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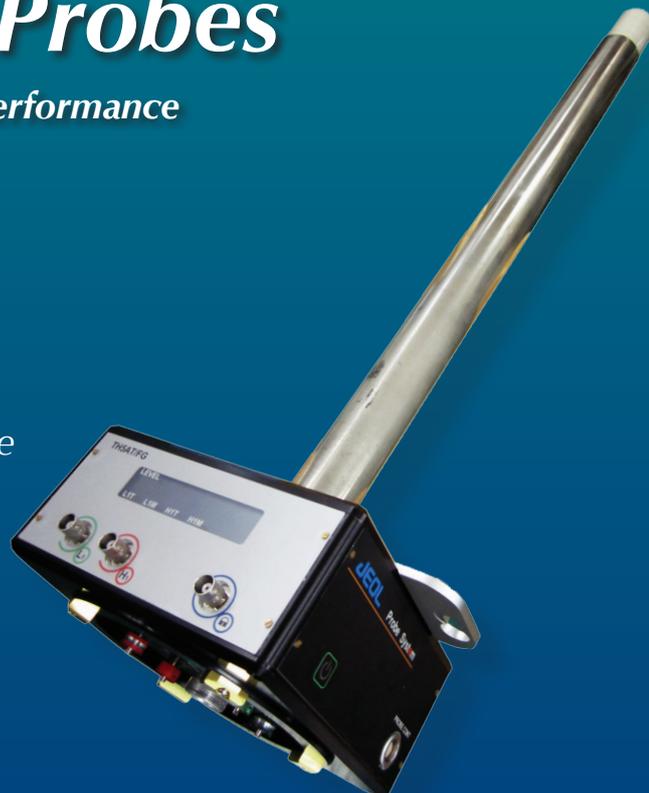


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It is not every issue that one of our articles starts with a quotation in medieval English, and it is appropriate as two of our articles cover the use of spectroscopy in cultural heritage. This is yet another field where the rich information provided by spectroscopy, along with its non-destructive nature (for many techniques), portability and ability to generate chemical images make it the answer to many questions. Kate Nicholson, Andrew Beeby and Richard Gameson are responsible for the medieval English at the start of their article "Shedding light on medieval manuscripts". They describe the general use of Raman spectroscopy for the analysis of historical artefacts, and, in particular, their work on medieval European manuscripts and 18th century watercolour pigments. They stress the importance of checking the actual laser power density to avoid damage to priceless artefacts.

Jean Robertson, Charles Shand and Estefania Perez-Fernandez update us on

the use of various spectroscopies for soil analysis in "The application of Fourier transform infrared, near infrared and X-ray fluorescence spectroscopy to soil analysis". Once again developments in portable instruments lead to greater ease of use and the ability to measure far more samples. They describe the application of FT-IR, NIR and XRF spectroscopies to the development of the National Soils Inventory of Scotland, and their work in developing the use of handheld instruments, particularly FT-IR spectrometers.

Returning to our cultural heritage theme, Bianca Jackson tells us about "TISCH—Terahertz Imaging and Spectroscopy in Cultural Heritage: applications in archaeology, architecture and art conservation science". Terahertz spectroscopy and imaging of Paleolithic cave etchings, 14th century paintings in a church and a mid-20th century Italian painting are all described. This helps demonstrate the versatility of the tech-

nique as well as its potential in cultural heritage preservation.

Tony Davies has interviewed Gerard (Gerry) Downey who has just retired from the Irish National Agriculture and Food Research Institute, Teagasc. Gerry will be known to many of you, particularly those who work in the fields of chemometrics, NIR spectroscopy and food & ag. I must have known Gerry for over 25 years and currently work closely with him on the publication of *NIR news*, so I am particularly delighted that Tony has chosen to highlight his career.

As well as our usual highlight of new spectroscopy products, we have included a section on many of the new product introductions at the recent American Society for Mass Spectrometry (ASMS) conference and exhibition.



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Soil is critical to life on Earth, and spectroscopy is playing an ever more important role its monitoring and our understanding of it, as described in the article starting on page 9.

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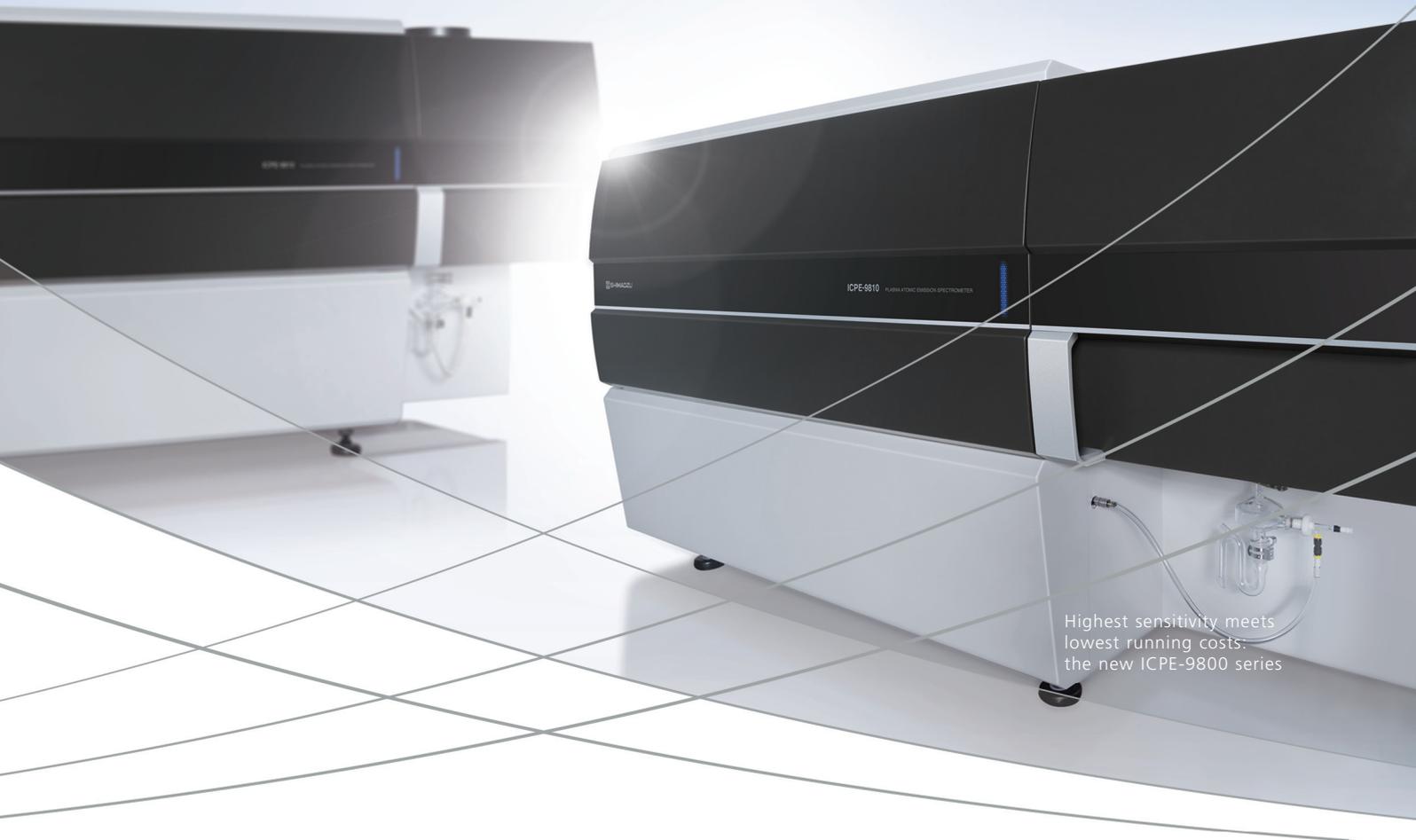
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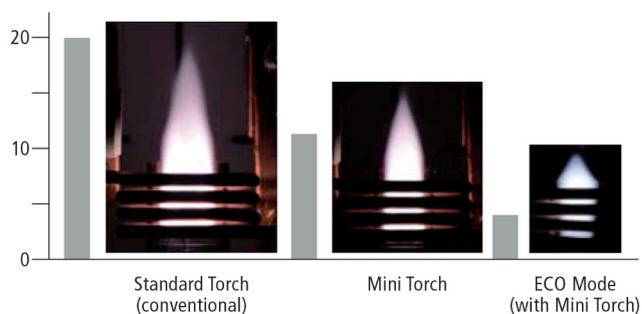


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Shedding light on medieval manuscripts

Catherine E. Nicholson,^a Andrew Beeby^b and Richard Gameson^b

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“Seo nydþearf feala læreð” –Necessity teaches many things.¹ *Durham proverbs*, DCL B_II_32 f.43–45

Introduction

Investigation of the pigments used by medieval illuminators is often piecemeal and slow, simply due to the logistics of uniting a medieval manuscript with a spectrometer. Insurance and conservation issues prevent the transport of precious books to scientific facilities for analysis, and the moratorium on sampling results in the fact that only optical spectroscopy (or those using electromagnetic radiation in a non-contact, non-invasive manner) can be used. The techniques of choice are Raman and diffuse reflection [also known as FORS, fibre-optic (visible and near infrared) reflectance spectroscopy] spectroscopies, multi- or hyperspectral imaging and X-ray fluorescence, XRF. Moving bulky equipment to the manuscripts has also been a logistical challenge but recent developments in portable equipment have allowed this area to flourish.

Extreme care must be taken when working with priceless artefacts; by working with conservators, safe exposure limits may be determined. In Raman spectroscopy studies for example, laser power density is the primary concern, with limits of $<0.02 \text{ mW} \mu\text{m}^{-2}$ classed as the safe limit to prevent degradation of photosensitive pigments in a confocal microscope.^{2,3} Often workers are not aware of the conditions they are using, and some commercial systems use far greater power densities to achieve good signal-to-noise ratio, and can rarely adhere to such strict limits. We would encourage anyone considering a purchase for this purpose to be mindful that the technology should not inadvertently damage their artefact.

The necessity for developing better systems has resulted in “Team Pigment” (see <http://www.durhamgospels.blogspot.co.uk> and [@teampigment](https://twitter.com/teampigment)) working

with the instrument manufacturers to develop custom solutions to allow for both portability and sensitivity at such low power densities, and by employing a selection of techniques such as Raman spectroscopy, multispectral imaging and reflection spectroscopy to identify pigments in use on a host of manuscripts.

Moving the mountain

For our initial study on the Northumbrian insular manuscripts of the 7th and 8th centuries,⁴ we used a Horiba LabRAM HR. This laboratory instrument was moved to the special collections library and was fitted with a re-engineered x,y sample stage to support large manuscripts beneath the microscope head. Neutral density filters allow for the power density to be reduced to safe limits and a 50× Leica LWD (Long Working

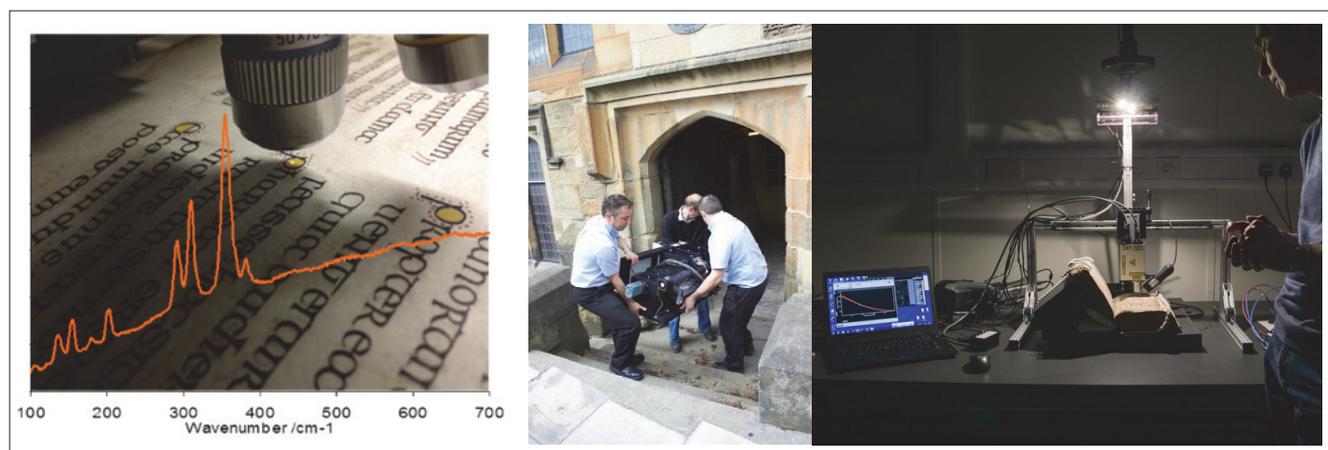


Figure 1. Left to right: manuscript under investigation, overlay of spectrum (orpiment As_2S_3) from yellow letter fill. Horiba engineers moving spectrometer into medieval dungeon at Palace Green Durham. Portable system in action.

Distance) objective kept a safe working distance away from the manuscript. This system also had the advantage of multiple lasers to choose from, thus if a particular pigment was fluorescent or absorbing in the region of our standard 633nm HeNe laser, a 785nm or 532nm laser could be used. The utmost care was taken to measure the laser power using a power meter placed at the focal point of the microscope prior to any measurements on manuscripts.

This early work was assisted by the generous provision of two engineers to move and re-align the spectrometer used in this project. Despite expert assistance this move required several days, and muscle power to physically move a laser, optical table and ancillary equipment. It was immediately apparent that whilst this system excelled in performance it was not practicable to move the instrument to other libraries where more work was needed to be done.

Superheads and supersmall spectrographs

The fixed microscope head of the Horiba LabRAM HR imposed some limitations on which areas of manuscripts could be accessed, hence a Horiba Superhead Raman probe which couples to the laser and spectrometer via fibre optics provided a logical evolution of the equipment. The disadvantage of the Superhead is that the filters are encased within the sealed unit, hence one per laser wavelength is required. However, this Raman probe does allow for coupling to an external laser source, and effectively any spectrograph/detector. Also, because of the fibre coupling of the laser, the spot size of this system is significantly larger than the LabRAM HR so is no longer strictly confocal. The spot is estimated to be 30 μm diameter, giving it a much lower power density at the sample, 0.5 $\mu\text{W}\mu\text{m}^{-2}$.

