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Raman spectroscopy of carious dental tissues
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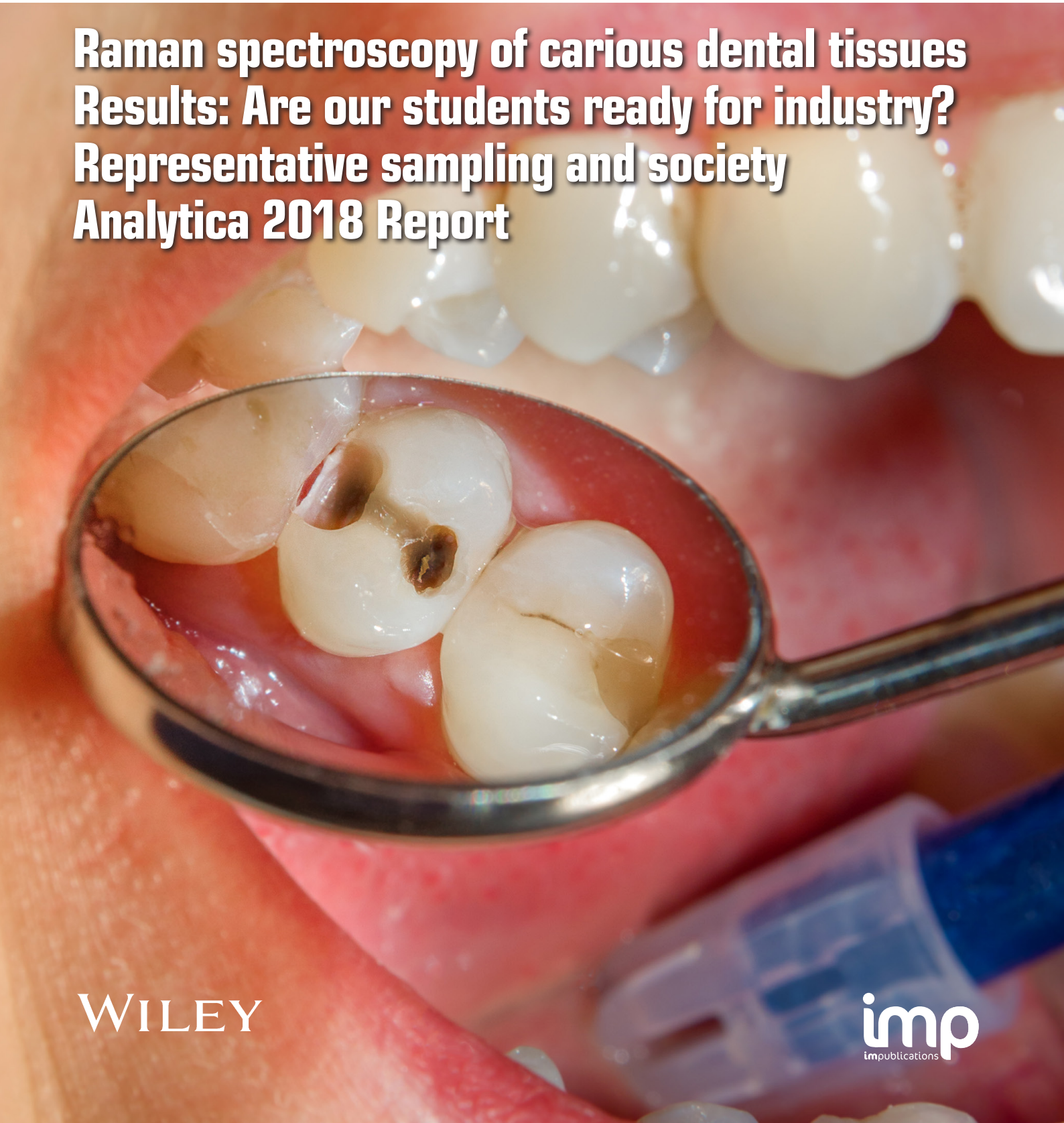

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EDITORIAL

Your subscription and new GDPR data protection regulations

I imagine that you, like me, will have received tens, if not hundreds, of e-mails asking you to consent to receive communications from organisations due to the new EU GDPR regulations that came into force on 25 May. You should have received some from me! The new regulations have an effect on how we contact you and I urge you to check and update your registration profile today. Whilst the choice of which communications you receive is, of course, yours, I would ask that you seriously consider giving us permission to send you information from carefully selected spectroscopy companies. This helps to make it possible to send you the publication without charge! Such mailings are not frequent, and we never release any of your details to these companies and always endeavour to ensure that only relevant information is sent to you. Of course, you can unsubscribe at any time.

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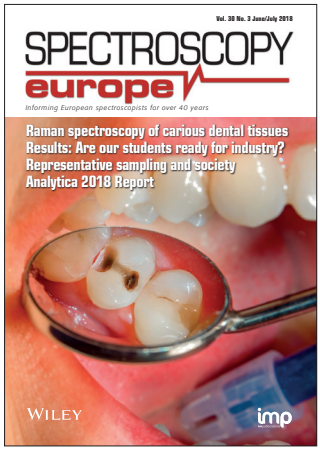

The suitability of confocal Raman microscopy for the characterisation of carious dental tissues is explored in the article starting on page 11.

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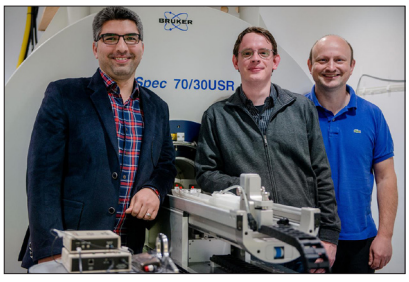
NEWS

Crocodiles have a taste for Bach according to fMRI

Crocodiles count among the most ancient species of vertebrates and have barely changed over the space of more than 200 million years. They constitute a link between dinosaurs and bird species today. "Analyses of crocodile brains thus provide deep insights into the evolution of the nervous system in mammals and may help us understand at which point certain brain structures and behaviours associated therewith were formed", explains Felix Ströckens of the Ruhr-Universitaet Bochum, Germany. A team of researchers from Iran, South Africa, France and Germany have studied Nile crocodiles using functional magnetic resonance imaging (fMRI) to ascertain the way sensory information is processed in their brain. "In the first step, we had to overcome a number of technical obstacles", says research team member Mehdi Behroozi. "For example, we had to adjust the scanner to the crocodile's physiology, which differs massively from that of mammals in several aspects."

Subsequently, the researchers exposed the animals to various visual and auditory stimuli, including classical music by Johann Sebastian Bach. At the same time, they measured the animals' brain activity. The results have shown that additional brain areas are activated during exposure to complex stimuli such as classical music—as opposed to exposure to simple sounds. The processing patterns strongly resemble the patterns identified in mammals and birds in similar studies. Consequently, the researchers assume that fundamental neuronal processing mechanisms of sensory stimuli formed at an early evolutionary stage and that they can be traced back to the same origins in all vertebrates.



For the first time Mehdi Behroozi, Felix Ströckens and Xavier Helluy (from the left) examined a cold-blooded reptile using functional MRI. © RUB, Marquard

By successfully deploying fMRI for the examination of a reptile for the first time, the researchers, moreover, demonstrated that the method does work for poikilothermic organisms. This non-invasive technology can thus be used for many other species that have not yet been studied in depth. Their work has been published in *Proceedings of the Royal Society B: Biological Sciences* (doi: 10.1098/rspb.2018.0178).

Gordon F. Kirkbright Bursary Award 2019

The Gordon F. Kirkbright bursary award is a prestigious annual award that assists a promising early career scientist of any nation to attend a recognised scientific meeting or visit a place of learning. (They define early career as being either a student, or an employee in a non-tenured academic post or in industry, within seven years of award of PhD excluding career breaks).

The fund for this bursary was established in 1985 as a memorial to Professor Gordon Kirkbright in recognition of his contributions to analytical spectroscopy and to science in general. Although the fund is administered by the Association of British Spectroscopists (ABS) Trust, the award is not restricted to spectroscopists, but is open to all involved with or utilising analytical science-based techniques.

Applications are invited for the 2019 Gordon Kirkbright Bursary. An Application Form can be downloaded from http://www.abstrust.org/kirkirkbright-bursary-award-application-form. For further information visit http://www.abstrust.org or contact abstrustuk@gmail.com.

The closing date for entries is 30 November 2018.

A new laser source for infrared chemical imaging

Sébastien Février, reader at the University of Limoges, France, and researcher at XLIM (CNRS/Université de Limoges), and his team have demonstrated that a bench-top, optical fibre-based laser source can be used to perform infrared spectromicroscopy with a precision rivalling, and in some regards even surpassing, that of experiments at large-scale synchrotron facilities.

Replacing the synchrotron with a compact laser source could unleash the potential of this technique and ease its implementation in the hospital, thus accelerating access to diagnosis and treatment. The results were published in *Optica* (doi: 10.1364/OPTICA.5.000378). The demonstration involved a consortium including

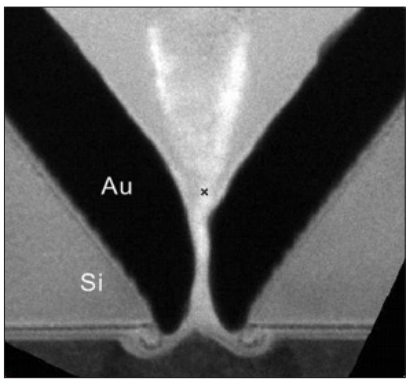
researchers from XLIM and the synchrotron Soleil in Saclay as well as engineers from the company Novae, a start-up founded in 2013 by researchers from the University of Limoges. Novae targets industrial and scientific markets such as laser-based bio-imaging and materials micro-processing. The infrared laser is now part of Novae's portfolio of products.

Direct optical reading of single-molecule DNA bases with SERS

imec have developed a new concept for direct identification of single DNA bases. The technique has the potential to detect, with unprecedented spatial resolution and without any labelling, the genetic code, as well as epigenetic variations in DNA. The combination of nanopore fluidics and surface enhanced Raman spectroscopy (SERS) makes it a promising tool for evolutionary biologists and for research on disease development.

Today, direct, real-time identification of nucleobases in DNA strands in nanopores is limited by the sensitivity and the spatial resolution of established ionic sensing strategies. In addition, established DNA sequencing techniques often use fluorescent labelling which is costly and time-consuming. In a paper published in *Nature Communications* (doi: 10.1038/s41467-018-04118-7), imec demonstrated a promising alternative with no need for labeling and with the ability to identify nucleobases, individually, and incorporated in a DNA strand. The technique is based on nanofluidics to drive the DNA strand through an engineered plasmonic nanoslit, and SERS to determine the adsorbed nucleobases. The spectroscopic signal is enhanced both by a gold coating on top of the nanoslit, and the engineered shape of the nanoslit. "The result reported here is an important step towards a solution for fast and direct sequencing up to the epigenetic level", stated Chang Chen, senior researcher at imec.

The signal generated by Raman spectroscopy holds a lot of information about the molecules and the molecular bonds. Not only can the DNA code be "read", but also base modifications such as methylation, histone acetylation and microRNA modification, which carry more detailed



The sub-10nm Nanoslit.

NEWS

information about epigenetic variations. Such variations are important for evolutionary studies as they influence gene expression in cells. Moreover, they have been shown to impact the origin and development of diseases such as cancer.

IR spectroscopy measures diabetes and renal insufficiency

Glyconics has signed an exclusive licensing deal with Ghent University in Belgium for its proprietary method for the measurement of diabetes and renal insufficiency using infrared (IR) absorption. Glyconics has also joined forces with the University to make use of future technology developed by the University Group in this key therapeutic area.

The diagnostic technology invented at Ghent University employs scanning the fingernails of diabetic versus control persons for post-translational modification of proteins using infrared spectroscopy for diabetes mellitus and renal insufficiency.

Under the terms of the license agreement, Glyconics has worldwide exclusive use of Ghent University's proprietary measurement algorithm, scientific and clinical support and proprietary know-how and database on age and gender reference values for diabetics and renal insufficiency patients.

"The exclusively licensed technology and R&D collaboration will significantly support our long-term goal to expand the applications of our hand-held IR point of care device and digital platform into other acute and chronic areas", said Dr Kam Pooni, CEO of Glyconics.

"Diabetes is a global major public health problem. According to the International Diabetes Federation (IDF) there are 425 million people with diabetes in the world and 1 in 2 adults with diabetes is undiagnosed. In Africa, for example the number of diabetics will increase from 14.2 million (2015) to 34.2 million in 2040. There is a huge need for affordable point of care diabetes diagnosis and monitoring. Infrared spectroscopy is an alternative, non-invasive way to assess glycation and offers information regarding the target organ damage caused by diabetes in vital organs (e.g. kidney, eye)", said Professor Joris Delanghe, Head of the Department of Laboratory Medicine, Ghent University.

MRI unlocks the benefits of Tai Chi

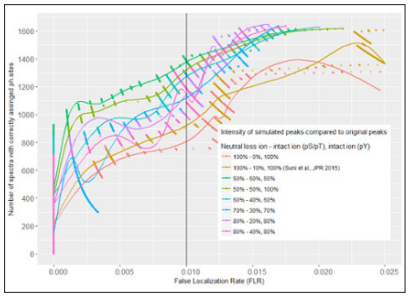
A new study in the *Journal of Neuroimaging* (doi: 10.1111/jon.12515) provides insights into the biochemical mechanisms by which Tai Chi, a mind–body exercise, may provide both physical and psychological benefits. Using magnetic resonance spectroscopy, tests conducted in six older adults enrolled in a twelve-week Tai Chi programme revealed significant increases in a marker of neuronal health in the brain and significantly improved recovery rates of a metabolite involved in energy production in leg muscles. Brain, ^{1}H, and muscle, ^{31}P, were scanned before and after the training, and post-processed to measure N-acetylaspartate to creatine (NAA/Cr) ratios and phosphocreatine (PCr) recovery time.

