Viavi have added Bluetooth capability to their MicroNIR OnSite, creating the MicroNIR OnSite-W. This can be connected to a tablet or PC by Bluetooth or USB, and runs the same software as the existing MicroNIR OnSite.

Viavi Solutions

- http://link.spectroscopyasia.com/31-031

Miniature NIR spectrometer

Hamamatsu's TF series C14486GA miniature NIR spectrometer has an InGaAs linear image sensor providing a wavelength range of 950–1700 nm. It is powered via a USB cable and so does not need an external power supply, weighs 88 g and has dimensions of 80 × 60 × 12 mm. The TF series incorporate a polychromator in a compact, thin case that houses the optical elements, image sensor and driver circuit. Light input is via a fibre-optic connection.

Hamamatsu

- http://link.spectroscopyasia.com/31-033

Ultra-compact NIR sensor

Hamamatsu's C14273 MEMS-FPI spectrum sensor weighs just 1 g and the ultra-compact sensor houses a MEMS Fabry–Perot interferometer (FPI) that can vary its transmission wavelength depending on the applied voltage and an InGaAs PIN photodiode in a single TO-5 package. Its spectral response range is 1750–2150 nm.

Hamamatsu

- http://link.spectroscopyasia.com/35-035

RAMAN

Rheo-Raman

TA Instruments announced the Rheo-Raman accessory for their Discovery Hybrid Rheometer product line. The accessory integrates with an iXR Raman spectrometer from Thermo Fisher Scientific, providing simultaneous collection of rheology and Raman data. This enables direct correlation between flow characteristics and chemical and morphology from Raman data.

TA Instruments

▸ http://link.spectroscopyasia.com/31-016

Particle analysis for Raman microscopy

WITec's ParticleScout is a particle analysis tool for the alpha300 Raman microscope series that finds, classifies, quantifies and identifies particles quickly and easily. It begins by surveying samples with bright and dark field illumination to view the particles they contain. Image Stitching combines many measured areas for a detailed overview of large areas and Focus Stacking allows larger particles to be sharply rendered for accurate outline recognition. The optical images lead to the creation of a mask which is used to physically categorise particles of interest and arrange them in a ranked list. A Raman spectrum is then automatically acquired from each particle. The Raman spectra are evaluated and the particles they correspond to can be identified manually or by using the WITec TrueMatch Raman database software. Finally, ParticleScout generates a report that features user-selectable combinations of filters and advanced algorithms to show the quantities of selected particles and their prevalence relative to other groups.

WITec

▸ http://link.spectroscopyasia.com/31-013

Raw material ID

Metrohm's Mira P is a version of their Mira hand-held Raman spectrometer for the pharmaceutical industry. It has enhanced resolution, new immersion sampling and validation accessories, and ergonomic improvements. New software features streamline verification routines and include an automated training set builder and improved model analysis tools. FDA compliance is catered for, and USP and EP guidelines can be followed with the new CVA (calibrate/verify accessory).

Metrohm

▸ http://link.spectroscopyasia.com/31-032

Miniature Raman spectrometer

The C14214MA from Hamamatsu is a similar configuration to the miniature NIR spectrometer above, but configured as a Raman spectrometer with a CMOS image sensor. A double grating and spectral resolution of 0.4 nm maintains low stray light. Spectral response is from 790 nm to 1050 nm.

Hamamatsu

▸ http://link.spectroscopyasia.com/31-034

Extended range Raman

The WP 785 ER Raman spectrometer series from Wasatch Photonics has an extended range to 200–3500 cm^{-1}. The instrument be configured with choice of slit size and sample coupling (fibre coupled or free space), and custom range models and more compact designs are available upon request. TEC-regulated and TEC-cooled detectors are available.

Wasatch Photonics

▸ http://link.spectroscopyasia.com/31-036

Handheld 1064 Raman

B&W Tek have introduced the NanoRam-1064 handheld Raman analyser. The reduced fluorescence from using 1064 nm light makes it suitable for identifying coloured samples, natural products and to differentiate between different grades of cellulose and polysorbate. The embedded software comes with method and library validation, instrument calibration, library and method development, and data storage/transfer functions.

