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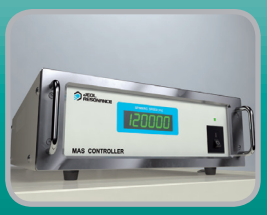

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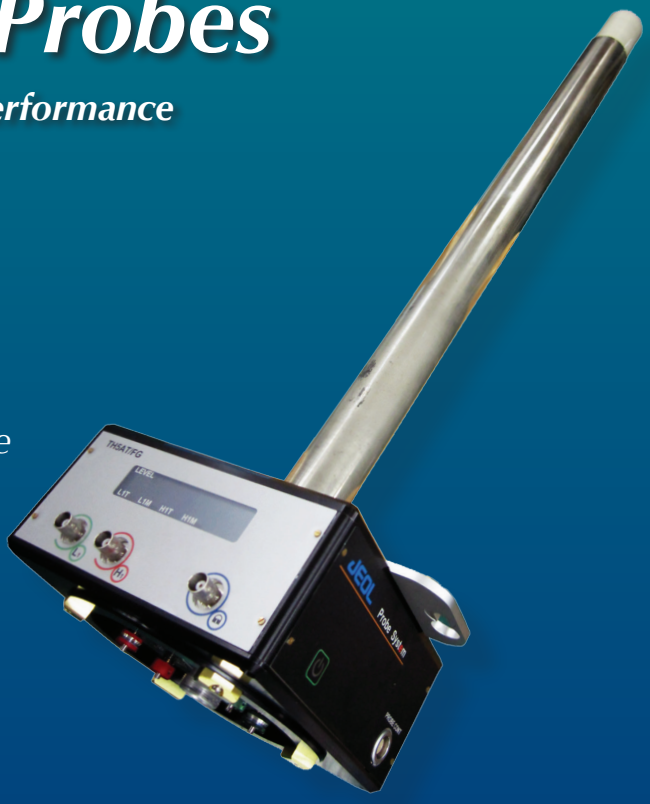

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EDITORIAL

It is not unusual to find that an idea, project or business is "ahead of its time". This might well be true of the EU 5th Framework project, Eurospec, that has been reported in these pages in the past. The idea was an excellent one: to capture the vast amount of spectral and associated data prepared for publication, and build a spectral database. Sources might be the usual scientific papers that we are all familiar with, or PhD or other theses. In the end, good idea or not, Eurospec did not gain enough traction to succeed, although all data collected has been preserved within the PubChem Project of the US National Library of Medicine. Now, Tony Davies and a number of others consider a not-too-dissimilar idea: collecting supplementary spectroscopic data. Like Eurospec, the plan is to use such supplementary data not only to enhance the published paper, but also to aid thorough peer-review by allowing reviewers access to the full data rather than, as Tony puts it, "low-resolution images of data". I'm sure you will be interested in a look at the future through "Simplifying spectroscopic supplementary data collection".

In the Quality Matters column, John Hammond also touches on a topic from the past pages of *Spectroscopy Europe*. In "Into the future (Part 2): changes to ISO 17025 and ISO Guide 34", he updates us on recent developments with the ISO 17xxx series of standards. John continues with news of standards particularly relevant to readers.

In the Sampling Column, Kim Esbensen and Claas Wagner continue their series of articles introducing readers to representative sampling and the Theory of Sampling. They have reached the area of process sampling and this issue consider "The variographic experiment". Variograms can provide valuable and unexpected insights into a process.

Sampling questions

Many readers may well be interested to learn more about representative sampling and the Theory of Sampling. To facilitate this, *Spectroscopy Europe* with the help of the editors of the Sampling Column will answer questions about specific sampling problems you may have or about theoretical aspects of the Theory of Sampling. If you have a question, please direct it to me (ian@impublications.com). You must be prepared for your question and the answer to be published, however, this can be anonymous (both individual and organisation) if you wish.

Each column and article on spectroscopyeurope.com has a commenting facility and you are welcome to use this to add your own comments or raise questions directly concerning the content of that article or column. Please note that you must be logged in use this facility.

Variograms can provide unexpected and valuable information about processes. Find out more in the Sampling Column starting on page 14.

