

Vol. 29 No. 3 June/July 2017

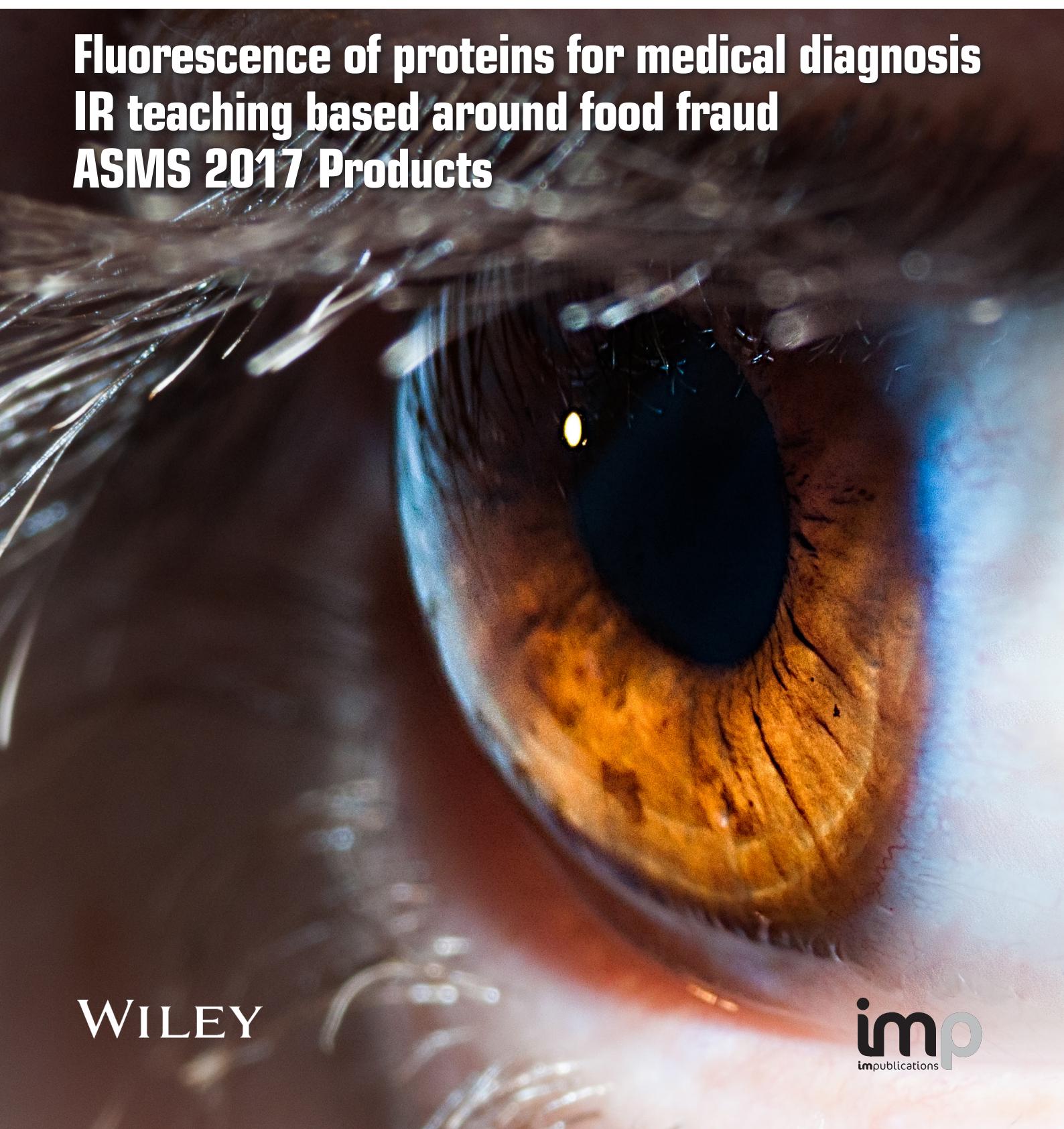
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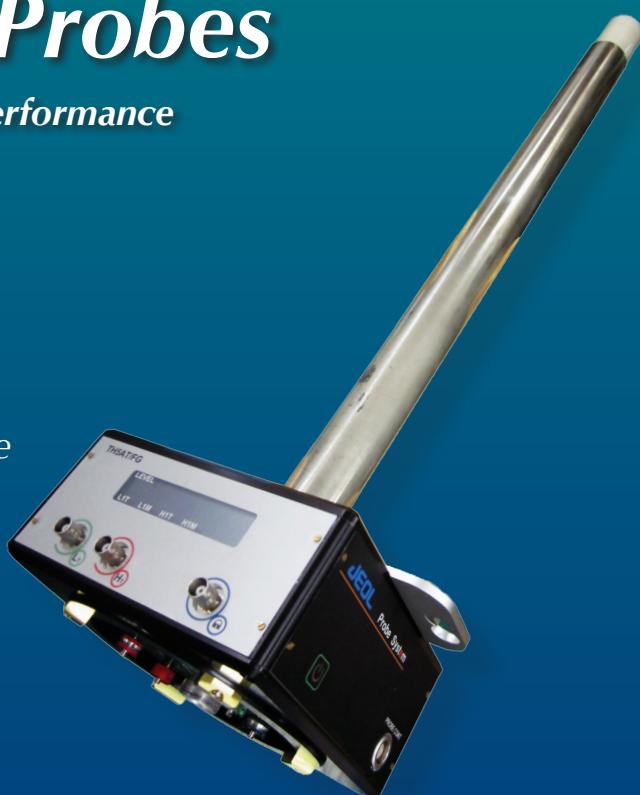


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EDITORIAL

There is a definite practical theme to this issue. Our regular columns all offer practical information and suggestions.

Dmitry Gakamsky and Anna Gakamsky start off this issue with their article on "Intrinsic fluorescence of proteins as a medical diagnostic tool". They describe how fluorescence may be used to diagnose cataracts in human eye lenses. Further, it may also be able to grade cataracts and monitor the disease's progress, which may help discover metabolic and ambient factors that influence the progress of the disease.

Colette Germon, Tony Davies and Paul Jones look at "Combining teaching chemometrics, with attenuated total reflection-infrared spectroscopy and food authentication". They describe a teaching project based around the detection of food fraud. It is a good example of teaching spectroscopic data handling

and advanced analysis techniques. They have investigated how adulteration and misrepresentation of meat and fish can be detected, as well as whether frozen and then thawed fish could be differentiated from chilled fish.

Peter Jenks and Alan Nichols embark on "ISO/IEC 17025: a never-ending journey". They describe what is behind this recent standard and give valuable advice as to what to expect from an audit. Newcomers may find the requirements daunting, but Peter and Alan's guidance will prove most helpful.

In the Sampling Column, Kim Esbensen and Claas Wagner continue their look at process sampling in "Process sampling: the importance of correct increment extraction". Following last issue's introductory column, in this issue they provide many practical examples and case histories demonstrating

the good and the terrible from real-world sampling.

There are also a three-page Product Focus on Imaging Spectroscopy, details on new products released at the major American Society for Mass Spectrometry (ASMS) conference, as well as more general new product introductions and an extensive diary of future events.

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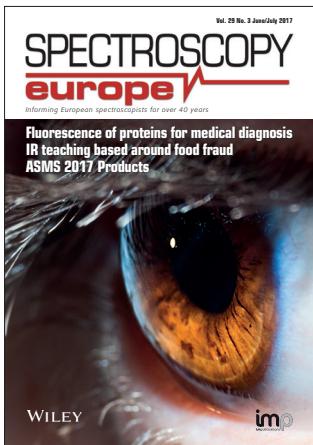
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Fluorescence may be used to diagnose cataracts in human eye lenses. Find out more in the article starting on page 6.

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Intrinsic fluorescence of proteins as a medical diagnostic tool

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Fluorescence methods have found a wide range of important applications in science and technology. Compared with absorption, fluorescence gives a many-fold higher sensitivity and specificity. In addition, fluorescence possesses several important parameters such as intensity, excitation and emission spectra, polarisation, lifetime, and quantum yield. These parameters are functions of solvent nature, temperature, polarity and viscosity, and can be used to research the structure and function of various systems and for analytical applications. For example, fluorescence polarisation and non-radiative resonance energy transfer are used for detection of biomarkers in *in vitro* medical diagnostics.¹

However, the use of fluorescence in *in vivo* diagnostics is hindered by the limited penetration of the visible light into living tissue or requires the use of fibre-optic probes. At the same time, proteins, being a major component of living organisms, should have diagnostic and prognostic potential.

The intrinsic fluorescence of proteins is caused by three amino acid residues with aromatic side chains: phenylalanine, tyrosine and tryptophan. Out of these three, the latter plays the most important role due to its excitation and emission spectra having the longest wavelength (near the UV range) and longest lifetime. These features simplify measurements of its fluorescence and allow for its selective detection. However, contrary to its universal

nature, tryptophan fluorescence of proteins has been predominantly used only in research to study protein conformational changes or protein–protein interactions. A question arises whether protein fluorescence can be used in medical diagnostics?

Success in understanding the role of protein conformation in homeostasis of living organisms² could provide solid support to this type of diagnostics. It has become apparent that protein post-translational modifications (PTM), causing protein mis-folding and aggregation, are responsible for a broad range of diseases, such as Parkinson's and Alzheimer's produced by degeneration in the brain tissue, cardiomyopathy caused by degeneration of the heart muscles or cataract caused by colouration and aggregation of the eye lens proteins.

Red-edge excitation of eye lens proteins

This generic basis for conformational disorders led us to conceive whether it would be possible to use protein fluorescence to detect changes in the eye lens structure. The eye lens created by nature is a perfectly transparent organ that represents an excellent experimental model for fluorescence measurements. A challenge in the use of tryptophan (Trp) fluorescence for cataract diagnostics is the incredibly high concentration of the eye lens proteins (crystallins) (200–400 mg mL⁻¹) which

makes the lens' optical density in the spectral range of the Trp absorption band (260–300 nm) a hundred of units. Such a high optical density does not allow the excitation light to penetrate deeper than a hundred of microns into the lens body. However, this experimental challenge can be overcome by the use of the so-called red-edge excitation of Trp; meaning excitation on the long-wavelength ("red") slope of the absorption band.³ First, due to the steepness of this slope, the optical density drops significantly and an excitation light of 317 nm wavelength travels throughout the lens with an attenuation of just about 25% (Figure 1, left panel).

Second, the red-edge excitation selectively brings to the excited state a fraction of Trp side chains situated in a polar environment ("red-shifted" fraction). This fraction correlates either with all side chains of misfolded proteins exposed to an aqueous environment, or with side chains of folded proteins situated on the surface or in hydrophilic "pockets". Hence, the combination of these two features gives the possibility to excite the "red-shifted" fraction throughout the lens.

Earlier, this method was successfully used to study the structure and function of class I Major Histocompatibility Complex proteins.⁴ With a view to applying this method to cataract diagnostics, we measured the fluorescence of soluble crystallins as a function of excitation wavelength. It was found that the fluorescence spectra exhibited

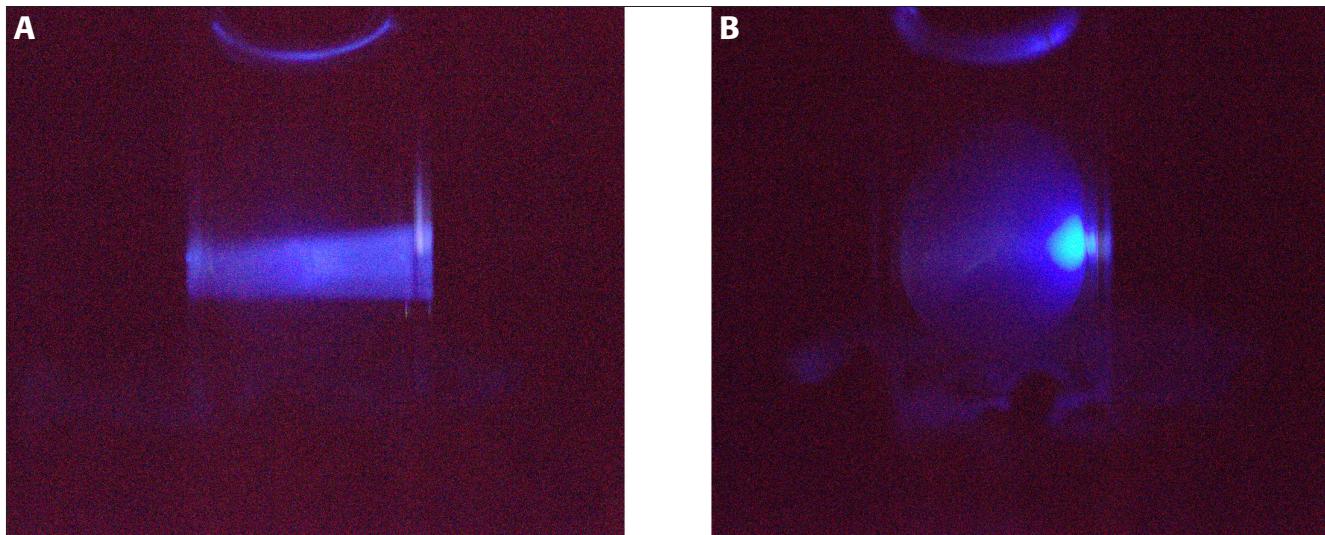


Figure 1. Excitation of eye lens fluorescence in a normal (A) and UV-irradiated (B) porcine lens by a 317 nm LED.

a gradual red shift proceeding along with the shift of the excitation wavelength towards the red edge of the Trp absorption spectrum (bathochromic shift). In accord with the prediction of the red-edge model, the emission spectrum was maximally shifted to the red position when the protein was dissolved in 8 M urea, which is known to have a strong denaturing property.⁵ This successful result encouraged us to employ the method to a whole eye lens. We compared the red-edge fluorescence of a normal and UV-irradiated porcine lens, which was used as a model of cataract. Results of this experiment are shown in Figure 2.

In part, these results are consistent with the model, as the emission band of the UV-irradiated lens showed a greater amplitude red-shift. However, there is a significant difference: the emission spectra of the normal and irradiated lenses show an unexpected additional band on the red slope of the emission spectrum. The UV irradiation decreased the amplitude of the Trp emission band and increased the intensity of the additional band. This situation seems to indicate that the red-shifted fraction of Trp converts to a newly formed fluorophore with emission maximum at ~440 nm. It was also found that the ratio of the 440 nm band to the Trp band positively

correlates with the irradiation dose⁵ and the sensitivity of this ratiometric parameter is much greater than the sensitivity of the slit-lamp method of light scattering. To be able to use this additional fluorescence band for diagnostic purposes, it is important to understand its chemical nature.