Bearing in mind the need for a portable system we chose to assemble a single wavelength mobile Raman spectrometer based upon a low power HeNe laser, the Horiba Superhead and an Ocean Optics QEPro spectrograph/camera as the detection system. This spectrometer, pre-set for operation at

633nm, has a small footprint, is lightweight and offered good sensitivity. Although limited to a single wavelength, this equipment is readily portable, can be set up in less than half an hour and retains its calibration after a journey.

The system is small enough to fit into a small suitcase and was taken to work in the field for a three-week campaign in the Fitzwilliam Museum in Cambridge. The overall sensitivity of this mobile system was lower than the benchtop system and required longer acquisition times (up to 120s compared to 20s on the LabRAM) which slowed progress. This modular system performed admirably and allowed a huge amount of data to be collected from late medieval European manuscripts.

Raman spectroscopy is a powerful technique for the identification of pigments; however, some materials do not readily yield a good spectrum, it can suffer from interference from fluorescent materials and can only analyse a sample on a point-by-point basis. To circumvent this we employ a combination of optical techniques including diffuse reflection and multispectral imaging which reveal the presence of additional pigments, for example carbon- and copper-based inks show low reflectivity in the near infrared spectral region, and cannot be readily detected with the 633nm portable Raman system at the low power densities considered non-damaging.

Optimisation and testing

Further investment to the "Team Pigment" project has allowed for further refinements to the portable system. We are currently using a deep-cooled, back-illuminated, deep-depletion CCD (charge-coupled device) camera (Andor iDus 416) which offers exceptionally low noise and high-efficiency allowing for reduced acquisition times (typically 20s) and the possibility of long exposures. Coupled to a spectrograph with a moveable and exchangeable grating (Andor Shamrock 163) this system has the advantage of being able to tune the system to any wavelength, allowing it to be used with a selection of laser wavelengths.

The performance of the Raman probe is an important consideration: several

pigments have characteristic bands at low wavenumber, hence they should have as low a low-wavenumber cut-off as possible: systems are now available that can operate at $>80\text{ cm}^{-1}$ for both 633nm and 532nm. For example, such a performance allows the identification of mixtures of the lead oxides red lead and massicot, that was previously only possible on a lab-based system.

A direct comparison of results collected using the same Raman probe, sample, fibre and incident laser power at the sample of 0.36mW from these portable systems is shown in Figure 2. In these normalised spectra, a clear improvement in the signal-to-noise ratio (S/N) can be seen with higher performance detection systems. Better S/N could readily be obtained using higher laser powers, but these tests of performance were carried out under similar conditions to those used in the conservation setting.

For the conservation community, Raman spectroscopy is not necessarily the silver bullet that permits the reliable identification of pigments, but a useful tool to complement the other techniques already in use. A preliminary study by our group of a selection of common 18th century water-colour pigments revealed that just over half of (24 of the 45) samples provided could be identified using Raman spectroscopy, with this number falling to 20 if just a single laser wavelength was used.

Another vital consideration is the expertise of the user—whilst many conservation scientists excel in a range of fields and are eager to be trained in using this technique, it is one that requires experience and time to perfect. Even after an intensive day-long training course, we find that students and conservators struggle to obtain spectra from test sheets with a thick layer of fresh pigment. This highlights the investment of time required to master the technique, and that it is currently far from a 'point, click and identify' solution. Conservator's time is stretched thinly as it is, and at present we recommend patience whilst the system is refined and optimised for this application rather than making an expensive purchase that may provide little information or, worse, may cause damage to the priceless artefacts they care for.

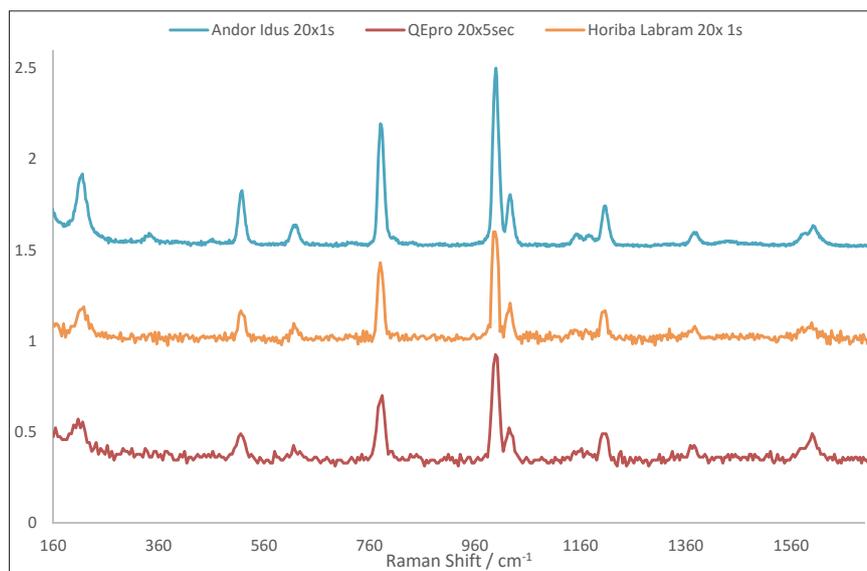


Figure 2. Comparable results are obtained from different portable detectors using the same collection conditions on liquid sample of toluene, Horiba Superhead and fibre-optic coupling, all using identical acquisition conditions (total power 0.36 mW, $0.5 \mu\text{W}\mu\text{m}^{-2}$).

Conclusion

Whilst Raman spectroscopy is far from its infancy in this field,^{5,6} it is only now becoming a fully-fledged technique that

can be applied *in situ* to any artefact without causing damage from the light exposure of the incident laser beam. Ongoing development of the equipment by

Table 1. Portable systems currently retailing. Note the authors strongly recommend that the laser power is always measured with a calibrated power meter and the laser power density calculated prior to any measurements on artefacts. (? indicates information not advertised on website.)

| Manufacturer | Model | Laser wavelength (nm) | Laser power (min) (mW) | Laser power (max) (mW) |
|-------------------|----------------------|-----------------------|------------------------|------------------------|
| B&W Tek | i-Raman Plus | 532 | Variable | 50 |
| B&W Tek | i-Raman Plus | 785 | Variable | 420 |
| B&W Tek | NanoRam | 785 | 30 | 300 |
| SciAps | Inspector 500 | 1030 | 300 | 300 |
| SciAps | Inspector 300 | 785 | 300 | 300 |
| Ocean Optics | IDRaman mini 2.0 | 785 | 50 | 100 |
| Rigaku | Progeny | 1064 | ? | ? |
| Metrohm | Mira | 785 | ? | 75 |
| Metrohm | Mira | 1064 | ? | 400 |
| Stellarnet | Various | Custom | Variable | 500 |
| BaySpec | Agility | 532 | Variable | 50 |
| BaySpec | Agility | 785 | Variable | 499 |
| BaySpec | Agility | 1064 | Variable | 499 |
| Bruker | Bravo | ? | ? | ? |
| Thermo Scientific | TruScan RM | 785 | 225 | 250 |
| Renishaw | RA100 Raman analyser | Custom | User specified | User specified |

instrument manufacturers (see Table 1) is leading towards new optimised modular spectrometers that can be deployed in the field yet retain or improve upon the performance of their lab-based counterparts at comparable low laser power densities. Development of this portable equipment has allowed relationships between conservation scientists, librarians and historians to grow. “Team Pigment” are pushing the development of the spectrometers in this application and working closely with the manufacturers to make advances in pigment identification in manuscripts.

The final word of caution that we would stress is that laser-based spectroscopic methods such as Raman spectroscopy must be used with the utmost care and consideration such that no damage is done to photosensitive pigments on priceless artefacts, and that conservation limits on light power density always be observed.

Acknowledgements

The authors would like to thank the many libraries, conservation scientists, curators and conservators of the collections we have visited and for allowing us access to the manuscripts in their care.

Notes and references

- As a trained chemist, quoting medieval English was not a prospect I ever imagined, however, spending the past three years as a founding member of “Team Pigment” and carrying out analysis on many manuscripts later, I would like to tip my hat to the original illuminators and scribes to whom I owe my current research interests.
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- This is the power density employed in a confocal system, but this does not scale linearly with spot size due to local heating effects.
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The application of Fourier transform infrared, near infrared and X-ray fluorescence spectroscopy to soil analysis

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Introduction

Soil is critical to life on earth and provides not only the key functions of food and energy production but also many other important functions, such as water regulation and carbon sequestration.¹ Soil is a highly complex material, consisting of an extremely variable mixture of minerals, organic matter, liquids and gases. Soils are heterogeneous on different scales: in the landscape they are heterogeneous both horizontally and vertically and generally occur in distinguishable layers termed horizons, as a result of modification of inputs and outputs over time.² On the microscopic scale, soil can be even more heterogeneous, moving, for example, over a very short distance from a discrete mineral grain to a soil microbe. Soils can range from a mineral soil with almost no organic matter content to an entirely organic soil or peat. In the context of productive and sustainable agriculture there is a need to know soil properties such as pH, organic matter, and nutrient and pollutant concentrations. Traditionally, many soil analyses have involved wet chemical methods with liquid extraction and subsequent analysis of solutions with laboratory-based instruments. For example, the determination of the micronutrient concentration of soil involves extraction with acids (typically HF/HNO₃ or HNO₃/HCl) and subsequent analysis by inductively coupled plasma (ICP)-based methods. Similarly, the determination of soil organic matter

concentration has traditionally involved wet oxidation, although many laboratories now use combustion with CHN analysers. There is now a drive towards using dry chemical methods such as X-ray fluorescence (XRF) and infrared (IR) spectroscopic analysis which minimise cost, improve speed and reduce environmental impact and waste. At the James Hutton Institute (and the legacy institutes of the Macaulay Institute and Scottish Crop Research Institute) we have a long history of expertise in soil science and spectroscopic techniques, particularly of IR spectroscopy in the mid-IR range. In recent years we have been developing methods for Fourier transform (FT)-IR, near infrared (NIR) and XRF spectroscopic analysis of soil and creating databases of soil spectral data and calibrations to predict soil properties. Currently we are working to move from laboratory-based analysis towards the development of methodology for field-based soil analysis using FT-IR and XRF spectroscopy.

Spectroscopic analysis of soil

Fourier transform infrared

The highly complex and variable nature of soil is reflected in the very different FT-IR spectra they produce in the mid-IR region (4000–400 cm⁻¹) arising from the fundamental vibrations of the components present. Usefully, the mid-IR spectra provide an overall chemical profile of the soil,

encompassing fundamental vibrations of both the organic and mineral components. The mineral components present in soil are predominantly silicates, including clay minerals (aluminosilicates), or carbonates, but can also include other types of minerals such as sulfates. Clay minerals play an important part in the properties of a soil and have free OH groups present in their structures³ (i.e. without hydrogen bonding). The O–H stretching bands for clay minerals (approximately 3700–3500 cm⁻¹) are therefore sharp bands which are highly diagnostic. Si–O stretching vibrations are strong bands found close to 1000 cm⁻¹, and those for the carbonate anion are close to 1400 cm⁻¹. When considered in combination with the bending vibrations, below 900 cm⁻¹, the individual minerals present can often be identified. For example, for carbonates, it is relatively easy to differentiate between calcite (calcium carbonate), aragonite (a different form of calcium carbonate) and dolomite (a calcium magnesium carbonate). Silicate minerals can also be identified from their bending vibrations, e.g. quartz can be readily identified by a sharp doublet at 797 cm⁻¹ and 779 cm⁻¹.^{4,5}

The organic components present largely originate from vegetation and so the IR spectral features of soil organic matter (SOM) have much in common with IR spectral features of plants,

although plants degrade to form other organic compounds such as humic and fulvic acids. A broad O–H stretch between approximately 3600 cm^{-1} and 3200 cm^{-1} is characteristic of SOM and the C–O stretch for polysaccharide is found at 1030 cm^{-1} , which can coincide with the silicate stretch if minerals are also present. The C–H stretching region can reveal whether long chain molecules are present or whether the organic material is more polysaccharide based. In addition, functional groups present in the SOM such as those arising from esters, carboxylic acid, amide (protein) and lignin can be identified and hence the SOM characterised.⁶ Interpretation of FT-IR spectra therefore allows a rapid assessment of the relative proportions and nature of both SOM and clay minerals present and also the determination of the underlying mineralogy.

Generally, FT-IR spectroscopic analysis of soil samples in the laboratory is carried out on dried, milled samples, with an optimal particle size $<2\ \mu\text{m}$, in order to avoid problems of reflection of the radiation, poor resolution of peaks and sloping baselines. An effective protocol for preparation of soil samples for FT-IR spectroscopic analysis, to allow the production of reliable and reproducible spectra, has been developed at the James Hutton Institute.⁷ Historically FT-IR spectroscopy of soils was carried out in transmission, using KBr discs prepared from the milled soil, but more recently, diamond attenuated total reflection (DATR) sampling accessories have become routinely used for soil analysis, having the advantage of allowing spectra to be recorded of unprocessed soil, automatically producing spectra of optimum intensity and being non-destructive. The spectra produced are similar in appearance to transmission spectra. Alternatively diffuse reflection or DRIFTS (diffuse reflection infrared Fourier transform spectroscopy) can be used for soil analysis. In this case the IR radiation is reflected from the external and internal surfaces of the sample, and this is also non-destructive and requires little sample preparation. DRIFTS spectra in the mid-IR region have a very different appearance to ATR or transmission

spectra⁸ and can be more difficult to interpret.

Near infrared

While the fundamental vibrations of molecular bonds and functional groups occur in the mid-IR region, the NIR region extends between 750 nm and 2500 nm (i.e. $12,500\text{--}4000\text{ cm}^{-1}$) and consists of broad absorption bands, overtones and combinations of the fundamental absorptions found in the mid-IR range. NIR spectra contain absorbance bands mainly due to chemical bonds of C–H (fats, oil, alkanes), O–H (water, alcohol) and N–H (protein). Other chemical bonds may exhibit overtone bands in the NIR region, but are generally weaker. NIR spectra of soil therefore reflect the SOM and clay minerals well, but provide much less information on the full mineralogy of the samples than their counterpart mid-IR FT-IR spectra.