B&W Tek

▸ http://link.spectroscopyasia.com/31-037

Stand-off, handheld Raman

The Pendar X10 has been designed for EOD, HAZMAT, narcotics and forensics use. It operates over a standoff distance of 1 m and readings can be taken through thick, translucent containers, closed plastic bags, fume cupboards and closed windows. It weighs 6 lbs and measures 11.5″ × 10.5″ × 5.5″, and is battery operated with 2 h continuous measurement time.

Pendar Technologies

▸ http://link.spectroscopyasia.com/31-039

Standoff Raman

The same standoff technology as the Pendar X10 is used in the Pendar XA, which is designed for use in the lab or in discovery and scale-up. It can be mounted on the lab bench, a microscope stand or adapted to the viewing port of a vessel. It measures through thick glass and translucent containers and includes visible and thermal cameras to record reaction turbidity and temperature.

Pendar Technologies

▸ http://link.spectroscopyasia.com/31-040

Handheld Raman

The Chem 200 from SciApps has been developed for military, law enforcement and first responder users. It is Android-based and has on-board HazMasterG3 decision support software. It includes a macro camera for photo documentation of samples tested and reading of 2D barcodes. It is completely touchscreen driven, useable with or without gloves. It features continuous and preset adjustable laser focus, which helps prevent the situation where the laser is focussed on the sample holder rather than the sample itself. The vial holder accommodates both 15 mL and 8 mL vials, and there is a right-angle adapter for bagged materials and the "adjustable pointer" for testing through thick plastic bags or plastic or glass bottles.

SciAps

▸ http://link.spectroscopyasia.com/31-048

Pollution monitoring/water quality

SAFTRA Photonics' PickMol technology is based on a plasmonic-enhanced Raman nanoparticle chip, can detect concentrations down to the single-molecule level in environmental, food and biological systems. The chip is read in the RAMASCOPE instrument.

SAFTRA Photonics

▸ http://link.spectroscopyasia.com/31-052

SOFTWARE

High-throughput experiments

ACD/Labs introduced Katalyst D2D, a web-based application to support high-throughput experiments. It has been developed to help ensure data integrity in high-throughput experiments (for reaction optimisation, process development, catalyst screening and scale-up), eliminating manual transcription through integration with third-party systems. Katalyst D2D integrates with analytical instrumentation to support execution of experiments, as well as processing and analysis of high-throughput data. Users can easily compare mass spectra, chromatograms and other analytical data with the array.

ACD/Labs

▸ http://link.spectroscopyasia.com/31-024

XGBoost added

Eigenvector have added XGBoost functionality to their PLS_Toolbox and Solo software. XGBoost models can be applied online with Solo_Predictor. XGBoost performs calibration and application of gradient-boosted decision tree models for classification. These are non-linear models which predict the probability of a test sample belonging to each of the modelled classes, hence they predict the class of a test sample.

Eigenvector

▸ http://link.spectroscopyasia.com/31-049

Transflectance probe

art Photonics has introduced the FlexiSpec, a dual-pass fibre optic probe for use with any fibre optic spectrometer or photometer in lab, pilot plant and process control. It provides high throughput in any part of the UV/vis and vis/NIR. Various versions are available with optical paths 2, 5 or 10 mm and the wavelength ranges of 200–1300 nm and 400–2200 nm.

art Photonics

▸ http://link.spectroscopyasia.com/31-025

UV/VIS

Craft beer QA

The BeerCraft software from Thermo Fisher Scientific works with the Genesys 50 and Genesys 150 UV/vis spectrophotometers to streamline quality assurance testing and batch-to-batch consistency for craft beer brewers. The combined system provides American Society of Brewing testing methods for more than 20 beer attributes, including colour, bitterness, protein, sugar, carbohydrate and polyphenol levels.

Thermo Fisher Scientific

▸ http://link.spectroscopyasia.com/31-021

Variable pathlength spectrometer

C Technologies introduced a lower-cost version of their variable pathlength UV/vis/NIR instrument, called the SoloVPM. This uses "slope spectroscopy" and has variable pathlengths from 0.010 mm to 12.00 mm and a wavelength range of 190–1100 nm. It is based around an Agilent Cary 60 spectral engine. VIPER software has been redeveloped specifically for variable pathlength measurements, controlling the instrument and providing results display.