"The benefits of Tai Chi have been well known anecdotally; however, recent research such as our study can quantify these improvements using objective measures", said senior author Dr Alexander Lin, of Brigham and Women's Hospital and Harvard Medical School, USA.

SimPhospho: an open source tool to enhance phosphopeptide analysis

Analytical chemists, including Garry Corthals from the University of Amsterdam's Van 't Hoff for Molecular Sciences (the Netherlands) and Veronika Suni of the University of Turku's Center for Biotechnology (Finland), have introduced SimPhospho, an open source tool for accurate simulation of phosphopeptide tandem mass spectra.

The biochemical process of protein phosphorylation plays a vital role in the regulation of many cellular processes including cell cycle, growth, apoptosis and signal transduction pathways. Given that the exact molecular site of a phosphorylation event determines its particular switching activity, validation of phosphorylation sites is of great importance. The leading technology to discover and confirm protein phosphorylation is tandem mass spectrometry. It has been successfully employed for two decades to identify sites of phosphorylation. However, unambiguous phosphosite assignment still is considered challenging. A further improvement of sophisticated phosphopeptide data analysis strongly depends on the ability to interpret more complex tandem mass spectrometry spectra.



Optimisation of intensity values of simulated peaks. False localisation rate (FLR) for two synthetic phosphopeptide mixes analysed with SpectraST 5.0 using simulated phosphopeptide spectral libraries. Image: HIMS. (187)

In an earlier study, the Dutch–Finnish team developed a method for tandem mass spectrometry interpretation based on the simulation of phosphopeptide spectral libraries, enabling highly sensitive and accurate phosphosite assignments. To promote more widespread use of this method, they introduced SimPhospho, a fast and user-friendly tool for accurate simulation of phosphopeptide tandem mass spectra. With SimPhospho, simulated phosphopeptide spectral libraries are used to validate and supplement database search results. It thus can improve reliable phosphoproteome identification and reporting. The program can be easily used together with the Trans-Proteomic Pipeline and can be integrated in a phosphoproteomics data analysis workflow.

SimPhospho is open source and it is available for Windows, Linux and Mac operating systems. The software and its user manual with detailed description of data analysis as well as test data can be found at https://sourceforge.net/projects/simphospho/. A description of SimPhospho has been published in *Bioinformatics* (doi: 10.1093/bioinformatics/bty151)

Specac receives prestigious award for export

Specac has won the Queen's Award for International Trade, recognising "outstanding continuous growth in overseas sales over the last six years".

The citation reads:

"Specac Limited is based in Orpington, Kent and has been in business since 1971. They design and manufacture accessories for spectrometers used in science and industry. In particular, they supply sample-analysis accessories, high-specification equipment using mirrors and crystal materials to direct infrared light. They sell to 70 countries across five continents, including the United States, China, Germany, Singapore and Japan."

"Innovation in new product development is key, with a target of three new products a year. Export represents 90% of their sales and the remaining 10% is often exported by original equipment manufacturers. Export has been the heart of the business since 2008 when they first travelled overseas to actively manage relationships, visit trade shows and boost sales. With growth in overseas sales, total sales and percentage overseas sales, whilst turning losses into profit, Specac Limited wins the Queen's Award for International Trade for Outstanding Continuous Growth in overseas sales over the last six years."

David Smith, Managing Director of Specac says, "I'm deeply honoured that

the business I've had the privilege to lead for the last ten years has won such a prestigious award. I believe it represents recognition at the highest level for a good commercial strategy, high quality in everything we design and make, and mostly, the hard work over a long period of an amazing team."

Rodney Appiah, Investment Director from Specac's majority shareholder, Foresight Group says, "To have been recognised for the Queens Award for International Trade is a testament to the dedication and effort of David and the talented staff at Specac. With the benefit of Foresight's support, Specac has continued to innovate and refine their offering both at home and abroad. We look forward to continuing our successful partnership over the coming years."

Jo Johnson, MP for Orpington, Minister of State at the Department of Transport, and until recently, Minister of State for Universities and Science says, "It is fantastic news that Specac has been recognised for its considerable contribution to international trade at the Queen's Awards for Enterprise. This prestigious award is an outstanding achievement of which the company and its employees should be very proud."

Specac are keen to place on record their appreciation of their key partners, both suppliers and customers, without whom this award would not have been possible.

Bruker acquires Anasys

Bruker has acquired Anasys Instruments Corp., a privately held company that develops and manufactures nanoscale infrared spectroscopy and thermal measurement instruments. This acquisition adds to Bruker's portfolio of Raman and FT-IR spectrometers, as well as to its nanoscale surface science instruments. Financial details of the transaction were not disclosed.

Anasys has pioneered the field of nanoprobe-based thermal and infrared measurements with its nanoIR™ products which recently increased performance with 10-nm resolution nanoIR imaging.

New CEO at CAMO Software

CAMO Software AS has appointed Raman Bhatnagar as the company's new Chief Executive Officer. Raman is an experienced international manager from senior positions in a range of companies: start-ups and established corporates within Norway and abroad.

Prior to joining CAMO, Raman was most recently Director of Strategic Projects at Intrum/Lindorff Group, Europe's leading Credit Management Services Company. Raman was also CEO at Big Data analytics company Cxense, where he managed a successful listing at Oslo Stock Exchange. More recently Raman co-founded Hjemmelegene, a successful startup disrupting Norwegian primary healthcare.

"Big Data, analytics and machine learning has globally created big value within the business data space and now the same technology will transform industrial and process data, and this is why CAMO is an interesting company for me," says Raman Bhatnagar.

Raman Bhatnagar replaces Shirley Henshall as CEO. "Shirley has done wonders with the Company over the last few years and will continue within a strategic capacity at CAMO Group with responsibility and focus on international business development and partners", says Erik Langaker, Chairman.

ARTICLE

Raman spectroscopy in the characterisation of carious dental tissues

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In this work we demonstrate the suitability of confocal Raman microscopy for the characterisation of carious dental tissues. Samples of enamel and dentine, presenting carious lesions in different stages of progression, were evaluated by comparing the depolarisation ratio of the PO_4^{3-} symmetric stretching band at 959 cm^{-1} in the different tissues. Both line and area scans were performed to gauge these variations. Moreover, the obtained results were compared with the tissues' behaviour when interacting with ultraviolet radiation, namely the induced fluorescence in some tissues. The depolarisation ratio has proven to be a valuable tool in recognition of demineralisation of both enamel and dentine due to caries. The analyses of the collagen bands in the dentine sample turned out to be more difficult to evaluate due to high fluorescence in the carious region.

Introduction

Most of us will, unfortunately experienced dental caries. These are caused by the release of acids (including lactic, acetic, formic and propionic) from bacterial metabolism diffusing into teeth and dissolving the mineral content of the dental tissues. This mineral is a carbonated hydroxyapatite with a complex crystal structure and containing defects, which is easily dissolved in acid.[1] The effect of acid starts demineralisation of the tooth at the atomic level on the crystal surface inside the enamel or dentine, and can continue until it produces a cavity. Fortunately, saliva in the mouth has a high buffer capacity and supersaturated composition in phosphate and calcium, which minimises the effect of acids.[2]

Damage to teeth from acid can be reversed in the early stages, before a cavity has formed, through remineralisation. This natural repair process relies on calcium and phosphate ions assisted by fluoride to rebuild a new tooth surface on crystal remaining in subsurface lesions after demineralisation. These remineralised crystals are acid resistant and are much less soluble than the original mineral.[1]

Two layers can be distinguished in a carious lesion in dentine: a superficial infected layer and another, deeper, affected layer. The first is completely demineralised and its collagen proteins are irreversibly denatured. The deeper layer is not infected by bacteria, has no denaturation of the collagen fibrils and is just partially demineralised, and is thus more ikely to undergo a remineralisation process. The removal of the infected and necrotic layer, and the maintenance of the affected layer as a substrate for a restorative procedure leads to less traumatic treatment, removing less tissue and leaving a thicker dentine layer between the restoration and the pulp tissue.[3]

It is increasingly important to recognise carious lesions in their early stages before cavitation occurs, while the process of mineral loss is still reversible or at least can be arrested. When more invasive treatment needs to be undertaken, the dentist will remove the infected tissue and fill the cavity with restorative material. Therefore, the identification and differentiation of infected/affected tissue is of great importance in a conservative approach, to guarantee that no further tissue than necessary is removed. Raman spectroscopy is an established spectroscopic technique in the evaluation of enamel's chemical composition modification due to demineralising agents such as acidic beverages[4] and whitening products, either used accordingly to the manufacturer's instructions[5] or in an abusive manner.[6] The analysis of the PO_4^{3-} symmetric stretching band at ~959 cm^{-1} and its polarisation anisotropy have also been shown to be sensitive markers of demineralisation, namely of early caries detection.[7] In this article we will demonstrate the suitability of Raman spectroscopy for the recognition and characterisation of carious dental tissue, namely, white spot lesions on enamel and carious dentine with different stages of progression, in order to differentiate between infected and affected tissue. The results will be compared with another emerging diagnostic technique in dental practice, illumination with ultraviolet (UV) light.

ARTICLE

Materials and methods

Specimen preparation

Six human molar teeth, extracted for periodontal or orthodontic reasons and stored in an aqueous solution of 0.4% chloramine, were selected by an expert and the inclusion criteria would be the presence of lesions, cavitated or not, including white spots. The teeth were cut in halves, perpendicularly to the occlusal surface, and the exposed surface was prepared for analysis by grinding with 1200- and 2500-grit SiC paper (Buehler, ref 30-5218-012 and 30-5218-025, respectively, Struers, Copenhagen, Denmark) under water refrigeration, and polished with a polycrystalline 1-µm diamond paste in a felt cloth. Between interventions, samples were sonicated for 1 min.

Confocal Raman microscope

Raman spectra of samples were obtained using a Horiba XploRA confocal microscope using a near infrared laser (785 nm) with a 1200 lines mm^{-1} grating. The spectral range investigated was from 300 cm^{-1} to 2200 cm^{-1} with spectral resolution of 4 cm^{-1}. Using an entrance slit of 100 µm and a confocal hole of 300 µm, the scattered light collected by the objective was dispersed onto the air-cooled charge coupled detector (CCD) array of an Andor iDus detector. Both 100× (N.A. = 0.9) and 10× (N.A. = 0.45) objectives were used as well as a 50% neutral density filter rendering a maximum incident power on the sample of 9.0 ± 0.4 mW (lasercheck®, Edmund Optics). Typical acquisition time for spot analysis was 15 s with 10 accumulations. Grids were constructed for line and area scans according to the region to be analysed.

In order to determine the depolarisation ratio (ρ) of the most intense band in the Raman spectrum, assigned to the symmetric stretching band of phosphate ions (~959 cm^{-1}), in each spot, spectra were recorded in two orthogonal polarisations of scattered light (perpendicular and parallel to the polarisation of the incident laser). The ρ_{960} was then determined according to Reference 7:

$$\rho_{959} = \frac{I_{959\perp}}{I_{959\parallel}}$$

where $I_{959\perp}$ is the intensity of the Raman band at ~959 cm^{-1} using perpendicular polarisation and $I_{959\parallel}$ is the intensity of the Raman band at ~959 cm^{-1} using parallel polarisation between the incident laser and the scattered radiation.

Spectra deconvolution was performed using LabSpec software (v5.58.25, Horiba, France), making use of a polynomial baseline correction to remove the background due to fluorescence. The intensities were determined by integrating the area under the bands.

Digital microscope with UV light

Images were acquired under UV illumination using the portable digital microscope AM4013-FVW DinoLite up to 215× magnification and UV LED light of 365 nm.

Results and discussion

Figures 1a and 1b present the combination of parallel-polarised and cross-polarised Raman spectra of sound and carious enamel, without background correction. As can be observed, the phosphate symmetric stretching band at 959 cm^{-1} drastically decreases in sound enamel, while in the carious spectrum, this decrease is not so evident due to a structural modification of the enamel and loss of anisotropy. Moreover, there is also an increase of the background in spectra of carious enamel due to fluorescence. Similar behaviour is seen when analysing carious dentine, with a significant increase of background in the Raman spectra as we collect spectra from sound dentine into denaturated dentine (represented by the arrow in Figure 2c). After background correction of the same spectra (Figure 1d) it is possible to observe the bands at 1240 cm^{-1} and 1270 cm^{-1} corresponding to the deformation bands of the amide III group, the bands from 1300 cm^{-1} to 1400 cm^{-1} from the methylene group or the band at ~1660 cm^{-1} corresponding to the C=C stretching mode, together with the bands corresponding to phosphate vibrational modes. As can be seen, the symmetric stretching band at 959 cm^{-1} decreases concomitantly with the decrease of signal-to-background ratio of collagen bands, almost impossible to deconvolute near the cavitated dentine.