Although NIR spectra do not have the resolution of the mid-IR spectra, NIR has the advantage of being a more energetic radiation that penetrates deeper into samples thus allowing the scanning of samples with little, or no, previous preparation. Nonetheless, samples are usually dried and sieved to 1–2 mm for homogenisation purposes. The most common spectral collection mode used is diffuse reflection, in which the light interacts with the sample and re-radiates diffuse reflected energy, which is detected (and plotted as $\log 1/\text{Reflectance}$) at a 45° angle in order to minimise specular reflection.

Its ease of use has given NIR spectroscopy some advantage over other techniques for soil analysis; however, the combinations and overtones that form the spectra conceal the sum of the numerous bands that correspond to functional groups present in the sample, making its interpretation more complex (Figure 1 illustrates the FT-IR and NIR spectra of the same peat sample). For this reason, NIR has traditionally relied on multivariate data analyses techniques (chemometrics) for the extraction of information and development of multivariate calibration models that correlate optical measure-

ments with soil chemical or physical attributes under study, for predictive purposes.⁹ As opposed to FT-IR spectroscopy in the mid-IR region, which has mainly been used qualitatively, NIR spectroscopy is mostly used as a quantitative technique that provides a very rapid means of simultaneously measuring multiple physical and chemical properties of soil.

X-ray fluorescence

Unlike the IR spectroscopic methods which are molecular, XRF using laboratory-based instruments has been a prime and widely used method for the determination of the elemental composition of soils. The main elements in soil expressed on a weight/weight basis are generally in the order O, Si, Al, Fe, C, Ca, K, Mg, Na, Ti, N and P. Soil also contains other minor elements, including those which are essential for plant growth such as Cu and Zn. The XRF method is based on excitation of the sample with a beam of X-rays resulting in the emission of secondary X-rays with energies characteristic of the elements in the sample (see, for example, Figure 3). To obtain reproducible and accurate data, soil samples are generally converted into a pressed disc or fused using a flux before pouring the melt into a mould to produce a glassy disc when cooled. These discs have a flat surface that is relatively homogeneous and so the sample is in a reproducible position in relation to the X-ray source and detector. With technological developments in devices for the production and detection of X-rays, portable XRF point and shoot instruments (PXRF) have become widely available and used on soil samples that have received little or no preparation apart from drying and milling. Because of the ease of use of PXRF, it is easy to obtain numerical data. However, appropriate calibration and checks are required to ensure accuracy of element concentrations. However, because of the low energies and absorption by air the determination of elements with atomic mass <12 by standard PXRF is challenging and requires the use of purging with He or use in a vacuum.

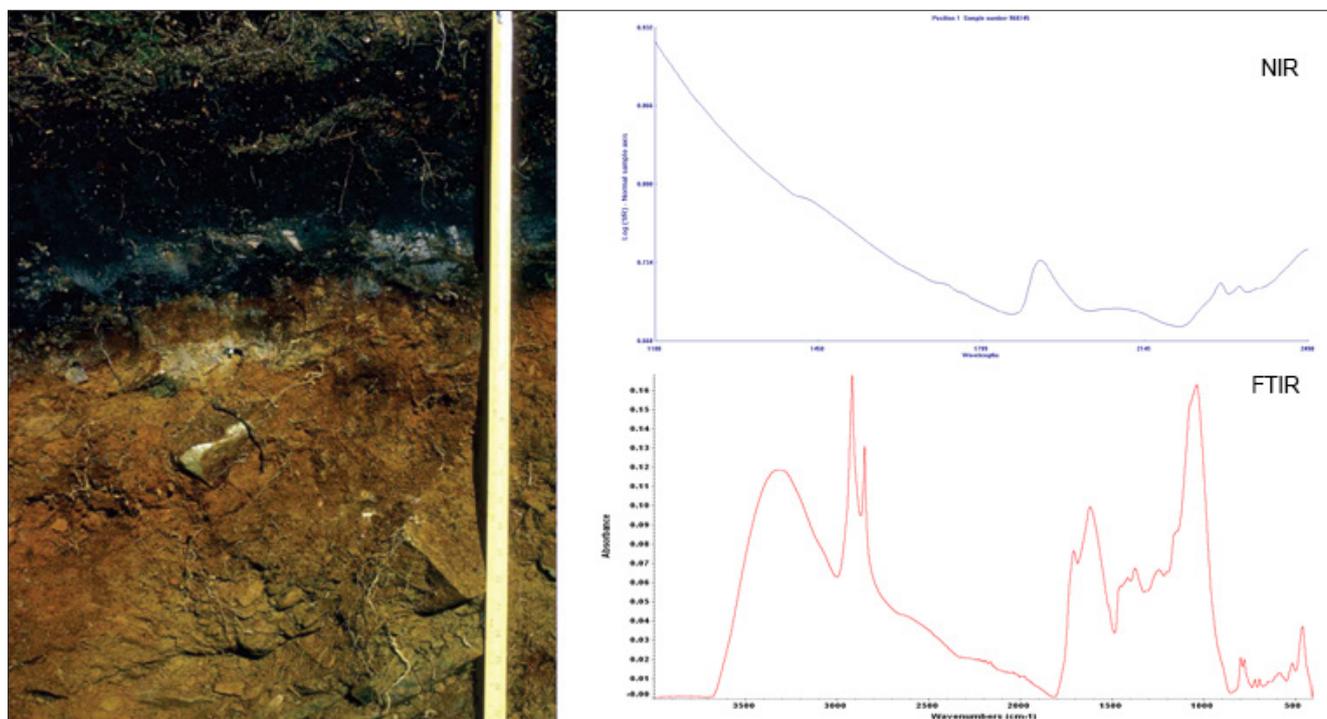


Figure 1. FT-IR and NIR spectra of the same highly organic soil sample with the soil profile.

Application of the spectroscopic techniques to the National Soils Inventory of Scotland dataset

The James Hutton Institute holds the samples and data for the National Soil Inventory of Scotland (NSIS), a spatial dataset of soils sampled on a 20 km grid throughout Scotland.¹⁰ Both recently sampled (NSIS2, 2007–2009) and legacy samples (NSIS1, 1978–1988) from each of the discrete horizons of a pit profile at the 183 different sites were available for the spectroscopic analysis. FT-IR spectroscopic and XRF analysis was carried out on the top horizons of each pit profile, while all the pit profile samples available were analysed by NIR spectroscopy. Prior to all the analysis, the soil samples were air-dried at ~30°C, passed through a 2-mm sieve to remove stones, large roots or other debris, and representative subsamples taken with a spinning riffler or by coning and quartering. Further sample preparation, as described above, was carried out for each individual technique. The samples were also analysed

by wet chemical methods for a wide range of analytes and properties, some by more than one method. Scottish soils have a great diversity and the

dataset had % C values ranging from 1% to 50%.

FT-IR spectra of the milled soils were recorded on a Bruker Vertex



Figure 2. Portable XRF instrument on stand with sample holder and film located under the radiation shield. The inset (bottom right) shows portable XRF being used in the field.

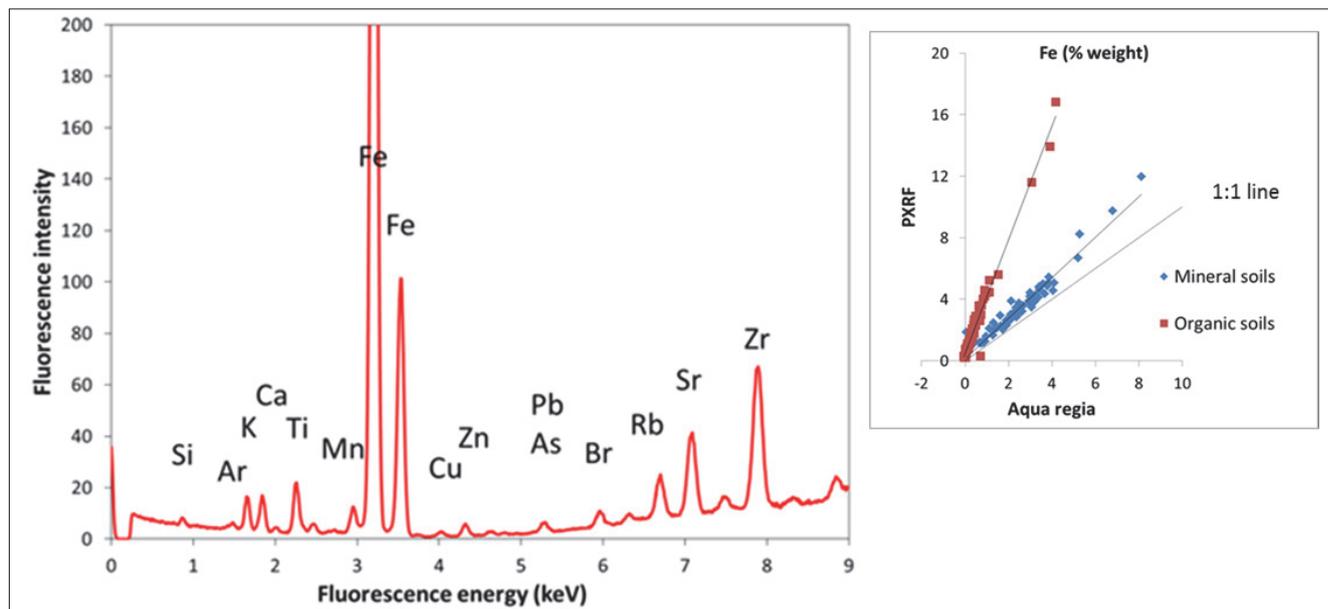


Figure 3. PXRF spectrum of a reference soil (left). Comparison of Fe concentration measured in mineral and organic soils by aqua regia extraction/ICP spectrometry, or directly by PXRF (see text for details).

70 FT-IR spectrometer using a DATR accessory over the range from 4000 cm^{-1} to 400 cm^{-1} (ATR and baseline corrected). High quality FT-IR spectra were achieved for the Scottish Soil Spectral Database and they were shown to be highly reproducible and representative by comparisons between spectra of recently sampled and legacy soils from the same sites, with differences relating primarily to the SOM. This provided validation of all the sampling and preparation procedures used and therefore showed that it was possible to look at change in the soil profile over time. In addition to providing a comprehensive FT-IR spectral database for Scottish soils, successful calibrations have also been achieved for prediction of a number of soil parameters, including soil bulk density.

NIR spectra were recorded on 2-mm sieved soils using a Foss NIRSystems 5000 between 1100 nm and 2500 nm. Successful NIR spectroscopy calibrations, using a NIR spectral database created from the NSIS soil samples, have been developed for the prediction of a wide range of essential soil parameters, some of which were measured using different analytical techniques

and therefore an interesting overview of the effects that different analytical techniques can have on calibration performance was provided.¹¹

We analysed the elemental composition of the dried and milled NSIS2 topsoils by PXRF, using a Bruker S1Turbo^{SD} and 25-mm diameter plastic cups with a 4- μm thick polypropylene covering¹² (Figure 2). The soil samples were also analysed for inorganic element concentrations by aqua regia extraction/ICP spectrometry. In relation to PXRF, mineral soils behaved differently from organic soils and a different calibration to the soils programme supplied with the instrument is required for organic soils. An example, for the determination of Fe is shown in Figure 3. Aqua regia extraction data is often classified as “pseudo” total but the efficiency of extraction for many elements is far from complete. A comparison of data obtained by total dissolution of a typical mineral and a typical peat soil using HF and aqua regia extraction showed that Fe is only 84% and 87% extracted by aqua regia for the mineral and peat soil, respectively. This discrepancy partly explains the difference between PXRF and aqua regia data shown in Figure 3.

The future—moving towards field-based spectroscopic analysis

Although most examples of soil IR spectroscopy are laboratory-based, another advantage is the potential adaptability of these techniques for field-based assessment of soils, a particularly relevant application nowadays given the increasing need for accurate and inexpensive spatial soil data for environmental monitoring and precision agriculture. NIR spectroscopic methodology for field analysis of soils is probably the most advanced of all three techniques¹³ discussed here, but at the James Hutton Institute we are concentrating on the potential for field-based FT-IR analysis.

Hand-held FT-IR instruments have relatively recently become readily available, with sampling accessories for both DRIFTS and DATR analysis, opening up the possibilities for field-based FT-IR spectroscopic analysis of soil. *In situ* analysis is on un-milled soil in the fresh state so in addition to particle size and inhomogeneity there are also moisture issues to deal with. Generally for ATR measurements of un-milled spectra there is a more sloping baseline, a lower intensity of most mineral bands and a greater relative intensity of bands due to clay

minerals and SOM, which can actually be an advantage. Currently no methods or robust protocols for the field-based FT-IR spectroscopic analysis of soils exist and we are working to develop suitable methodology which will allow soil analysis in the field for a range of purposes including soil monitoring, agricultural and forensic work.

The technological advances in XRF have permitted the widespread use of affordable PXRF analysers, opening up XRF analysis to a wider audience of soil and environmental scientists and replacing the traditional methods of soil analysis involving chemical dissolution and subsequent analysis by ICP methods.¹⁴ PXRF can be used in the field directly on the soil surface (Figure 2). At the James Hutton Institute we are investigating this approach but surface roughness, heterogeneity and wetness are known¹⁵ to compromise performance. However, often in soil analysis, semi-quantitative data or data that reflect composition changes between sampling points are sufficient to meet the requirements. With an analysis time of <2min it is possible to analyse >20 soil samples per hour. The detection limits for hand-held instruments are poorer by orders of magnitude than traditional wet chemical method involving analysis by ICP but they are often adequate for measurement of elements in soil that are subject to legislation governing maximum concentrations.

Acknowledgements

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TISCH—Terahertz Imaging and Spectroscopy in Cultural Heritage: applications in archaeology, architecture and art conservation science

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Introduction

Spectroscopy and imaging have become well-established tools in the evaluation and conservation of drawings, paintings, sculptures and many other art forms. Electromagnetic radiation-based measurement techniques exploit the fact that materials reflect, absorb and emit radiation in ways that depend on their molecular composition. Unlike chemical analysis, these techniques can be used non-invasively and therefore rarely require specimens to be removed from the art sample, which is beneficial to the preservation of the work of art being studied. However, some of the more powerful forms of radiation for imaging, such as X-ray, gamma-ray, proton and neutron, are ionising and usually available only through external specialised laboratories or large research installations, which can be both financially and logistically challenging for heritage conservators. Because it is non-ionising, moderate exposure to terahertz radiation poses significantly less long-term risk to the molecular stability of the historical artefact and humans than other forms of radiation. Also, portable terahertz systems are becoming increasingly available and affordable.