C Technologies

▸ http://link.spectroscopyasia.com/31-053

IMAGING

Broadband infrared emitter for hyperspectral imaging applications

Lumileds has introduced the LUXEON IR ONYX LED for use in spectroscopy and hyperspectral imaging applications. This is a continuous broadband infrared (IR) emitter from 650 nm to 1100 nm. The IR spectrum consists of a broad, flat emission without any peaks, enabling ease of calibration. The LED comes in an industry standard 2720 package and small footprint of 2.7 mm × 2.5 mm for integration in existing designs. The broadband IR emission is produced by new proprietary phosphor materials developed and manufactured by Lumileds. Radiometric power is 50 mW IR over the range 600–1050 nm, and more than 80 µW nm^{-1} over a broad range (750–1000 nm) enabling hyperspectral analysis with high signal-to-noise ratio.

The new LED opens up new possibilities for miniaturisation of spectroscopy and hyperspectral imaging applications in, for example, hand-held devices for mobile, industrial and medical applications.

Lumileds

- http://link.spectroscopyasia.com/31-012

INFRARED

ATR mode certified polystyrene reference films

Starna now supply an "ATR" set of polystyrene film references to assist compliance with the new European Pharmacopoeia Chapter 2.2.24. This is supplied as a kit of two films: a RM-1921/38 film certified film for normal transmission measurements and an accompanying film specifically certified for "ATR only". This new set expands the Starna range of polystyrene film references for use in FT-IR, mid-IR and NIR wavelength calibration to include both transmission and ATR modes. Existing films are available in two thicknesses: RM-1921/38 is a 38 µm polystyrene film with 14 certified peaks from 540 cm^{-1} to 3080 cm^{-1} (18.5–3.25 µm) whose values are traceable to NIST SRM 1921b. A thicker version, RM-1921/65, is 65 µm thick and in addition to the 14 peaks in the mid-IR, eight peaks are certified in the NIR from 3060 cm^{-1} to 8750 cm^{-1} (3.25–1.15 µm). These peaks are traceable to NIST SRM 2065.

The reference films comply with the latest revisions of the European Pharmacopoeia Chapter 2.2.24, and US Pharmacopoeia General Chapters 854 and 1854 on Mid-Infrared Spectroscopy. They are presented as card-mounted films in the conventional industry pattern; ATR film unmounted. These references are produced under Starna's ISO 17034 Reference Material Producer accreditation and certified under ISO/IEC 17025 for Calibration.

Starna

- http://link.spectroscopyasia.com/31-044

MAGNETIC RESONANCE

CryoProbe for biological solids

The BioSolids CryoProbe from Bruker is optimised for biological solids, such as membrane proteins or disease aggregates at physiological temperatures. An increase in x-nucleus sensitivity by a factor of four reduces experiment time by a factor of up sixteen. It is available for 600 MHz systems in H/C/N configuration and supports high-power decoupling as well as CP and double CP based solid-state NMR experiments.

Bruker

- http://link.spectroscopyasia.com/31-056

Automated MAS probe

Bruker has introduced new new iProbes. The iProbe CP-MAS has been designed to support automated workflows and has automated magic angle calibration, auto tuning and matching for solid-state magic angle spinning experiments, and support for autochangers. It is available for 400, 500 and 600 MHz systems in double-resonance H/X channel configurations with 4.0 mm rotor diameter for MAS up to 15 KHz. The iProbe TBO is a higher-sensitivity, true triple-resonance broadband NMR probe for the study of fluorinated compounds. It can observe any nucleus from ^{31}P to ^{109}Ag with simultaneous decoupling on ^{1}H and ^{19}F, eliminating the need for probe changes. Auto-tuning and matching capability allows liquids NMR automation.