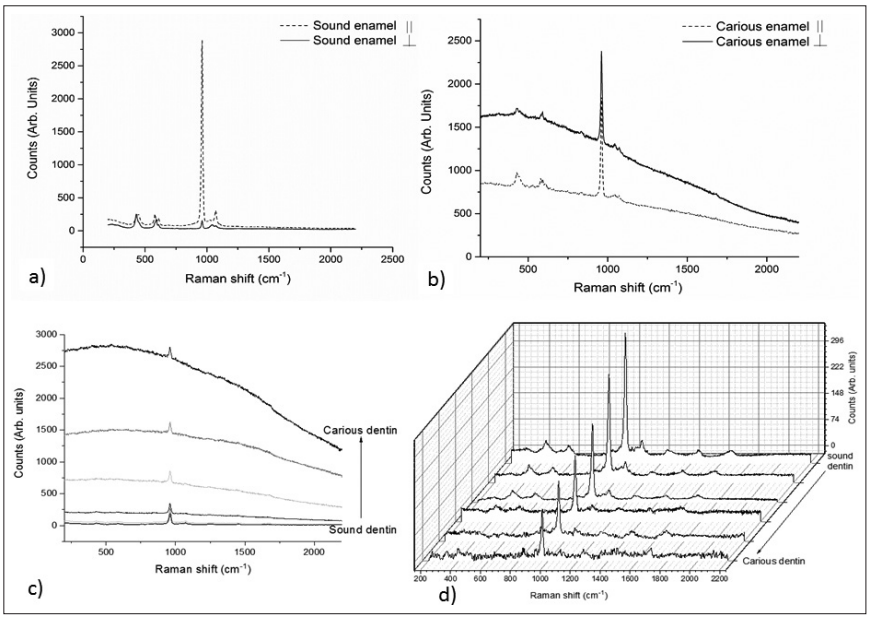

Figure 1. Raman spectra obtained for a) sound enamel with parallel and cross-polarisation; b) carious enamel with parallel and cross-polarisation; c) comparison of spectra obtained in sound through carious dentine without background correction and d) comparison of spectra obtained in sound through carious dentine after background correction.

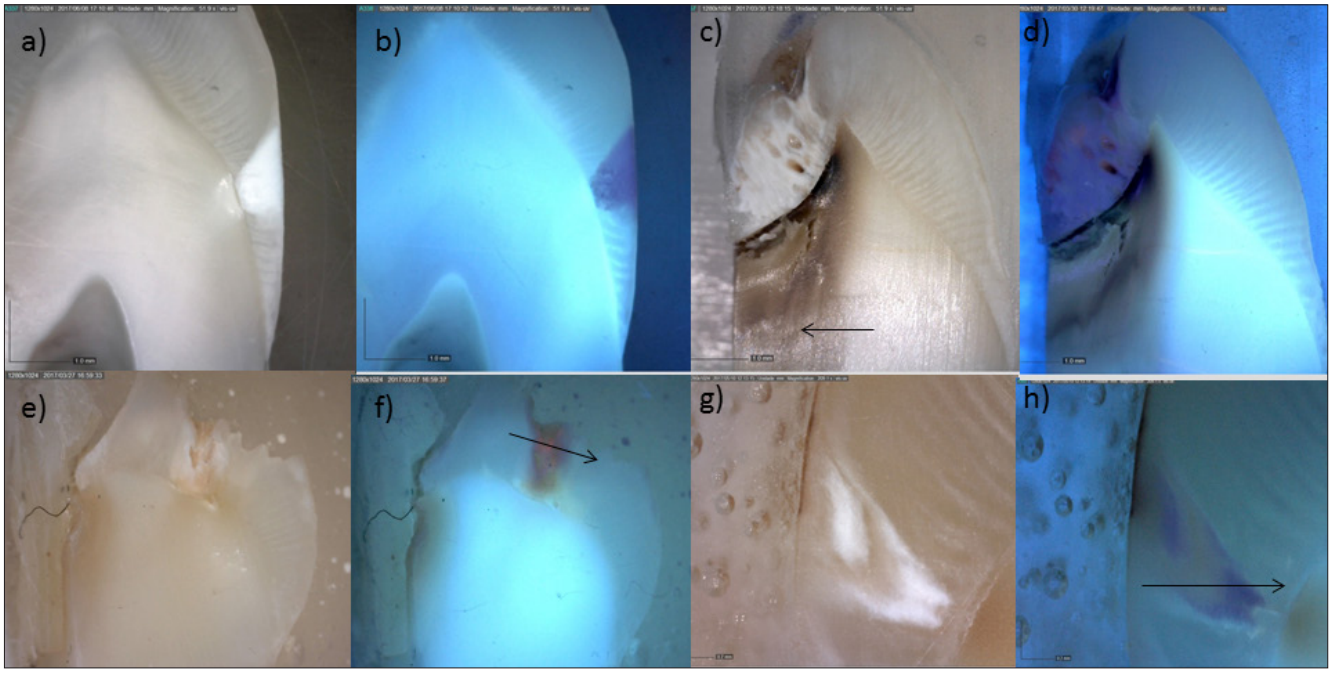

Figure 2. Comparison of the images obtained with digital microscope with and without UV illumination for four of the studied samples.

Figure 2 shows the images obtained with the digital microscope with and without UV light for four of the analysed samples (samples 1–3 and 5). Regarding Figure 2a, a typical "white spot" lesion is clearly visible in the enamel. This type of incipient lesion is considered to be the initial stage of evolution of a carious lesion. Ultraviolet irradiation of the same sample (Figure 2b) shows two different behaviours. On the one hand we have the bluish/green fluorescence induced in the collagen proteins of dentine; on the other hand, under ultraviolet light, enamel with white spot lesions is darker compared to the adjacent luminescent sound enamel. Similar results were obtained by Walsh *et al.*[8] when studying dental biofilms and caries under different UV wavelengths. Regarding Figure 2c corresponding to a carious lesion in a more advanced stage of progression, reaching well into the dentine and resulting in cavitation and detachment of the amelodentinal junction, we can see distinguish three events. There is the healthy dentine with bluish fluorescence, but there is also a region where the UV radiation is completely absorbed in the dentine suggesting complete denaturation of collagen, and another region, more opaque without the fluorescence of collagen, suggesting some alteration of these proteins, but possibly recoverable.

Regarding Raman analysis of the samples, line scans were performed in order to gauge the demineralisation stages of the enamel and non-cavitated dentine. Figures 3a and 3b show the variation of the depolarisation ratio obtained for the lines depicted in Figures 2f and 2h, respectively.

As can be observed, in sound enamel the depolarisation ratio is ~0.05, while there is a significant increase of the depolarisation ratio in the areas that correspond to the white spot lesions. Moreover, it was determined that in the region nearer to the surface of the tooth, the depolarisation ratio is very low (Figure 3b) which could be related with the contact of these tissues with saliva and, therefore, superficial remineralisation. Area scans were also performed, although these are very time consuming and more prone to defocusing during acquisitions. Similar behaviour was observed in the area scans obtained for samples 4 and 6, with higher depolarisation ratio in the carious lesion region.

Conclusion

With this work we have demonstrated the suitability of Raman spectroscopy, namely by means of the depolarisation

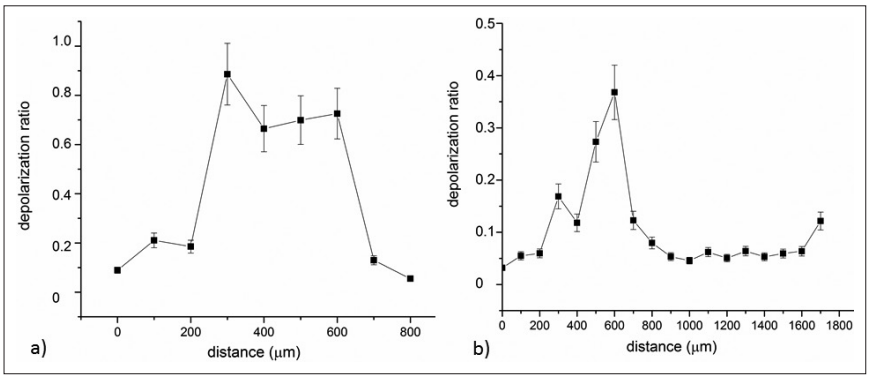

Figure 3. Plot of the depolarisation ration obtained in line scans of two of the studied samples.

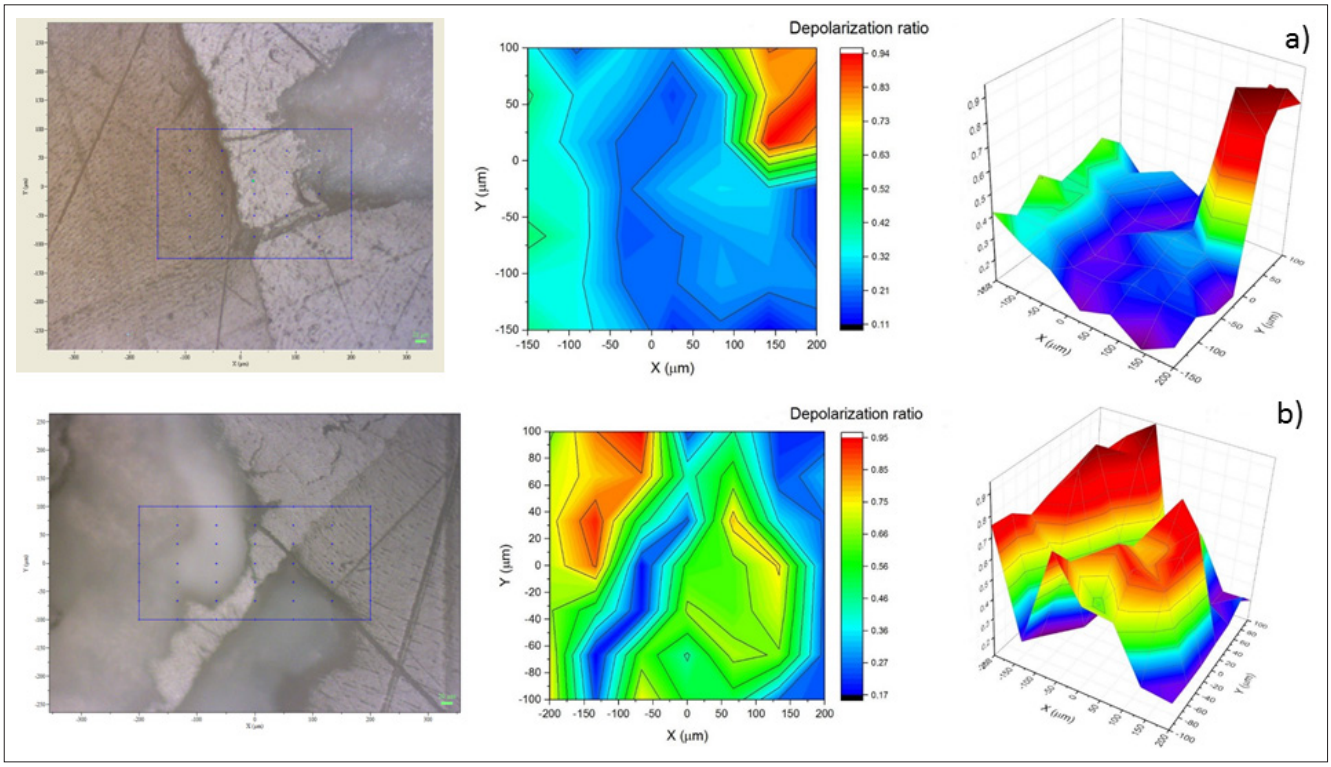

Figure 4. Plot of the depolarisation ratio obtained in are scans of two of the studied samples in 2D and 3D. Image obtained in the Raman microscope is represented for guidance.

ratio of the symmetric stretching of the phosphate band, as a powerful tool for carious detection even in early stages. Mappings proved very useful in the delimitation of carious tissues, however, the analysis of a representative area is very time consuming considering that the areas should be scanned twice with different polarisations, and if the area is too big there is a greater risk of defocusing. This way, we should find a good compromise between time of acquisition for good signal-to-noise ratio and the dimensions of the XY array. Moreover, the area to be sampled should also be completely plane or a setup with an automated Z-axis should be used.

The fluorescence induced by illumination with UV radiation also proved a versatile tool for the rapid recognition and delineation of demineralised tissue, as well as showing promise for differentiation between infected and affected dentine. With Raman analysis, on the other hand, it was more difficult to evaluate the denaturation of the collagen bands due to the low signal of the bands and the high fluorescence of the spectra in the carious region.

Acknowledgements

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Preliminary results from the "Training future analysts" survey

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In this column we would like to explore the initial results extracted from the survey into the training the next generation of colleagues currently receives in analytical chemistry. The background and some details around the survey were provided in the previous column and will not be repeated here.[1]

First, a great vote of thanks from all three of us to those who have so far participated in the survey. Roughly equal numbers have completed the academics' and industrialists' surveys. This gives us the ability to let you know that the average time taken to complete the industrialists' survey was just over nine minutes and the academics' survey just over four minutes so if you have not does so yet—it is not too late as the links remain open… please go to the survey links below.

Assessing the academic responses—taught courses

As I started to look at the results I realised that some decisions would have to be made on how to weight and visualise the answers we were receiving. As the survey has been crafted to harvest as much information as possible whilst consuming as little of your precious time as possible, it does not dig deeply into the content of what is actually being taught or requested. At the extremes of the response scales there are obviously no problems—a subject being the topic of a compulsory course is clearly ranked the highest and a topic not being taught at all the lowest. However, how do you value the perceived importance being given to a topic which is covered only in a supplementary course which a student may well opt not to take, as opposed the same topic being mentioned—but not the main topic—in a mandatory course all students need to attend.

Interestingly, this mirrors, to a certain extent, the discussions around the types of analysts we are looking to recruit in the future. I am personally very much in the camp of looking for "T-shaped analysts". Stolen from the business concept of T-shaped managers, this has nothing to do with recruiting colleagues based on the hours per-day they spend in the gym. I like to look for people who can not only contribute to our teams by bringing new deeper insights on a specific field, but have the experience and personality to be able to contribute across teams and expertise areas sharing lessons learnt. In the past, I have often seen cases where a spectroscopist will continue to struggle with a complex problem using the tools at their disposal, sometimes for months, just because they were asked a specific question but did not have the experience or network to know that a different group even just down the corridor could actually solve the problem in a fraction of the time. So where does that leave us? I have concluded for this column, maybe a little controversially, that being exposed during your academic training to the strengths and weaknesses of many different analytical techniques will probably be of greater value later in your industrial career than spending too much time going deeper into only a few techniques. Sorry if you disagree!

So, if we look at Figure 1 you can see how I have assessed the responses to the first question for academics on the coverage of analytical techniques likely to be encountered in industry.