Decomposition: a key approach for spectra analysis

Mass spectrometry of irradiated porcine lens solubilised proteins and solubilised human post-operative protein samples revealed that, together with tryptophan

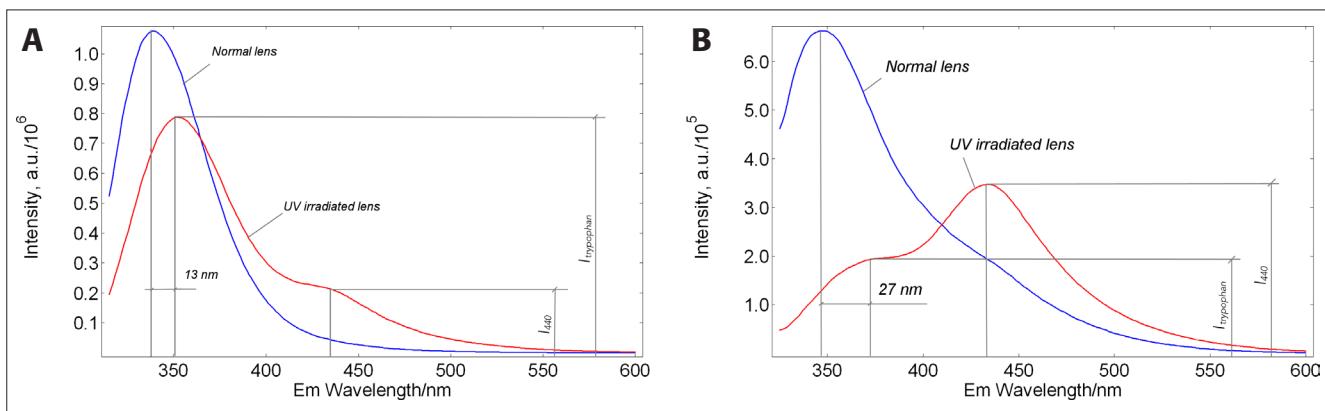


Figure 2. Red-edge excitation of eye lens proteins. Corrected fluorescence spectra of a normal and UV-irradiated porcine lens measured in a FLS980 spectrometer in 90° geometry. Excitation at 305 nm (A) caused a red shift of Trp emission by 13 nm and the appearance of a low-intensity, additional emission band at 440 nm ($I_{440}/I_{Trp} < 1$). While upon excitation at 315 nm (B) the Trp emission peak is shifted by 27 nm and the relative intensity of the addition band is increased ($I_{440}/I_{Trp} > 1$).

residues, these proteins contain two primary products of Trp: hydroxytryptophan (OH-Trp) and N-formylkynurenine (NFK) and two downstream products, kynurenine (Kyn) and hydroxykynurenine (OH-Kyn). In addition, a fluorescent derivative of arginine, argyrimidine (ArgP), was identified.⁶ Importantly, all the fluorophores could be excited by the same wavelength of 317 nm, which was earlier found as a trade-off wavelength for deep lens penetration and Trp excitation.

To make this method semi-quantitative, we need to normalise the non-Trp emission against a reference signal. This signal should vary to the same extent as the emission of the fluorescent PTMs as a function of experimental conditions (intensity of excitation, geometry etc.). Since the concentration of Trp remains nearly constant in spite of the modifications (1–2%), emission

of its "red-shifted" fraction ideally fits this purpose.

Knowledge of the spectral properties of each fluorescence component greatly simplifies calculations of concentration of the individual components, which can be determined by decomposing the total emission spectrum. Figure 3 shows a typical example of the spectral decomposition emission spectrum measured from a post-operative emulsified sample with the second grade of nuclear cataract (NC++). The quality of the decomposition given by the shape and amplitude of the residuals function suggests that the elementary spectral components were correctly determined. We found that, for a statistically representative number of experimental samples, emission of OH-Trp, NFK and ArgP comprised the major portion of the total emission spectra. Assuming that the accumulation of PTMs causes

cataractogenesis, we correlated the cumulative contribution of these three components with the grade of cataract measured by a slit-lamp.⁶ The data revealed a Pearson's coefficient of correlation of 0.93. A smaller (0.68), but still significant, coefficient was found for the correlation of the cumulative emission of these fluorescent modifications with donors' age for 17 post-mortem lenses. Thus, this method can be used for a non-invasive, semi-quantitative cataract diagnosis, with greatly increased sensitivity over current techniques.

A wide range of PTMs in crystallins was identified by mass spectrometry and it is likely that all modifications may contribute to protein degradation. A question therefore arises—why does the fluorescent fraction, from all possible PTMs, correlate with cataract grade and age? While the significance of every PTM is not clearly understood, we

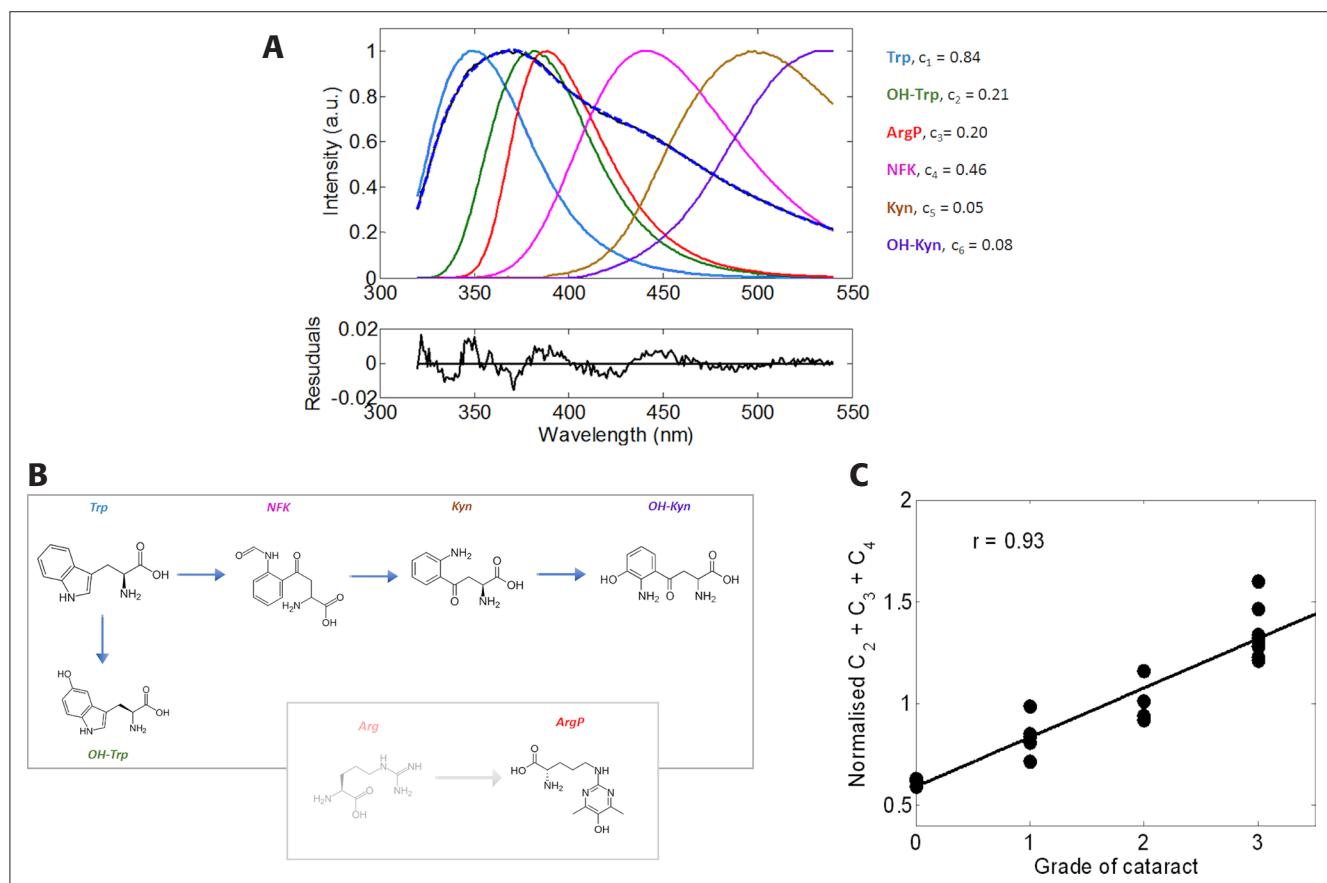


Figure 3. Fluorescent spectrum of the insoluble fraction of emulsified cataractous sample (A, black) and its decomposition determined from spectra of identified fluorescent derivatives of Trp and ArgP (B). Correlation of cataract grade with the normalised cumulative fraction for 21 emulsified eye lens proteins (C).

hypothesise that the fluorescent fraction represents the total modification statistics. Moreover, some specific fluorescent PTMs has been shown to play important roles in cataractogenesis by changing the stability and interactions of proteins. Ghosh *et al.*⁷ demonstrated that the interaction between the *N*-terminal W60 and the core domain R123 plays a role in the monomeric interaction of α -crystallins involved in the formation of the α -crystallin oligomeric structure. The assembly of α -crystallins into large oligomeric complexes is believed to be central to the chaperone-like function of this protein.

The formation of NFK from Trp is mediated by the interaction with singlet oxygen and, therefore, the concentration of NFK can be used as a marker of protein oxidative stress. Moreover, NFK possesses photosensitising properties, which make it the most biologically important photo-product of Trp because its formation facilitates the production of hydrogen peroxide in irradiated Trp solutions. Hence, the formation of NFK can stimulate modifications of other side chains.

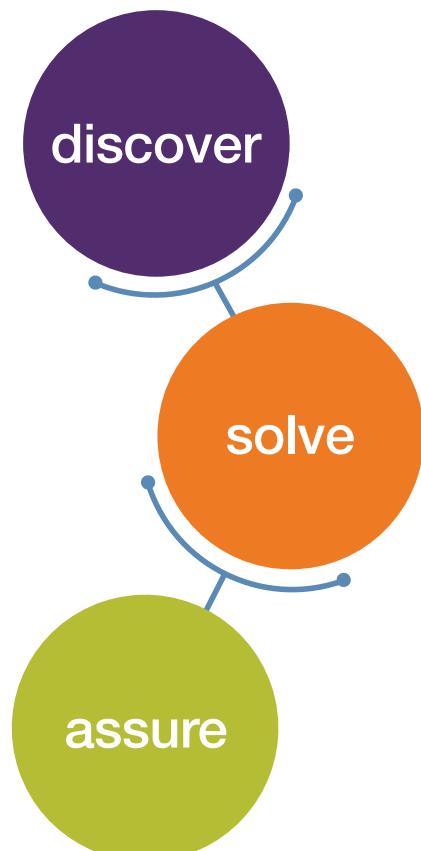
We found abundant formation of ArgP in α -crystallins and, in particular, the conversion of Arg120 to ArgP in α -crystallin B is likely to affect its chaperone-like function. Vicart *et al.*⁸ identified the Arg120Gly mutation in α -crystallin B as responsible for desmin-related myopathy in a French family. It has also been shown that cataract and myopathy pathologies in α -B-Arg120Gly knock-in mice share common mechanisms, and mutation of the Arg120 residue in the human α -crystallin causes a partial loss of its chaperone-like activity. All these findings strongly suggest that the concentration of Arg120 should negatively correlate with the chaperone-like function of α -crystallin and hence may be used as a marker of cataract.

In summary, we discussed here a novel, non-invasive method of semi-quantitative determination of the concentrations of fluorescent PTMs

in the lens based on simultaneous measurements of the fluorescence emission spectra of Trp, its photodegradation products and ArgP, which can be used for diagnostics of cataract at the molecular level. This makes the method useful for cataract grading and for monitoring cataractogenesis over a period of time. The latter may help in elucidation of various metabolic and ambient factors contributing to cataractogenesis. The possibility to monitor changes in the lens structure at the molecular level may also facilitate the development of cataract medications, aimed at slowing down the cataractogenic processes and prolonging lens homeostasis.

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Combining teaching chemometrics with attenuated total reflection–infrared spectroscopy and food authentication

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With numerous food-fraud cases being revealed by the media and catching significant public attention, a training project which embodies the establishment of "facts" amongst all the hype is a very good idea. Intergovernmental regulations also control fish catch quotas, which has led to some fraudulent mislabelling of cheaper fish, which then also brings the accuracy of the fish catch data and subsequent fisheries management into doubt. Rapid, simple and robust analytical spectroscopic techniques have the potential to unmask these food fraudsters. Recently, I have enjoyed being involved on the edges of a very nicely crafted and fun experimental project which cleverly brings together learning goals around analytical science, more advanced spectroscopic training, as well as fundamental understandings around food authentication and the applicability of chemometrics techniques.

The problem posed

As part of an MSc project, a challenge was set to see how attenuated total reflection–infrared spectroscopy (ATR-IR) could be used as part of a simple

testing methodology for adulteration of food. The experimental design looked not only at mislabelling the source of meat or fish, but was also extended to investigate if the technique could help identify the selling of frozen and then thawed food products as "fresh". One of the teaching goals is, of course, that you need to sample as widely as possible if you are going to fully cover the scope of the problem. However, this is after all a teaching opportunity rather than a full-scale national screening programme and the lessons learnt would be equally applicable at national or international level.

Representative meat samples chosen

The size of the experimental design can be very nicely scaled to the amount of laboratory instrument time available at the teaching location, as most of the lessons learnt will be valid regardless of the breadth of samples sourced. As several months were available in the current course example, a wide range of meats and fish were added to the design. Processed foods are tough products to clearly characterise and the

project started off on pork (shoulder) and beef (rump) samples from a reputable local source of traceable meat. The raw materials were made up into experimental beef burgers of varying mixture concentrations to simulate label fraud from pure beef to pure pork in 10% increments. Two different locations on each sample burger were sampled and three repeat measurements were taken at each location.

These measurements allowed the student to look first for isolated peaks which might be capable of being quantified (not possible) and then to realise the value of chemometric analyses in classifying adulterated vs non-adulterated and creating a regression model for the degree of adulteration. This was a nice combination of practical manual laboratory sample preparation work, analytical spectroscopy using a modern simple accessory and more advanced data analysis applications.

For "unknown" samples, luxury-branded, high-end supermarket outlet burgers were taken and analysed using the same methodology of two locations on the burger and three repeat measurements.