Terahertz spectroscopic imaging is a nascent technique—established in the 1990s, and developed only in the last several years for cultural heritage applications. Terahertz (THz) radiation—designated between the microwave and infrared (IR) regions—penetrates most non-polar, non-metallic media. Many dielectric materials that are opaque or highly scattering at optical frequencies are transparent at terahertz frequencies. It is the combination of material characterisation, time-of-flight imaging and the penetration of optically opaque materials that gives rise to applications for sub-surface imaging of many culturally significant objects. Moreover, the variety and adaptability of the many electronic, photonic and hybrid terahertz sources allows for versatile approaches to measurements. Spatial resolution can be scaled from tens of micrometres to several millimetres, providing the possibility of taking measurements without necessitating sample extraction—either in the laboratory or in the field. In addition, THz radiation is considered non-destructive because its low photon energy is non-ionising and molecular heating—due to absorption—is low. Therefore, it is appropriate for scientists to develop THz measurement techniques in order

to facilitate, qualify and quantify the non-destructive evaluation of objects in ways in which other measurement techniques may not.¹ Examples of some applications of THz spectroscopic measurements in cultural heritage are outlined in the sections below.

Methodology

Our terahertz time-domain spectroscopic (TDS) imaging system consisted of a commercially-available ultrafast, optically-excited, fibre-coupled photoconductive emitter and receiver pair by Picometrix, Inc. For both the transmission and reflection geometries, the terahertz beams were focused onto the surface using 1" (2.54 cm) focal length lenses. The antennas were raster-scanned across the painting in 1-mm increments. Each pixel acquired was an average of 25 time-domain waveforms plus Coif 5 wavelet denoising, and each pixel spectrum was obtained via fast Fourier transform with a tapered cosine apodisation window. Due to the limited scan range of the XY translation stages and the size of the dataset, artworks are often scanned in multiple sections, sometimes over a couple of days. This results in some variation in signal quality and alignment, which are addressed in the post-processing stage.

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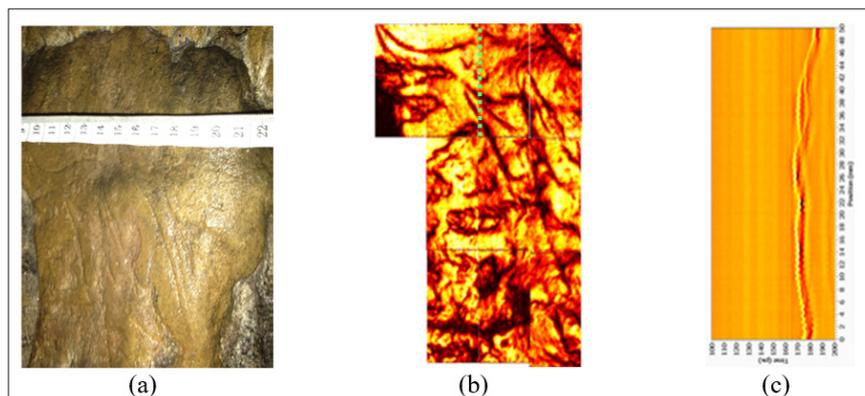


Figure 1. (a) Photograph of panel of bird etchings in Church Hole cave, (b) composite of scanned sections of the bird etching and (c) selected b-scan cross-section.

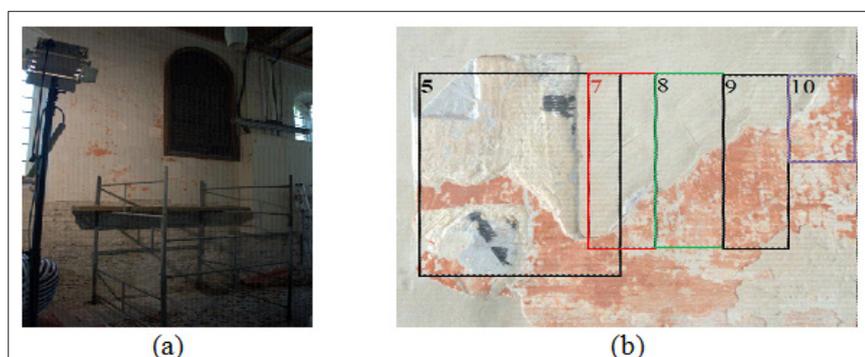


Figure 2. (a) Nave, North Mural second bay and (b) close-up of zones 5 and 7–10.

Paleolithic cave etchings at Creswell Crags, UK

In 2002, the first evidence of prehistoric cave art in Great Britain was discovered at the Creswell Crags, on the Derbyshire–Nottingham border in the UK.² Much of this art comprised of etchings—or patterns directly engraved into the rock using a sharp implement—which, unlike paintings, are difficult to recognise or see without a practiced eye. True prehistoric etchings can be distinguished from contemporary graffiti by the presence of a rock patina, due to prolonged weathering, exposure and precipitation, and the uranium-series dating of the flow rock, layers of calcium precipitate deposits, that overlie the art and Magnesian limestone. The figures are estimated to be approximately 12–15 k years old. We were given access to one such panel in the Church Hole cave at Creswell Crags (see Figure 1a). The figures are series of semi-paral-

lel lines, generally accepted to represent birds of indeterminate type. The lines are v-shaped grooves of depths and widths ranging from hundreds of microns to three millimetres.

Figure 1b shows the composite of several contiguous sections of the panel. The *en face* images were generated from peak amplitude signal. The lines from the etching are clearly distinguishable from the other features of the rock. The more rounded, cloud-like shading could be a result of the non-flat surface of the cave due to weathering or flow rock. The dotted, black line denotes the location of the extracted cross-section in Figure 1c, where the horizontal axis represents the time delay of the THz pulse which correlates to depth within the rock. Here we can see variations in the signal suggesting two separate layers—the limestone subsurface with the calcite flow rock filling into the grooves.



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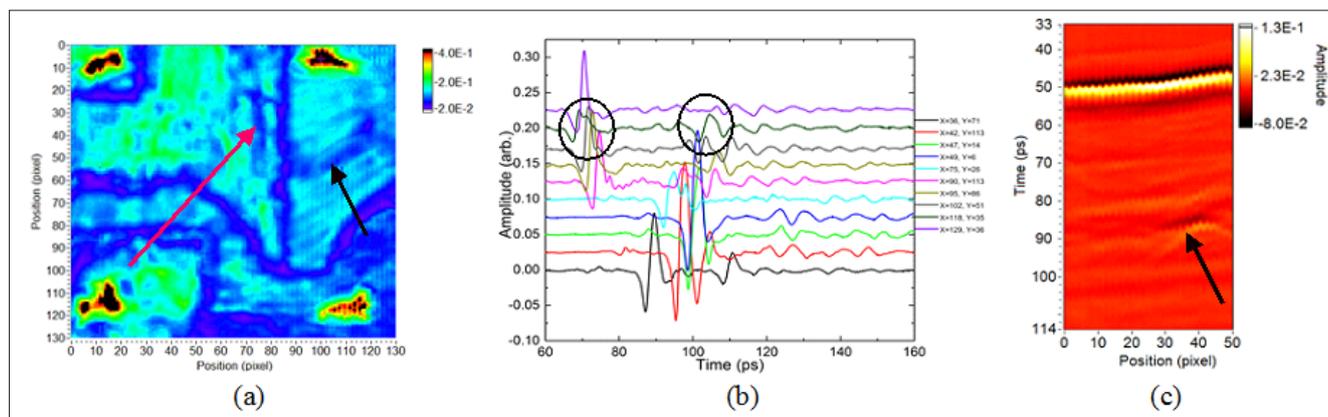


Figure 3. (a) Zone 5 peak-to-peak amplitude map of entire time-domain signal, (b) select time-domain waveforms and (c) a b-scan cross-section showing strong, possibly metallic, sub-surface feature in Zone 7.

St Mary's Church in Chalgrove, UK

Situated in Chalgrove, Oxfordshire, UK, St Mary's Church was founded by a Benedictine monk in the early 12th century CE. Paintings are believed to exist dating as far back as 1320 CE, however, they were all covered during the Protestant Restoration period (1500s to mid-1700s), though many remarkable ones were rediscovered during renovations in 1858. The church was awarded a £1M grant for renovations and the restoration of their Medieval paintings. Before the work was started, we were invited to examine a region situated on the north nave wall between the window and a plaque. The section was comprised of multiple exposed layers, including the layer suspected of being from the Medieval era (the black motif). This region was

broken up into five scanning zones (5 and 7–10; see Figure 2b).

Figure 3a shows an image of zone 5 generated from the peak-to-peak amplitude of the largest terahertz pulse in the time-domain signal for each pixel. The dark blue lines accentuate the boundaries of the exposed layers. The yellow ochre-painted region has a higher reflectivity than the red ochre-painted region, despite the red ochre region seeming smoother. There is a slight vertical groove about 1 cm to the left of the covered region, which shows up in the THz image as indicated by the pink arrow. It may also be possible to see the lower reflectivity of the black paint in the same area, although it is not well resolved. The black arrow points to a broad stripe that is visible by eye in the most modern layer. However, looking at the time-domain waveforms in Figure 3b, there is a notice-

able increase in the size of the second major pulse compared to the first surface pulse where the stripe is (see circled regions). This strongly suggests that the source of the surface defect is something highly reflective, probably metallic, below the surface (Figure 3c). The time-of-flight delay of this second pulse is within reason to come from the same depth as the layer containing the Medieval motif. The black arrow points to a second major pulse beneath the red ochre-painted region. It may also be the same layer we are interested in, despite the difference in the time-of-flight between the main and second pulse.

After Fishing by Ausonio Tanda

We examined the mid-20th century Italian painting *After Fishing* (Figure 4a) by Ausonio Tanda using terahertz

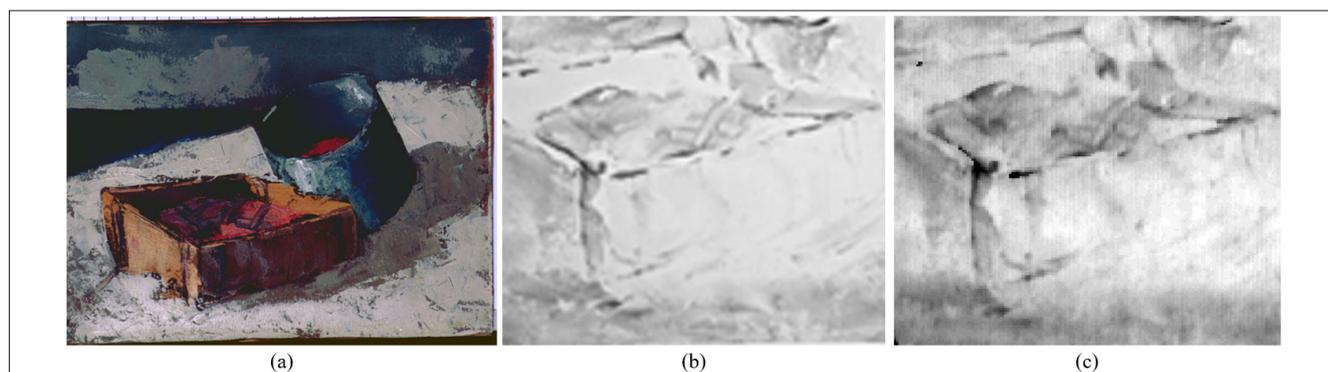


Figure 4. (a) Visible photograph of *After Fishing* by Ausonio Tanda, and region-of-interest enlargement of (b) X-ray density image and (c) terahertz minimum peak time-of-flight image.

time-domain spectroscopic imaging (THz-TDSI) for systematic comparison with multi-spectral imaging (UV, RGB visible, tri-band IR) and X-ray. The painting's binder is oil—however, the pigments have not yet been identified—and the substrate is unbleached compressed paperboard.

In transmission, qualitative comparisons were made between the X-ray density image (Figure 4b) and THz images and minimum peak time-of-flight (Figure 4c). The linear greyscales for the terahertz images were optimised for qualitative comparability to the X-ray radiograph. Overall, the terahertz images are not as sharp as the X-ray images; however, that is to be expected given the difference in diffraction-limited spatial resolution. The spectral bandwidth of the THz-TDS system was not optimised, so the 1/2e amplitude was approximately 0.7THz, with the peak frequency around 0.15THz. However, it should be noted that most of the features present in the X-ray image are present in the terahertz images such that a localised section of the painting shows high correlation between the two techniques. Moreover, in terahertz images not shown here, there are many small spots that do not appear at all in the X-ray image. These spots are a result of defects in the porous cardboard substrate, which we speculate to be oil and/or some kind of biological growth. As such, they are undetectable by standard X-ray systems.

Outlook

The examples discussed above are just a few of many examples of the use of

terahertz imaging and spectroscopy in cultural heritage. In the ten years since this research area blossomed, the number of scientists and conservators investigating this technique has grown from a few to dozens around the world, including a few cross-disciplinary PhDs specialising in both! This technique can be applied to objects ranging from paintings to mummies to sculptures, from plaster to wood to metals. With hope, one day it too will be a standard technique.

Acknowledgements

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Gerry Downey: an authentic spectroscopist

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This year has seen the retirement of Gerry Downey from active service with the Irish National Agriculture and Food Research Institute, Teagasc¹ in Dublin. As one of Europe's leading innovative spectroscopic chemometricians and a great positive personality to have as a project partner, we thought it appropriate to dedicate a column to Gerry's career, however embarrassed he may be about the idea!

Background

Gerry, you graduated from Queen's University Belfast in 1972 so you studied Biochemistry right through the worst time of the troubles in Northern Ireland and the introduction of direct rule from London. How much did this experience effect your decisions to move south of the border to Galway to start your PhD and your later career move to Dublin?