These results were somewhat surprising in that I would have assumed the main chromatography techniques would have been at the heart of all analytical chemistry teaching. The lack of priority given to some of the key sample preparation techniques which must be mastered as a matter of course, since spectroscopists are constantly driven to deliver lower and lower limits of detection, is worrying.

Focussing on the spectroscopic techniques, the results are probably a little less surprising for me with the exception of the weakness in the teaching of atomic absorption and emission spectroscopies.

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Assessing the academic responses—practical courses

Here again, I have imposed an arbitrary weighting on the responses for the visual representation of the importance of the topic shown in Figure 2. I have given particular weight to the techniques which are mandatory for a student to carry out in the laboratory during their education. I have applied somewhat less weight if this hands-on experience is not mandatory. Much less weight has been given if they only carry out the sample preparation steps and hand the sample over to be measured for them, or if they only have the method demonstrated to them and do not actually get to touch the equipment themselves.

As mentioned in the first column on this survey, we may now actually see the cost of running academic laboratories coming in as a bad, if unavoidable, influencing factor in the selection of topics being taught to students in the laboratory.

Do the industrialists agree?

Well, if we look at Figure 3—unfortunately in many areas they do not. I have not tried to weight these responses as I found I was effectively looking for answers which agreed with my prejudices! I have let the numbers speak for themselves. For me the biggest revelation is the strong preference for employers in a broad theoretical knowledge across pretty much all the techniques mentioned in the survey. This goes against what we see from the academics, where students may well not have been taught many of the subjects important in the industrial labs by the time they finish university.

Industrialists also clearly believe that a much greater level of practical skills is to be expected from students they are recruiting than is reflected both in the breadth and in the depth of what they receive at university.

As to the other skills being taught to future industrial analytical chemists, the prioritisation of the most wanted skills is not too different from the ranking placed by the educationalists (Table 1).

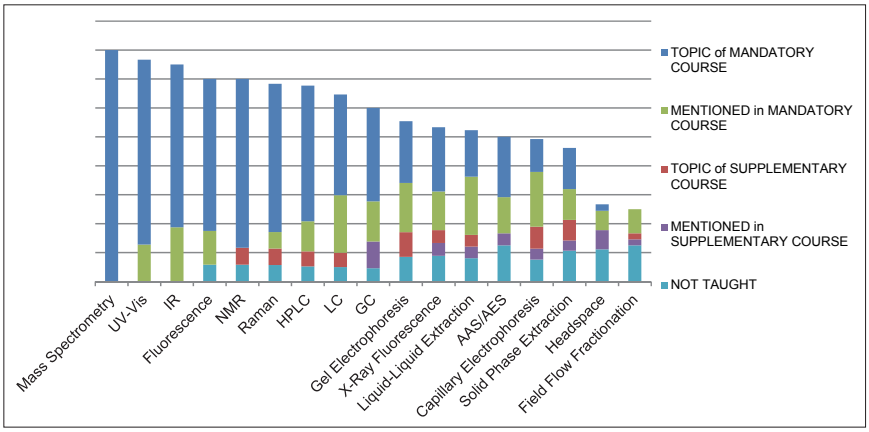

Figure 1. Weight given to teaching different analytical techniques.

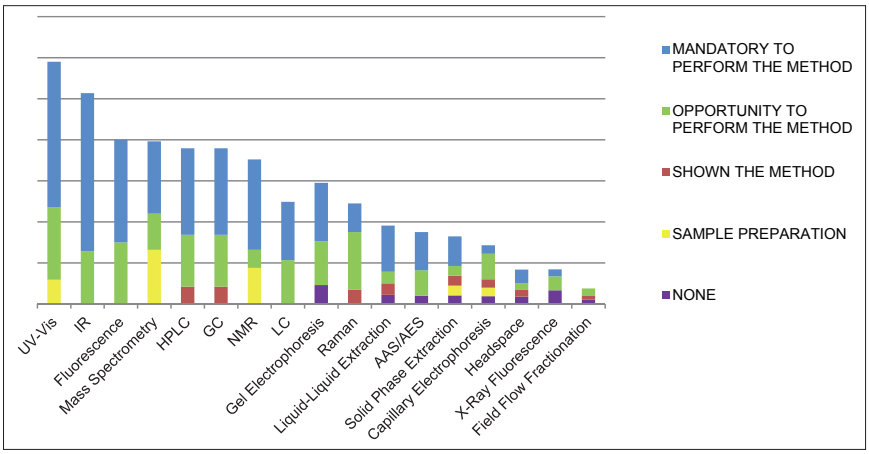

Figure 2. Weight given to laboratory-based training in the different analytical technqiues.

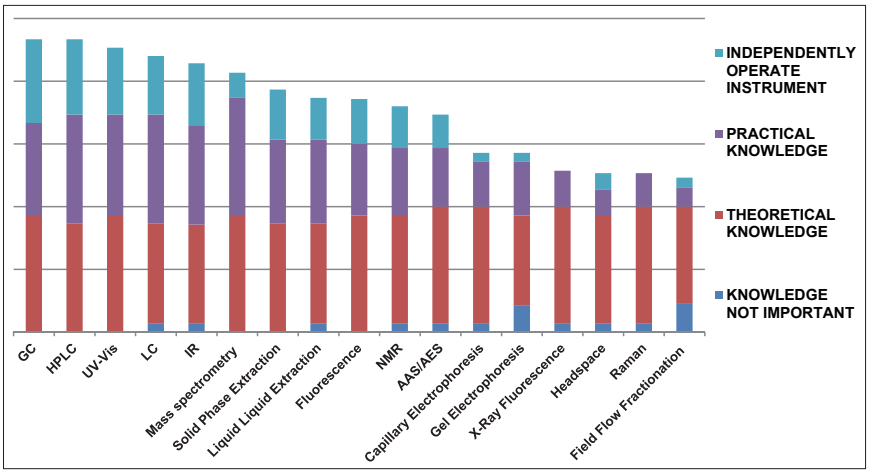

Figure 3. Weight given by industrialists to knowledge in the different analytical technqiues.

However, there was a very interesting comment made by one of the industrialists' survey responses around the balance of priorities between "soft skills" and hard technical ones. An area the structure of the survey didn't address…

"…There could be more focus on other skills such as communication (all kinds), influencing, idea generation, but also executing ideas etc… skills next to "analytical thinking". In general, we looking into these

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Table 1. Prioritisation of other skills between educators and employers.

Other skills prioritisation	
Academic	Industrial
Problem solving and critical thinking	Critical thinking and problem solving
Literary research	Ability to work in a team
Communication skills	Communication skills
Sample handling	Ability to work independently
Design of experiment	Time management
Sampling	Ability to perform efficient literature searches and information retrieval
Laboratory management	Knowledge of statistical procedures
Project management	Project management
High throughput screening	Design of experiment

Table 2

	Prioritisation		
Rank	Industrial	Academic teaching	Academic laboratories
1	GC	Mass spectrometry	UV-Vis
2	HPLC	UV-Vis	IR
3	UV-Vis	IR	Fluorescence
4	LC	Fluorescence	Mass spectrometry
5	IR	NMR	HPLC
6	Mass spectrometry	Raman	GC
7	Solid phase extraction	HPLC	NMR
8	Liquid–liquid extraction	LC	LC
9	Fluorescence	GC	Gel electrophoresis
10	NMR	Gel electrophoresis	Raman
11	AAS/AES	X-ray fluorescence	Liquid–liquid extraction
12	Capillary electrophoresis	Liquid–liquid extraction	AAS/AES
13	Gel electrophoresis	AAS/AES	Solid phase extraction
14	X-ray fluorescence	Capillary electrophoresis	Capillary electrophoresis
15	Headspace	Solid phase extraction	Headspace
16	Raman	Headspace	X-ray fluorescence
17	Field flow fractionation	Field flow fractionation	Field flow fractionation

skills rather than knowing how an LC works."

Some respondents did also complain that the courses seemed to deliver too much "soft-skill" training as opposed to the analytical skills. Another interesting point in exactly this area, but also one not addressed in the survey, was around the underlying assumption that we were trying to match graduate skills against their future employment environment. However, one respondent pointed out… *"University graduates do not usually get a position at the lab bench in my company, but are working as project managers. The softer skills such as project and time management, communication etc. do not seem to get a lot of attention in their academic training. Also, the analytical chemistry knowledge usually does not completely match with what is important in our industry and a lot has to be learned on the job. Problem solving skills and analytical thinking are usually well developed."*

Summary

Table 2 shows a summary of the weighted assessment of the different priorities given to different topics by industrialists, academics planning lecture courses and academic practical laboratory work.

As I feared there does seem to be a need to re-align priorities. More emphasis on the preparation techniques for handling samples in the academic arena is needed to ensure that graduates of the future are better suited to the world in which they will need to find employment. As to the availability of more expensive spectroscopic techniques, I think there could also be lessons to be learnt around industrialists understanding the financial pressures that universities find themselves under. They might decide to take concrete steps to help ensure access for students to facilities their universities can no longer justify maintaining on cost grounds. Additionally, the weighting between hard analytical skills and the softer workplace integration type of skills seems to be of concern.

Finally, if you have not yet completed the survey please find some time today to do so. As mentioned in the title, this is just a quick preliminary look at the results that have come in to-date and a much stronger statistical base from respondents from a wider geographical area would be greatly appreciated!

The surveys

To access the **Academics' Survey** please use this link:
nl.surveymonkey.com/r/8HVCMR5

To access the **Industrialists' Survey** please use this link
www.surveymonkey.com/r/MYSKVMG

Reference

1. J.R.J. Dania, J.I. Zahradnik and A.N. Davies, "Training future analysts", *Spectrosc. Europe* **30(2),** 20–22 (2018). http://bit.ly/2rXcb4A

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Representative sampling and society

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The last sampling columns have focused on the advantages the Theory of Sampling (TOS) can bring to companies, producers and manufacturers significantly reducing costs due to inferior sampling, and maximising efficiency and logistics. Here instead we take a look at sampling from the point of view of buyers, consumers and from a broader societal perspective, exploring the economic benefits and other advantages (e.g. transparency) that can be obtained through proper sampling. We address the point of view of the ultimate users and beneficiaries of TOS, on the market place or elsewhere. We are going to explore the other side of the coin, the one linked to the ethical and moral obligations that pertain to decision-makers of responsible public and governmental bodies, which indeed should apply equally also to producers and manufacturing companies.

Sampling: from the point of view of buyers, consumers, citizens

Let us start by thinking of the role of sampling from the point of view of consumers dealing with market products which are essential in terms of both *security* and *safety*, primary examples would be food, agricultural commodities, beverages, drugs and other medicinal products, air, soil and water quality. Here inferior sampling may not only threaten economic optimisation in the narrow production and commercial sense, but also result in a potentially negative impact on public health, for example. Quantitative and analytical data are used daily all over the world to take important decisions which ultimately affect every single citizen; and single citizens have no other choice than to *trust* that such decisions are made on the best available basis and knowledge. The question is how, and on what basis, are decisions made regarding product and commodity safety or environmental thresholds regarding maximally allowed pollution levels? Upon reflection, there are very many such decisions that are dependent upon proper sampling… usually hidden far away in early stages of causal pathways, e.g. "from-field-to-table".

The problem is linked to the concept of "best available knowledge" for which a universal definition cannot be identified, even though it is often used to claim/guarantee quality in the interest of consumers, stakeholders and, ultimately, society at large.

However, often what is "best available" is just not good enough.

During the last fifteen years we have provided documented evidence of sampling situations where "the best available" was, and sometimes still is, insufficient. A few examples can be found in References 1–4, where the critical issue of proper sampling for GMO detection and quantification was treated in a series of papers in *Trends in Analytical Chemistry*.[2–4] In the food and feed realm, a major achievement was the 2015 special issue section of *Journal of AOAC International*: "Representative Sampling for Food and Feed Materials" presenting a compact handbook for this important societal sector,[5] complete with many consumer, user and societal viewpoints. There has also been a consistent critique of existing "sampling" sections and paragraphs in current ISO standards. Indeed, this topic remains highly critical: *much* of what is presented in international standards does not meet what is required to guide towards, far less guarantee, "representative sampling". The very wide spectrum of recommendations offered ranges from acceptable (not often) to "home-grown statistics" (quite often), which, although maybe correct w.r.t. the statistical formulations, do not apply to the harsh reality of heterogeneity.[4,5]

Despite such first forays, representative sampling is not yet recognised as one of the key tools needed to ensure that the quantitative analytical data used to take subject-matter decisions are truly the "best available". As responsible scientists, we must be realistic and accept that, on the present basis, claims identifying the Theory of Sampling (TOS) as the *only* frame for correct sampling may not always be understood; there is much more work to be done before significant impacts on the general population will be achieved. A newly released report dealing with a topic that runs parallel to the present (indeed it overlaps significantly: proper sampling is a critical prerequisite to circular economy)[6] shows this compellingly. Another, "Barriers to the circular economy: evidence from the European Union" by Kircherr *et al.*[7] reveals the complexity and immensity of this kind of awareness and educational endeavours.

Sampling champions feel a moral obligation to find innovative ways and means to incorporate representative sampling as a key criterion for any quality statement, ensuring a step-forward in

the correct application of scientific knowledge to practice.

So, two basic questions arise:

1) **Who** should decide when "the best available" is indeed the best?
2) **How** can we convince stakeholders and citizens that correct sampling is a necessary pre-requisite, among others, to ensure security and safety of the relevant products and services essential for society?