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Table 1

Fish samples	
Common name	Latin name
Mackerel	<i>Scomber scomber</i>
Sea bass	<i>Dicentrarchus labrax</i>
Salmon	<i>Salmo salar</i>
Smoked haddock	<i>Melanogrammus aeglefinus</i>
Cod	<i>Gadus morhua</i>
Smoked river cobbler	<i>Pangasius hypophthalmus</i>
Haddock loin	<i>Melanogrammus aeglefinus</i>
British hake	<i>Merluccius merluccius</i>
Plaice	<i>Pleuronectes platessa</i>
Pollock	<i>Pollachius</i>
Lemon sole	<i>Microstomus kitt</i>
Sea bream	<i>Sparidae</i>
Halibut	<i>Hippoglossus hippoglossus</i>

The final issue this piece of work was configured to address was the question of frozen then thawed meat potentially entering the food chain under the mislabelling of fresh. Essentially the same experimental design as above was conducted but using meat which had been frozen at -12°C for three weeks, including the supermarket brand products for comparison, yielding 84 samples for analysis.

Something fishy on the spectrometer

Moving on to fish samples allowed a broad range of samples to be analysed whose spectra were at times extremely similar (see Table 1). Some fish samples had undergone "pre-processing", such as smoking or had other distinguishing claims such as the location of the source on the fish itself—presumably claims which were intended to imply added quality to the labelling of the product and hence increased price.

Keeping with the theme of processed foods being the easiest product type with which to hide food fraud, the fish samples were all homogenised and prepared into fishcakes before undergoing infrared analysis using the same methodology as in the meat case. Again, three shop-bought "cod" fishcakes were

used as "unknowns" against which to test. Finally, fish stock samples were also frozen for a period of weeks to test for the fresh vs frozen/thawed storyline and the measurement sequence repeated.

Equipment and software

The spectra were recorded using a Perkin-Elmer UATR Two FT-IR spectrometer with a one-bounce diamond crystal ATR accessory. Data were acquired by accumulating four scans of 500–4000 cm^{-1} and the background recorded every six spectra. The cell was thoroughly cleaned between samples. As ATR spectra can be pressure sensitive this was tested for the samples in this study at two different pressures and as no noticeable difference was found

the lower pressure was selected to reduce sample compression.

The Unscrambler software package from CAMO was used to carry out the chemometric analyses using partial least squares (PLS) for the quantitative analysis and principal component analysis (PCA) for classification. The only pre-processing considered was wavelength selection at four different ranges, 4000–400 cm^{-1} , 4000–1000 cm^{-1} , 4000–2500 cm^{-1} and the fingerprint region (1850–1000 cm^{-1}). A "leave-one-out" full cross-validation was used to test the models created.

Some meaty results

The PLS analysis of the beef/pork mixtures went well (see, for example, Figure 1). Regardless of the wavelength range selected or whether the frozen/thawed samples were analysed, the R^2 values showed good calibrations were obtained, ranging from 0.97 to 0.99. The best results were obtained for the 4000–1000 cm^{-1} wavelength range with 0.99.

The supermarket burgers when analysed, pleasingly showed good correlation between the label values, however, Figure 2 clearly shows that these burgers contained significantly more fat at the cost of the protein levels than those prepared from the fresh meat.

Some fishy results

The study results for the potential fish adulteration also delivered excellent calibration results (e.g. Figure 3 for Cod with Haddock adulteration with R^2 value of 0.99). This issue occasionally rises its head in the normal newspapers for public consumption, such as

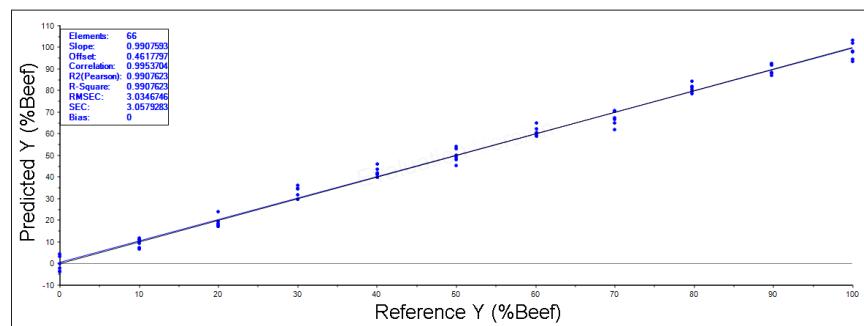


Figure 1. PLS analysis of the fresh meat.

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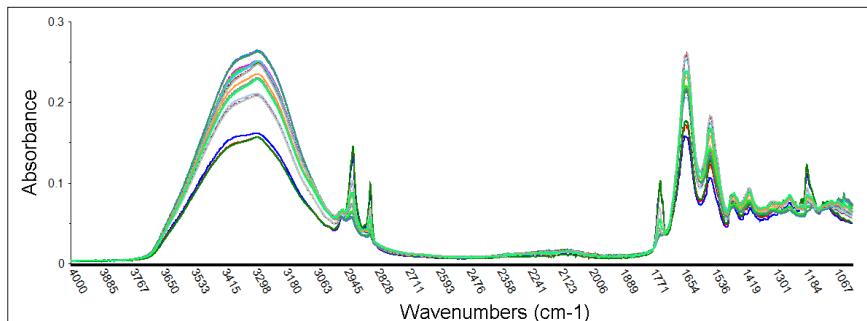


Figure 2. Variation of spectra obtained from the supermarket luxury branded beef burgers at wavelength range 4000–1000 cm⁻¹.

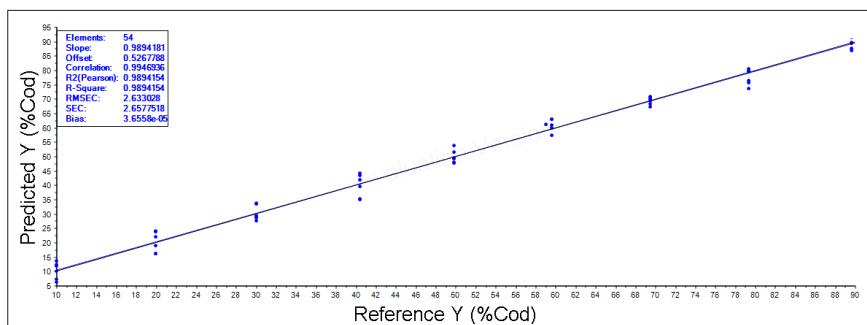


Figure 3. PLS regression for frozen/thawed Cod with Haddock adulteration (10–90%) calculation data.

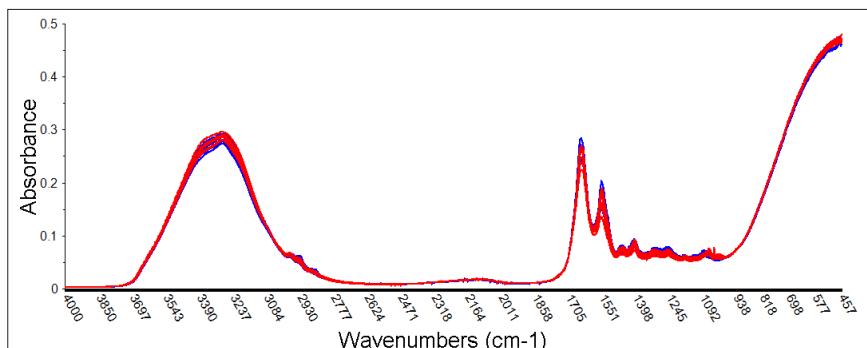


Figure 4. The similarity of the infrared spectra of two fish species is substantially greater than between the two meat sources analysed.

a report on figures supplied by councils to the UK Food Standards Agency indicating that 41 of 303 checks on packaged frozen or chilled fish and in catering businesses did not meet labelling requirements.¹ They reported that

in 27 cases the fish described as Cod was another species, such as Haddock, Whiting or Pollock. Other types of fish were also incorrectly described among other breaches of labelling rules. In Ireland, one DNA testing study

reportedly found that 28% of the fish labelled as Cod from 226 products in 131 supermarkets, fishmongers and takeaways were actually substitutes, such as Pollock and Whiting.

Figure 4 shows that the infrared spectra of some of the fish species selected are remarkably similar, in this case Cod and Haddock. This makes the classification of species difficult.

Summary

Before all our food scientists leap to their Facebook and Twitter accounts to decry the breadth of the work done, it is worth reminding ourselves that this is an innovative approach to helping teach and embed understanding in students of some pretty complex and difficult topics. If we look into the literature, one of the interesting challenges in, for example, the area of fish labelling is that the common names for fish vary from location to location. FishBase^{2,3} is a great source of information in this respect and, when searched, showed that "Cod" was used in the USA alone for six different species, only one of which is the same as used in Europe. Also, there is no species overlap between what you will be served in the USA and Europe and Australia where "Cod" may be two different species, one of which is a Perch.

All in all, I was very impressed with the development of this particular project and its potential future use as a teaching tool for spectroscopic data handling and advanced analysis techniques.

If you have similar examples which we can learn from please get in touch!

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ISO/IEC 17025: a never-ending journey

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It seems that there is no limit to the number of laboratories seeking and maintaining accreditation to ISO/IEC 17025. Why is this?

Properly described as "ISO/IEC 17025 General Requirements for the Competence of Testing and Calibration Laboratories", this standard has been around since 1999, but its origins lie in ISO Guide 25 and European Standard EN4501.

The increase in accreditation to ISO/IEC 17025 started in around 2000 and is driven by the demands of both regulatory authorities and users of laboratory testing services who each want to be certain that the data they "buy" is fit for purpose. The generally accepted means of achieving this objective is to require that laboratories demonstrate, via third party attestation, a certain level of competence and that they have in place a process that ensures that they are on a never-ending journey of improvement to the quality system. The most popular route to do this is, at least within the measurement and testing environment, accreditation to ISO/IEC 17025.

In common with other accreditation standards of the ISO 17000 series (and unlike most ISO standards for management systems), ISO/IEC 17025 requires continual improvement. Regular internal audits are intended to reveal opportunities to improve the test or calibration procedure, reducing, for example, uncertainty and increasing consistency. In addition, an accredited laboratory is expected to keep abreast of scientific and technological advances in areas

relevant to the test method or procedure.

Third party auditing (assessment) of an accredited laboratory is normally carried out by the national organisation responsible for accreditation, in the UK this is UKAS, the United Kingdom Accreditation Service. Laboratories are therefore accredited under ISO/IEC 17025, rather than certified or registered as in the ISO 9000 series).

The first laboratory accreditation bodies to be established were NATA in Australia (1947) and TELARC in New Zealand (1973). Most other bodies around the world are based on the NATA/TELARC model including UKAS! In most countries, excluding the United States of America and Canada, there is a single, national Accreditation Body. In the USA there are, at the time of writing, five and in Canada, two.

In short, accreditation differs from certification by adding the concept of a third party, the accreditation body (AB) attesting to technical competence within a laboratory in addition to its adherence and operation under a documented quality system, specific to a Scope of Accreditation.

The originators of ISO/IEC 17025 had a philosophy that accreditation to this new standard should ensure that data from an accredited testing laboratory would be accepted by everyone, so to make it possible for accreditation bodies to recognise each other's accreditations, the International Laboratory Accreditation Cooperation (ILAC) worked to establish methods of

evaluating accreditation bodies against another ISO/CASCO Standard, ISO/IEC 17011.

Around the world, geo-political regions such as the European Community, and Asia-Pacific, the Americas and others, established regional co-operatives to manage the work needed to achieve mutual recognition. These regional bodies (all working within the ILAC umbrella) include:

- European Accreditation Cooperation (EA),
- Asia Pacific Laboratory Accreditation Cooperation (APLAC),
- Southern Africa Accreditation Cooperation (SADCA) and
- Inter-American Accreditation Cooperation (IAAC).

ISO/IEC 17025 has become the foundation for a quality management system that covers all the activity that a laboratory may want to undertake and provides the structure against which it can be accredited by the AB. Like most ISO/IEC Standards in the "17000" series it includes the following five main sections:

- Scope,
- Normative references,
- Terms and definitions,
- Management requirements and
- Technical requirements.

The two main sections in ISO/IEC 17025 are Management Requirements and Technical Requirements. Management Requirements are primarily related to the operation and effectiveness of the quality management system within the laboratory. Technical

QUALITY MATTERS

Requirements include factors which determines the correctness and reliability of the tests and calibrations performed in the laboratory.

As more testing laboratories achieve accreditation to ISO/IEC 17025, those that do not will find their options in the marketplace limited, hence the steady stream of laboratories seeking accreditation. To the inexperienced the pathway to accreditation can seem daunting to the laboratory: indeed, the ISO/IEC 17025 standard has many management and technical requirements that may be new to a routine analytical laboratory. A common misconception among laboratories seeking accreditation is that prior to the initial assessment they only have to write a Quality Manual and develop some procedures. This is far from the case, as the reality is that the AB's assessor will be looking for objective evidence that the laboratory meets the requirements of the standard. Therefore, the laboratory must be operating fully to the standard **prior to** the initial assessment. To be able to do so inevitably requires either the external training of an in-house project lead or the appointment of a third-party consultant.

This need for external support has led to a sophisticated industry of training and consultant support aimed at "helping" testing laboratories achieve and maintain accreditation to ISO/IEC 17025. Most such services are far from free, it is possible to spend extravagantly on preparation for accreditation to ISO/IEC 17025!

As well as demonstrating competence a lab must show that the associated paperwork and records are all correct and up to date. The main documentation areas given below.

Quality manual

The quality manual is the heart of any quality management system. Anyone assessing a lab needs to have a copy available. Needless to say, it must be fit for purpose!

Standard operating procedures

An assessor will want to verify that you have a SOP for all procedures relevant

to your proposed scope of accreditation and that they are up to date and relate back to the methods listed in the scope of accreditation.

Normative documents

Any ISO or ILAC Document referenced in your QM should be available for inspection and should be the most up to date version!

Scope of accreditation

A lab's scope of accreditation is the best advertisement it can use. Make sure that it is always up to date and available for assessors as they will use it when assessing the competency of your laboratory personnel and capability.

Master document list

Your master document list references all of the documents that form your quality management system. As with your Scope, it must be up to date.

Approved subcontractors list

If you subcontract tests and(or) calibrations, you must have a list of your approved subcontractors and it must be up to date and available. It should also include a copy of the subcontractor's scope of accreditation.

Approved suppliers list

As with the Subcontractors list, it must be up to date and available.