That was a very difficult period for everyone, particularly in Belfast, although arguably the worst period of the Troubles came a few years later. Anyway, yes it did play a role in my move south of the border to Galway in the Republic of Ireland but it wasn't the only reason. A desire to get away from the entrenched bigotry and discrimination that was still present in everyday life was perhaps the main reason. Thankfully things are much better now after the Good Friday Agreement, but many political arguments in the North remain circular and "what-aboutery" is still a disappointing feature of public discourse. Having moved to Galway and getting married to a Belfast woman (Geryllyn, who I met when I was

16) during my time there, I focussed on employment opportunities in both Northern Ireland and the Republic. Opportunities arose in the Republic when I moved briefly to Cork and then to Dublin. By that stage, we had children and even though we both had close family and friendship relationships with Belfast, we were reluctant to move our children back up given that violence was still a daily reality there. So, in the end, we remained in Dublin and, though we still consider ourselves as Belfast people, we have been happy here in Dublin. At that point I worked for An Foras Talúntais (a precursor of Teagasc) while Geryllyn was an occupational physiotherapist with Aer Lingus.

I've experienced many of the ups and downs of relocating to another country when work calls, but what were the best and worst experiences you had in relocating?

That is a difficult question to answer because I am not sure we encountered very many difficulties. I suppose the biggest thing would be the general outlook of people in the Republic as compared to the North. Here, life is generally much more relaxed and that applies to also to operational efficiencies in the public sector; but I have to say that this country has changed dramatically in the last 20–30 years and I can say that levels of business performance and general professionalism equal or even surpass those in the North. Perhaps the best experience we had was when a local woman in Dublin became a housekeeper and third granny to our kids while

we worked—this was before the days of organised childcare. Mrs Browne never missed a day's work in over 30 years with us and she was a rock for us and the kids. Ironically, she died just a few days ago but all our children were happy to play a role in her funeral mass.

Biochemist to spectroscopist to top chemometrician—how come?

After moving to Galway to start your PhD you joined An Foras Talúntais (Agricultural Research Institute) in Dublin at a critical time for the cereals industry with major changes in the way farmers were to be paid and the value of their crops calculated?

In fact, while I moved from Belfast to Galway to work towards a PhD, I never obtained one from that university—personal difficulties between myself and my supervisor made it a fraught time for me. But you are correct about the cereals industry. Just at that time there had been a major swing in Ireland and the rest of Europe in the cultivation of wheat. Winter wheat varieties were increasingly being grown because of the better yields associated with them, but this was problematic from the flour millers' point of view because most winter-sown varieties were not of bread-making quality. The milling industry had no test which could discriminate between winter- and spring-sown crops at grain intakes, nor had the merchants who made the purchase decision in the first instance. However, it was known that these wheat types differed in their protein content so measurement

TONY DAVIES COLUMN

of this constituent was the only way to achieve segregation of feed from bread quality wheats.

This led directly to your role in establishing NIR spectroscopy and multi-variate data analysis as a trusted tool responsible for the financial success of an entire agro-industrial sector replacing the old Kjeldahl methodology that had been trusted since 1883!² How scary was that project to work on knowing the consequences of failure?

As we all know, Kjeldahl was the reference protein measurement at that time and it was quite unsuitable owing to its complex nature, requirement for laboratory staff and general slow speed. Luckily, NIR (near infrared) spectroscopy emerged just at that time and it was viewed as being the only real solution to this testing need. Replacing it was a very daunting task but I was far from alone in achieving this goal. At that time, the Irish Flour Millers Association had very competent technical people working in the flour mills and they, in combination with Technicon, devised an elegant and effective experimental exercise to develop calibrations and to demonstrate the transferability of these calibrations to similar instrument and wheat grinder combinations. To be honest, I was only an observer in this work. I became involved at the behest of the Irish Farmers' Association who, while understanding the requirement for the test, wanted assurance that it was working effectively and did not unfairly penalise any of their members. So I had to devise a mechanism for checking both the operation and performance of the equipment, instruments and calibrations during the harvest over the first three years of its operation. This was paid for by both the milling and farming organisations; once they were both happy, they withdrew funding and grain merchants paid for that service on an individual basis for the next 20 years. Thankfully, there were no major problems with either calibrations or instruments apart from routine maintenance of the latter and occasional bias adjustments of the former.

In the past you have hinted of some stories about mice and water at this time—what was all that about?

One of the really valuable lessons I have learned during my work with the cereals industry and NIR spectroscopy is that there is no substitute for actually going out to the site where measurements are being taken to fully understand the issues which can arise when a laboratory method is transferred to the real world. In this case, I visited the grain merchants (around 40 premises at the high point of the harvest monitoring exercise). These were rough and ready places at which the person doing the rapid grain testing was also the forklift driver or a summer student earning some holiday pay. They all understood fully what they needed to do (we also trained them) but the equipment was generally used during the harvest and then put away somewhere until the following year. In one instance, we were present when a NIR instrument was removed from its storage in an apparently safe place under a bench in the makeshift laboratory and found to be full of water having been placed under a tap which, unknown to the company owner, had a small but significant leak over the winter!! In another location, the grinder operator (we used a Kamas grinder—big and bulky with a metal mesh but effective) complained of difficulty in getting the correct grind and we opened it to find that a poor unfortunate mouse had made a home for itself there unaware of the hazards involved in residing in a grinder. You can imagine how unhappy the operator was when we pointed out the mess inside the grinder which he had to clean up!!

This early encounter with the interface between analytical spectroscopy and high-value agro-industrial production clearly inspired you to carry on work in this area, expanding into food quality, food authenticity and adulteration, in fact the food fraud topic in general—well before the European Union decided this needed to be a priority! Even as late as 2013 European Parliament motion³ seems still to have been bemoaning

the lack of concrete action in fields which you had identified as being of particular concern and been researching for many years. Table 1 shows their citation of the work of Spink and Moyer showing the Top Ten products that are most at risk of food fraud.⁴

I think I am right to say you have published food quality spectroscopic analytical research on most of the systems identified. Which matrix did you find the most challenging and why?

It is true that we have examined many authenticity issues, although we did not do any work on tea, spices, organic foods or wine. It is also important to remember that since I worked for a publicly-funded organisation, all my research was aimed at demonstrating the potential of vibrational spectroscopy to address authenticity issues rather than to develop robust and accurate predictive models. For most of the foods that we studied, the greatest challenge was always to obtain representative sample sets collected over a number of years and with provenance that we could be sure of. In this context, work we did on honey and fruit purées was possibly the most satisfying. We received good national funding for this work and were able to obtain large sample sets from producers on the island of Ireland which we could trust. Maybe the most difficult, but also

Table 1. Is based on Spink *et al.*⁴ and information from retail and branch organisations.⁵

| | |
|----|--|
| 1 | Olive oil |
| 2 | Fish |
| 3 | Organic foods |
| 4 | Milk |
| 5 | Grains |
| 6 | Honey and maple syrup |
| 7 | Coffee and tea |
| 8 | Spices (such as saffron and chilli powder) |
| 9 | Wine |
| 10 | Certain fruit juices |

TONY DAVIES COLUMN

interesting, was some work in which we collaborated with a large team assembled by the United States Pharmacopeia (USP) which wanted to investigate non-targeted methods for detection of adulterants in milk powders. The focus was on melamine adulteration of course and it turned out that the way in which melamine was incorporated into the powder had a significant effect on our ability to detect it. This work is being published soon and it highlights another apparently trivial but crucial issue that we have now learned to address early in our work—what really is the issue that we are trying to address? In authenticity studies it is very easy to conflate problems especially those dealing with geographic provenance and the problem one is trying to solve may in fact mask other issues of quality which need to be well thought out and tackled using rigorous experimental designs.

Your skills have made you a popular partner in international projects, especially funded through the European Union—in fact that is how we first met many years ago in Paris, I was surprised that you have collaborated with the USP in Washington, DC.

How did that come about?

Thank you for the praise but it has always been important to me to make and retain strong working relationships with international partners. In a small island off the west of Europe, it has historically not been easy to work at or near the forefront of science, but membership of the EU and access to competitive funding has enabled me to join groups of excellent scientists who are not only expert in their field but have, in my experience, always been ready and willing to help people like me to understand the tools, especially in chemometrics, that they use. Such collaborations have always been rewarding on a personal level too and I count myself lucky that I can probably lift the phone and ask for help from most of the global leaders in vibrational spectroscopy and chemometrics. The USP collaboration has been interesting and it really originated in a telephone call from a senior staffer in that organ-

isation. As I mentioned above, they were involved in research into methods for non-targeted adulteration in milk powders with the long-term goal of developing and demonstrating appropriate techniques and then supplying standards to support them. They had developed a really large team looking at techniques ranging from dye-binding to nuclear magnetic resonance and including NIR spectroscopy. Having assembled a small sub-group of people to produce samples and NIR data, they were looking for help in interpreting the data and ensuring their interpretations were valid. For no specific reason that I know of, they contacted me, had an extended telephone call to discuss my work and some of theirs and then followed up with an invitation to join the collaboration. It has been really interesting to work with a group like this that has considerable firepower to bring to an analytical problem and a global reach. The work continues although given my retirement my involvement is reduced slightly.

... and how did it compare with working on multi-lateral EU projects?

I suppose that the biggest difference was that regular travel to meetings and other laboratories was a constant and, in my view, critical feature of the EU collaborations. Right from the beginning when we were involved in what were called EU Concerted Actions which had money for meetings and training but none for research, the value of the scientific exchanges facilitated by this money was incalculable. Actually, most of the people I go to for help and advice were involved in the very first Concerted Action dealing with spectroscopic analysis of food—QUEST. Effectively coordinated by our good friend Chris Scotter of what was then called Campden Food Research Institute, this project laid the basis for many subsequent research partnerships which were successful in obtaining EU funds. On a personal level, the EU projects were learning experiences in the broadest sense in which we all learned to understand the different dynamics behind the different national positions around the research

table and hopefully developed tools to allow us to operate as effective teams by bringing the different strengths of partners from a now very expanded pool of countries. The final EU bonus was of course that there was always money available in these projects which was to be used for training; this allowed me to spend time in laboratories such as that of Dominique Bertrand in Nantes which was a very effective way to learn first-hand about chemometrics.

Tomas Hirschfeld Award

This dedication, to what was clearly becoming a very important field for us all, led in 2007 to the International Committee for Near Infrared Spectroscopy honouring you with the prestigious Tomas B. Hirschfeld Award for your application of NIR spectroscopy to the qualitative analysis of foodstuffs.⁵ Apart from the American Chemical Society's *Chemical and Engineering News* not being able to distinguish between Dublin and Belfast,⁶ how did this honour affect you and your work?

That was indeed a very nice moment and I think it is important to recognise that we all appreciate a pat on the back from our peers no matter what age we are. For me it was a very important milestone professionally as it represented a validation of my research efforts by the global body representing NIR spectroscopists at a time when such recognition was not so forthcoming nationally and funding to continue my endeavours was getting harder to come by. Given my subsequent exposure to American scientific societies in a different field, I have come to appreciate their focus on rewarding achievement in a particular field as a way of recognising scientific excellence outside an institutional setting. Of course, having the award probably helps to some degree in obtaining research funding although I cannot be sure of that.

Collaboration with the University College Dublin

Clearly your work hasn't only attracted the attention of the agro-industrial food sector as you were honoured



Gerry Downey receiving the 2007 Tomas Hirschfeld Award.

with a DSc by your alma mater, Queen's University Belfast in 2005, and after a number of joint research publications you became adjunct Professor supporting research in the UCD School of Biosystems and Food Engineering at UCD in 2009. How would you compare the work at UCD to the daily schedule at Teagasc?

Well I think that the two are quite different and there are pros and cons associated with each. One advantage of



Gerry Downey with his parents after receiving a DSc at Queen's University, Belfast.

working in Teagasc is that one is a full-time researcher with no distractions associated with lecture schedules and examinations which are the essence of working in a university. Of course, how much full-time research is actually full-time nowadays with the incessant grant application and reporting requirements associated with the job is a moot point, but I suppose this problem affects both research institutes and academia. The potential downside of working in an applied institute as opposed to a university is that one's freedom to explore scientific problems that are not directly associated with the agriculture and food industries in one's country can be a significant issue, but one that I have had to cope with for many years. Looking objectively at the Irish food industry, it is not at all evident at first glance why work on the authenticity of olive oil is of relevance! For me also there is the question of scholarship or the advancement of science as an end in itself. I know that this is under pressure in many of our universities now as education becomes a commodity to be bought and sold in the marketplace but I do still believe that science as an end in itself to describe and understand the universe which we inhabit still has a place in academic institutions.



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TONY DAVIES COLUMN

Workplace values

On a different topic, many scientists are often so buried in their work that they fail to see—or want to see—the societal issues around them. You are not one of these people and if I remember rightly have involved yourself in the support of fellow colleagues in the workplace?

I have always been involved in my trade union and served as an officer for several years. I have also been significantly involved in the introduction of a bullying and harassment policy for Teagasc and have acted as a mentor to research students on my campus and as a support to staff who find themselves bullied or otherwise badly treated in the workplace. While never being a rabid socialist, I have always felt the need to have some mechanism or mechanisms in the workplace to, at the very least, articulate the concerns of temporary or permanent employees with the overall goal of making the workplace a better environment and therefore enhancing the performance and happiness of both the organisation and its staff. Working in the public sector, I think that these values are present in most organisations but that sometimes the management of these bodies need reminding of their responsibilities and the general advantages of working with staff rather than trying to solve issues by diktat. It is regrettable that as a result of the economic maelstrom in which we in Ireland have found ourselves that some of these attitudes have hardened and we have had to take backward steps in some of our industrial relations, but it is my hope that these losses will prove to be temporary. Probably because of my experience in Galway, I have always felt a particular responsibility to post-graduate students who have placed a lot of trust and time in a supervisor and a system in order to advance their career.

Inheritance...

Teagasc is known as a world-class facility in infrared and NIR spectroscopy specialising in multivariate data

analysis: hopefully you have left behind a strong successor to keep up this tradition?

Ironically, perhaps, the answer to this is no! As an organisation Teagasc is perhaps not very good at succession planning but even without that I think it is fair to say that I operated as a lone wolf and that I probably was unable to convince my organisation of the merit in retaining expertise in this area. This also applies to the chemometric expertise which I have accumulated—despite banging a drum about the need to move from the default univariate analysis to multivariate exploration and modelling of data, I am not sure that the desirability of at least one person on the campus with this expertise will materialise.