Addressing both questions

1) Normally consumers decide quality, but this rule is difficult to apply when the quality under discussion is not the one of the final product(s), but rather of the *process* used to manufacture process or deliver products (or services). Suddenly quality becomes *invisible* for the consumer. This is why *individual citizens* can only trust that market decisions taken for essential products are made on the best available knowledge and must be happy (if not happy… at least willing) to pay taxes so that public control systems have sufficient resources to protect them! This admittedly oversimplified scenario is meant to illustrate the ethical responsibility that regulatory science bears towards society, a complex responsibility. But when one accepts this logic, we can easily answer the first question, **who** should decide when "the best available" is indeed the best? Only those having sufficient competence and knowledge of the process leading to a product can decide if "the best available" information is sufficient. If we project these considerations to sampling, it becomes clear that the quality of the sampling used in the decision-making regarding products essential for society cannot be assessed by the individual final costumer. Assessment of sampling quality relies on the professional integrity, expertise and objectivity of those controlling the production process. This completely changes the frame within which sampling problems are addressed and resolved, making it incomparable to that faced by TOS consultants working in the commercial realms, where the quality of their work is assessed directly by their clients. The part of the TOS community interested in engaging in sampling of societally essential products must be fully aware of these additional difficulties and responsibilities, which can frustrate (hopefully only temporarily) even the most motivated and determined sampling expert.

"Where it all begins." The dominating errors behind the final analytical uncertainty are always largest at the primary sampling step. Here soy beans are off-loaded from a cargo ship's holds. It is decidedly not a trivial issue how to sample this type of lot in a documented representative fashion—professional TOS competence is needed.

2) However, even if society in its role as final consumer of essential goods cannot monitor the quality of processes, it should be educated and aware (enough) to fully appreciate the practical relevance and implications that representative sampling has, even if oftentimes invisible to its final consumers. Here is a fact simple enough to be intuitively understandable **by all**: if sampling is not representative it is futile, indeed useless, to analyse the ensuing "samples", because it has no meaning to produce such analytical results without a clear provenance; the sampling + analytical uncertainty becomes totally unknown. This issue has been well illustrated in previous columns and has been explained many times in various fora. So much so that gradually various international normative documents now do mention that "good sampling *should be* representative". True, this is a much milder and timid version of "non-representative sampling is useless", but whether we like it or not, this is currently the only reward the sampling community has received for some 15–20 years of hard work. Now is the time to explore new strategies to speed up progress and ensure that representative sampling becomes a central element in the list of the essential quality criteria. But exactly **how to do so** requires careful thinking, because it will unavoidably entail identification and correction of deficiencies in current practices, which of course is never popular. Examples of the first steps in this direction could be References 8 and 9, against which there is non-trivial resistance. These issues were plentifully illustrated in the recent Sampling Column: "Sampling—*Pro et Contra*".[10]

The way forward: some proposals

First, we should better *substantiate* the claim that TOS is the **only** sampling frame universally applicable to any type of material and heterogeneity. We should demonstrate, with empirical evidence that this is in fact the case.

The KeLDA project[2–4] did so ten years ago, but no other examples of simi-

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lar dimension (outside the mining and minerals processing sectors) have been produced ever since. No misunderstanding regarding the mining sector: from here comes the evergreen "How much TOS saves you in monetary terms" publication paper *par excellence* by Carrasco, Carrasco and Jada: "The economic impact of correct sampling and analysis practices in the copper mining industry",[11] which was summarised in the previous column.[12]

The sampling community has provided seminal books and many excellent scientific papers explaining with various degrees of complexity and comprehensibility the mathematics upon which TOS is rooted, and where TOS is currently technically progressing. The series of Proceedings, from eight consecutive World Conferences on Sampling and Blending, in which applications to a much broader societal field are presented, especially in the later three editions constitutes further progress in such direction.

Still the sampling community must continue to make extra efforts to put itself on the side of society, where intimidating mathematical formulae are respected, but only occasionally understood and where practical/direct examples are seen as the primary evidence that allows seeing the light in what is perceived as an intricate forest of technical and scientific complexity. History teaches that significant, mass-scale changes in attitude towards scientific innovation have only taken place when triggering explanations were simple, clear and self-evident. The TOS community has not yet found a fully comprehensive, winning formula to achieve this. But two previous columns made serious attempts.[10,12] What a challenge—one cannot wait to contribute! Below follows a few views on what *can* perhaps be done to trigger increased societal attention to sampling.

Beyond traditional application fields

The use of fortified foods, food supplements and "functional foods" is on the rise. This may result in a higher intake of nutrient substances, which *could* turn into a concern if intake levels become sufficiently high to induce adverse effects. Nutrients, in contrast to contaminants, are essential for human/animal health and have their positive nutritional effects within specific concentration ranges, governed by homeostatic mechanisms in the human/animal body. Adverse health effects may occur due to over-consumption or may lead to deficiency symptoms in case of under-consumption. Therefore, upper intake levels (ULs) of nutrients from food sources by humans/animals not inducing adverse health effects and minimal required intake levels should be identified in order to avoid such effects. Obviously proper sampling methods to be applied in various stages of production and processing of these foods are needed in order to be able to correctly determine actual intake levels of nutrients by humans and compare these with the established upper safety limits and minimal required intake levels.

Another well-known fact is the increased spread of *pathogens* in the food production chain, presumably due to globalisation of trade and to the migration of people.[13] New pathogenic micro-organisms have been detected and characterised, as well as an increase in antibiotic-resistant bacteria, presumably due to massive (over-) use of antibiotics for human therapy. Ingestion of pathogens or their toxins may induce a variety of diseases in humans/animals, ranging from acute illness like diarrhoea to many chronic diseases and death. Specific guidance for risk assessment of microbial food and feed contamination has been developed[14] and the importance of the dynamics of microbiological growth, survival and the (rapid) transfer of micro-organisms throughout the food production chain in many types of foods, raw or processed, and further spread in the environment has been underlined. Exposure assessment is of critical importance for risk assessment and consequently also for definition of suitable sampling plans, that take into account the specific distributional characteristics of microbial populations and of their spreading dynamics. These issues are of the utmost importance to allow an effective safety evaluation of food and feed commodities.

Consumption and request for *niche and brand* products, e.g. mono-cultural products, extra-virgin olive oil, mozzarella cheese, designed to capture the interest of an elite portion of consumers, is also increasing, at least in wealthy countries. In such cases, proper sampling may raise interest in **both** producers and society. For producers, correct sampling may facilitate the conquest of a portion of the market at the global level, ensuring/proving specific quality standards of unique products. Indeed, producers are aggregating into consortia with the objective of facilitating their business. For society the same holds true: representative sampling becomes a tool to ensure that the final niche-product on the market, possibly at a higher price to cover the specific production costs, indeed has the

Pathogens (or toxins), irregularly distributed in the lot (material).

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For niche and/or brand product proper sampling actually benefits both sides of the traditional producer–consumer issue equally.

compositional, organoleptic and nutritional properties it should have. Here proper sampling benefits both sides of the traditional producer–consumer issue equally.

The TOS community needs to accept that sampling is up against a series of inherent difficulties linked to the nature of products in a wide societal sense, in particular beyond TOS' traditional target fields of mining, minerals processing and cement. The great diversity in food and feed sources and commodities and the different kinds and degrees of food/water contaminations are just a few examples, focussed on the difficulty for society to directly verify the quality of the production processes involved.

Here is a problem that only a few want to entertain today: the sampling frameworks currently used for quality assessments too often rely on *specific* statistical distributional assumptions (i.e. "homogeneous distributions" of compounds/test materials, "assumed" normal distributions), but which are very nearly *never* **verified** in practice, as current protocols do not even stipulate characterisation of inherent heterogeneity patterns stemming from the specific properties of the targeted materials. Moreover, current quality assessment protocols do not provide estimates of the risk associated with the sampling surveys *themselves*, nor do they address the uncertainties associated with spatially irregular distributions (material distributional heterogeneity).

Conclusions

Above, it is underlined that representative sampling is **key** in order to reduce the possibilities of either misestimating actual exposure levels for humans and animals or, worse, underestimating the risks for consumers to exceed tolerable intake levels. We need to prove this correct framework understanding with real data.

When you go to a wine cellar or wine store, you taste (***sample***) the wine before buying it: you do not ask the seller **if** the wine is good. The TOS community cannot expect to be listened to if they cannot also document our claims with **facts**, compelling visual, graphic and quantitative facts. This calls for superior examples and resources to support well-thought out research and demonstration projects with the same purpose. Examples from these frontlines will be presented in sequel columns.

Disclaimer

Claudia Paoletti is employed by the European Food Safety Authority (EFSA). The positions and opinions presented in this article are those of the authors alone and do not necessarily represent the views or scientific works of EFSA. Kim H. Esbensen is an independent researcher.

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PRODUCT FOCUS

Product Focus on Imaging Spectroscopy

Andor

Tel: +44 (28) 9023 7126
quote@andor.com
www.andor.com/spectroscopy

PRODUCT: Kymera 328i Intelligent and Multi-Modal Spectrograph Platform for Physical and Life Science
APPLICATIONS: Raman ▪ Luminescence ▪ LIBS ▪ Absorption ▪ Non-linear optics ▪ Transient spectroscopy ▪ Micro-spectroscopy ▪ Material science ▪ Chemistry ▪ Biomedical ▪ Plasma studies
KEY FEATURES: 328 mm focal length ▪ Adaptive focus (patented) ▪ Quad grating turret & RFID ▪ Dual input and dual detector outputs ▪ TruRes™ spectral resolution enhancement ▪ µ-Manager software for microspectroscopy

PRODUCT: iStar sCMOS Ultrafast Platform for Nanosecond Time-resolved Imaging and Spectroscopy
APPLICATIONS: Plasma studies ▪ Time-resolved fluorescence ▪ Photoluminescence ▪ Flow analysis / combustion ▪ PLIF imaging ▪ Hyperspectral imaging
KEY FEATURES: 5.5 megapixel sCMOS ▪ 50 fps full frame, 4000 sps ▪ High dynamic range at full speed ▪ Integrated triple output DDG ▪ Photocathode QE up to 50% ▪ Integrate-On-Chip gating up to 500 kHz ▪ USB 3.0 interface

BaySpec

Tel: 408 512 5928
lchandler@baySpec.com
www.BaySpec.com

PRODUCT: Aerial Hyperspectral Imager (OCI™--UAV)
APPLICATIONS: Precision agriculture ▪ Remote sensing ▪ Environmental monitoring ▪ Geological survey ▪ Food inspection ▪ Security/defence
KEY FEATURES: Super lightweight ▪ Compact size ▪ 110 bands, VISNIR 475–975 nm, fully automatic operation ▪ Stitching multiple images without GPS/IMU

PRODUCT: Hyperspectral Imagers OCI™-F Series for 400–1700 nm
APPLICATIONS: Precision agriculture ▪ Remote sensing, environmental monitoring, geological survey, food inspection, security/defence and mining
KEY FEATURES: Lightweight ▪ Compact size ▪ High spectral resolution ▪ Up to 220 bands ▪ VIS/SWIR 400–1000 nm ▪ Fully automatic operation ▪ Stitching multiple images without GPS/IMU

PRODUCT: SnapShot Imager OCI™-D2000 for 475–975 nm
APPLICATIONS: Online material sorting with instant feedback ▪ *In vivo* biomedical imaging ▪ Precision agriculture ▪ Remote sensing, environmental monitoring, geological survey, food inspection, security/defence
KEY FEATURES: Online material sorting with instant feedback ▪ Video rate ▪ *In vivo* biomedical imaging ▪ Precision agriculture ▪ Remote sensing, environmental monitoring, geological survey, food inspection and security

Bruker Optik GmbH

Tel: +49 (0)7243-504 2000
info.bopt.de@bruker.com
www.bruker.com/optics

PRODUCT: FTIR Spectrometer INVENIO
APPLICATIONS: Research & Development ▪ Pharma ▪ Polymers and chemistry ▪ Surface analysis ▪ Material science ▪ Semiconductors
KEY FEATURES: Integrated touch panel ▪ MultiTect detector technology ▪ Transit measurement channel ▪ Spectral range from 15 cm^{-1} to 28,000 cm^{-1} ▪ Unique Bruker FM technology

PRODUCT: FT-NIR Spectrometer MPA II
APPLICATIONS: Food and feed industry ▪ Pharmaceutical and cosmetics industry ▪ Chemical industry
KEY FEATURES: Easy operation ▪ User-friendly software ▪ Long-life light source ▪ Solid state laser for highest wavenumber accuracy ▪ Hassle-free maintenance ▪ GMP and 21 CFR Part 11 compliance

Headwall Photonics, Inc.