Complaint log

Any assessor will want to be certain that complaints are logged and documented in accordance with the quality manual.

Non-conformity reports

Assessors like to know what non-conformity events a laboratory has encountered and what corrective and(or) preventative actions, including root cause analysis, have been implemented to control them.

Corrective and preventative actions

Prepare copies of all corrective action records and make them available for your assessors to review.

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Internal audits

Internal Audits are at the heart of a quality manual and assessors want to see any findings from internal audit. Again, make sure that copies are available.

Management reviews

Assessors want to see that company management is involved in the quality of laboratory operations. Therefore, it is important to evidence management reviews and their findings.

Training records and qualifications

How well laboratory staff are trained and qualified is important and assessors will ask to see their training records. They will want to know how training goals are formulated, implemented and monitored.

In this series of articles we will focus on the key Technical Requirements of ISO/IEC 17025 and look in some detail at the requirements for and the use of Traceability, Proficiency Testing and Uncertainty: the aim is to start to demystify the process and in so doing help our readers better prepare and communicate with those involved with achieving accreditation.

We will start with a topic which has engaged and engrossed the authors for more than 20 years, Reference Materials and Certified Reference Materials. Previous articles have described how a RM or CRM should be selected and the pitfalls to avoid. Here we look at the use of RMs in demonstrating Traceability within an ISO/IEC 17025 accredited laboratory.

The way a laboratory uses Reference Materials (RMs) and Certified Reference Materials (CRMs) is one of the key laboratory activities that will be assessed for accreditation. There are many different types of RM and CRM and each have specific uses: the most common forms are single and multi-component analytes in a solution form and matrix RMs and CRMs, where the analytes are present in a matrix that is similar to the type of matrix that forms the sample to be tested, for example pollutants in soil.

RMs have many uses in the analytical laboratory, including instrument qualifica-

tion and calibration, method validation, within and between batch QC checks etc.

ISO/IEC 17025 requires that measurements be Traceable to the SI, a National Metrology Institute (NMI) or in some cases a recognised Authoritative organisation (e.g., the United States Pharmacopeia or the European Pharmacopoeia). Originally this meant that the laboratory must obtain its RMs and CRMs directly from an NMI, but in recent years it means that sourcing is normally from an ISO Guide 34/ISO 17034 accredited Reference Material Producer or an Authoritative organisation.

How does a laboratory choose between using a CRM or an RM? The answer is simple: check with the accreditation body! Most if not all Accreditation Bodies require the use of Certified Reference Materials (CRMs) if they are reasonably available and only when no such CRM is available can a RM be substituted.

In many industries and especially in academic research it has been traditional to use "home-made standards". This practice is generally discouraged in accredited laboratories, primarily because in-house production of RMs generally does not meet the Traceability requirement, unless the laboratory produces them in compliance with the requirements of ISO Guide 34/ISO 17034. In 2014, ISO published ISO Guide 80, that outlines the essential characteristics of reference materials for quality control (QC) purposes, and describes the processes by which they can be prepared by competent staff within the facility in which they will be used. The preparation of QCMs should involve homogeneity and stability assessments, and a limited characterisation of the material to provide an indication of its relevant property values and their variation, prior to use. It is important to understand that QCMs are not usually considered suitable for instrument qualification and calibration or method validation use.

It is common, when a laboratory is first assessed to find instances of the use of in-house RMs that do not meet the Traceability requirement. Typically, the

laboratory has been preparing in-house RMs for a long time, has technically valid procedures and has difficulty understanding why this is not acceptable. It is also very unusual to find that their procedures fulfil the requirements of a CRM as defined by ISO Guide 34/ISO 17034. It is also common to find a laboratory using procured RMs that is believed to be CRMs. Unfortunately, the marketplace is confusing and not always easy to distinguish CRMs from RMs. It is also not uncommon for an ISO Guide 34/ISO 17034 accredited organisation to issue RMs that do not meet the Traceability requirements, so assumptions are not advisable.

So, what is a laboratory to do? First, be aware of the meaning of the Traceability requirement. Accreditation Bodies may have different policies on the stringency of their interpretation. Try to find CRMs for all RM needs, either from an NMI, an Accredited Reference Material Producer or an Authoritative organisation. If a suitable CRM cannot be found, be sure to document the effort in order to justify the use of RMs. Next, look at Certificates from suppliers that might supply CRMs. Look for the terms "Accredited to ISO Guide 34 or ISO 17034". You can also review their Scope of Accreditation, typically found on the website of their AB.

Things to be wary of:

- Designating a CRM without any mention of Accreditation to ISO Guide 34/ISO 17034.
- Accreditation to ISO/IEC 17025 only.
- Reference to ISO 9001 Quality System.
- Claims to traceability to NIST, without any accreditation credentials.

In conclusion, a laboratory properly using RMs and CRMs for its analytical measurements should have no problem meeting the Traceability requirement for the use of Reference Materials in their Accreditation Assessment.

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SAMPLING COLUMN

Process sampling: the importance of correct increment extraction

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After the previous column's introduction to the *why*, the *how* and the *technicalities* involved in process sampling and variographic analysis, it is time for a bonanza of applications and case histories covering as broad a practical scope as possible. In this column, we introduce the critical *prerequisites* for the *variographic experiment*, by focusing on the importance of TOS-correct increment extraction for proper variographics. This issue cannot be overemphasised.

Moving, or static, 1-dimensional lots: increment cutting must be TOS-correct

Figures 1 and 2 illustrate how focus is on the extension dimension in process sampling (aka one-dimensional sampling), as long as each increment complies with TOS' stringent demand for a *complete slice* of the two width–height dimensions. By securing increments of this geometric configuration, there is only the extension dimension heterogeneity left, i.e. the longitudinal in-between increment spatial heterogeneity (DH = distributional heterogeneity). All variographic

characterisation is aimed at describing, and managing DH_{process}.

If this demand is not observed, see Figures 3 and 4, it is clear how there will be a fundamental compositional imbalance (see incorrect sampling errors in earlier sampling columns) from one increment to another, which therefore should not be used for the purpose of characterising the 1-dimensional DH.

Correct planar–parallel or curvy–planar cross-sections of a moving stream is the **only** correct delineation of process sampling increments, Figure 5 (cases "A" and "C") and Figure 6 top panel, eliminating a potential incorrect delineation

error [one of the three potential incorrect sampling errors (ISE)].

Incorrect increment delineation, and extraction, will give rise to an inflated nugget effect in variographic process sampling characterisation (see below and the previous sampling column). Non-compliance with these basics will give rise to incorrect sampling errors (IDE; IEE: Incorrect Delineation Error; Incorrect Extraction Error) which are **unnecessary** and which **can** in fact be eliminated from the sampling process.

Manual increment extraction is nearly always a bad idea, and can never be



Figure 1. Dynamic (moving) 1-dimensional lots, from left to right: a conveyor belt transporting coal to a power plant, a pipeline, a series of produced goods). Photo credit: Hans Møller, with permission, and KHE.

SAMPLING COLUMN



Figure 2. Stationary 1-dimensional lots produced in a laboratory scale-study of internal distributional heterogeneity (DH) as a function of the specific laying up process. Photo credit: KHEC teaching collection.

TOS-correct in practice, see horrific examples in Figure 7. Whenever all Incorrect Sampling Errors (IDE, IEE, IPE, IWE) have not been eliminated, the sampling process will invariably be fraught with a fatal, inconstant sampling bias, which can

be never be corrected for, see, for example, References 1 and 2.

There is actually no excuse for not getting the fundamental increment sampling right—and from the first time. Figure 8 shows three examples that are



Figure 3. Examples of irregular, unacceptable, partial cross-section slices compared to a correct full slice of the moving stream; the first two do not comply with the definition of correct increments. Observe also the marked asymmetrical load on the conveyor belt, which would wreak havoc with either of the partial cross-sections. The insert shows when this adverse issue is taken to its extreme, with no observance of the need of securing a balanced cross-section of the moving stream. Indeed, here the objective here seems to be “get a full bucket with the least hassle”, which does not make for representativity—it is grab sampling plain and simple. Photo credit: KHEC teaching collection.



Figure 4. Evidence of a very irregular “sampling” in effect only *grab sampling* from one side of a conveyor belt, cf. Figure 3. Also shown is a trace of what *would have been* a correct cross-stream increment. Photo credit: KHEC teaching collection.

all completely TOS-correct, which is the first condition for sampling representativity.

Only representative increment sampling processes are of interest in science, technology and industry. All examples shown in Figure 8 allow proper variographic process characterisation. Any violation of these simple requirements affects a given sampling process and will lead to an inflated nugget effect, see further below.

Observe above how 1-dimensional lots of both types, static and dynamic (moving), must live up to the same demands concerning the fundamental increment cutting requirements.

“Sooner or later” ...

Sooner or later, however, we are ready to perform proper process sampling—enter *variographics*. The variogram was introduced in the previous column in some detail, so most of what is lacking is simply a basic understanding of what the variogram portrays with respect to the process, and how this comes about. A very small matter of a mathematical equation is all it takes: the professional sampler has to understand the meanings and implication of the variographic master equation,, all will be revealed in the next column.



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Figure 5. Illustration of the “stopped belt” situation in which it is possible to extract a perfect, TOS-correct cross-belt slice (central panel). The geometric delineation may be as in “A” or “C”, but never “B”, which depicts an unbalanced cross-cut. Example taken from a calibration test of an on-line sampler at a coal power plant (not shown), to be validated against the representative samples extracted as illustrated. Photo credit: Hans Møller; with permission.



Figure 7. Horrific examples of extremely unbalanced, IDE/IEE-ridden attempts of manual increment process sampling—always doomed to fail. Manual process sampling is pretty much always a fatal give in to practical complacency. Photo credit: KHEC teaching collection.

For readers who have been inspired to know more about variographics, and who can't wait, there is salvation in the two standard references^{1,2} as well as the new professional introduction published recently by Minnitt & Esbensen.³ This latter also takes you through the mathematical intricacies; well suited as a follow-up to the present columns.

This column has presented the critical issue of correct increment delineation and extraction in great detail (eliminating the otherwise fatal Incorrect Sampling Errors contributing to a sampling bias)—for a good reason. Full attention to these issues is absolutely necessary before embarking on the powerful variographic

process characterisation. The next two columns are filled with practical case histories in which both benefits and throwbacks will be revealed.

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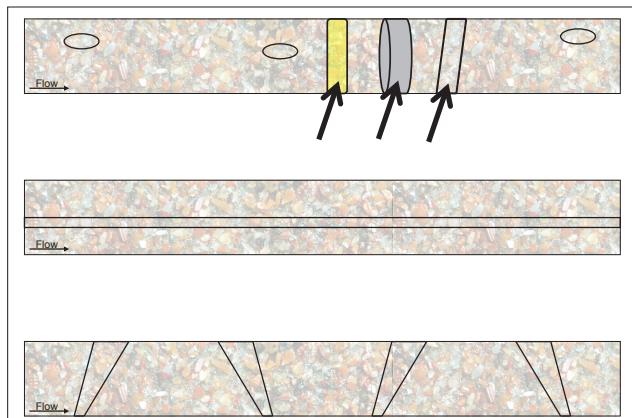


Figure 6. The “complete stream slice” dictum: only a *complete* cross-section of the moving stream of matter will satisfy TOS’ principles re. correct increment extraction. This illustration can be thought of both as looking down on the top surface of a conveyor belt, or as a longitudinal cross-section of a pipeline. Observe that the “oblique” trace (rightmost slice) which is the practical realisation of all cross-cutter samplers when working “on-line”. Illustration credit: KHEC teaching collection.

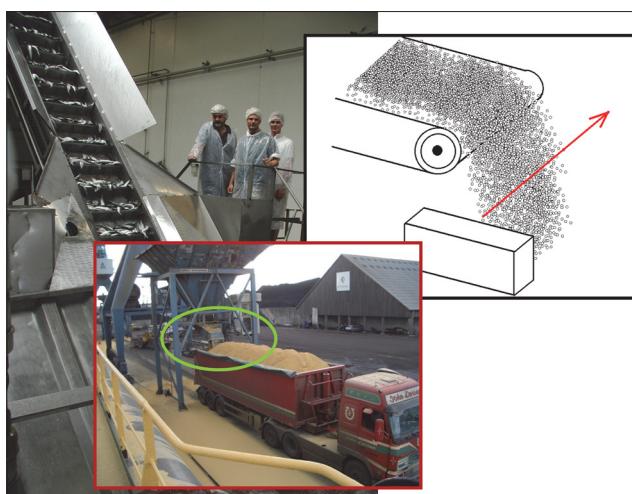


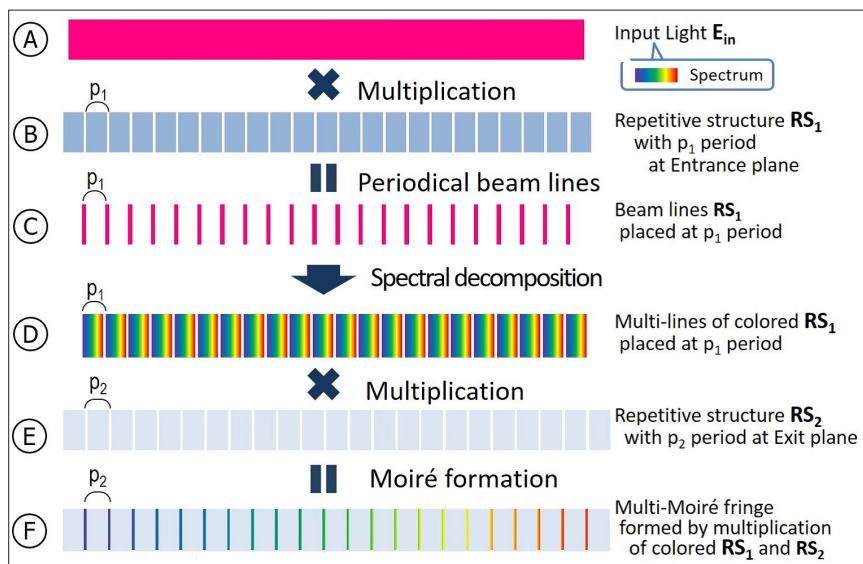
Figure 8. Examples of TOS-correct increment delineation/extraction. Left: a “fish stair case” transporter is functioning as a correct increment “cross stream” cutter (even if the unit particles in this case are *unusually* large). Centre: the bottom outlet opening of a grain off-loading hopper also functions so as to delineate increments without IDE/IEE. Right: a role model “cross-stream” cutter at work at the terminal end of a conveyor belt. All increment sampling process shown here are representative. Credit: KHEC teaching collection.