Bruker

- http://link.spectroscopyasia.com/31-055

MASS SPEC

Q-ToF LC/MS system

Agilent Technologies has announced a range of new mass spectrometry products. The new Agilent 6546 quadrupole time-of-flight LC/MS system includes Q-RAI (Quadrupole-Resolved All Ions), a data-independent acquisition mode which reduces the complexity of MS/MS spectra while maximising the accuracy and quality of the data acquired. MassHunter software complementing the Agilent 6546 LC/Q-TOF includes MassHunter Quantitative Analysis 10.0 software with new features that allow quicker and more accurate screening of complex sample sets for both target and suspect compounds in a single workflow. New MassHunter Classifier software which complements the enhanced method development workflow in the Mass Profiler Professional (MPP) software, enabling faster testing for food authenticity with results that are easier to review. MassHunter Lipid Annotator that presents theoretical lipid MS/MS annotations for Q-TOF results with support through the MassHunter Mass Profiler Professional Lipidomics workflow.

Agilent also announced the new Agilent Bravo Metabolomics Sample Prep Platform, which provides consistent and accurate preparation of human plasma samples for metabolomics analysis via LC/MS.

Agilent

▸ http://link.spectroscopyasia.com/31-047

PaperSpray ion source

The Thermo Scientific VeriSpray PaperSpray ion source is a high-throughput direct sampling system with an interface that is simple to operate, regardless of the analyst's experience. The system offers simple clean-up and a disposable interface, eliminating the potential for carry-over and contamination. The autosampler simply adds sample and solvent to the paper cartridge and loads it into the system for analysis. The VeriSpray is compatible with Thermo Scientific TSQ Quantis, TSQ Fortis, TSQ Altis, TSQ Endura and Quantiva TSQ mass spectrometers.

Thermo Fisher Scientific

▸ http://link.spectroscopyasia.com/31-058

NIR

Cloud-connected spectroscopy

ZEISS has developed, jointly with Microsoft, a spectroscopic solution that uploads real-time pro-duction data from spectroscopic analysis to the cloud. A ZEISS Corona process spectrometer is mounted directly on the production line, and the data from this is fed into Microsoft's cloud platform, Azure. The information is available to all individuals responsible for monitoring and optimising production. Real-time spectroscopic measurement and data upload to the cloud is part of the move towards a "connected factory", also known as "Industry 4.0". ZEISS has been involved in these developments in connected production and manufacturing. Real-time spectroscopic analysis allows for proactive process optimisation, leading to consistent quality and productivity.

ZEISS

▸ http://link.spectroscopyasia.com/31-045

UV/VIS

Miniature visible OEM spectrometer

Ibsen Photonics has launched the compact PEBBLE VIS OEM spectrometer, which has a size of 17 × 15 × 8 mm with high resolution and sensitivity as well as environmental ruggedness. The PEBBLE VIS is based on the same diffraction grating technology used in all other Ibsen spectrometers, which enables the PEBBLE to be manufactured in high quantities with very small unit-to-unit performance variation. The core of the PEBBLE is a highly efficient transmission grating manufactured in-house. Furthermore, the PEBBLE utilises a new, fast and sensitive CMOS detector array with 256 pixels. When combined with a large numerical aperture of 0.22 (low f-number of f/2.2) the PEBBLE provides high sensitivity for a spectrometer of its size. A key benefit of using a transmission grating inside the PEBBLE is a high resolution of 6 nm across the full 380–850 nm wavelength range.

Ibsen Photonics

▸ http://link.spectroscopyasia.com/31-015

DIARY

Conferences

2019

2–5 June, Nara, Japan. **15th International Symposium on Applied Bioinorganic Chemistry (ISABC 15).** 🕸 http://web.apollon.nta.co.jp/isabc15/.

2–6 June, Atlanta, Georgia, United States. **67th ASMS Conference on Mass Spectrometry.** ✉ office@asms.org, 🕸 https://www.asms.org/conferences/annual-conference.

9–14 June, Mexico City, Mexico. **Latin American Meeting on Laser-Induced Breakdown Spectroscopy (LAMLIBS).** ✉ mayo.villagran@icat.unam.mx, 🕸 http://www.csi2019mexico.com/index.php/lamlibs.

9–14 June, Mexico City, Mexico. **Colloquium Spectroscopicum Internationale XLI (CSI XLI).** ✉ info@csi2019.mexico.com, 🕸 http://www.csi2019mexico.com/.