Tel: +1-978-353-4100
sales@headwallphotonics.com
www.headwallphotonics.com

PRODUCT: Nano-Hyperspec
APPLICATIONS: Crop disease detection ▪ Environmental monitoring ▪ Remote sensing
KEY FEATURES: VNIR (400–1000 nm) ▪ Internal 500 GB solid state storage ▪ Smallest and lightest airborne hyperspectral imaging sensor ▪ 270 spectral bands and 640 spatial bands

PRODUCT: Application-specific holographic diffraction gratings
APPLICATIONS: Colour measurement ▪ Biotech ▪ OEM spectral imaging instruments
KEY FEATURES: Low stray light ▪ High signal-to-noise ▪ Aberration-corrected optics ▪ Small size ▪ Planar, concave, convex

PRODUCT FOCUS

Kratos Analytical Ltd
Tel: +44-161-888-4400
surface.sales@kratos.co.uk
www.kratos.com

PRODUCT: AXIS Supra
APPLICATIONS: Elemental & chemical state XPS imaging ▪ Thin film characterisation ▪ Monitoring surface modification ▪ R&D
KEY FEATURES: X-ray photoelelectron spectroscopy (XPS) ▪ Secondary electron microscopy (SEM) ▪ Scanning Auger microscopy (SAM)

Thermo Fisher Scientific
Tel: +1-561-688-8700
info.spectroscopy@thermofisher.com
www.thermofisher.com/spectroscopy

PRODUCT: Thermo Scientific™ DXR™ 2xi Raman Imaging Microscope

APPLICATIONS: Chemical imaging across advanced materials, pharmaceutical and biological samples
KEY FEATURES: Real-time chemical identification with ultra-fast mapping and visual answers ▪ Compare and contrast multiple areas and visually rank features of interest ▪ Configure settings in seconds without tools

PRODUCT: Thermo Scientific™ Nicolet™ iN™ 10 MX Infrared Imaging Microscope

APPLICATIONS: Identify materials and contaminants for product quality assurance, failure analysis and counterfeit analysis
KEY FEATURES: Minimise learning process with intuitive software for busy labs ▪ Improve speed and sensitivity of routine single point-and-shoot measurements ▪ Optional MicroTip ATR and motorised visible polariser

WITec GmbH
Tel: +49(0)731 140 700
info@witec.de
www.witec.de

PRODUCT: alpha300 R Confocal 3D Raman Imaging System
APPLICATIONS: Materials research ▪ Pharmaceutics ▪ Semiconductor and PV ▪ Life science ▪ Geosciences, coatings & thin films, polymer research, low-dimensional materials
KEY FEATURES: Cutting-edge 3D chemical Raman imaging while maintaining the highest measurement speed and spectral quality ▪ Confocal setup: highest spatial resolution (200 nm) ▪ Correlative Raman Imaging easy possible

PRODUCT: TrueSurface Microscopy
APPLICATIONS: Large-area investigations ▪ Characterisation of rough & inclined surfaces
KEY FEATURES: Topographic confocal Raman Imaging ▪ Precise tracing of the true surface while acquiring Raman imaging data in a one-pass measurement process ▪ Virtually no sample preparation of large samples

PRODUCT: RISE Microscopy – Raman SEM Imaging
APPLICATIONS: Materials research ▪ Pharmaceutics ▪ Nanotechnology ▪ Life science ▪ Geoscience
KEY FEATURES: Correlative Raman-SEM imaging integrated in one system ▪ Quick and convenient switching between Raman and SEM measurement on the same position ▪ Correlation of the measurement results and image overlay

PRODUCT: apyron - Automated Raman Imaging System
APPLICATIONS: Materials research ▪ Pharmaceutics ▪ Forensics ▪ Life science ▪ Geoscience
KEY FEATURES: Push-button principle for high performance 3D Raman imaging ▪ TruePower automated absolute laser power determination ▪ Outstanding spectral & spatial resolution ▪ Streamlined measurement workflow

PRODUCT: alpha300 Ri inverted Raman Imaging Microscope
APPLICATIONS: Life sciences ▪ Biomedical research ▪ Living cell analysis ▪ Aqueous samples
KEY FEATURES: Inverted beam path allows liquid samples to be placed on the stage for quick and repeatable measurements ▪ Compatible with other microscopy techniques including: fluorescence, DIC, phase-contrast

ANALYTICA 2018

ATOMIC

LC-ICP-MS

Analytik Jena has introduced an HPLC module, the PQ LC, for its PlasmaQuant MS ICP-MS system. HPLC separation enables many routine analyses to be performed more efficiently, quickly and accurately. There are three versions of the PQ LC modules: the compact PQ LC for routine applications in small labs, the version of the PQ LC for routine and special applications and the PQ IC ion chromatography system.

Analytik Jena

- http://link.spectroscopyeurope.com/30-W-063

novAA 800 atomic absorption spectrometer

Analytik Jena introduced the novAA® 800 atomic absorption spectrometer with flame, graphite furnace and hydride technologies on one platform. A wide range of accessories is also available. The novAA 800 is especially designed for industrial process labs, for example in the food, environmental or chemical industries where moderate sample quantities need to be analysed. The atomiser can be changed easily benefitting labs that measure both high- and low-concentration ranges. The novAA 800 is available in three models: the novAA 800 with flame and hydride technology; the novAA 800 G with graphite furnace and hydride technology; and the novAA 800 D, which integrates all three technologies in one system.

Analytik Jena

- http://link.spectroscopyeurope.com/30-W-058

CHEMICALS AND RMS

Romil-UpS ultra-purity solvents

Romil have introduced a range of ultra-purity solvents, Romil-UpS, for high-sensitivity techniques. Applications such as environmental analysis now require routine detection of trace amounts of pollutants, and hyphenated techniques need a solvent quality matched to the requirements of all the configured detectors. Purification techniques of the new solvents are more exacting and each batch is carefully use-tested. Product is filled into bottles which have been specially pre-treated to ensure that trace metal impurities are kept as low as when freshly manufactured. Thus, not only is the original purity controlled but also the actual purity when opened some time later.

Romil

- http://link.spectroscopyeurope.com/30-W-065

ICP and ICP-MS standards in 25 mL bottles

Ultra Scientific have added the option of 25 mL bottles to their range of ICP and ICP-MS standards. The 25 mL size avoids extra shipping costs for hazardous materials.

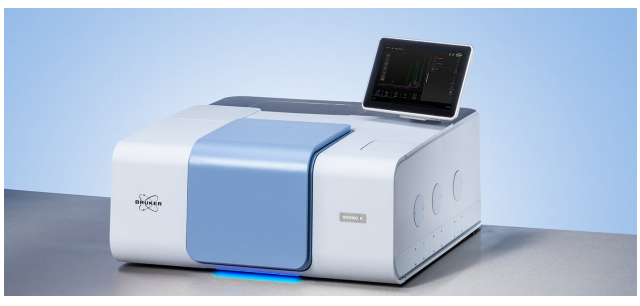
Ultra Scientific

- http://link.spectroscopyeurope.com/30-W-068

INFRARED

INVENIO FT-IR R&D spectrometer

Bruker has launched the new INVENIO™ FT-IR research spectrometer; the successor to the VERTEX 70 FT-IR for advanced R&D applications. The INVENIO combines new features with Vertex 70 technologies, such as unique FM technology for simultaneous mid- and far-IR spectroscopy. The new MultiTect™ technology allows for control of up to five internal detectors, covering the spectral range from far infrared to Vis/UV. A DigiTect™ detector slot enables additional flexibility for even more detectors. The smart INVENIO beam path further improves optical throughput and spectroscopic sensitivity. An integrated touch panel enables intuitive configuration set-ups and workflows for R&D



applications, and the system can also be switched to notebook operation. The Transit™ channel allows for easy transmission measurements, without removing experiments from the sample compartment. Intelligent spectrometer features include electronically coded beam windows with magnetic mount, an automated internal attenuator wheel and an eight-position validation wheel for standards and customer-specific filters.

Bruker

http://link.spectroscopyeurope.com/30-W-061

Atmos gas cells

Specac has introduced a new range of fixed, long pathlength gas cells, Atomos, for measuring the infrared spectra of gases and vapours. They are designed for use over a wide range of temperatures and pressures, and are suitable for operation in all modern

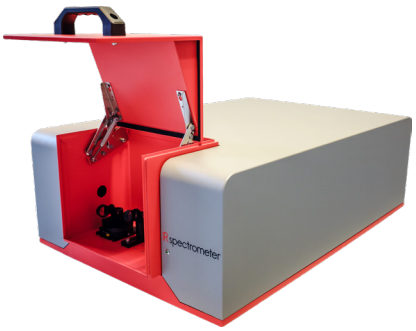
FT-IR spectrometers. The cells are available, as standard, with a metal body for operation at ambient temperatures and pressures ranging from vacuum to 125 psi. Models are available covering pathlengths from 2.5 m to 20 m.

Specac

http://link.spectroscopyeurope.com/30-W-066

Mid-IR frequency comb spectrometer

IRsweep showed the latest version of their mid-IR frequency comb spectrometer, the IRisF1. This allows for the simultaneous measurement of the whole laser spectrum without requiring tuning of the source, enabling high spectral and temporal resolution in a single-shot measurement. Applications include reaction kinetics, protein-folding, photocatalysis and high-throughput. Time-resolution is in microseconds and spectral resolution 0.25–0.5 cm^{-1}.



IRsweep

http://link.spectroscopyeurope.com/30-W-070

MASS SPECTROMETRY

4500 MiD chip-based mass spectrometer

Microsaic Systems has introduced the 4500 MiD® chip-based mass spectrometer, which is designed for point-of-need analyses. The 4500 MiD combines the vacuum system, electronics and computer in one box, with no need for a floor pump. The new system offers an increased mass range (50–1400 *m/z*), a completely tool-less front-end and intuitive user interface. In addition, a change in front-end alignment has strengthened system uptime whilst reducing the deposition of contaminants downstream.

Microsaic Systems

http://link.spectroscopyeurope.com/30-W-064

Nitrogen generator for LC-MS

Peak Scientific has introduced a new addition to its Solaris Nitrogen range, the new Solaris XE. Solaris XE can deliver up to 35 $Lmin^{-1}$, at purity levels of up to 99.5% making it suitable for LC-MS applications. The Solaris XE has variable purity in relation to outlet flow and pressure, and so is also capable of supplying compact MS instruments or multiple evaporative light scattering detector instruments simultaneously. The Solaris XE has been specifically designed to provide nitrogen to laboratories that utilise an external source of compressed air and its compact chassis allows it to be placed on a benchtop or on a wall.

Peak Scientific

http://link.spectroscopyeurope.com/30-W-060

Dry scroll pumps

Agilent were keen to emphasise the sustainability initiatives they have put in place. These include a 1% reduction in energy use and 2% reduction in water each year, with 10% and 20% reduction by 2024, respectively, and a 100% diversion of solid waste from landfill by 2010. They will achieve these through enabling better recycling and reuse, reduction in energy, water and gas consumption of instrumentation, and reducing both hazardous and non-hazardous waste.

An example of this in practice is their new range of IDP dry scroll pumps which are oil-free, compact and quiet vacuum pumps with longer maintenance cycles. IDP pumps use a single-sided scroll design that only requires an annual, 15-min maintenance procedure with simple tools. IDP pumps have the motor and all bearings completely isolated from the vacuum path, which extends the bearing life and provides clean, dry vacuum to the application.

Agilent

http://link.spectroscopyeurope.com/30-W-078

ANALYTICA 2018

NIR

Miniature NIR spectrometer module

SiWare systems' latest miniature spectrometer is the NeoSpectra Micro; a chip-sized, self-contained NIR spectral sensor. It is designed to be the basis of a complete system as an OEM module. It has a wavelength range of 1250–2500 nm. The module contains the optical head for sample illumination and collection, ASIC chips for system control and data processing and the optical core module that contains a monolithic MEMS Michelson interferometer and a single-element uncooled InGaAs photodetector.

Si-Ware Systems

http://link.spectroscopyeurope.com/30-W-072

RAMAN

BLAZE spectroscopy cameras

Princeton Instruments were showing their high-performance BLAZE cameras, which use two new sensors. BLAZE LD-Sensors are deep-depletion devices designed for high sensitivity and low dark current, making them suitable for low-light applications. BLAZE HR-Sensors are "super-deep-depletion" devices manufactured from high-resistivity bulk silicon to yield the highest NIR quantum efficiency. BLAZE LD and HR cameras are both offered in 1340 × 100 or 1340 × 400 formats with 20 µm pixels. Applications include Raman spectroscopy, photoluminescence, nanoparticle research, carbon nanotube studies, pump–probe experiments, fluorescence and micro-spectroscopy.

Princeton Instruments

http://link.spectroscopyeurope.com/30-W-073

SOFTWARE

Data acquisition software for J&M spectrometers

J&M have introduced a new version, TIDASDAQ3, of the TIDASDAQ software that runs their TIDAS UV/vis/NIR spectrometers. This introduces data exchange with SCADA systems with an integrated OPC server. A scripting option allows the data acquisition and processing to be adapted to complex processes, such as baseline correction, multi-channel acquisition etc. Different user access levels and user interfaces can be defined.

J&M Analytik

http://link.spectroscopyeurope.com/30-W-071

UV/VIS

Stand-alone spectrometers

J&M have launched a new all-in-one range of their TIDAS diode-array spectrometers, the TIDAS L. These spectrometers have an integrated PC with a large touchscreen and run the TIDASDAQ software. They can be operated on their own or connected to a network. A number of different wavelength ranges are available, including UV and NIR.

J&M

http://link.spectroscopyeurope.com/30-W-069

X-RAY

Apex quick release XRF dies

Specac's Apex range of quick release XRF dies produce sample pellets of 32 mm and 40 mm diameter. A patented auto-ejector sleeve allows release of the finished pellet without needing to reset the die in an inverted position at the mid-point of the pressing cycle. After compression of the sample, release of the load causes the ejector tabs to swivel over and capture the sleeve in release position. Re-applying a load causes the finished pellet to be pushed clear of the die body. When used with Specac's Atlas Autotouch press, this process can be automated.

Specac

http://link.spectroscopyeurope.com/30-W-067

Automatic dosing for XRF flux

Fluxana were showing their BORAMAT automatic dosing machine for flux in XRF analysis. It is designed to allow the user to weigh faster and monitor every weighing. It is compatible with all common laboratory scales, avoiding the need to invest in a new scale. It has three weighing modes: sample/flux ratio, catch weight and absolute weight.

Fluxana

http://link.spectroscopyeurope.com/30-W-074

CTX portable XRF analyser

Bruker's new CTX™ X-ray fluorescence (XRF) elemental analyser is a portable Counter Top XRF (CTX) instrument. The self-contained CTX weighs less than 7 kg and has a footprint of 14 cm wide. The CTX uses a 4 W X-ray source, a high-performance silicon drift detector (SDD), as well as Wi-Fi, Bluetooth and USB connectivity. The CTX's touchscreen user interface provides measurement control and results display. Additionally, Bruker's Toolbox PC software enables remote operation of the CTX and optional PC software includes Artax™ for advanced qualitative, semi-quantitative composition analysis, as well as EasyCal™ for user-defined empirical correlations. The CTX is available in several configurations, such as minerals and mining, food safety and agriculture, pharmaceutical raw materials, precious metals, polymers and marine fuel oil analysis. It is specifically designed for applications which require sample preparation and/or sample presentation in a cup or bag, as well as for small samples and samples which require measurement times of more than a few seconds. The CTX is also suited to central labs and on the factory floor for quick pre-screening or routine analysis, and as a back-up for larger XRF or ICP/AA systems.