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Super-resolution spectral imaging to monitor dynamic processes in real time

A common goal of spectroscopy is improved spectroscopic resolution to provide more detailed information about dynamic processes. Multichannel spectrometers are widely used in spectroscopy because they are compact, strong and capture high-speed images. However, the resolution of multichannel spectrometers is limited. Improvement of this resolution is currently restricted by the inability to make the entrance slit width smaller than the pixel size; known as the "pixel Nyquist limit."

Researchers at Osaka University recently developed a way to increase the resolution of multichannel spectrometers beyond the pixel Nyquist limit using Moiré patterns. A Moiré pattern is an interference pattern created between two similar overlapping patterns with



Principle of the proposed method for super spectral resolution beyond pixel Nyquist limits.

slightly different pitch, displacement or rotation.

"We used the Moiré effect to enhance the spectral resolution in a multichan-

nel spectrometer", says Tsuyoshi Konishi, lead author of the recently published report on the study. "This allowed us to achieve resolution beyond the pixel

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 - Food and agriculture
 - Pharmaceuticals

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NEWS

Nyquist limit in a multichannel spectrometer for the first time."

The team created the Moiré effect in a commercial multichannel spectrometer using a pair of slit arrays with periods of 100 µm and 180 µm positioned at the entrance and exit of the spectrometer. The overlap of the patterns from the pair of slit arrays created a Moiré fringe. The image sensor of the spectrometer had a pixel Nyquist limit of 50 nm, so the resolution needed to be smaller than this value. The Moiré fringe generated by the modified spectrometer was able to resolve a wavelength change of just 0.31 nm, overcoming the pixel Nyquist limit. This means that the spectral resolution of the spectrometer was improved by a factor of more than ten from its original resolution of 4.63 nm.

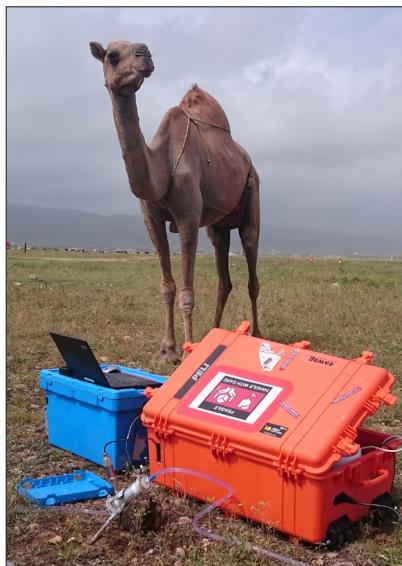
The approach was tested using both a single-wavelength light source and a polychromatic light source consisting of two laser beams of different wavelength. In both cases, the generated Moiré fringe provided resolution beyond the pixel Nyquist limit. Importantly, the developed approach is simple and can be adapted to suit various situations.

This research represents an important step toward the goal of real-time high-resolution monitoring of dynamic events in fields ranging from biology to astronomy. They have published their work in *Optics Express* (<https://doi.org/10.1364/OE.24.026583>).

Portable mass spectrometer allows on-site gas analysis

A portable mass spectrometer, developed by scientists from EAWAG, the Swiss Federal Institute of Aquatic Science and Technology, weighs 13 kg and is mounted in a wheeled suitcase. It can operate autonomously, providing continuous measurements of a wide range of gases; long-term operation is also possible. The instrument is described in a paper in *Environmental Science & Technology* (<https://doi.org/10.1021/acs.est.6b03669>).

For example, the EAWAG team took two weeks to complete a groundwater analysis project in Australia. With conventional methods and instruments,



The portable mass spectrometer deployed in Oman.

EAWAG environmental physicist Matthias Brennwald estimates the team would have required about six years in the lab.

The precision of the new system's measurements is high, with an analytical uncertainty of 1–3% (cf. 1–1.5% for a lab-based spectrometer). Other advantages offered by the system are its low power consumption (50W) and maintenance-free operation.

Now, two years after the instrument was first deployed, eight more instruments are in use—a total of five at EAWAG and four at the Universities of Geneva and Tübingen and the Mont Terri rock laboratory. Following numerous enquiries, it was decided to establish a spin-off. Since April, the spin-off company Gasometrix has been producing the instruments commercially. Their first client is the University of Oxford.

Optical spectroscopy improves predictive assessment of kidney function

A new technique developed by researchers at Lawrence Livermore National Lab promises to improve accuracy and lower costs of real-time assessment of kidney function, reports an article published in *Journal of Biomedical Optics* (<https://doi.org/10.1117/1.JBO.22.5.056001>). The paper explores the use of multimodal autofluorescence and light scatter-

ing to evaluate functional changes in the kidneys after ischemic injury. Conditions including accumulated arterial plaque or blood clots restrict the flow of oxygen and glucose to organs, and prolonged periods of such ischemia can compromise function.

While other current work in this area uses expensive multiphoton and laser-based techniques, the authors reduced expenses by switching to camera-based imaging. Currently, there is no real-time tool to measure the degree of ischemic injury incurred in tissue or to predict the return of its function. The inability to decisively determine tissue functional status runs two great risks: that dysfunctional tissue may be transplanted, increasing the morbidity and mortality of the patient; and that much-needed functional kidney tissue may be discarded.

In their study, Rajesh Raman of Lawrence Livermore National Lab and co-authors Christopher Pivetti and Christoph Troppmann of the University of California Davis, Rajendra Ramsamooj of California Northstate University, and Stavros Demos of Lawrence Livermore acquired autofluorescence images of kidneys *in vivo* under 355 nm, 325 nm and 266 nm illumination. Light-scattering images were collected at the excitation wavelengths while using a relatively narrow band light centred at 500 nm.

The images were simultaneously recorded using a multimodal optical imaging system. The recorded signals were then analysed to obtain time constants, which were correlated to kidney dysfunction as determined by a subsequent survival study and histopathological analysis. Analysis of the light-scattering and autofluorescence images suggests that variations in tissue microstructure, fluorophore emission and blood absorption spectral characteristics, combined with vascular response, contribute to the behaviour of the recorded signals. These are used to obtain tissue functional information and enable the ability to predict post-transplant kidney function. This information can also be applied to the prediction of kidney failure when visual observation cannot, almost immediately following an injury.

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APPLICATIONS: Precision agriculture ▪ Remote sensing ▪ Environmental monitoring ▪ Geological survey ▪ Food inspection ▪ Security/defence

KEY FEATURES: Super lightweight ▪ Compact size ▪ 110 bands, VIS/NIR 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: +49-7243-504-2000
info.bopt.de@Bruker.com
www.bruker.com/optics

PRODUCT: LUMOS FT-IR Microscope

APPLICATIONS: Identification of particles ▪ Analysis of defects and contaminations ▪ Surface analysis ▪ Investigation of multilayer structures ▪ Fibre identification ▪ Determination of the chemical composition

KEY FEATURES: Stand-alone FT-IR microscope with full automation ▪ Highly comfortable and easy in use ▪ Motorised ATR crystal ▪ Fully automated measurement in transmission, reflection and ATR mode

PRODUCT: BRAVO Handheld Raman Spectrometer

APPLICATIONS: Incoming goods control especially in the Pharmaceutical industry ▪ In mobile laboratories for advanced applications

KEY FEATURES: SSE™—patented fluorescence mitigation ▪ Duo LASER™ excitation ▪ IntelliTip™—automated measuring tip recognition ▪ Laser class 1M ▪ Intuitive and guided touch screen operation ▪ Automated batch

Energetiq Technology
 Tel: +1 (781) 939-0763
info@energetiq.com
www.energetiq.com



PRODUCT: EQ-77 Laser-Driven Light Source

APPLICATIONS: Semiconductor metrology & inspection ▪ UV-Vis-NIR spectroscopy ▪ Materials characterisation ▪ Thin film measurements ▪ Advanced imaging



KEY FEATURES: Radiance >40 mW/mm².sr.nm ▪ Very low noise & excellent spatial stability ▪ Extreme high brightness across UV-Vis-NIR (170–2100 nm) ▪ Electrodeless operation ▪ Electronic optical output control

PRODUCT FOCUS

HORIBA
Scientific

Tel: +33 1 69 74 72 00
info-sci.fr@horiba.com
<http://www.horiba.com/scientific/>



PRODUCT: Raman EasyNav Package

APPLICATIONS: Any sample surface, even very rough

KEY FEATURES: The new EasyNav package makes it easy to navigate through your image and acquire sharp, and 3D topography images in real-time delivering a powerful user experience for all Raman users.

PRODUCT: CLUE Series

APPLICATIONS: Electrical and compositional properties, quality control and failure analysis, defects, impurities, dopants, vacancies, contaminations and inclusions, zoning analysis in zircons

KEY FEATURES: The universal extensions for cathodoluminescence, photoluminescence and Raman spectroscopy to gain unique insight into the chemical and electronic properties of materials with nanoscale resolution.

Infometrix, Inc.

Tel: +1-425-402-1450
info@infometrix.com
<https://www.infometrix.com>

PRODUCT: Pirouette

APPLICATIONS: Chemometrics • Calibration modelling • Multivariate classification • Chemical profiling • Data exploration

KEY FEATURES: Partial least squares • Principal component analysis • Soft independent modelling of class analogies • Alternating least squares • Hierarchical cluster analysis

PRODUCT: InStep

APPLICATIONS: Multivariate statistical process analysis • Process automation • Routine quality analytics • Hierarchical chemometrics • Decision tree analytics

KEY FEATURES: Multivariate predictions • PLS/regression/discriminant analysis, PCA • SIMCA • KNN • ALS

Kratos Analytical Ltd

Tel: +44 (0) 161 888 4400
info@kratos.co.uk
<http://www.kratos.com/se>



PRODUCT: AXIS Supra

APPLICATIONS: XPS surface analysis • Materials characterisation • Surface homogeneity • Quantitative imaging

KEY FEATURES: Surface sensitive XPS imaging • Quantitative elemental and chemical state imaging • Spectromicroscopy sub-micron XPS from a pixel • Variable fields of view from 2mm to 200 µm • Complimentary Auger microscopy

McPHERSON

Tel: 1-978-256-4512
MCP@McPhersonInc.com
<http://www.McPhersonInc.com>

PRODUCT: Deep UV Imaging Spectrometer

APPLICATIONS: Energy • Environmental • Semiconductor • Basic Research • Teaching

KEY FEATURES: Works up to 10 eV • Astigmatic optical design • Large focal plane • High throughput • Many diffraction gratings available

PRODUCT: Soft X-ray EUV imaging Monochromator

APPLICATIONS: High harmonic generation • PES/ARPES • Laser produced plasma physics • Basic research • Teaching

KEY FEATURES: Works up to 150 eV • Astigmatic optical design • Conical dispersion • High throughput • Many diffraction gratings available

Moxtek, Inc

Tel: 1 (801) 225-0930
info@moxtek.com
<http://www.moxtek.com>



PRODUCT: Mox-HPC X-Ray Tubes

APPLICATIONS: Mox-HPC x-ray tubes are compact, high power x-ray tubes intended for XRF applications. These air cooled tubes have continuous power ratings from 100W up to 350W at 75 kV.

KEY FEATURES: The total weight is only 2.2kg compared to ~ 17kg for equivalent liquid cooled x-ray tubes. (Engineering samples are available)

PRODUCT: MAGPRO 60 kV & 70 kV

Sources

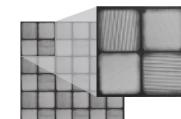
APPLICATIONS: Moxtek MAGPRO 60 kV & 70 kV x-ray sources are ideal for XRF, XRD and small imaging applications. These compact sources include an air cooled tube with an integrated power supply.



KEY FEATURES: The MAGPRO can achieve 12W of power and is designed for close coupling to detectors. 70 kV samples now available. Size: 35 × 70 × 164 mm. Weight: ~800 g.

PRODUCT: Pixelated Wire Grid Polarisers

APPLICATIONS: Moxtek's Pixelated Polarisers enable real-time polarised imaging without the difficulty of separate camera image overlay. Applications: target identification, facial recognition and oil on water.



KEY FEATURES: Pixelated polarisers are available as two, three and four-state devices in both visible and IR wavelengths. Customisable pixel pitches are available for specific CCD/CMOS sensor arrays.

PRODUCT: Mox-Micro X-ray Tubes

APPLICATIONS: Mox-Micro x-ray tubes have a focal spot of $\leq 50 \mu\text{m}$ with up to 30W continuous power. Mox-Micro can be used with or without a poly-capillary optic for x-ray imaging and x-ray spectroscopy applications.



KEY FEATURES: A variety of targets are available to match your application needs. Size: 40 × 65 × 102 mm (+ cable) Weight: ~225g. (Engineering samples are available)

PIXELTEQ

Tel: +31-652-557-997
info@pixelteq.com
www.pixelteq.com

PRODUCT: SpectroCam: Multispectral Camera (UV-VIS, VIS-NIR, NIR-SWIR, multispectral conversion kit)

APPLICATIONS: Aerospace & security • Biomedical & life science • Food & water safety • OEM & industrial • Scientific & research

KEY FEATURES: 6 to 8-band sequential multispectral cameras-integrated sensor & software • Versions for UV-VIS / VIS-NIR / NIR-SWIR wavelength ranges • Interchangeable standard and custom dichroic filters • Multispectral conversion kit-user-provided camera & integration • Customised OEM modules and cameras available

PRODUCT FOCUS

PRODUCT: PixelCam: Multispectral Camera (simultaneous multi-band acquisition at video rates)

APPLICATIONS: Aerospace & security ▪ Biomedical & life science ▪ OEM & industrial ▪ Remote sensing ▪ Unmanned vehicles

KEY FEATURES: Application-specific cameras-data-rich multispectral imaging ▪ Simultaneous multi-band acquisition-no scene change or pixel shift ▪ Passive spectral filtering-integrate into mobile & aerial devices ▪ Small footprint-same size, weight & power as monochrome ▪ Scalable production for cost-effective OEM multispectral cameras

Princeton Instruments

Tel: +1 609 587 9797
info@princetoninstruments.com
www.princetoninstruments.com

PRODUCT: FERGIE Spectrograph

APPLICATIONS: Raman ▪ Fluorescence ▪ Absorption ▪ TERS ▪ Microspectroscopy

KEY FEATURES: Aberration-free optical design ▪ Perfect imaging performance ▪ Modular accessories ▪ TE-cooled back-illuminated CCD ▪ Powerful software



PRODUCT: SpectraPro HRS 300

Spectrographs

APPLICATIONS: Raman ▪ LIBS ▪ Photoluminescence ▪ Plasma diagnostics ▪ Absorption

KEY FEATURES: ResXtreme spectral deconvolution ▪ Multiple exit ports for versatility ▪ Intelligent wavelength calibration ▪ AccuDrive grating drive system yields up to 3x improvement in wavelength accuracy



Renishaw plc

Tel: +44 (1453) 524 524
raman@renishaw.com
<http://www.renishaw.com/raman>

PRODUCT: inVia™ confocal Raman microscope

APPLICATIONS: Biological imaging ▪ Materials science (e.g. graphene/batteries/semiconductors) ▪ Pharmaceuticals (particle identity/size/distribution) ▪ Complex geological structures ▪ Art and heritage investigation.