Advice for those entering their careers

Finally, with I believe five children and several grandchildren you have clearly ensured your pension pot will remain filled, but what advice would you have for offspring or young graduates looking for help in making their first career steps? Is spectroscopy still the exciting place of opportunity to plant your career flag as it was when you left Galway?

Wow, keeping the easy ones to the last Tony! First, the grandson tally is now five and GERALYN and I are hoping more than ever for a grand-daughter, but of course we have no say in these matters! On your main question, I have always thought of science as a vocation rather than a simple career choice. There has to be some connection between a student and the inherent beauty of scientific experimentation and theory as a way of understanding the world. And for that reason, if one exists then I would encourage some-one to follow this path. However, I think that a research career is something else. I have advised several students who asked about a PhD that the only reason I could see for doing it was to have a career in research; while it is true that people with PhD degrees can make it out of the technical side of

science-based companies, I feel that such a route is the exception rather than the rule. If financial success of executive power is the goal, then a science degree followed by a business qualification is always my suggestion.

Regarding spectroscopy, I still think that it is an exciting field of study. With the continued development of better, more accurate and stable instruments which may in the future obviate any need for calibration transfer and the improved performance of miniaturised equipment, I believe there is much excitement ahead. And let's not forget developments in chemometrics and general field of big data. I suppose the one risk is that, as in so many other scientific fields, the days of the specialist in any specific technology are fading rapidly as career paths are more diverse and scientists are increasingly called upon to use spectroscopic techniques as but one of a number of other techniques in their analytical armoury. But the world keeps on turning and change is more of a constant than ever before so our young scientists will, I have no doubt, rise to these challenges.

Thanks Gerry, and sorry for embarrassing you!

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NEW PRODUCTS

Industrialised proteomics

Sciex have introduced their Next-Generation Proteomics (NGP) platform which is designed to handle industrialised performance levels, and adds new tools to analyse larger sample sets. Components of the NGP platform include new sample prep automation with the Beckman Coulter Biomek NX with protein preparation kits; microflow SWATH acquisition; SWATH performance kits; OneOmics autoloader; and SWATH to MRM builder. The combination of these technologies enables reproducible protein quantitation for thousands of proteins in hundreds of samples.

Sciex

▶ link.spectroscopyeurope.com/28-04-101

Biopharma software

BioPharmaView Software 2.0 from Sciex is designed for automated biotherapeutic data processing, to simplify and speed up biologics characterisation. Updates in this version include improvements in processing speed for intact mass and peptide mapping workflows; ability to process SWATH acquisition data for complete high-resolution MS/MS data to be acquired and analysed in a single run; automated drug-to-antibody ratio calculation for antibody–drug conjugates; automated post-translational modification ratio calculations for a quick view of unmodified/modified peptide ratios; ability to define custom modifications, including proprietary linkers and drug conjugates; batch processing functions and automated flagging for simplified comparability assessments; and comprehensive reports in multiple output formats.

Sciex

▶ link.spectroscopyeurope.com/28-04-102

Large molecule bioanalysis

The Sciex BioBA Solution has been expanded to include the QTrap 6500⁺ LC-MS system with Selexion⁺ ion mobility, as well as new options and programs to enhance workflows. Further additions include: the Sciex M3 MicroLC; automated sample prep with the Beckman Coulter Biomek FX^P lab automation workstation; and a BioBA certification training

programme for large molecule bioanalysis.

Sciex

▶ link.spectroscopyeurope.com/28-04-103

LC-MS/MS

The QTrap 6500⁺ LC-MS/MS system from Sciex has improved sensitivity and selectivity for small molecule quantitation and integrates with their BioBA solution for large molecule quantitation. New features include the multi-component IonDrive technology with the new IonDrive high energy detector; its increased detection area produces sensitivity improvements in positive-ion ionisation and significant ones in negative mode in the low mass region. The scan function of MS³ adds an additional level of mass filtering, and the new Selexion⁺ ion mobility technology (which now has a 2× increase in ion transmission) provides an orthogonal separation prior to mass separation.

Sciex

▶ link.spectroscopyeurope.com/28-04-104

MALDI-ToF/ToF

Bruker's rapifleX MALDI-ToF/ToF system has new ToF/ToF optics and smartbeam 10 kHz laser technology, which provide higher speed, better mass resolution and accuracy, and a significantly enhanced MS/MS mass range. The rapifleX can also be used for mass spectrometry imaging offering improved spatial resolution, image contrast and quality, as well as a new ion source for superior robustness and throughput. The laser and ion optics can be dynamically adapted to research or analytical needs. The MS/MS ion optics can be removed from the ion path for imaging, intact protein and peptide applications. Its three-stage grid-less ion reflector is software adjustable to MS/MS and intact molecular weight measurements. A 10-bit digitiser improves dynamic range for quantitative applications.

Bruker

▶ link.spectroscopyeurope.com/28-04-105

Fast ion source

The Luxon ion source from Phytronix Technologies is now powered by fibre-coupled optics for greater precision, accuracy and speed. It can provide sample



Phytronix' Luxon ion source.

analysis in less than 1 s per sample with 24/7 runtime capability. The new ion source can be combined with rapid liquid handling and the new Phytronix automated LazWell transfer process to offer a fast high throughput screening workflow.

Phytronix Technologies

▶ link.spectroscopyeurope.com/28-04-106

New separation technology for Orbitraps

908 Devices' ZipChip microfluidics separation technology can be combined with Thermo Fisher's Exactive, Q Exactive and LTQ Orbitrap Hybrid FT mass spectrometers. The ZipChip can separate biological samples in three minutes or less prior to MS characterisation, and uses only a few nL of sample. Two chip types, ZipChip HS for small molecule analysis and peptide mapping and ZipChip HR for intact large molecules, are available.

Thermo Fisher Scientific and 908 Devices

▶ link.spectroscopyeurope.com/28-04-107

Biopharmaceutical characterisation

Thermo Fisher Scientific's Q Exactive BioPharma MS/MS hybrid quadrupole-Orbitrap mass spectrometer supports three protein characterisation workflows: denatured and native MS intact analysis, subunit and top/middle-down analysis and peptide mapping. It has a new high mass range mode which adds the ability for intact monoclonal antibody and antibody–drug conjugate analysis, under both native intact and denatured intact conditions.

Thermo Fisher Scientific

▶ link.spectroscopyeurope.com/28-04-108

NEW PRODUCTS

Software and cloud solutions

Thermo Fisher Scientific introduced a number of software and cloud solutions. TraceFinder 4.1 software is for quantitation and screening of both small and large molecules, now with support for peptide/protein quantitation. Compound Discoverer 2.0 software is for small molecule identification and characterisation using high-resolution, accurate mass Orbitrap data. Proteome Discoverer 2.1 provides data analysis for quantitative and qualitative proteomics research using a node-based processing framework. Additional support for large data sets, new user interface and enhanced capabilities for TMT quantitation workflows. BioPharma Finder 1.0 is designed for in-depth characterisation of biotherapeutic proteins. Automates analysis of peptide digests and intact proteins, providing relative quantitation of proteins, sequence variants, disulfide bonds and low level modifications. LipidSearch 4.1 provides an automated solution for the identification and relative quantitation of lipids. It has an enhanced database, improved lipid annotation and support for HCD and CID data in the same search. mzCloud Advanced Mass Spectral Database is equipped with twice as many compounds as before, triple the number of spectra and automatic batch search tools.

Thermo Fisher Scientific

▶ link.spectroscopyeurope.com/28-04-109

Triple quad ICP-MS

Agilent Technologies introduced the second-generation, 8900 triple quadrupole ICP-MS system which adds MS/MS



The 8900 triple quadrupole ICP-MS from Agilent.

mode for controlled and consistent interference removal in reaction mode. Other new features are controlled reaction chemistry, resolution of isobaric overlaps and low detection limits, even for S, Si and P; four-channel cell gas control as standard; and precursor/product ion scan modes to clarify reaction processes.

Agilent Technologies

▶ link.spectroscopyeurope.com/28-04-110

Self-cleaning ion source

Agilent's JetClean is a self-cleaning ion source to keep their GC-MS systems free of matrix deposits. It uses a carefully controlled hydrogen flow and greatly reduces or even eliminates the need for source cleaning on Agilent single- and triple-quadrupole GC-MS systems.

Agilent Technologies

▶ link.spectroscopyeurope.com/28-04-111

Arsine/phosphine analyser

This GC-MS system from Agilent Technologies is capable of ultra-trace (single-digit ppb levels) of arsine/phosphine contaminants in high-purity ethylene and propylene. It consists of the necessary hardware, consumables, calibration system and standards, and methods.

Agilent Technologies

▶ link.spectroscopyeurope.com/28-04-112

Water screening analyser

Agilent Technologies' Water Screener GC-MS analyser fast data review and reporting of water pollutants and screens for unknown compounds. It is preconfigured with hardware, consumables and software, allows fast implementation of screening methods for the identification of over 1000 known water pollutants via Agilent's retention time and spectral database, and unknown pollutants via NIST search.

Agilent Technologies

▶ link.spectroscopyeurope.com/28-04-113

New databases

Agilent also introduced updates to several software tools. Agilent MassHunter BioConfirm Software now includes a new walkup version of the drug-to-antibody calculator, which enables characterisa-

tion of antibody drug conjugates by non-expert LC/MS users. Agilent MassHunter Profinder Software speeds up recursive feature extraction and performs simultaneous analysis of multiple data files from quadrupole time-of-flight mass spectrometers used in tandem with gas or liquid chromatographs. New analytical features, such as improved reporting, are available on Agilent MassHunter Quant Software, as well as support for national pharmacopoeia system suitability testing and a new metabolomics database and method for dynamic multiple reaction monitoring. Several personal compound databases and libraries in water purity assessment, extractables and leachables, for food and pharmaceuticals, were also announced. Additions were made to existing PCDLs for pesticides, veterinary drugs and forensic toxicology.

Agilent Technologies

▶ link.spectroscopyeurope.com/28-04-114

IMS metabolite profiling library

Waters has introduced a metabolic profiling reference library for use with ion mobility research. The Metabolic Profiling CCS Library includes more than 900 measurements of collision cross-section (CCS) values, which measure the gas-phase three-dimensional shape of a molecule for additional information to confirm analytical results. The library also includes more than 600 MS/MS spectra.

Waters

▶ link.spectroscopyeurope.com/28-04-115

Automated metabolite ID

ACD/Labs has launched MetaSense, an automated metabolite identification platform. It combines comprehensive metabolic transformation prediction with analysis of LC-MS analytical measurements to identify, visualise and report chemical biotransformations. It is built on the ACD/Spectrum platform and provides knowledge management capabilities that allow the information from metabolite studies to be applied in other areas of R&D. The live data environment and new web-based visualisation components help decision support and knowledge sharing.

ACD/Labs

▶ link.spectroscopyeurope.com/28-04-116

NEW PRODUCTS

ATOMIC

Small ICP-OES

PerkinElmer describe the new Avio 200 as the smallest ICP-OES on the market, measuring 65cm wide and 81cm high. It has a RF generator with Flat Plate technology which can generate a matrix-tolerant plasma with half the argon of other systems (it uses 9 Lmin^{-1}). Its patented Dual View capability measures every wavelength with no loss of light or sensitivity, and a full-wavelength-range CCD array detector measures the wavelengths around the emission line of interest simultaneously. Setup is fast, with the spectrometer ready in 10 minutes from powering it on. The Avio 200 is available in two configurations of nebuliser and spray chamber: Scott/Cross Flow or Cyclonic/Meinhard.

PerkinElmer

▶ link.spectroscopyeurope.com/28-04-120



PerkinElmer's Avio 200 small ICP-OES

FLUORESCENCE

High sensitivity spectrofluorometer

Horiba Scientific has added the PTI QuantaMaster 8000 to its line of spectrofluorometers with a signal-to-noise ratio of 30,000:1 RMS for water Raman. It is a modular, research-grade spectrofluorometer for steady state and lifetime measurements. It accommodates up to four excitation sources and six detection channels, triple grating turrets for extended wavelength range, and can be used with single or double monochromators. TCSPC can be added to increase flexibility, and offering a tuneable UV/vis/NIR supercontinuum laser from 260 nm to 2000 nm. The instrument can provide spectral and phosphorescence lifetime detection coverage up to 5500 nm.

Horiba Scientific

▶ link.spectroscopyeurope.com/28-04-121

IMAGING

Multispectral wheel camera

Pixelteq's SpectroCam VIS-SWIR 640 multispectral imaging camera is suitable



The SpectroCam VIS-SWIR 640 imaging camera.

for imaging in tissue and biological material. It has an InGaAs sensor, full frame 640×512 pixel resolution, $15\text{-}\mu\text{m}$ pixel pitch and can produce live processed images of six spectral bands at 25 frames per second.

Pixelteq

▶ link.spectroscopyeurope.com/28-04-122

UAV-based VNIR camera

The HySpex Mjolnir-1024 from Norsk Elektro Optik is a hyperspectral camera



NEO's Mjolnir-1024 hyperspectral camera for use with UAVs.

for UAV applications. The system includes the camera, computer and Applanix APX-15 UAV (GNSS-Inertial component) inside a small chassis weighing $<4.5\text{ kg}$. Its spectral range is 400–1000 nm with 200 spectral bands, and its optical architecture is based on HySpex's high-end ODIN system.

Norsk Elektro Optik

▶ link.spectroscopyeurope.com/28-04-123

MASS SPEC

Orbitrap GC-MS

The Exactive GC Orbitrap from Thermo Scientific is a GC-MS system for both targeted and non-targeted analysis,

NEW PRODUCTS

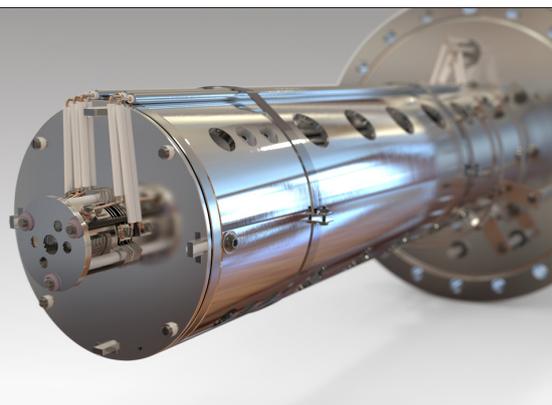
along with quantitation capability. It can be used with TraceFinder software and mass spectral libraries for analyte screening and quantitation. A new Orbitrap GC-MS Contaminants Library contains more than 700 compounds significant for food and environmental analysis.