Bruker

http://link.spectroscopyeurope.com/30-W-062

NEW PRODUCTS

ATOMIC

Upgraded SpectroTest mobile metal analyser

A major upgrade to Spectro's SpectroTest mobile metal analyser introduces a new, more-advanced readout system, which is a prerequisite for the introduction of iCAL 2.0—an enhancement of the instrument's proprietary iCAL calibration logic system. iCAL 2.0 ensures the analyser's stability during ambient temperature changes. With pre-defined calibration packages and the iCAL 2.0 diagnostics software, the upgraded SpectroTest allows users to perform a single-sample standardisation (in less than five minutes) at the start of the day's testing. The iCAL diagnostics ensure stable performance through a typical day, and, now, the software helps maintain the same standardisation, regardless of most temperature shifts.

Spectro Analytical Instruments

▸ http://link.spectroscopyeurope.com/30-W-046

INFRARED

New protein characterisation system

RedShift BioAnalytics has launched the AQS^{3}™pro, a new protein characterisation platform with integrated bioanalytics software that provides automated spectroscopic analysis for the development, formulation and manufacture of biotherapeutics. Its ability to provide multiple attribute data reduces or eliminates the need to perform separate measurements across different tools. The AQS^{3}pro uses the patented technique of microfluidic modulation spectroscopy (MMS), which combines mid-infrared laser spectroscopy with microfluidics and advanced signal processing to measure the secondary structure of proteins. It provides direct, label-free measurements over the concentration range 0.01–200 mg mL^{-1}, characterising samples under all the conditions routinely encountered in biopharmaceutical development and manufacture, without sample dilution.

RedShift BioAnalytics

▸ http://link.spectroscopyeurope.com/30-W-054

LUMINESCENCE

Cryostat inside integrating sphere for photoluminescence

Edinburgh Instruments have introduced the Cryosphere for the FLS1000 spectrometer, which enables measurement of the photoluminescence quantum yield from 77 K to 500 K. The Cryosphere features a software-controlled cryostat inside an integrating sphere and allows measurements of solids and powders. The absolute quantum yield as a function of temperature is easily obtained using Fluoracle software.

Edinburgh Instruments

▸ http://link.spectroscopyeurope.com/30-W-055

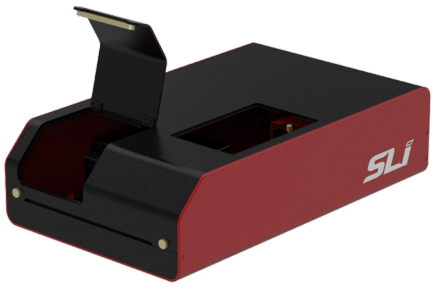
NEW PRODUCTS

New fluorimeter

Spectrolight has introduced the FWS fluorimeter, which combines their tungsten halogen lamp, Mighty Light and Flexible Wavelength Selector to provide a high power, tuneable monochromatic beam for excitation. The detection part uses a high signal-to-noise CCD. Currently, three models are available based on the sensitivity of different detector platforms.

Spectrolight

http://link.spectroscopyeurope.com/30-W-077



MASS SPEC

Software to streamline multiple-attribute methods

SCIEX has released BioPharmaView™ Software 3.0 solution for LC-MS Multiple Attribute Methodology (MAM) workflows, which enable in-depth characterisation of biologics by mass spectrometry. The SCIEX Workflow for MAM makes it easier for organisations to move to LC-MS-based MAM workflows. Currently, two SCIEX mass spectrometers are designed to integrate with the MAM Workflow: the SCIEX X500B QTOF and the SCIEX TripleTOF® 6600 systems. BioPharmaView Software 3.0 comes with new features for performing a complete MAM workflow in a single software suite, along with the ability to automate core biologics characterisation workflows, such as intact mass, subunit mass and peptide mapping analyses.

SCIEX

http://link.spectroscopyeurope.com/30-W-076

NIR

New NIR analyser for food

FOSS has announced the FoodScan™ 2, a new-generation near infrared (NIR) analyser which provides a result in as little as 25 s—approximately 50 % faster than the first FoodScan. Besides the traditional information about content of fat, protein, moisture and collagen, FoodScan 2 also provides new parameters such as saturated fat, carbohydrates, sodium and energy. A single test gives all information required to fulfil, for example, the EU requirements for product labelling. Colour is becoming an increasingly important consumer choice parameter, and the FoodScan 2 can perform a colour measurement simultaneously with compositional tests. This offers a convenient and time-saving alternative to separate colour measurement equipment or subjective assessment by eye with visual charts. The new option is achieved by the use of both NIR transmittance and transflectance technology in the one unit.

FoodScan 2 is available in a number of models including a Lab TS for laboratory operation, a Pro model for use in the production environment and Lab model with a keyboard for users not requiring the touchscreen interface.

FOSS

http://link.spectroscopyeurope.com/30-W-057

PHOTONICS

Smart picosecond laser driver

PicoQuant has released the Taiko PDL M1 smart laser driver, which is able to monitor and control most laser head parameters such as optical output power or laser head temperature. It offers a wide range of repetition rates, burst patterns, continuous wave operation and external triggering. A local one button control scheme and a remote user interface are provided, and the two interfaces are synchronised and can be used simultaneously. The Taiko PDL M1 enables time-resolved applications to be carried out on time scales ranging from very short (fluorescence lifetime investigations) to very long (study of phosphorescence dynamics).

PicoQuant

http://link.spectroscopyeurope.com/30-W-056

RAMAN

New inverted confocal Raman microscope

WITec has launched the alpha300 R*i* inverted Raman microscope. It combines the advantages of data acquisition from below with 3D confocal Raman imaging. Research applications in the fields of life sciences, biomedicine and pharmaceutics will benefit in particular from the new setup. The inverted beam geometry of the alpha300 R*i* delivers advantages in sample access and handling. Specimens in aqueous environments, such as cell cultures, can be examined more effectively. Standardised liquid sample holder formats can be quickly and easily mounted and measured. This accelerates the experimental workflow and helps ensure consistency. Investigations in materials science will be aided by the very large working area that can accommodate bulky samples and the set focal plane. The motorised sample stage also facilitates the mounting of environmental enclosures and other accessories.

Many modular components and upgrade possibilities developed for the WITec alpha300 series are compatible with the R*i* version. Other microscopy techniques associated with inverted microscopes, such as fluorescence, differential interference contrast (DIC) and phase-contrast can also be easily integrated.

WITec

http://link.spectroscopyeurope.com/30-W-045

Narcotics-focused handheld Raman analyser

Rigaku Analytical Devices has introduced the Progeny ResQ FLX, handheld Raman analyser, specifically designed for narcotics identification. Based on the Progeny ResQ 1064 nm Raman analyser released in 2015, the Progeny ResQ FLX provides law enforcement agencies with greater flexibility for use in the widespread opioid epidemic and increase in drug trafficking. The response time is less than one minute and the analyser can scan through glass and plastic.

It has a standard library of <1000 narcotics and cutting agents, as well as features important to law enforcement, such as: on-board digital camera to add pictorial evidence to results; smartphone pairing to rapidly transfer results; tamper-proof reports with digital signatures (21 CFR Part 11 compliant); accepted as a Class A analytical technique by the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG); and free library updates. Additional libraries (TICS, explosives, chemical warfare agents), custom applications, Reachback support and 4C technology mode to warn of threat combinations are also available.

Rigaku Analytical Devices

http://link.spectroscopyeurope.com/30-W-047

OEM spectrometer for spectral domain OCT

Ibsen Photonics's Eagle OCT-S spectrometer platform provides high optical throughput and a compact size due to the use of the company's in-house produced wide bandwidth transmission gratings. The wavelength range of the standard EOS-121 version is 810–900 nm, but can be customised to other ranges. Eagle OCT-S is supplied with the new Teledyne E2V OctoPlus camera with 2048 tall pixels. The Eagle platform is suited for OEM integration into industrial grade instruments for applications like Raman and SD-OCT.

Ibsen Photonics

http://link.spectroscopyeurope.com/30-W-052

Update to Raman software

Tornado Spectral Systems has released an update to its SpectralSoft Raman software. Version 2.8 adds security of access and data, multi-channel operation, remote access and control, as well as developments to boost measurement precision. The Security Module complies with US FDA 21 CFR Part 11. The Productivity Module enables users to configure and control multi-channel fibre-switching hardware for monitoring up to eight channels. The Industrial Control Module has a Modbus TCP interface for DCS connectivity. In addition to the add-on modules, v2.8 improves productivity via auto-calibration and increases data signal-to-noise ratio.

Tornado Spectral Systems

http://link.spectroscopyeurope.com/30-W-075

NEW PRODUCTS

Raman spectrometer for pharmaceutical applications

B&W Tek's QTRam performs solid dosage content uniformity testing to confirm the concentration of the active ingredients in finished products, even through sample coatings. It can be used for applications including blend and content uniformity, formulation development and counterfeit detection. The QTRam has the ability to quantify multiple components in a single scan for at-line monitoring and final product release. The QTRam comes with the portable lab-grade high-throughput Raman spectrometer system, the QT-Sampler quantitative transmission module, 21 CFR Part 11 compliant BWAnalyst™ software that can be operated using the onboard touchscreen and two standard sample holders. Users are able quickly to build methods, perform routine analysis and obtain results, with the data saved to a secure database and reports accessible immediately through the software. B&W Tek also offers customisable sample holders to accommodate any sample dimension of the finished products, such as tablets or gel capsules.

B&W Tek

http://link.spectroscopyeurope.com/30-W-053

UV/VIS

New UV-Vis spectrophotometer

Shimadzu has released the UV-1900 UV-vis spectrophotometer, which is equipped with an ultrafast scan function that enables data acquisition of 29,000 nm min^{-1} (the visible region can be measured in three seconds). The UV-1900 has a large, easy-to-use colour touch panel, through which all functions are accessible with large and easy to understand icons. In addition, patented LOW-RAY-LIGH® diffraction grating technology ensures low stray light with high resolution and one of the largest ranges of linearity.

While the UV-1900 can be operated as a standalone instrument, the new LabSolutions UV-Vis (Shimadzu's UV-Vis control software released simultaneously) offers further features, including data pass/fail judgements via its spectral evaluation functions. Data transfer to spreadsheet software and batch text export of multiple data sets are easy. The UV-1900 can connect with Shimadzu's analysis data management systems (LabSolutions DB/CS) in order to provide integrated data management with other analytical instruments, meeting the various guidelines and regulations relating to electronic records and electronic signatures such as the FDA's 21 CFR Part 11.

Shimadzu

http://link.spectroscopyeurope.com/30-W-049

Jenway launches micro-volume spectrophotometer

Cole-Parmer Ltd have announced that Jenway® has introduced its new micro-volume spectrophotometer, the 7415 Nano. Designed to measure micro-volume samples accurately, the 7415 Nano spectrophotometer is suitable for measuring DNA and RNA concentrations and purity. It enables micro-volume samples as small as 0.5 µL to be directly pipetted onto the read head, reducing the need for dilutions and eliminating the requirement for cuvettes. The 7415 Nano has a 7" high definition colour touchscreen display and an Android operating system. It succeeds the Genova Nano, and has multiple USB ports for data transfer and printer connectivity and multi-language options in English, French, German, Spanish and Italian. With the new 74 range Jenway also has introduced CP LIVE, the free Cole-Parmer web and mobile app that enables scientists to transfer and store data, protocols and results in one place. One administrator login can grant rights to other users to access the data, wherever they are located.

Jenway

http://link.spectroscopyeurope.com/30-W-050

Conferences
2018

17–20 June, Seattle, WA, United States. **International Association for Spectral Imaging (IASIM) Conference 2018.** http://www.iasim18.iasim.net/.

17–22 June, Dublin, Ireland. **24th International Conference on Spectral Line Shapes ICSLS 2018.** ICSLS2018@dcu.ie, https://www.icsls2018.com/.

18 June–22 February, Santiago de Compostela, Spain. **ISEAC-40 International Conference on Environmental & Food Monitoring.** info@iseac40.es, https://www.iseac40.es/.

19–22 June, Brest, France. **XVIIIth International Symposium on Luminescence Spectrometry (ISLS 2018).** isls2018@sciencesconf.org, https://isls2018.sciencesconf.org/.

20–21 June, Manchester, United Kingdom. **The Proteomics Methods Forum (PMF).** https://www.proteomicsmethodsforum.org.uk/.

20 June, London, United Kingdom. **Analytical Research Forum 2018.** http://www.rsc.org/events/detail/29031/analytical-research-forum-2018-arf18.

20–22 June, Rome, Italy. **7th World Congress on Mass Spectrometry.** https://www.massspectra.com/europe/.

24–28 June, Seattle, Washington, United States. **Metabolomics 2018.** info@metabolomics2018.org, http://metabolomics2018.org/.

24–29 June, Ljubljana, Slovenia. **European Conference on X-Ray Spectrometry (EXRS 2018).** Matjaz Kavcic, exrs2018@ijs.si, https://exrs2018.ijs.si/.

25–29 June, Halifax, Canada. **XVII Chemometrics in Analytical Chemistry (CAC).** Peter Wentzell, peter.wentzell@dal.ca, https://www.cac2018halifax.com/.

25–26 June, Tokyo, Japan. **6th RamanFest Symposium (RamanFest 2018).** ramanfest.jp@horiba.com, http://www.ramanfest.org/ramanfest2018.htm.

26–29 June, Pau, France. **14th European Workshop on Laser Ablation (EWLA 2018).** Christophe Pecheyran, https://ewla2018.sciencesconf.org/.

1–5 July, Nantes, France. **European Magnetic Resonance Meeting (EUROMAR) 2018.** info@euromar2018.org, http://www.euromar2018.org.