KEY FEATURES: LiveTrack™ focus-tracking technology ▪ Flexibility, configurable with multiple lasers and can couple with other analytical techniques ▪ Streamline™ rapid generation of images with no sample damage.

PRODUCT: RA802 Pharmaceutical Analyser

APPLICATIONS: Particle identity, size and distribution investigation of pharmaceuticals ▪ Coating uniformity analysis ▪ Contamination identification and analysis ▪ Counterfeit investigation ▪ Polymorph screening.

KEY FEATURES: LiveTrack™ focus-tracking technology ▪ Ultra-fast data collection with Streamline™ Rapide ▪ Queuing capability, run samples unattended ▪ Sample flexibility, image formulations without preparation.

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

www.spectroscropyeurope.com

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

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info@witec.de
<http://www.witec.de>



PRODUCT: alpha300 R Confocal 3D Raman Imaging System

APPLICATIONS: Materials research ▪ Pharmaceutics ▪ Semiconductor and PV ▪ Life science ▪ Geosciences, Coatings & Thins 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 easily 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

Xenics

Tel: +32 16 38 99 00
sales@xenics.com
www.xenics.com

PRODUCT: Lynx: smallest SWIR line-scan cameras

APPLICATIONS: R&D spectroscopy ▪ Food inspection ▪ Sorting ▪ Industrial web inspection

KEY FEATURES: Smallest SWIR line-scan camera with small pixel pitch ▪ Multiple line resolutions: 512, 1024 or 2048 ▪ Full flexibility in integration time settings ▪ Broad range of pixel sizes, square and rectangular ▪ Extended trigger functionality ▪ Standard GigE Vision, Power over Ethernet or CameraLink interface

PRODUCT: Cougar: extreme SWIR imaging

APPLICATIONS: Raman spectroscopy ▪ High resolution imaging spectroscopy ▪ R&D spectroscopy

KEY FEATURES: Lowest noise (~20 e-) and high sensitivity for measurements of low-light signals ▪ High resolution 640 × 512 InGaAs detector ▪ Liquid nitrogen (LN₂) cooled at 77K ▪ Long integration times of several hours

PRODUCTS AT ASMS 2017

Agilent Technologies introduces new GC/Q-TOF system

Agilent Technologies have introduced a new high-resolution, accurate-mass system designed for laboratories doing food and environmental testing, life science research, forensics and chemical analysis. The Agilent 7250 GC/Q-TOF system combines gas chromatography and quadrupole time-of-flight mass spectrometry with a low-energy electron ionisation source that enables greater exploration of unknown chemical samples. The 7250 GC/Q-TOF system will allow labs to quickly and easily identify volatile and semi-volatile compounds that, in the past, would require them to perform alternative techniques, or longer sample preparations to detect and deter-



The Agilent 7250 GC/Q-TOF high-resolution, accurate-mass system.

mine the compounds present in their samples. Furthermore, with low energy electron ionisation, scientists will be better able to elucidate chemical structures.

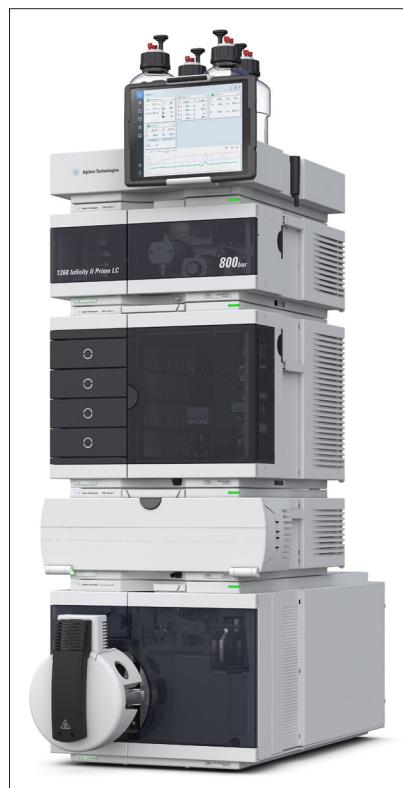
Agilent Technologies

► link.spectroscopyeurope.com/29-W-027

LC-MS triple quadrupole mass spectrometer

Agilent Technologies has introduced a new member to its family of triple quadrupole liquid chromatography mass spec-

trometers (triple quad LC/MS). The Ultivo triple quad is optimised for the food and environmental routine testing segments employing triple quad LC/MS systems



Agilent's Ultivo triple quad LC/MS system.

for quantitative analyses. Ultivo delivers robust performance, superior uptime and easier serviceability, in a footprint that is 70% smaller than previous instruments. Greater ion transmission efficiency leads to optimised sensitivity; and improved, intelligent diagnostics use intuitive read-backs that can quickly identify issues, ensuring optimum uptime. Furthermore, Ultivo's new VacShield vacuum provides vent-less ion injector exchange capabilities that reduce wear and tear and facilitate rapid front-end maintenance.

Agilent Technologies

► link.spectroscopyeurope.com/29-W-019

New metabolomics software and workflows

Bruker introduces its third-generation metabolomics research and validation solution, MetaboScape® 3.0, which has

new features for discovery metabolomics, including support for direct-injection (DI) or MALDI Magnetic Resonance Mass Spectrometry (MRMS) for high-throughput phenomics translational research and validation. Innovations include a novel algorithm called Time-aligned-Region-complete-eXtraction ("T-ReX"), which automatically extracts all relevant information in sample cohorts in a "region complete" manner. Included in MetaboScape 3.0 are workflows that support evaluating high-throughput, chromatography-free DI-MRMS or MALDI-MRMS data, enabling two extreme mass resolution techniques that enable higher sample throughput for profiling complex metabolic extracts. The speed and high throughput of these MRMS methods yields advantages for validating larger sample cohorts, and enabling larger-scale longitudinal studies.

Bruker

► link.spectroscopyeurope.com/29-W-021

Proteoform characterisation solution

Bruker's Proteoform Profiling™ 1.0 solution enables a new life-science research and translational research workflow, i.e. the systematic, large-scale, label-free study of all expressed proteoforms, including protein mutations, splice variants, post-translational modifications, as well as protein processing or degradation products. Detailed proteoform characterisation is of tremendous importance in cell biology and in clinical proteomics research, where traditional bottom-up proteomics analysis of digested proteins scrambles key biological information. While the human genome only has about 25–30,000 coding sequences, or "genes", for transcription and translation into protein families, the human body may have up to 1 billion different proteoforms expressed.

Bruker

► link.spectroscopyeurope.com/29-W-023

Applied toxicology and forensics software

Bruker announced the release of TargetScreener 3.0HR (high-resolution), which includes TASQ™ 1.4 (Target Analysis for Screening and Quantitation)

PRODUCTS AT ASMS 2017

software to provide a unified software platform for automated screening and quantitative applications in forensic, food and environmental safety markets. Bruker also launched the Toxtyper 2.0E solution for routine, high-throughput forensic toxicology with further improved capabilities and database updates to enhance productivity. Further improvements in the new Toxtyper 2.0E solution integrate Bruker's newly launched line of Elute UHPLC liquid chromatography systems. With an expanded curated toxicology screening database and new automated software for LIMS sample table I/O, automated parallel processing with TASQ, and automated reporting of results, these solutions enable increased throughput while minimising false positives and increasing confidence for routine "push-button" forensic toxicology.

Bruker

► link.spectroscopyeurope.com/29-W-022

Pharmaceutical and translational mass spectrometry imaging

Bruker have introduced new SCiLS Cloud and SCiLS Lab mass spectrometry imaging (MSI) software solutions, now with MultiVendor Support. MALDI imaging has rapidly developed as a label-free technique for spatially resolved molecular analysis of proteins, glycans, lipids, as well as drugs and their metabolites. MALDI imaging is finding rapidly increasing use in pharmaceutical drug development, in tissue-resolved biomarker research (e.g. glycans on cell surfaces as cancer markers), as well as in translational pathology research to complement immunohistochemistry (IHC). The new SCiLS Cloud software offers web-based tools to facilitate distributed workflows, where data and analysis results can be shared, viewed and manipulated with a web browser through secure access. SCiLS Lab provides advanced and user-friendly solutions for data handling, visualisation and computational analysis for Bruker MALDI imaging data sets, and now also offers support for data acquired from non-Bruker mass spectrometers.

Bruker

► link.spectroscopyeurope.com/29-W-020

www.spectroscopyeurope.com

New multi-application nitrogen generator system

Peak Scientific has unveiled the new Infinity XE 50 Series nitrogen generator. It is designed to cater for numerous applications across a typical laboratory, from a single source solution, and provides a variable flow of nitrogen gas ranging from 11 Lmin^{-1} to 432 Lmin^{-1} and at purities up to 99.5%. The Infinity XE 50 Series is suited for a wide range



Peak Scientific's new Infinity XE 50 Series nitrogen generator.

of applications including LC-MS, ELSD, sample evaporation, NMR, FTMS and gloveboxes, with the potential of providing nitrogen for multiple applications across an entire lab. The generator can also be used for industrial applications such as Modified Atmosphere Packaging and wine bottling. This new line represents a significant evolution from its predecessor, Peak's highly successful Infinity 50 Series, with greater performance range available across a streamlined range of four models (5011, 5021, 5031, 5041) and new features including purity monitoring with optional failsafe shutdown and eco mode for maximum energy efficiency and reduced running costs.

Peak Scientific

► link.spectroscopyeurope.com/29-W-026

Prosolia DESI 2D molecular imaging now compatible with Agilent Technologies

Prosolia has introduced a new desorption electrospray ionisation (DESI) 2D model compatible with Agilent TOF, Q-TOF and IM-Q-TOF LC/MS systems. With no sample prep required, DESI 2D enables molecular imaging without matrix by mass spectrometry. DESI 2D integrates real time, micro-scale solvent extraction in fast-moving droplets with electrospray ionisation for direct sample analysis. DESI 2D incorporates Prosolia's proprietary DESI technology and is currently used in preclinical and clinical research for determining the distribution of drugs, metabolites and biomarkers of disease, as well as, a variety of chemical analysis applications.

Prosolia

► link.spectroscopyeurope.com/29-W-025

SWATH technology for routine analyses

SCIEX has launched its SWATH® data independent acquisition (DIA) technology for the new X500 series mass spectrometers, enabling it use on a routine system. SWATH Acquisition allows the simultaneous and comprehensive identification and quantification of virtually every detectable compound in a sample, from a single analysis. SWATH Acquisition has unique capabilities for quantitative accuracy, offering high reproducibility across multiple samples with wide dynamic range. The technology enables the creation of a permanent digital record of quantitative MS/MS data for the entire sample. Following the implementation of SWATH for proteomics research, this technology can be used in other fields, including forensics, food testing, environmental analysis and biologics.

SCIEX

► link.spectroscopyeurope.com/29-W-012

New Orbitrap mass spectrometer

The Thermo Scientific Q Exactive HF-X Hybrid Quadrupole Orbitrap mass spectrometer has improved depth of analysis, quantitative accuracy and reproducibility. It aims to provide sensi-

PRODUCTS AT ASMS 2017



The Thermo Scientific Q Exactive HF-X Hybrid Quadrupole Orbitrap mass spectrometer.

tive, accurate and reproducible analyses of highly complex samples for various aspects of translational research and biopharma applications. This includes comprehensive proteome profiling and quantitation, biomarker discovery and verification, and full characterisation of complex biotherapeutics. For R&D scientists, the Q Exactive HF-X instrument delivers fast and accurate mass analysis, plus two-to-three-fold sensitivity improvements, delivering the same number of protein identifications in half of the time required for previous models. For biopharma scientists, the Q Exactive HF-X instrument provides up to eight times better signal-to-noise ratio for native, intact monoclonal antibody mass determination, glycoprofiling and purity checks.

Thermo Scientific

► link.spectroscopyeurope.com/29-W-017

Enhancements to Thermo Scientific Tribrid mass spectrometer

Thermo Scientific have added enhancements to their Orbitrap Fusion Lumos Tribrid mass spectrometer that extend its power, performance and versatility. The Integrated Ultraviolet Photodissociation (UVPD) allows researchers to perform large and small molecule structure determination on an LC time scale. Now an optional feature on Orbitrap Fusion Lumos systems, this fragmentation mode is designed to improve sequence coverage and antibody characterisation,

decrease scrambling in top-down hydrogen deuterium exchange (HDX) experiments and to be a complete solution for structural characterisation of lipids and other metabolites. A new Advanced Peak Determination (APD) algorithm is designed to improve the performance of most proteomic workflows with high peptide and protein identification rates in data-dependent experiments. 1M resolution is also a new option, used to obtain unique structural and quantitative information for a wide range of compound classes.

Thermo Scientific

► link.spectroscopyeurope.com/29-W-014

New software and cloud-based solutions for metabolomics and proteomics

Thermo Fisher Scientific have introduced new software and cloud-based solutions for metabolomics and proteomics. The new Compound Discoverer 2.1 software supports metabolomics research insight into the biochemical phenotype of organisms. The latest software release of Proteome Discover 2.2 software has a new XlinkX node with a fully integrated cross-linked peptide search engine, for use with the Thermo Scientific Orbitrap Fusion and Fusion Lumos Tribrid mass spectrometers, a new algorithm for label-free quantification and new tools for statistical analysis. ProSightPC 4.0 software is for researchers performing top-down and middle-down proteomics experiments. The new Xcalibur 4.1 software now supports the latest Thermo Scientific Orbitrap Fusion Lumos UPVD. The FreeStyle 1.3 software now features improved usability and offers elemental composition information using MS/MS. New cloud-based software applications, for proteomics and genomics research and applied markets, are now available through the Thermo Fisher Connect cloud-based platform. The Sample Profiler application helps identify unknown compounds in high-resolution accurate mass spectrometry sample data. The new Pathway Overrepresentation application helps prot-

eomics researchers detect significant pathways within genes or proteins. The new Omics Comparator allows users to rapidly identify overlap and uniqueness when comparing protein or gene lists.