Thermo Scientific

► link.spectroscopyeurope.com/28-04-124

Quadrupole system

Hiden have introduced the DLS-20 mass spectrometer uses a design based on Hiden's established triple-stage mass filter technology and incorporates enlarged molybdenum rods of 20-mm diameter for increased mass resolution and sensitivity with particular application to precision measurement of low molecular weight species. It is particularly suited to refined nuclear and fusion process applications. The system oper-



Hiden's DLS-20 mass spectrometer uses enlarged molybdenum rods.

ates in both the Zone I and Zone II stability regions. Zone I tuning is for general gas analysis over a broad mass range. Zone II enables high mass resolution for light gases, typically up to 10 amu. It can switch smoothly for operation in either region.

Hiden Analytical

► link.spectroscopyeurope.com/28-04-125

MISCELLANEOUS

Turbopump

Pfeiffer Vacuum have introduced the HiPace 300 H, a high compression



The Exactive GC Orbitrap from Thermo Scientific is a GC-MS system for both targeted and non-targeted analysis.

turbopump working at 300Ls^{-1} , and with a compression ratio of 10^7 for hydrogen, making it suitable for high and ultra-high vacuum. It has a high backing pressure compatibility of 30 hPa, which helps the pump achieve ultra-high vacuum when operating with high backing pressure in combination with diaphragm pumps. An "intermittent operation" function switches on a backing pump only when the backing pressure is no longer sufficient; this lowers energy consumption of the entire vacuum system by up to 90%.

Pfeiffer Vacuum

► link.spectroscopyeurope.com/28-04-126

NEAR INFRARED

Unity Scientific introduces M18 moisture analyser

Unity Scientific has introduced the M18 moisture analyser, which is a new type of moisture meter that is designed for at-line use in manufacturing plants in support of process control. It has a 30-second analysis time for immediate feedback to process control, and scanning technology for measurement over a wide range of product types. The sealed case and rugged design allow use at-line, and various sample accessories are available for maximum flexibility. The analyser

also makes use of graphical software and touch screen operation for ease of use.

Unity Scientific

► link.spectroscopyeurope.com/28-04-127

High sensitivity compact NIR spectrometers

Avantes has introduced the AvaSpec-NIR 2.5-HSC, which has greater sensitivity, less weight and a smaller size. The spectrometers are based on a 100 mm optical bench with a NA of 0.13. The 2.5-HSC series feature 256- or 512-pixel InGaAs detectors and are available in multiple configurations. These instruments are suitable for grain, corn, wheat, soya and



Avantes' AvaSpec-NIR 2.5-HSC high sensitivity, compact NIR spectrometer.

NEW PRODUCTS

polymer analysis, as well as for medical uses, process monitoring and other analysis. The 256-pixel detectors offer best sensitivity for most applications. If resolution is particularly important, or more datapoints for modelling are required, the 512-pixel detector will be the best choice. A range of gratings are available enabling the instrument to be tailored for optimal performance in a particular application and the instrument is equipped with a replaceable slit.

Avantes

▶ link.spectroscopyeurope.com/28-04-128

RAMAN

Improved handheld analyser for threat response

Rigaku Analytical Devices has enhanced its Progeny ResQ handheld chemical identification analyser with a new feature, 4CTechnology, which indicates the overall threat level posed by the presence of multiple individual chemicals. Although



The Progeny ResQ handheld Raman analyser from Rigaku Analytical Devices.

individually the chemicals may not be a threat, their combined presence could indicate the presence of something worse. 4CTechnology comes as standard with new instruments and can be downloaded for free to upgrade existing units.

Rigaku Analytical Devices

▶ link.spectroscopyeurope.com/28-04-129

Silver TERS probes

Horiba Scientific's Omni silver TERS probes for nanoRaman systems enable all modes of TERS operation: top, side and bottom optical access. They are made of bulk noble metal (STM tips) or with a multilayer coating on AFM tips. When used with nanoRaman systems they are guaranteed to produce Raman signal enhancement at 633/638 nm on a reliable test sample. Tests have shown that the probes can reach >40 times improved contrast (tip down, near-field Raman), versus tip up (far-field Raman), leading to an enhancement factor up to 10^6 .

Horiba Scientific

▶ link.spectroscopyeurope.com/28-04-130

SOFTWARE

Batch monitoring

Camo have released a Batch Modelling add-on for the Unscrambler X that uses an improved approach using principal component analysis, accommodating uneven batch lengths and different chemical or biological starting points. The method models the data in relative time and is also independent of the actual sampling rate between the batches.

Batch Modelling can also be used with Camo's process monitoring software, Unscrambler X Process Pulse II.

Camo Software

▶ link.spectroscopyeurope.com/28-04-131

X-RAY

Microanalysis software

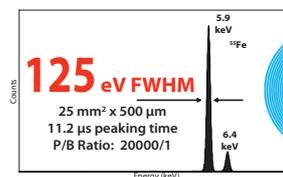
Thermo Scientific have introduced Pathfinder X-ray microanalysis software that process incoming data and provides a real-time statistical map of the chemical constituents within a sample. Compass phase mapping classifies statistically distinct phases and combines ED and WD analysis with structural and morphological information from the electron microscope. A spectral match database automatically identifies and maps analysed regions, whilst algorithms for background subtraction, peak deconvolution and quantitative analysis help provide accurate data analysis. A set of 29 image filters provide new data enhancement tools to provide users with a clear picture of their SEM/EDS and SEM/WDS data.

Thermo Scientific

▶ link.spectroscopyeurope.com/28-04-132

Silicon Drift Detectors

XRF Experimenter's Kit



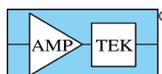
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Conferences 2016

14–19 August, Fortaleza, Brazil. **25th International Conference on Raman Spectroscopy (ICORS 2016)**. ✉ www.icors2016.org.

14–19 August, West Dover, Vermont, USA. **Gordon Research Conference on Molecular Structure Elucidation**. ✉ www.grc.org/programs.aspx?id=17262.

16–18 August, Campinas, Brazil. **The 6th IASTED International Conference on Modelling, Simulation and Identification—MSI 2016**. ✉ calgary@iasted.org, ✉ <http://iasted.org/conferences/cfp-840.html>.

20–26 August, Toronto, Ontario, Canada. **21st International Mass Spectrometry Conference**. ✉ contact@imsc2016.ca, ✉ www.imsc2016.ca.

21–25 August, Philadelphia, Pennsylvania, USA. **American Chemical Society National Fall Meeting & Exposition**. ✉ www.acs.org.

21–26 August, Kyoto, Japan. **International Conference on Magnetic Resonance in Biological Systems (ICMRBS XXVII)**. ✉ icmrbs2016@ics-inc.co.jp, ✉ www.icmrbs2016.org.

21–24 August, Los Angeles, California, USA. **8th Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing (WHISPERS)**. ✉ www.ieee-whispers.com.

23–26 August, Moscow, Russia. **International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS 2016)**. ✉ mps2016@sinp.msu.ru, ✉ www.mps2016.ru.

24–25 August, Kuta, Bali, Indonesia. **2nd International Seminar on Photonics, Optics, and Applications (ISPHOA 2016)**. ✉ isphoa2016@ep.its.ac.id, ✉ www.isphoa2016.org.

24–26 August, Reims, France. **14th Biennial HITRAN Database Conf. & 13th Atmospheric Spectroscopy Applications (ASA) Meeting**. Maud Rotger, ✉ maud.rotger@univ-reims.fr, ✉ www.univ-reims.fr/site/evenement/asa-hitran/home-accueil,18642,32042.html.

26–28 August, Xi'an, China. **9th International Symposium on Photonics and Optoelectronics (SOPO 2016)**. ✉ sopo@sopoconf.org, ✉ www.sopoconf.org/2016.

27 August–4 September, Cape Town, South Africa. **35th International Geological Congress**. Danie Barnardo, ✉ barnardo@geoscience.org.za, ✉ www.35igc.org.

28 August–2 September, Irkutsk, Russia. **Asia-Pacific EPR/ESR Symposium (APES 2016)**. Dr Dmitriy Polovyanenko, ✉ apes2016@nioch.nsc.ru, ✉ www.apes2016.org.

28 August–1 September, San Diego, California, USA. **SPIE Optics + Photonics**. ✉ <http://spie.org/x30582.xml>.

29–31 August, Raleigh, North Carolina, USA. **Conference on Detection Limits**. Mike Brisson, Savannah River National Laboratory, Aiken, SC, USA, ✉ mike.brisson@srs.gov, ✉ www.astm.org/D22ConferenceAug2016.

29 August–4 September, Helsinki, Finland. **9th International Conference on Nuclear and Radio-Chemistry**. Jukka Lehto, ✉ risto.koivula@helsinki.fi, ✉ <http://nrc9.it.helsinki.fi>.

30 August–3 September, Prague, Czech Republic. **24th International Conference on High Resolution Molecular Spectroscopy (PRAHA2016)**. Professor Štěpán Urban, University of Chemistry and Technology, Faculty of Chemical Engineering, Technická 5, CZ-16628 Praha 6, Czech Republic, ✉ paha16@vscht.cz, ✉ www.chem.uni-wuppertal.de/conference.

31 August–2 September, Edinburgh, UK. **Ultra Fast Imaging of Photochemical Dynamics**. ✉ www.rsc.org/events/detail/19765.

4–8 September, Potchefstroom, South Africa. **International Symposium on the Industrial Applications of the Mössbauer Effect (ISIAME 2016)**. Prof. Frans Waanders, ✉ frans.waanders@nwu.ac.za, ✉ www.medc.dicp.ac.cn/news/201512/20151208_30000025.php?id=30000025.

4–9 September, Ghent, Belgium. **Joint European Stable Isotopes User Group Meeting**. Ogarit Uhlmann, ✉ jesium2016@fu-confirm.de, ✉ www.jesium2016.eu.

4–7 September, Gdansk, Poland. **TraceSpec 2016 15th Workshop on Progress in Trace Metal Speciation for Environmental Analytical Chemistry**. ✉ chemanal@pg.gda.pl, ✉ www.chem.pg.edu.pl/tracespec.

4–8 September, Torino, Italy. **10th Conference of the European Federation of EPR Groups (EFEP)**. ✉ efep2016@unito.it, ✉ www.efep2016.unito.it.

4–9 September, Bayreuth, Germany. **54th European High Pressure Research Group International Meeting (EHPRG 2016)**. ✉ www.ehprg2016.org.

5–9 September, Jasná, Slovakia. **20th Slovak–Czech–Polish Optical Conference on Wave and Quantum Aspects of Contemporary Optics**. ✉ scpoc2016@lm.uniza.sk, ✉ <https://lm.uniza.sk/~scpoc2016>.

5–8 September, Leeds, UK. **Photon16**. Joanne Hemstock, ✉ joanne.hemstock@iop.org, ✉ www.photon.org.uk/home.

6–9 September, Chiba, Japan. **JASIS 2016 (4th)**. ✉ www.jasis.jp/en.

6–9 September, Shenzhen, Guangdong, China. **18th China International Optoelectronic Expo (CIOE 2015)**. ✉ www.cioe.cn/EN.

11–15 September, Seville, Spain. **6th EuCheMS Chemistry Congress**. ✉ <http://euchems-seville2016.eu>.

11–14 September, La Jolla, California, USA. **SMASH 2016: Small Molecule NMR Conference**. ✉ www.smashnmr.org.

11–14 September, Dresden, Germany. **20th European Symposium on Polymer Spectroscopy**. ✉ www.ipfdd.de/ESOPS20.

11–16 September, Antwerp, Belgium. **5th International Conference on Vibrational Optical Activity**. Prof. Dr Christian Johannessen, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium, ✉ voa5@uantwerpen.be, ✉ www.voa5.org.

12–16 September, Chamonix-Mont Blanc, France. **9th International Conference on Laser Induced Breakdown Spectroscopy (LIBS 2016)**. Conference office, Université Claude Bernard Lyon 1, Cellule Congrès de l'UCBL, LIBS 2016, 43, bd du 11 Novembre 1918, 69622 Villeurbanne Cedex, France. ✉ contact@libs2016-france.org, ✉ www.libs2016-france.org/en.

12–15 September, Siegen, Germany. **25th ICP-MS User Meeting, 12th Symposium on Mass Spectrometric Techniques for Trace Element Analysis**. Carsten Engelhard, ✉ www.icpms-anwendertreffen.de.

13–15 September, Eastbourne, UK. **37th Annual Meeting of the British Mass Spectrometry Society (BMSS 2016)**. ✉ www.bmss.org.uk/meetings.shtml.

18–23 September, Minneapolis, Minnesota, USA. **2016 SciX Conference (formerly FACSS)**. ✉ facss@facss.org, ✉ <https://www.scixconference.org>.

18–21 September, Florianópolis, Brazil. **18th Brazilian Meeting on Analytical Chemistry**. ✉ enqa2016@contato.ufsc.br, ✉ <http://enqa.paginas.ufsc.br>.

18–21 September, Dallas, Texas, USA. **130th AOAC International Meeting and Exposition**. ✉ www.aoac.org.

19–22 September, Warsaw, Poland. **European Materials Research Society (E-MRS) 2016 Fall Meeting**. Marek Godlewski, Institute of Physics, Polish

Academy of Sciences, Al. Lotników 32/46 02-668, Warszawa, Poland, ✉ godlew@ifpan.edu.pl, 🌐 www.european-mrs.com/meetings/2016-fall.

25–30 September, Copenhagen, Denmark. **41st International Conference on Infrared, Millimeter, and Terahertz Waves (IRMMW-THz 2016)**. 🌐 www.irmmw-thz2016.org.

26–29 September, Edinburgh, UK. **SPIE Security & Defence**. 🌐 <http://spie.org/conferences-and-exhibitions/security-and-defence>.

26–28 September, Ulm, Germany. **13th Confocal Raman Imaging Symposium**. Dr Karin Hollricher, WITec GmbH, Lise-Meitner-Str. 6, 89081 Ulm, Germany, ✉ Karin.Hollrichr@witec.de, 🌐 www.witec.de.