2–4 July, London, United Kingdom. **19th Biennial National Atomic Spectroscopy Symposium (BNASS-2018).** http://www.rsc.org/events/detail/26021/bnass-2018-the-19th-biennial-national-atomic-spectroscopy-symposium.

2–4 July, Tihany, Hungary. **16th Hungarian–Italian Symposium on**

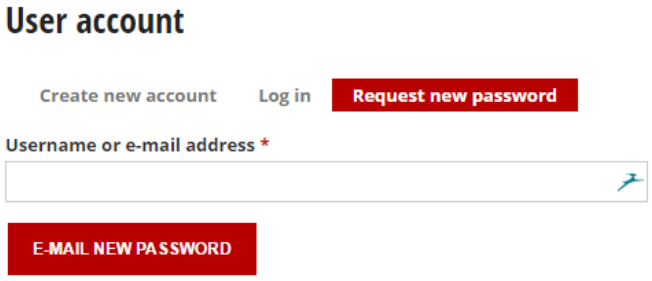
A New Website for *Spectroscopy Europe*

The *Spectroscopy Europe* website which works well on all devices from large screens to smartphones. The URL remains www.spectroscopyeurope.com.

We have migrated all users/readers from the old website but it was impossible, due to built-in security, to transfer users' passwords. I hope you have received an e-mail with a link to log in and reset your password. If you have not or are having any difficulty, here is how to log into the new site.

1) Use the Lost Password facility

From any page, click LOGIN in the main menu, and then "Request new password" to the right of the white-on-red "Log in". Enter your e-mail address and you will receive an e-mail with a "one-time" link that you can use to log in and then change the password to one you want to use. Please also check your details whilst you are in your Profile.

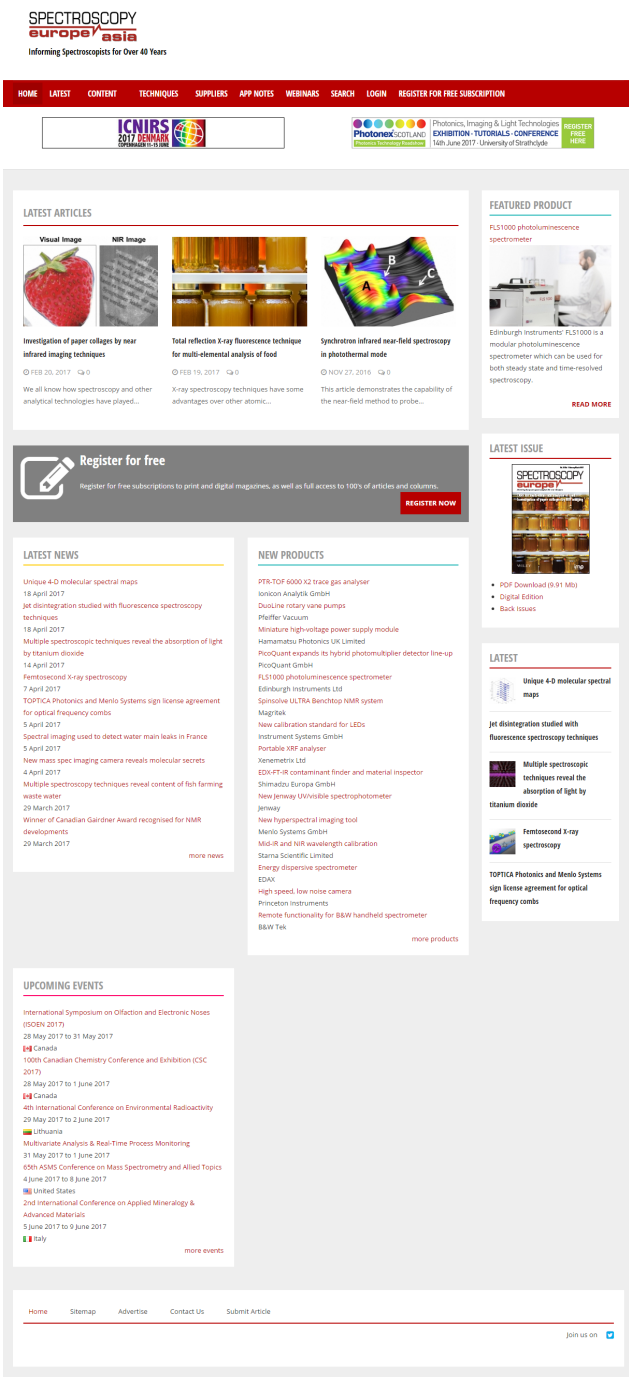


The e-mail usually arrives within seconds; if you do not see it, check your spam folder(s): these types of e-mails are often mistaken for spam.

If this does not work, perhaps because your e-mail address has changed:

2) Ask for help

Just e-mail katie@impublications.com who will check if you have an account and help you log in.



Of course, if you or a colleague don't have an account, you can quickly create one and ensure your continued access to the print version of *Spectroscopy Europe* as well as online access.

www.spectroscopyeurope.com

Spectrochemistry. Viktor G Mihuez, vgmihuez@chem.elte.hu.

2–4 July, London, United Kingdom. **Attosecond and Free Electron Laser Science 2018.** Dr Agapi Emmanouilidou, a.emmanouilidou@ucl.ac.uk, https://eventbooking.stfc.ac.uk/news-events/afels-2018.

9–11 July, Bradford, United Kingdom. **British Society for Proteome Research (BSPR) Annual Scientific Meeting.** http://www.bspr.org/event/bspr-meeting-2018.

15–20 July, Andover, NH, United States. **The Gordon Research Conference on *In Vivo* Magnetic Resonance.** https://www.grc.org/in-vivo-magnetic-resonance-conference/2018/.

15–19 July, Pohang, Korea. **The 15th International Surface X-ray and Neutron Scattering Conference (SXNS15).** Secretariat, sxns15th@gmail.com, www.sxns15.org.

16–18 July, Leeds, United Kingdom. **UPPCON 2018: 15th Uppsala Conference on Electron Capture and Transfer Dissociation Mass Spectrometry.** https://kuhmassy.wixsite.com/uppcon18.

22–26 July, Snowbird, Utah, United States. **Solid-State NMR Symposium.** http://www.rockychem.com/conference/solid-state-nmr-symposium.html.

22–27 July, Utah, United States. **59th Annual Rocky Mountain Conference on Magnetic Resonance.** info@rockychem.com, http://www.rockychem.com/.

23–25 July, Milan, Italy. **2nd World Congress on Pharmaceutical and Chemical Sciences.** pharma@colossalfacet.com, http://colossalfacet.com/pharma-conference/.

29 July–2 August, Chambersburg, PA, United States. **The International Diffuse Reflectance Conference (IDRC) 2018.** info@cnirs.org, www.idrc-chambersburg.org/.

6–10 August, Westminster, Colorado, United States. **67th Annual Denver X-ray Conference (DXC 2018).** dxc@icdd.com, http://www.dxcicdd.com/.

9–10 August, Vancouver, Canada. **ICSSA 2018: 20th International Conference on Spectroscopy and Spectral Analysis.** https://waset.org/conference/2018/08/vancouver/ICSSA/home.

18–24 August, Dublin, Ireland. **XXVIII International Council on Magnetic Resonance in Biological Systems (ICMRBS) Meeting.** icmrbs2018info@keynotepco.ie, www.icmrbs.org.

19–24 August, Coimbra, Portugal. **XXXIV European Congress on Molecular Spectroscopy (EUCMOS 2018).** Rui Fausto, rfausto@ci.uc.pt, http://www.qui.uc.pt/eucmos2018/.

21–24 August, Budapest, Hungary. **International Conference on Many Particle Spectroscopy of Atoms, Molecules, Clusters and Surfaces (MPS 18).** mps2018@atomki.mta.hu, http://ekho94.hu/en.

26–31 August, Florence, Italy. **XXII International Mass Spectrometry Conference (IMSC 2018).** Secretariat, info@imsc2018.it, www.imsc2018.it.

26–31 August, Jeju, Korea. **The 26th International Conference on Raman Spectroscopy (XXVI ICORS).** icors2018@icors2018.org, http://www.icors2018.org/.

26–30 August, Liverpool, United Kingdom. **7th EuCheMS Chemistry Congress.** www.euchems2018.org.

31 August–1 September, Toronto, Canada. **18th International Conference on Pure & Applied Chemistry (IPAC 2018).** appliedchemistry@conferenceescanada.org, https://pureappliedchemistry.conferenceseries.com/.

3–7 September, Bilbao, Spain. **25th International Conference on High Resolution Molecular Spectroscopy (BILBAO2018).** http://www.chem.uni-wuppertal.de/conference/.

3–7 September, Portsmouth, United Kingdom. **8th International Conference on Synchrotron Radiation and Neutrons in Art and Archaeology-SR2A-2018.** Emma Clarke, events@diamond.ac.uk, http://www.diamond.ac.uk/Conference/SR2A-2018.html.

9–13 September, Brescia, Italy. **6th International Conference on Vibrational Optical Activity (VOA-6).** www.voa6.org.

9–13 September, Berlin, Germany. **1st International Conference on Ion Analysis (ICIA 2018).** Dr Wolfgang Frenzel, https://www.icia-conference.net/.

10–13 September, Cambridge, United Kingdom. **39th BMSS Annual Meeting 2018.** Lisa Sage, bmssadmin@btinternet.com, http://www.bmss.org.uk/bmss2018/bmss2018.shtml.

16–19 September, Philadelphia, United States. **Small Molecule NMR Conference (SMASH 2018).** https://www.smashnmr.org/.

17–21 September, Rennes, France. **14th International Conference on the Applications of Magnetic Resonance in Food Science.** mrfood2018@irstea.fr, https://www.foodmr.org/.

17–20 September, Warsaw, Poland. **European Materials Research Society (E-MRS) Fall Meeting.** https://www.european-mrs.com/meetings/2018-fall-meeting.

23–26 September, Amsterdam, Netherlands. **9th Workshop on Hyperspectral Image and Signal Processing: Evolution in Remote Sensing (WHISPERS).** http://ieee-whispers.com.

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- ☐ Medical Sciences
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DIARY

24–28 September, Kazan, Russia. **Modern Development of Magnetic Resonance.** Secretariat, mdmr.kazan@yandex.ru, www.kfti.knc.ru/mdmr/2018.

24–26 September, Ulm, Germany. **15th WITec Confocal Raman Imaging Symposium.** https://witec.de/resources-and-education/events.

29 September–1 October, London, Ontario, Canada. **30th Annual Moot NMR Conference.** mootnmr@gmail.com, http://www.mootnmr.org/.

30 September–3 October, Orlando, FL, United States. **17th Human Proteome Organization World Congress–HUPO 2018.** Secretariat, office@ushupo.org, http://hupo2018.org/.

5–8 October, Tokyo, Japan. **Functional Near-Infrared Spectroscopy (fNIRS 2018).** http://fnirs2018.org/.

10–11 October, Coventry, United Kingdom. **Hyperspectral Imaging and Applications Conference (HSI2018).** Brenda Hargreaves, brenda@xmark-media.com, https://www.hsi2018.com/.

15–16 October, Paris, France. **World Congress on Advanced Laser, Optics and Photonics.** https://lasers-optics-photonics.pulsusconference.com/.

16–17 October, Galveston, TX, United States. **Gulf Coast Conference 2018.** https://www.gulfcoastconference.com/.

21–26 October, Atlanta, GA, United States. **45th Annual Conference of Federation of Analytical Chemistry and Spectroscopy Societies (SciX2018).** facss@facss.org, http://www.scixconference.org.

21–26 October, Long Beach, CA, United States. **AVS 65th International Symposium and Exhibition.** https://www.avs.org/symposium.

2–6 November, Pacific Grove, California, United States. **34th Asilomar Conference on Mass Spectrometry: Quantitative Analysis of Posttranslational Modifications by Mass Spectrometry.** info@asms.org, http://www.asms.org/conferences/asilomar-conference/asilomar-conference-homepage.

4–7 November, Washington, DC, United States. **American Association of Pharmaceutical Scientists (AAPS) 2018 Annual Meeting.** aaps@aaps.org, www.aaps.org/annualmeeting/.

7 November, Stuttgart, Germany. **European Photonics Industry Consortium (EPIC) Meeting on Hyperspectral Imaging at VISION.** http://www.epic-assoc.com/epic-meeting-on-hyperspectral-imaging-at-vision/.

12–14 November, Princeton, New Jersey, United States. **Eastern Analytical Symposium and Exposition EAS 2018.** askEAS@eas.org, http://easinc.org/wordpress/.

Courses

2018

8–14 July, Dubrovnik, Croatia. **12th Summer School in Mass Spectrometry in Biotechnology and Medicine (MSBM).** Prof. David Goodlett, msbm.dubrovnik@gmail.com, www.msbm.org.

Exhibitions

2018

27–28 June, Essen, Germany. **Plastics Recycling World Exhibition.** www.plasticsrecyclingworldexpo.com/eu/.

23–26 September, Amsterdam, Netherlands. **Spectro Expo: Science. Technology. Applications.** http://www.spectroexpo.com/.

21–22 November, Telford, United Kingdom. **WWEM 2018: The 8th International Conference and Exhibition on Water, Wasterwater & Environmental Monitoring.** info@ilmexhibitions.com, https://www.ilmexhibitions.com/wwem/.

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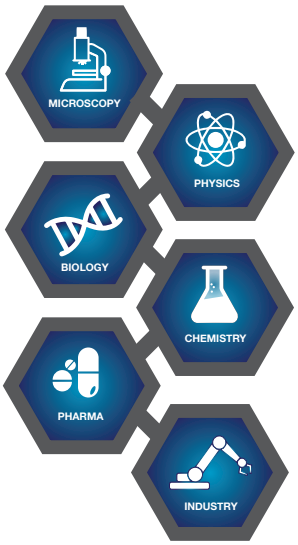

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