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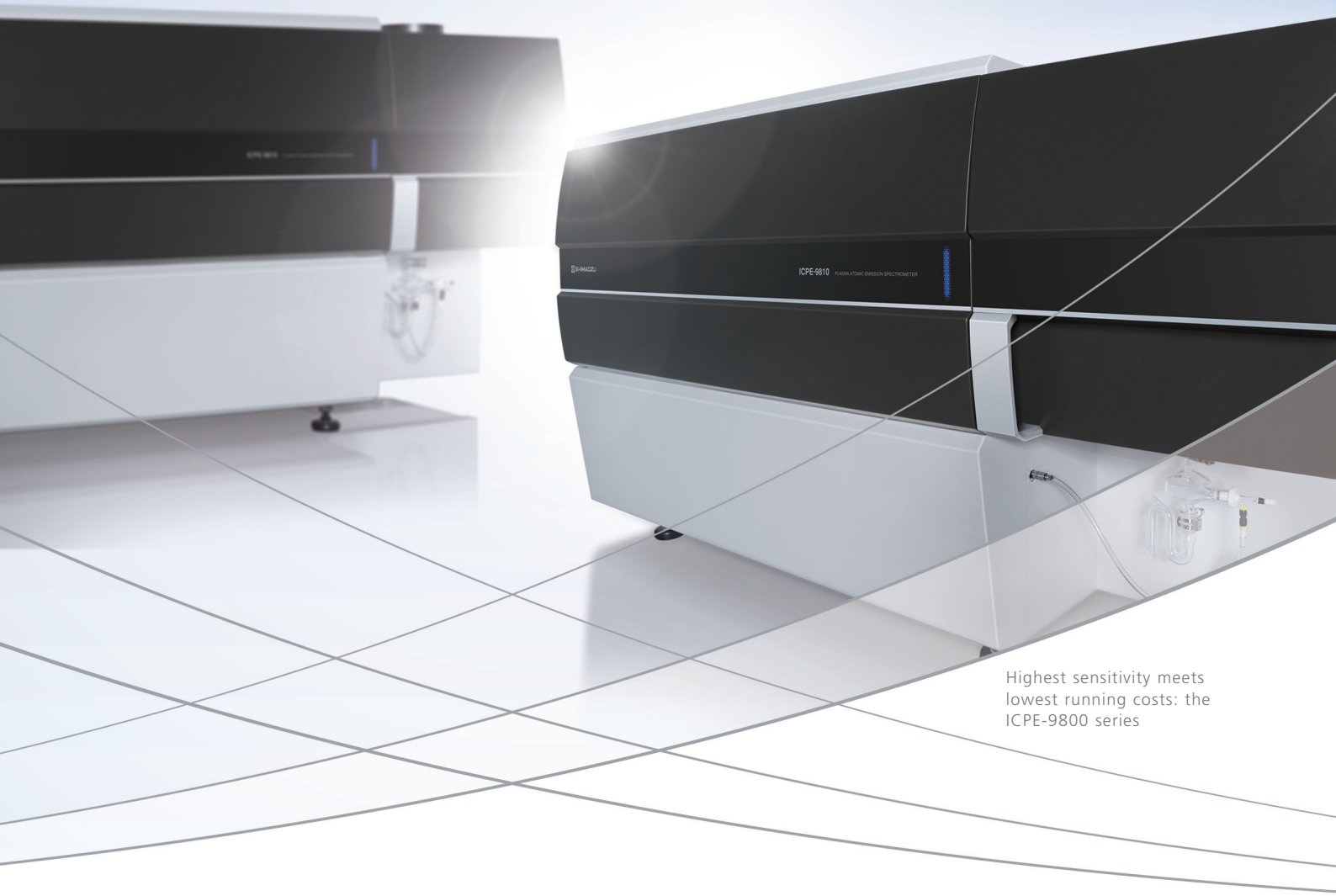

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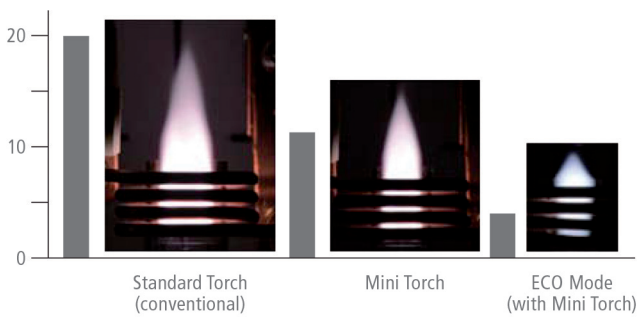