Available as both a cloud and mobile app, the new MS Instrument Connect enables researchers to monitor their LC-MS and GC-MS analyses remotely.

Thermo Fisher Scientific

► link.spectroscopyeurope.com/29-W-016

Ready-to-use mass spectrometric kit simplifies insulin bioanalysis workflows

Thermo Scientific's new, ready-to-use InsuQuant mass spectrometric immunoassay kit incorporates all the necessary reagents and consumables needed in the pre-analytical stage of the LC-MS



The ready-to-use InsuQuant mass spectrometric immunoassay kit from Thermo Scientific.

workflow in a convenient, easy-to-use platform. The kit is designed to eliminate the need for researchers to make buffers and match reagents, thus saving resources and reducing the risk of human errors in complex protocols, which can be costly and impact productivity. It uses proprietary microcolumn technology to enable advanced detection of endogenous insulin and its exogenous analogues in the tip of a pipette, while also reducing background and improving reproducibility. The mass spectrometric immunoassay (MSIA) methodology has demonstrated pg mL^{-1} levels of detection while yielding simultaneous qualitative and quan-

PRODUCTS AT ASMS 2017

itative data from complex biological matrices, making it well suited for use with plasma.

Thermo Scientific

► link.spectroscopyeurope.com/29-W-018

New triple quadrupole mass spectrometers from Thermo Scientific

Thermo Scientific has introduced the TSQ Altis triple stage quadrupole and



Thermo Scientific has introduced the TSQ Altis triple stage quadrupole mass spectrometer.

TSQ Quantis triple stage quadrupole mass spectrometers for targeted quantitation assays. The TSQ Altis mass spectrometer offers sensitivity, selectivity and speed while providing the analytical flexibility and reproducibility for demanding applications.

The TSQ Altis and TSQ Quantis systems are engineered for high-resolution single reaction monitoring (SRM) capabilities, which enables ion transmission and consistency for reproducible results across instruments. In addition, both systems are equipped with Active Ion Management (AIM+) technology that includes redesigned ion source housing, segmented quadrupoles, new RF electronics and an enhanced dual-mode electron multiplier detector.

Thermo Scientific

► link.spectroscopyeurope.com/29-W-013

Waters introduces LiveID software for real-time food analysis

Waters has introduced LiveID™ Software for near-instantaneous, direct-from-sample measurement and classification of food products including meat and crops by Waters' quadrupole, time-of-flight (QToF) mass spectrometers. The new software enables mass spectrometers equipped with an iKnife™ sampling device, rapid evaporative ionisation mass spectrometry (REIMS) ion source and MassLynx® mass spectrometry software to help laboratories detect food fraud. In recent years, QToF mass spectrometry has emerged as a promising technique for detecting food fraud. Faster than conventional techniques like immunoassay and PCR, mass spectrometry with LiveID Software produces definitive results in seconds. With iKnife Sampling and REIMS, no sample pretreatment or separation is typically necessary. When the hand-held iKnife sampling device comes in contact with a sample of animal or plant tissue or other processed foodstuffs such as butter, it creates smoke containing compound-specific molecules which are directed to the REIMS source where the molecules are ionised and then

passed on to be detected by the mass spectrometer. The LiveID software then creates a molecular profile or chemical fingerprint of the sample, compares it to a user-generated database of reference fingerprints and then classifies the sample as belonging to one of a number of sample types or groupings.

Waters

► link.spectroscopyeurope.com/29-W-024

Latest version of Progenesis QI for proteomics software

Waters has introduced the latest version of Progenesis® QI for proteomics software. This latest version is designed to keep Progenesis QI for proteomics compatible with current mass spectrometry approaches, while also increasing flexibility and usability. New features include: Spectral library searching, SONAR Support, Automatic thresholding for data independent acquisition, mzIdentML export, Proteolabels connectivity and Symphony connectivity. The new version of Progenesis QI for proteomics will be available worldwide from July 2017.

Waters

► link.spectroscopyeurope.com/29-W-028

Silicon Drift Detectors

XRF Experimenter's Kit

125 eV FWHM

OEM Components

FAST SDD®

Count Rate >1,000,000 CPS

Complete X-Ray Spectrometer

OEM's #1 Choice for XRF

XRF System

www.amptek.com

AMETEK
MATERIALS ANALYSIS DIVISION

NEW PRODUCTS

FLUORESCENCE

Automating time-resolved fluorescence spectroscopy

A recent software upgrade adding a remote interface to PicoQuant's modular FluoTime 300 spectrometer makes it possible to interface it with external accessories, such as the liquid handling automation workstation Biomek NXP from Beckman-Coulter. This simplifies recording spectra for high-throughput



The remote interface added in a recent system software update allows interfacing the time-resolved fluorescence spectrometer FluoTime 300 with accessories such as the Biomek NXP liquid handling automation workstation from Beckman-Coulter.

applications in a convenient and reproducible manner. Additionally, it also allows obtaining spectroscopic snap shots at well-defined time points of reactions being carried out in the cuvettes of the liquid handling automation workstation.

PicoQuant

► link.spectroscopieurope.com/29-W-036

INFRARED

Table-top, frequency comb spectrometer

IRsweep have introduced the IRspectrometer, a table-top, frequency comb spectrometer with μs time-resolution, a large spectral bandwidth and high spectral resolution. The use of dual-comb spectroscopy can overcome the limitations around speed, resolution and signal-to-noise ratio inherent in Michelson FT-IR spectrometers. The

IRspectrometer has time-resolution of $1\ \mu\text{s}$ for a full spectrum, and the brightness of the laser frequency-comb source provides a large dynamic range, enabling the analysis of highly absorbing samples. The spectrometer also delivers μs resolution at high bandwidths, and has signal-to-noise ratios above 1000 per data point with $<1\text{ ms}$ acquisition.

Potential applications include time-resolved bio-spectroscopy, high-throughput IR analysis and chemical composition determination of gaseous, liquid and solid samples.

IRsweep

► link.spectroscopieurope.com/29-W-001

Sentera introduces multispectral Double 4K sensor

Sentera has announced the release of its multispectral Double 4K sensor, offering five spectral bands: blue, green, red, red edge and near infrared (NIR). This sensor enables users to collect visual band imagery as well as vegetation indices based upon the addition of NIR or Red Edge, including normalised difference vegetation index (NDVI) and normalised difference vegetation red edge (NDRE).

Sentera

► link.spectroscopieurope.com/29-W-037

NMR

Magritek launch the 80MHz Spinsolve 80

Magritek has announced the Spinsolve 80, an 80 MHz benchtop NMR using 5 mm NMR tubes. The higher field enables a large chemical shift spread which, combined with a high resolution (0.5 Hz/20 Hz), makes it possible to



The Spinsolve 80 NMR spectrometer from Magritek.

resolve close NMR peaks. It also gives a sensitivity of 1% Ethyl Benzene > 200:1 dual channel. Through its software, users can perform multiple advanced 2D NMR methods such as COSY, HSQC-ME and HMBC. Its benchtop size and weight (72 kg) means it can be conveniently placed almost anywhere. All Spinsolve models have almost zero running costs as they do not require any cryogens.

The Spinsolve 80 Carbon spectrometer includes a selection of pulse sequences for the multi-nuclear probe which can measure ^1H , ^{19}F and ^{13}C nuclei. Other nuclei and newer pulse sequences are available on request.

Magritek

► link.spectroscopieurope.com/29-W-009

MASS SPEC

Mass spectrometry integrated into clinical analyser

Thermo Fisher Scientific has introduced the Thermo Scientific Cascadion SM Clinical Analyser, which combines the ease of use of clinical analysers with the selectivity and sensitivity of liquid chro-



The Thermo Scientific Cascadion SM Clinical Analyser.

matography-tandem mass spectrometry (LC-MS/MS). The fully automated analyser is designed for use in a variety of settings, including hospital laboratories, and to provide results for a range of clinical tests. The Cascadion will be commercially available in Europe, followed by the US, once regulatory approvals have been received. The Cascadion system was completely designed and built using Thermo Fisher products and technologies. Featuring turnkey operation, it is

NEW PRODUCTS

designed to be used by laboratory staff with no specialised knowledge required.

Thermo Fisher Scientific

► link.spectroscopyeurope.com/29-W-030

NIST upgrades mass spectral library

NIST have added mass spectra from more than 25,000 compounds to the Mass Spectral Library, bringing the total number to more than 265,000. Among the compounds whose mass spectra are included in this upgrade are many dangerous drugs. These include dozens of synthetic cannabinoids—"synthetic marijuana"—which can cause psychotic episodes, seizures and death. Also included are more than 30 types of fentanyl, the synthetic opioid that is driving an epidemic of overdoses in the USA.

NIST

► link.spectroscopyeurope.com/29-W-034

RAMAN

NanoRam update readies instrument for new FDA data integrity guidance

The NanoRam is a handheld instrument used for non-destructive identification and verification of materials such as active pharmaceutical ingredients (APIs), excipients and intermediates. These software updates provide improvements on data integrity, security and activity tracking through the Audit Trail to make user experience with the NanoRam safe and secure. These updates are being released in compliance with the future publication of the Data Integrity and Compliance with CGMP Guidance for Industry, the purpose of which is to clarify the role of data integrity in current good manufacturing practice (CGMP) for drugs, as required in 21 CFR parts 210, 211 and 212. The guidance provides the FDA's current thinking on the creation and handling of data in accordance with CGMP requirements, and the NanoRam software updates ensure these guidelines are followed.

B&W Tek

► link.spectroscopyeurope.com/29-W-033

www.spectroscopyeurope.com

Enhancements to handheld Raman analyser

Rigaku Analytical Devices has enhanced the features of its Rigaku Progeny ResQ handheld 1064 nm Raman analyser. Recent updates to the Progeny ResQ Raman analyser include an expanded library that includes latest fentanyl strands, the ability to pair a smartphone to view live field analysis, customised setting applications specific to analysis conditions and identification of lower concentrations using a SERS signal enhancement kit.

Rigaku Analytical Devices

► link.spectroscopyeurope.com/29-W-031

X-RAY

Bruker launches the S8 TIGER Series 2 WDXRF system

Bruker has launched its new S8 TIGER Series 2 wavelength dispersive X-ray fluorescence (WDXRF) spectrometer. The new S8 TIGER Series 2 introduces HighSense technology which improves linear dynamic range, thus enabling higher precision levels for process and quality control in cement, minerals, mining, metals, glass and ceramics applications. In addition, measurement times are significantly reduced, sample throughput is increased and time-to-result is improved, typically by 25%. The



Bruker's new S8 TIGER Series 2 WD XRF spectrometer.

S8 TIGER Series 2 also features XRF2 small spot mapping for detailed maps of elemental distributions in materials. With a 300-µm spot size, XRF2 makes the S8 TIGER Series 2 an excellent system for both industrial QC labs as well as for industrial and academic research and methods development laboratories.

In addition, the S8 TIGER Series 2 new HighSense X-ray optics improves both sensitivity and spectral resolution. This benefits a wide range of applications including recognition of foreign particles, optimisation of mineral beneficiation processes in mining, analysis of material properties in metals, semiconductors and nanotechnology. A new multilingual TouchControl interface offers intuitive and robust operation.

Bruker

► link.spectroscopyeurope.com/29-W-010

Benchtop X-ray diffraction instrument

Rigaku Corporation has announced the sixth generation of their Rigaku MiniFlex benchtop X-ray diffraction (XRD) instrument. The new MiniFlex X-ray diffractometer is a multipurpose analytical instrument that can determine phase identification and quantification, percent (%) crystallinity, crystallite size and strain, lattice parameter refinement, Rietveld refinement, and molecular structure. The new MiniFlex system has increased speed and sensitivity with new technologies, including the HyPix-400 MF 2D hybrid pixel array detector (HPAD) together with an available 600W X-ray source and new eight-position automatic sample changer. This new direct photon counting detector enables high-speed, low-noise data collection and may be operated in 0D and 1D modes for conventional XRD analysis and 2D mode for samples with coarse grain size and/or preferred orientation. A variety of X-ray tube anodes—along with a range of sample rotation and positioning accessories, together with a variety of temperature attachments—are offered to ensure coverage of a broad range of samples, whether performing research or routine quality control.

Rigaku

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DIARY

Conferences 2017

23–28 July, Québec City, Canada. 20th International Society of Magnetic Resonance Conference (ISMAR 2017). <http://www.ismar2017.org>.

30 July–4 August, Montreal, Quebec, Canada. 23rd International Symposium on Plasma Chemistry. Sylvain Coulombe, McGill University, Dept of Chemical Engineering, Montreal, Quebec, Canada, <http://ispc23.conference.mcgill.ca>.

31 July–4 August, Florianopolis, Brazil. 18th International Conference on Biological Inorganic Chemistry (ICBIC18). Ademir Neves, University of Santa Catarina, <http://icbic18.weebly.com>.

31 July–4 August, Singapore, Singapore. 12th Conference on Lasers and Electro-Optics Pacific Rim (CLEO-PR 2017). <http://www.cleopacificrim.com>.

13–17 August, Santa Fe, NM, United States. 2017 International Conference on Optical MEMS and Nanophotonics (OMN2017). Mary Lou Norris, marylou.norris@nist.gov, <http://bit.ly/2p8AARV>.

13–18 August, Paris, France. Goldschmidt 2017. Le Palais des Congrès de Paris, 2 place

de la Porte Maillot, 75017 Paris, France, helpdesk@goldschmidt.info, <https://goldschmidt.info/2017>.

14–17 August, Vienna, Austria. 6th International Symposium on Metallomics. Gunda Köllensperger, gunda.koellensperger@univie.ac.at, <http://www.metallomics2017.at>.

14–15 August, Didcot, United Kingdom. International Workshop on Improving Data Quality in XAFS Spectroscopy (Q2XAFS 2017). Emma Clarke, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, UK, emma.clarke@diamond.ac.uk, www.q2xafs.com.

20–25 August, Cancun, Mexico. XXVI International Materials Research Congress (IMRC 2017). webmaster@mrs-mexico.org.mx, <https://www.mrs-mexico.org.mx/imrc2017/index.php>.

21–25 August, Lausanne, Switzerland. Microscopy Conference 2017. Marlen Schiller, marlen.schiller@conventus.de, <http://www.mc2017.ch/>.