26–30 September, Minsk, Belarus. **SPIE International Conference on Coherent and Nonlinear Optics and The Lasers, Applications, and Technologies Conference (ICONO/LAT 2016)**. 🌐 <http://avh.phys.msu.su/index.php/ICONO-LAT-2016/main>.

26–30 September, Berlin, Germany. **European Optical Society Annual Meeting (EOSAM 2016)**. 🌐 www.myeos.org/events/eosam2016.

26–29 September, Edinburgh, UK. **SPIE Remote Sensing**. 🌐 <http://spie.org/conferences-and-exhibitions/remote-sensing>.

27–30 September, San Diego, California, USA. **Mass Spec 2016: 12th Symposium on the Practical Applications of Mass Spec in the Biotechnology Industry**. 🌐 www.casss.org/?MS1600.

28–30 September, Orlando, Florida, USA. **7th International Conference and Exhibition on Analytical & Bioanalytical Technique**. 🌐 <http://analytical-bioanalytical.pharmaceuticalconferences.com>.

29–30 September, Vienna, Austria. **4th Workshop on Field-Flow Fractionation – Mass Spectrometry**. Stephan Wagner, ✉ nanoanalytics@univie.ac.at, 🌐 <http://umweltgeologie.univie.ac.at/hofmnan-group/workshops>.

1–5 October, Oludeniz, Turkey. **4th International Multidisciplinary Microscopy and Microanalysis Congress & Exhibition (InterM2016)**. Prof Dr. A. Yavuz Oral, ✉ chair@interm2015.org, 🌐 <http://2016.intermcongress.org>.

2–6 October, Merida, Mexico. **14th International Congress of Toxicology**. Hernández-Ochoa, ✉ mihernandez@cinvestav.mx, 🌐 www.ict-mexico2016.org.

2–7 October, Palma de Mallorca, Spain. **20th International Conference on Flow**

Injection Analysis and Related Techniques. ✉ laura.ferrer@uib.es, 🌐 www.icfia2016.org.

4–6 October, Chania, Crete Island, Greece. **2016 IEEE International Conference on Imaging Systems and Techniques (IST)**. 🌐 <http://ist2016.ieee-ims.org>.

11–12 October, Houston, Texas, USA. **Gulf Coast Conference**. 🌐 <http://gulfcostconference.com>.

12–14 October, Milan, Italy. **7th Italian Symposium on NIRS**. ✉ segreteria@sisnir.org, 🌐 www.sisnir.org.

12–14 October, Beijing, China. **SPIE/COS Photonics Asia**. 🌐 <http://spie.org/conferences-and-exhibitions/photonics-asia>.

12–13 October, Coventry, UK. **Photonex 2016 Exhibition Roadshow & Conference**. 🌐 www.photonex.org/index.php.

13–16 October, Paris, France. **Functional Near Infrared Spectroscopy (fNIRS) Conference**. 🌐 <http://fnirs.org/conferences/fnirs2016-conference>.

14–18 October, Pacific Grove, California, USA. **Asilomar Conference on Mass Spectrometry: Novel Instrumentation in Mass and Mobility Spectrometry**. 🌐 www.asms.org.

16–20 October, San Diego, California, USA. **International Congress on Applications of Lasers & Electro-Optics (ICALEO)**. 🌐 www.lia.org/conferences/icaleo.

16–20 October, Liptovský Ján, Slovakia. **21st Slovak–Czech Spectroscopic Conference**. 🌐 www.spektroskopia.sk/scsc/index.htm.

19–22 October, Amherst, Massachusetts, USA. **32nd Annual International Conference on Contaminated Soils, Sediments and Water**. Brenna Lockwood, ✉ brenna@aehs-foundation.org, 🌐 www.aehsfoundation.org.

19–20 October, Geel, Belgium. **Feed 2016 International Conference**. ✉ Feed2016@semico.be, 🌐 www.feed2016.eu.

3–4 November, Baltimore, Maryland, USA. **ASMS Fall Workshop: Sample Preparation for Analysis of Real-World Samples for Mass Spectrometry: The Common Denominator for Quality Data**. 🌐 www.asms.org/conferences/fall-workshop/fall-workshop-homepage.

5–8 November, Lucknow, Uttar Pradesh, India. **6th International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2016)**. Prof. Poonam Tandon, Convenor, ICOPVS-2016, Physics Department, University of Lucknow, Lucknow-226 007, India. ✉ contact@icopvs16.com, 🌐 www.icopvs16.com/index.php.

6–10 November, Orlando, Florida, USA. **7th SETAC World Congress; SETAC North American 37th Annual Meeting**. ✉ setac@setac.org, 🌐 <http://orlando.setac.org>.

6–11 November, Nashville, Tennessee, USA. **AVS 63rd International Symposium & Exhibition**. 🌐 <http://avs.org/Meetings-Exhibits>.

8–9 November, Berlin, Germany. **6th Annual Lab Automation & Robotics (ELA 2016)**. 🌐 <https://selectbiosciences.com/conferences/index.aspx?conf=LABAR2016>.

10–12 November, Osaka, Japan. **55th Annual Meeting of the Society of Electron Spin Science and Technology (SEST2016)**. 🌐 www.sci.osaka-cu.ac.jp/~sest2016/indexe.html.

11–13 November, Nanjing, China. **10th International Conference on Sensing Technology**. 🌐 www.ieee.org/conferences_events/conferences/conferencedetails/index.html?Conf_ID=38001.

13–17 November, Denver, Colorado, USA. **American Association of Pharmaceutical Scientists (AAPS) Annual Meeting and Exposition**. 🌐 www.aaps.org/annualmeeting.

13–18 November, Panama City, Panama. **XVth Latin American Conference on the Applications of the Mössbauer Effect (LACAME 2016)**. ✉ LACAME2016@up.ac.pa, 🌐 www.viceipup.up.ac.pa/Lacame2016.

14–16 November, Somerset, New Jersey, USA. **Eastern Analytical Symposium and Exposition (EAS 2016)**. 🌐 www.eas.org.

22–25 November, Piracicaba, São Paulo, Brazil. **XI Workshop on Sample Preparation**. Francisco José Krug, ✉ wpa2016@cena.usp.br, 🌐 <http://sitenovo.cena.usp.br/wpa2016>.

22–25 November, Taipei, Taiwan. **17th International Symposium on Luminescence Spectrometry (ISLS 2016)**. 🌐 www.isls2016.com.tw.

27 November–2 December, Boston, Massachusetts, USA. **Materials Research Society Fall Meeting & Exhibit**. 🌐 www.mrs.org/fall2016.

28–30 November, Atlanta, Georgia, USA. **5th International Conference and Exhibition on Lasers, Optics & Photonics**. 🌐 <http://optics.conferenceseries.com>.

28–30 November, Mumbai, India. **14th International Symposium on Metal Ions in Biology and Medicine and 4th Green Health Conference**. Vijay Chaudhari, ✉ metalions2016@gmail.com, 🌐 www.metalions2016.com.

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5–7 December, Caparica, Portugal. **2nd Caparica Christmas Conference on Sample Treatment.** José-Luis Capelo-Martínez, ✉ jlcapelom@bioscopegroup.org, ☞ www.sampletreatment2016.com.

12–16 December, San Francisco, California, USA. **2016 AGU Fall Meeting.** ✉ meeting-info@agu.org, ☞ www.agu.org/meetings.

2017

19–22 January, Clearwater Beach, Florida, USA. **Sanibel Conference on Mass Spectrometry, "Peptidomics: Bridging the Gap between Proteomics and Metabolomics by Mass Spectrometry.** ☞ www.asms.org/.

28 January–2 February, San Francisco, California, USA. **SPIE Photonics West.** ☞ <http://spie.org/conferences-and-exhibitions/photonics-west>.

4–8 February, Washington, DC, USA. **Society for Laboratory Automation and Screening 6th Annual Conference and Exhibition (SLAS2017).** ☞ www.slas2017.org/.

13–18 February, New Orleans, Louisiana, USA. **2017 AAFS 69th Annual Scientific Meeting.** ☞ www.aafs.org.

19–24 February, Sankt Anton am Arlberg, Austria. **European Winter Conference on Plasma Spectrochemistry.** ☞ www.wcps2017.at.

20–23 February, Hilton Head Island, South Carolina, USA. **PANIC 2017– 5th Annual Practical Applications of NMR in Industry Conference.** ☞ www.panicnmr.com.

27 February–1 March, Porto, Portugal. **5th International Conference on Photonics, Optics and Laser Technology (Photoptics 2017).** ✉ photoptics.secretariat@insticc.org, ☞ www.photoptics.org.

27 February–2 March, North Bethesda, Maryland, USA. **31st International Forum on Process Analytical Chemistry (IFPAC Annual Meeting).** ✉ info@ifpacnet.org, ☞ www.ifpacglobal.org.

5–10 March, Chicago, Illinois, USA. **The Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (PITCON 2017).** ☞ www.pitcon.org.

13–17 March, New Orleans, Louisiana, USA. **American Physical Society March Meeting.** ☞ www.aps.org/meetings/march.

2–6 April, San Francisco, California, USA. **American Chemical Society National Spring Meeting & Exposition.** ☞ <https://www.acs.org/content/acs/en.html>.

2–8 April, Vitoria, ES, Brazil. **14th Rio Symposium on Atomic Spectrometry.** Maria Tereza, ✉ riosymposium2017@ufes.br.

11–15 June, Copenhagen, Denmark. **ICNIRS 2017.** ✉ icnirs2017@mci-group.com, ☞ www.icnirs2017.com.

11–16 July, Victoria, Canada. **9th International Conference on Advanced Vibrational Spectroscopy (ICAVS-9).** ☞ www.icavs.org/icavs-9.

23–28 July, Québec City, Canada. **20th International Society of Magnetic Resonance Conference (ISMAR 2017).** ☞ www.ismar2017.org.

8–13 September, Santa Fe, New Mexico, USA. **2017 SciX Conference (formerly FACSS).** ✉ facss@facss.org, ☞ www.facss.org.

13–15 November, Somerset, New Jersey, USA. **Eastern Analytical Symposium and Exposition (EAS 2017).** ☞ www.eas.org.

Courses 2016

26–30 September, Genoa, Italy. **School of Experimental Design.** Riccardo Leardi, ✉ ricea@difar.unige.it, ☞ www.difar.unige.it/images/Chimica_Analitica/program_2016.pdf.

7–10 November, Berlin, Germany. **14th European Short Course on Time-resolved Fluorescence Spectroscopy.** ✉ trfcourse@picoquant.com, ☞ www.picoquant.com/trfcourse.

23–25 November, Utrecht, Netherlands. **Multivariate Analysis of Spectroscopic Data.** ☞ www.camo.com/training/more/en/spectroscopy.html?id=726&tid=20&po=1.

Exhibitions 2016

7–9 September, Chiba, Japan. **Japan Analytical Scientific Instruments Show (JASIS 2016).** ☞ www.jasis.jp/en.

11–15 September, Seville, Spain. **6th EuCheMS Chemistry Congress.** ☞ <http://euchems-seville2016.eu>.

10–12 October, Shanghai, China. **Analytica China 2016.** ☞ www.analyticachina.com.

12–13 October, Coventry, UK. **Photonex 2016.** Laurence Devereux, ✉ ld@photonex.org, ☞ www.photonex.org.

20–22 October, Hyderabad, India. **India Lab Expo.** ☞ www.indialabexpo.com.

2017

2–10 March, Chicago, Illinois, USA. **Pitcon 2017.** ✉ pitconinfo@pitcon.org, ☞ www.pitcon.org.

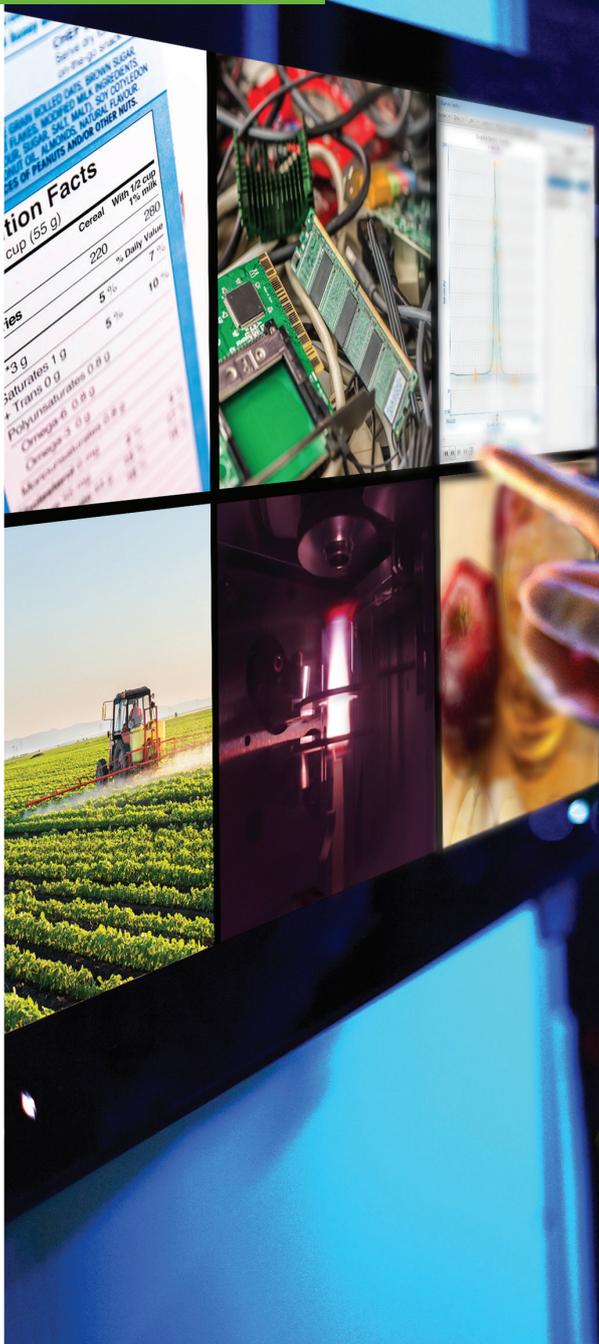
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