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TONY DAVIES COLUMN

Simplifying spectroscopic supplementary data collection

Antony N. Davies,[a,b] David Martinsen,[c] Henry S. Rzepa,[d] Charles Romain,[d] Agustin Barba,[e] Felipe Seoane[e], Santiago Dominguez[e] and Carlos Cobas[e]

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One of the interesting initiatives discussed during the IUPAC General Assembly[1] a few weeks ago in Sao Paulo was the renewed push for more efficient and simpler ways of submitting supplementary spectroscopic data. IUPAC Division 3 were particularly keen on enabling better NMR supplementary data submission. It emerged that there have been some interesting efforts made to radically simplify such submission. Mestrelab Research have developed a solution called Mpublish which has been tested and deployed at Imperial College London, aimed at lowering the barriers to the submission of supplementary full spectroscopic data. Along the lines of the EuroSpec project,[2,3] the submission system also handles the most complicated data needing submission—multi-dimensional nuclear magnetic resonance spectra. Henry Rzepa's blog discusses the background and submission process and provides a link to his guide to setting up and uploading files to the Imperial College HPC Data Repository as well as to the "FAIR" principles… (findable, accessible, inter-operable and re-usable).[4]

Issues to be overcome

As has been discussed extensively, it is crazy that in an internet age, scientists asked to review publications are expected to make decisions on the appropriateness of the work being presented by studying low-resolution images of data. In their day-to-day work in their own labs, the reviewers would have far better tools available to support their decision making. Regulatory compliance agencies are concentrating more on data integrity and the overall desire for better fraud prevention, making available the actual spectroscopic data which is the evidence for claims made within publications is clearly desirable. The benefit for funding bodies has been reflected in, for example, the EU Guidance on access to research data which explains the rules around open access that all beneficiaries of Horizon 2020 funding have to follow.[5]

However, such a process brings with it a not insignificant amount of additional work for the submitter of a publication. This includes collating, annotating and submitting what—for example in a synthetic organics chemistry paper—could well be quite a large number of files. Not to mention the issue of which format should the electronic data be submitted in—and how to match that submitted with what each reviewer can actually read.

Outline solution

So any new attempt to reduce the barriers to submission of more real supplementary spectroscopic data is to be welcomed. The solution outlined here is the result of a collaborative approach using tools from Mestrelab Research S.L. in a project to see if an end-to-end simplification was possible.

Figure 1 outlines the individual stages that such a solution needs to embody, with each step being more or less independent of one another. Now, this figure is mainly focussed on the submission process, but the results of the peer review can be many and varied. One example cited by Angie Hunter of *Organic Letters* is that the reviewers may well request the authors to provide more or corrected supplementary information having reviewed the originally submitted paper. The outcome may still not be approval to publish, as the re-submitted paper with or without additional supplementary data can, of course, also fall short of the standard required for a particular journal.

In this solution. they addressed one of the more complex data types. Figure 2 shows a typical example of the spectroscopic information content required for an organic chemistry journal, *Organic Letters*. Their guidance for authors describes what is required concerning spectra (see "Spectra in manuscript" text box).

So, the "User Requirements" for the submission of supplementary spectroscopic data that any author should follow are not new and give clear guidance as to the direction a solution provider must follow! Further details are given below.

The Mpublish project with Mestrelab has one major advantage in that the software partner, as with many third-party NMR analytical software providers, already has many of the tools required