26–29 August, Bodrum, Turkey. 3rd International Turkish Congress on Molecular Spectroscopy (TURCMOS2017). Pınar Tekbaş Çam, Leon Congress, Turkey, info@leoncongress.com, <http://turcmos.com>.

28 August–1 September, Stockholm, Sweden. 19th Euroanalysis 2017 Conference. Ulrika Örn, ulrika.orn@kemisamfundet.se, <http://euroanalysis2017.se>.

31 August–2 September, Rhodes, Greece. 15th International Conference on Environmental Science and Technology (CEST2017). Secretariat, University of Aegean, Voulgaroktonou Str. 30, 11472 Athens, Greece, cest@gnest.org, <http://cest.gnest.org/cest2017/about>.

3–8 September, Berlin, Germany. International Conference on Ion Analysis (ICIA). wolfgang.frenzel@tu-berlin.de, <http://www.icia-conference.net>.

3–8 September, Berlin, Germany. 4th International Conference on Radioecology and Environmental Radioactivity (ICRER). Laureline Fevrier, Institut de Radioprotection et de Surete Nucléaire (IRSN), laureline.fevrier@irsn.fr, <http://www.icrer2017.com/>.

4–7 September, Munich, Germany. International Conference on Enhanced Spectroscopies (ICES) 2017. Achim Hartschuh, achim.hartschuh@lmu.de, <http://www.lmu.de/ices2017>.

4–8 September, Herceg Novi, Montenegro. 19th Annual Conference of the Materials Research Society of Serbia. Materials Research Society of Serbia, P.O. Box 433,

11001, Belgrade, Serbia. [✉](mailto:yucomat@mrs-serbia.org.rs) [★](http://www.mrs-serbia.org.rs/index.php/yucomat-2017m)

5 September, Manchester, United Kingdom. **BMSS Careers in MS Workshop.** Lisa Sage, [✉](mailto:bmssadmin@btinternet.com), [★](http://www.bmss.org.uk/bmss2017/careersWorkshop.shtml)

5–7 September, Manchester, United Kingdom. **The 38th BMSS Annual Meeting.** Royal Northern College of Music, Manchester, UK, [★](http://www.bmss.org.uk/meetings.shtml)

9–12 September, Boston, United States. **14th Symposium on the Practical Applications of Mass Spectrometry in the Biotechnology Industry.** [✉](mailto:info@casss.org), [★](http://www.casss.org)

10–14 September, Berg en Dal, Netherlands. **7th International Chemometrics Research Meeting ICRM2017.** Organisers, [✉](mailto:ICRM2017@DutchChemometricsSociety.nl), [★](http://www.DutchChemometricsSociety.nl/icrm-2017)

13–15 September, Berlin, Germany. **23rd International Workshop on "Single Molecule Spectroscopy and Super-resolution Microscopy in the Life Sciences".** Jana Bültner, [✉](mailto:workshop@picoquant.com), [★](http://www.picoquant.com/events/detail/single-molecule-workshop)

17–21 September, Heraklion, Crete, Greece. **10th International Conference on Instrumental Methods of Analysis (IMA-2017).** Konstantinos Simeonidis, National Technical University of Athens, Lab. of Inorganic & Analytical Chemistry, Athens, Greece, [✉](mailto:ima2017@chemistry.uoc.gr), [★](http://www.ima2017.gr)

17–21 September, Dublin, Ireland. **16th Human Proteome Organisation World Congress (HUPO 2017).** Conference Partners, Suites 11-13, The Hyde Building, The Park, Carrickmines, Dublin 18, Ireland. [✉](mailto:hupo2017@conferencepartners.com), [★](http://www.hupo2017.ie)

17–22 September, Thessaloniki, Greece. **European Congress and Exhibition on Advanced Materials and Processes (EUROMAT 2017).** [✉](mailto:euromat2017@afea.gr), [★](http://euromat2017.fems.eu)

24–27 September, Atlanta, Georgia. **131st Association of Official Agricultural Chemists (AOAC) International Annual Meeting and Exposition.** AOAC International, 2275 Research Blvd, Suite 300, Rockville, MD 20850-3250, USA. [✉](mailto:lchelf@aoac.org), [★](http://www.aoac.org)

25–27 September, Ulm, Germany. **14th Confocal Raman Imaging Symposium.**

Dr Sonja Breuninger, [✉](mailto:Sonja.Breuninger@WITec.de) [★](http://www.raman.net)

25–29 September, Oxford, United Kingdom. **9th International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources (WIRMS-2017).** Emma Clarke, [✉](mailto:WIRMS2017@diamond.ac.uk), [★](http://www.wirms2017.com)

28–29 September, Vienna, Austria. **5th Workshop on Field-Flow Fractionation-Mass Spectrometry (FFF-MS).** Stephan Wagner, [✉](mailto:nanoanalytics@univie.ac.at), [★](http://umweltgeologie.univie.ac.at/hofmann-group/workshops/)

1–4 October, Naples, Italy. **10th International Symposium on Biological Monitoring in Occupational and Environmental Health (ISBM-10).** Secretariat, [✉](mailto:info@centercongressi.com), [★](http://www.centercongressi.com/isbm10/splashscreen.php)

3–4 October, Houston, Texas, United States. **Gulf Coast Conference (GCC) 2017.** Gulf Coast Conference, 13921 Highway 105 W #163, Conroe, TX 77304, USA, [★](http://www.gulfcoastconference.com)

4–6 October, Budapest, Hungary. **EuroFood Chem XIX Conference.** [✉](mailto:eurofood-chem2017@mke.org.hu), [★](http://www.eurofoodchem2017.mke.org.hu/)

4–5 October, Blacksburg, VA, United States. **3rd Annual ICP Conference: Back to Basics-Drilling Down.** [★](https://www.inorganicventures.com/icp)

4–6 October, Reims, France. **International Workshop on Spectroscopy and Dynamics of Ozone and Related Atmospheric Species.** [✉](mailto:maud.rotger@univ-reims.fr), [★](http://www.univ-reims.fr/ozone2017)

8–13 October, Reno, Nevada, United States. **44th Annual Conference of Federation of Analytical Chemistry and Spectroscopy Societies (SciX2017).** [✉](mailto:facss@facss.org), [★](http://www.scixconference.org)

11–13 October, Berlin, Germany. **EXSA Workshop on Quantitative Methods in X-ray Spectrometry.** [✉](mailto:quant2017@exsa.hu), [★](https://www.exsa.hu/quant2017)

11–13 October, Bologna, Italy. **5th Mass Spectrometry (MS) Food Day.** Dr. Davide Garbini, [✉](mailto:davide.garbini@coopitalia.coop.it), [★](http://www.spettrometriadimassa.it/Congressi/5MS-FoodDay/)

16–18 October, Menorca, Spain. **2nd International Conference on Ionization Principles in Organic and Inorganic Mass Spectrometry.** Yngvar Thomassen, [✉](mailto:yngvar.thomassen@stami.no), [★](http://www.ipioms.com)

17–19 October, Calabar, Nigeria. **SETAC Africa 8th Biennial Conference.** SETAC North

America, 229 S. Baylen Street, 2nd Floor, Pensacola, FL 32502, USA, [✉](mailto:setaceu@setac.org), [★](https://saf2017.setac.org)

18–20 October, Barcelona, Spain. **Environmental Omics, Integration and Modelling.** [✉](mailto:wenvomics2017@idaea.csic.es), [★](http://wenvomics2017.info)

18–19 October, Osaka, Japan. **6th Global Conference on Mass Spectrometry (MASSSPECTRA2017).** [✉](mailto:massspectra@chemistryconferene.org), [★](http://www.massspectra.com/asia-pacific)

22–25 October, Seattle, Washington, United States. **Geological Society of America (GSA) 2017 Annual Meeting.** Geological Society of America, [✉](mailto:meetings@geosociety.org), [★](http://www.geosociety.org/meetings)

24–28 October, Évora, Portugal. **9th International Congress on the Application of Raman Spectroscopy in Art and Archaeology (RAA2017).** [✉](mailto:raa2017@uevora.pt), [★](http://raa2017.uevora.pt)

25–27 October, Lahore, Pakistan. **2017 International Conference on Agricultural and Food Science.** Secretary, [✉](mailto:info@icbb.vu.edu.pk), [★](http://www.icbb.vu.edu.pk/)

7–10 November, Prague, Czech Republic. **8th International Symposium on Recent Advances in Food Analysis (RAFA2017).** [✉](mailto:jana.hajslova@vscht.cz), [★](http://www.rafa2017.eu)

12–16 November, San Diego, California, United States. **American Association of Pharmaceutical Scientists (AAPS) 2017 Annual Meeting.** AAPS, 2107 Wilson Blvd, Suite 700, Arlington, Virginia 22201-3042, USA, [✉](mailto:aaps@aaps.org), [★](http://www.aaps.org/annualmeeting/)

12–16 November, Minneapolis, MN, United States. **SETAC North America 38th Annual Meeting.** SETAC North America, [✉](mailto:setac@setac.org), [★](https://msp.setac.org)

12–17 November, Matsue-City, Shimane, Japan. **7th Asia-Pacific Winter Conference on Plasma Spectrochemistry (APWC).** Takafumi Hirata, Koyo University, Kitashirakawa, Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan. [✉](mailto:ht1@kueps.kyoto-u.ac.jp), [★](http://www2.es.titech.ac.jp/okino/pdf/17APWPoster.pdf)

13–15 November, Somerset, New Jersey, United States. **Eastern Analytical Symposium and Exposition (EAS 2017).** [✉](mailto:askEAS@eas.org), [★](http://www.eas.org)

2018

8–13 January, Amelia Island, Florida, United States. **2018 Winter Conference on Plasma Spectrochemistry.** Ramon Barnes, [✉](mailto:wc2018@chem.umass.edu), [★](http://icpinformation.org)

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19–24 February, Seattle, Washington, United States. **American Academy of Forensic Sciences (AAFS) 70th Annual Scientific Meeting.**  www.aafs.org.

18–22 March, New Orleans, United States. **255th American Chemical Society National Meeting.**  natlmtgs@acs.org,  www.chemistry.org.

26–29 March, Santa Fe, New Mexico, United States. **International High Power Laser Ablation Symposium (HPLA 2018).** Amy Walker,  awalker@blue52productions.com,  www.usasymposium.com/hpla.

8–13 April, Vienna, Austria. **European Geosciences Union (EGU) General Assembly 2018.** EGU Executive Office,  secretariat@egu.eu,  www.egu.eu.

14–18 April, Chicago, IL, United States. **Annual Meeting American Association for Cancer Research.** AACR,  aacr@aacr.org,  www.aacr.org.

15–19 April, Estepona (Málaga), Spain. **6th International Congress on Operando Spectroscopy (Operando VI).** Secretary,  info@operandoconference.com,  <http://www.operandoconference.com/index>.

16–20 April, Berlin, Germany. **4th International Glow Discharge Symposium (GDS).** Silke Richter,  silke.richter@bam.de,  <http://ew-gds.com/>.

21–25 April, San Diego, CA, United States. **Experimental Biology 2018.** Experimental Biology,  eb@faseb.org,  <http://experimentalbiology.org>.

28 April–2 May, Prague, Czech Republic. **33rd Congress International Society for Advancement of Cytometry.**  infor@cytoconference.org,  <http://cytoconference.org>.

3–7 June, San Diego, CA, United States. **66th ASMS Conference on Mass Spectrometry.**  office@asms.org,  www.asms.org.

10–13 June, Leon, Norway. **9th Nordic Conference on Plasma Spectrochemistry.** Yngvar Thomassen,  yngvar.thomassen@stami.no,  www.nordicplasma.com.

10–15 June, Glasgow, Scotland, United Kingdom. **10th International Conference on Clinical Vibrational Spectroscopy (SPEC-2018).**  <http://spec2018.com/>.

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

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

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

19–23 August, Boston, MA, United States. **256th American Chemical Society National Meeting.**  natlmtgs@asc.org,  www.chemistry.org.

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

26–29 August, Toronto, Ontario, Canada. **132nd Association of Official Agricultural Chemists (AOAC) International Annual Meeting and Exposition.**  meetings@aoac.org,  www.aoac.org.

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

4–8 November, Washington, DC, United States. **American Association of Pharmaceutical Scientists (AAPS) 2018 Annual Meeting.**  aaps@aaps.org,  www.aaps.org/annualmeeting/.

Courses

2017

30 July–5 August, Kloster Neustift, Brixen/Bressanone, Italy. **11th European Summer School Advanced Proteomics.** Shabaz Mohammed,  info@proteomic-basics.eu,  <http://www.proteomic-basics.eu>.

18–25 August, Dresden, Germany. **International Summer School Spectroelectrochemistry.** Evgenia Dmitrieva, IFW Dresden, Helmholtzstrasse 20, 01069, Dresden,  summerschool@ifw-dresden.de,  <https://www.ifw-dresden.de/institutes/iff/events/4th-summer-school-spectroelectrochemistry/>.

4–5 September, Manchester, United Kingdom. **BMSS Introduction to MS Short Course.** Lisa Sage,  bmssadmin@btinternet.com,  <http://www.bmss.org.uk/bmss2017/msCourse.shtml>.

9–11 October, Berlin, Germany. **EXSA Autumn School on Quantitative Methods in X-ray Spectrometry.**  quant2017@exsa.hu,  <https://www.exsa.hu/quant2017/>.

12–13 October, Birmingham, United Kingdom. **Quality Assurance and Quality Control in Metabolomics.** David Epps,  d.epps@bham.ac.uk,  <http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/quality-phenotyping.aspx>.

16–20 October, Montpellier, France. **Seventh Annual Eigenvector University Europe.** Barry Wise,  bmw@eigenvector.com,  http://eigenvector.com/courses/EigenU_Europe.html.

6–9 November, Berlin, Germany. **15th European Short Course on "Principles and Applications of Time-resolved Fluorescence Spectroscopy".** Nicola Kasse,  trfcourse@picoquant.com,  <http://www.picoquant.com/events/details/fluorescence-course>.

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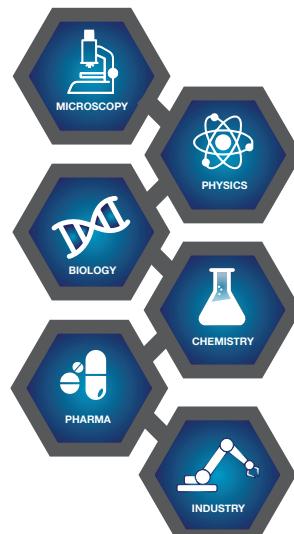
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