16–20 June, Split, Croatia. **5th International Sclerochronology Conference (ISC2019).** Melita Peharda, ✉ isc2019@izor.hr, 🕸 http://jadran.izor.hr/isc2019/index.html.

18–20 June, Minneapolis, United States. **2019 Analytics Solutions Conference.** 🕸 https://www.camo.com/analyticsconference/.

23–27 June, Munich, Germany. **Laser World of Photonics Congress.** Ellen Richter-Maierhofer, ✉ nfo@photonics-congress.com, 🕸 https://www.photonics-congress.com/about/conferences/index.html.

24–25 June, Oxford, United Kingdom. **RamanFest 2019: Conference on Advanced Applied Raman Spectroscopy.** ✉ ramanfest.uk@horiba.com, 🕸 https://www.ramanfest2019.com/.

25–28 June, Dorval, Canada. **63rd International Conference on Analytical Sciences and Spectroscopy (ICASS).** Diane Beauchemin, ✉ diane.beauchemin@chem.queensu.ca, 🕸 http://www.csass.org/ICASS.html.

25–28 June, Dorval, Quebec, Canada. **Spectr'Atom 2019.** Diane Beauchemin, ✉ diane.beauchemin@chem.queensu.ca, 🕸 http://www.csass.org/SpectrAtom2019.html.

25–27 June, San Jose, California, United States. **OSA Optical Sensors and Sensing Congress.** 🕸 https://www.osa.org/en-us/meetings/osa_meetings/optical_sensors_and_sensing_congress/.

27–29 June, Amsterdam, Netherlands. **18th Annual Congress on Pharmaceutics & Drug Delivery Systems.** ✉ clarajane567@gmail.com, 🕸 https://pharmaceutics.annualcongress.com/.

30 June–3 July, Warsaw, Poland. **7th International Symposium on Metallomics.** Ryszard Lobinski, ✉ sekretariat@metallomics2019.pl, 🕸 http://metallomics2019.pl/.

7–13 July, Dubrovnik, Croatia. **13th Mass Spectrometry in Biotechnology and Medicine (MSBM).** 🕸 http://www.msbm.org/.

8–12 July, Auckland, New Zealand. **International Conference on Advanced Vibrational Spectroscopy (ICAVS10).** ICAVS Secretariat, Podium Conference Specialists, 2661 Queenswood Drive, Victoria, BC, Canada, V8N 1X6. 🕸 http://www.icavs.org/2019-conference/.

15–18 July, Honolulu, Hawaii, United States. **15th International Congress of Toxicology (ICTXV).** ✉ sothq@toxicology.org, 🕸 https://www.toxicology.org/events/ict/index.asp.

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

28 July–2 August, Singapore, Singapore. **16th Annual Meeting Asia Oceania Geosciences Society (AOGS).** ✉ info@asiaoceania.org, 🕸 http://www.asiaoceania.org/society/index.asp.

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

12–13 August, Auckland, New Zealand. **7th Asia Pacific Congress on Chemical and Biochemical Engineering.** ✉ asiachemical2019@gmail.com, 🕸 https://www.chemicalengineeringconference.com.

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

25–29 August, San Diego, CA, United States. **258th American Chemical Society (ACS) National Meeting & Exposition.** ✉ NationalMeetings@acs.org, 🕸 https://global.acs.org/events/258th-acs-national-meeting-exposition/.

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

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.

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

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/.

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

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22–25 September, Phoenix, Arizona, United States. **2019 GSA Annual Meeting.** ✉ meetings@geosociety.org, 🌐 http://www.geosociety.org/GSA/Events/Annual_Meeting/GSA/Events/2019info.aspx.

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

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.

24–26 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/.

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.

23–27 February, San Diego, United States. **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://global.acs.org/events/259th-acs-national-meeting-exposition/.

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

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

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

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

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

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

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.

Courses

2019

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

Exhibitions

2019

9–11 July, Johannesburg, South Africa. **Analytica Lab Africa.** Barbara Kals, ✉ barbara.kals@messe-muenchen.de, 🌐 https://www.analytica-africa.com/.

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/.