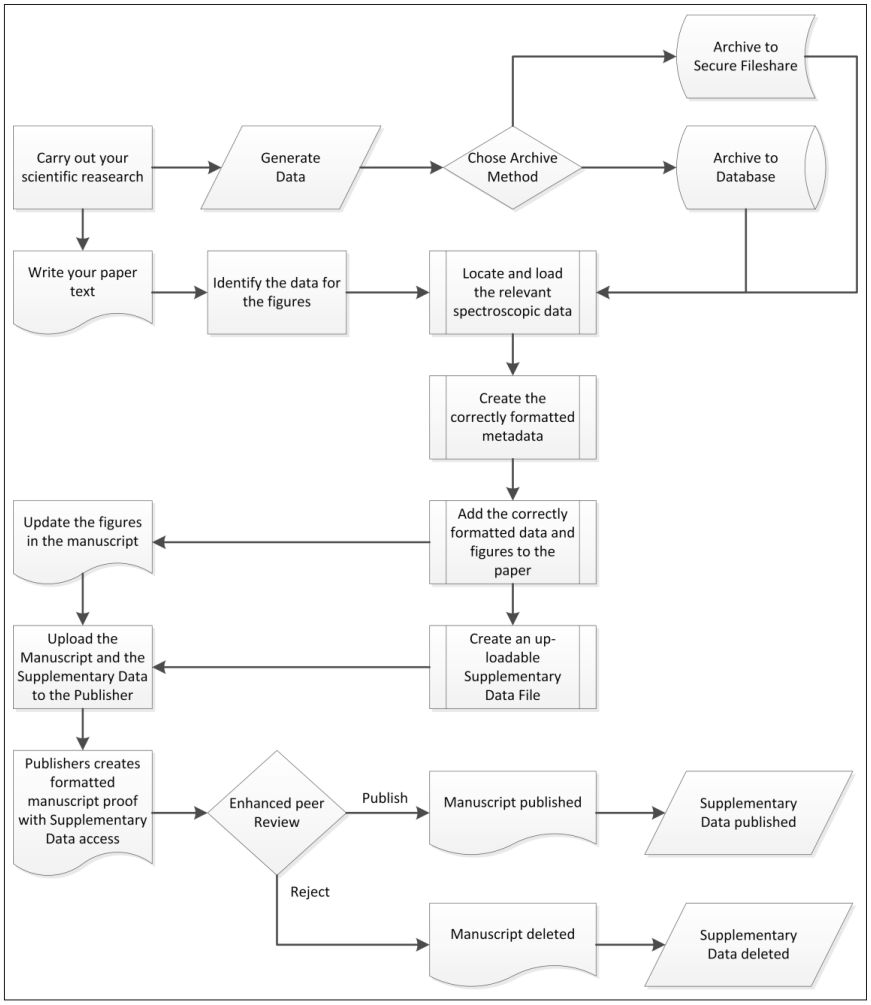


Figure 1. Enhanced publishing workflow with supplementary data capture and submission.

to deliver the formatted annotations and data rendering in their software solutions. Scientists who already work with their tools either with or without the associated databases already have installed most of the functionality required for the initial steps in the flowchart.

The additional functionality in the workflow revolves around the reporting tools and automation targeted specifically at manuscript submission.

Documentation reporting tools and packing supplementary data

These requirements are critical to getting widespread acceptance by the publishing authors as they represent an essentially "non-productive" overhead in their already stressful lives. Automation of the creation of the journal-specific peak position, coupling constant etc. information

Spectra in manuscript

Spectra will be published in the body of the manuscript only when concise numerical summaries are inadequate for the discussion. A brief summary of spectral data can be provided in the Letter as a footnote.

- Letters dealing primarily with interpretation of spectra, and those in which band shape or fine structure needs to be illustrated, may qualify for an exception
- When presentation of spectra within the paper is essential, only the pertinent sections, prepared as figures should be presented

Full data and images of spectra should be included in the Supporting Information (see Compound Characterization and Spectra Standards for details).

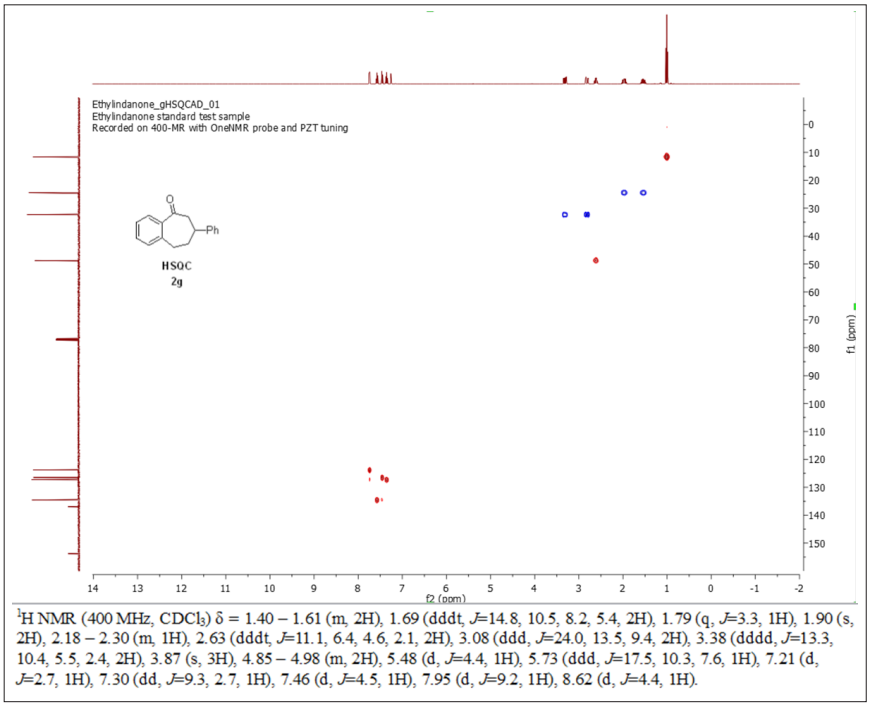
TONY DAVIES COLUMN

tables already saves NMR spectroscopists much effort and formatting/re-formatting in the correct manner for submission to a specific journal. Should the authors then decide to change publishers, it is even more welcome.

Figure 3 shows the reporting part of the solution where the specific files, loaded either from the local database or from specific individual saved files are selected before loading into the automated processing and reporting phase where the figures are generated and the entire files saved in an open document file format for later editing if required.

With the figures now ready, the data packer has the capability to carry out one of the most arduous submission tasks. *Organic Letters* specifies in their guidance section details on how to submit the spectra as shown in the "Primary NMR data files" text box.[6]

I will not attempt to work out how much time this takes to do manually, but fortunately the data packer has now automated this process and, after politely asking you if you want to create a .ZIP file with all the raw data used in the document, generates the .ZIP file with individual subdirectories for each of the figures in the documents named appropriately for easy identification (Figure 4). You now have everything ready to submit to the journal with almost no additional effort over a conventional publication submission without accompanying supplementary data. Fortunately, Henry Rzepa's data publishing workflow is much simpler but arises from a different ethos around academic institutions being considered data publishers—something to be detailed elsewhere!



^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.40 – 1.61 (m, 2H), 1.69 (dddt, *J*=14.8, 10.5, 8.2, 5.4, 2H), 1.79 (q, *J*=3.3, 1H), 1.90 (s, 2H), 2.18 – 2.30 (m, 1H), 2.63 (dddt, *J*=11.1, 6.4, 4.6, 2.1, 2H), 3.08 (ddd, *J*=24.0, 13.5, 9.4, 2H), 3.38 (dddd, *J*=13.3, 10.4, 5.5, 2.4, 2H), 3.87 (s, 3H), 4.85 – 4.98 (m, 2H), 5.48 (d, *J*=4.4, 1H), 5.73 (ddd, *J*=17.5, 10.3, 7.6, 1H), 7.21 (d, *J*=2.7, 1H), 7.30 (dd, *J*=9.3, 2.7, 1H), 7.46 (d, *J*=4.5, 1H), 7.95 (d, *J*=9.2, 1H), 8.62 (d, *J*=4.4, 1H).

Figure 2. Typical spectroscopic data expected to support a manuscript in *Organic Letters*.

And how to review?

So, we now only have to find a solution for the final section of the workflow.

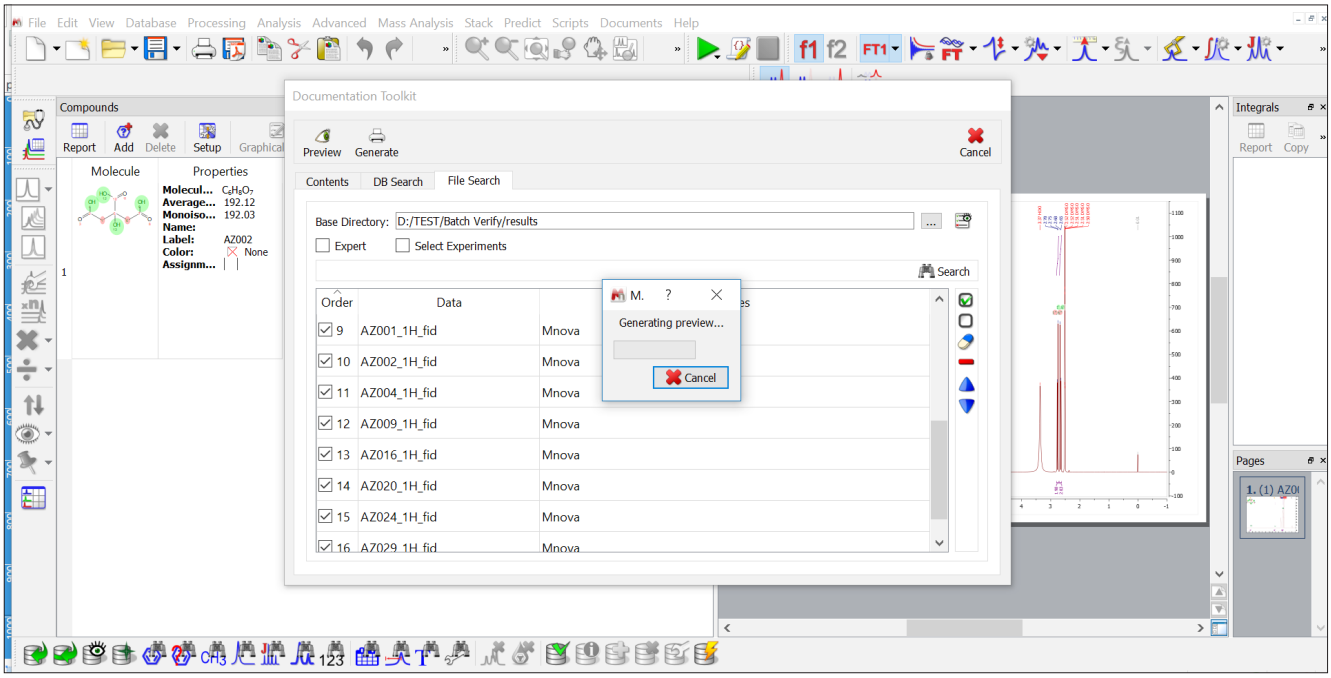


Figure 3. Automated reporting starting with the saved analytical spectra and chemical structure files.

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Primary NMR data files

Submission of primary NMR data files (FID files, acquisition data, processing parameters) is highly recommended. All original primary NMR data supporting a submission should be retained and provided if requested.

When submitting FID files:

- One folder should be created for each compound
- Folder should be named clearly, using the compound number
- Include the FID files, acquisition data and processing parameters for each experiment
- Name each spectrum according to the type of nucleus measured: ^{1}H, ^{13}C, DEPT, COSY, etc.
- NMR files should be compressed into zip file(s)

In a text document, include the name of the manufacturer of the spectrometer used to collect the data, the acquisition software and processing programs used to analyse the data, and the field strength used to measure each nucleus (i.e., 300 MHz ^{1}H or 50 MHz ^{13}C). Include a structure file that shows the structure and compound identifier for each provided dataset. MolFile is the recommended format and is strongly preferred.

Here the generosity of the software vendors has provided a surprisingly simple solution to what could have been a nasty sticking point. As Peter Lampen rightly pointed out when reviewing this solution, it appears to be too closely linked to authors, reviewers and publishers buying a specific software product.[7] As the uploaded supplementary data are in the native format of the original measuring spectrometer, it would be possible to read the files with any vendor's solutions that are capable of parsing these raw data files. The vendor in this project has, however, come up with a nice solution.

The final stage of the workflow requires the publishers to digitally sign the submitted supplementary data file using a public/private key certification service. Reviewers are then able to download a free version of the software used to create the files in the first place and upon reading the digitally signed file, the full capability of the software is unlocked allowing the enhanced review to take place on the full supporting data. Access to the full data in this manner also strongly enhances the ability of the publishers and reviewers to spot data fraud or unwanted manipulation.

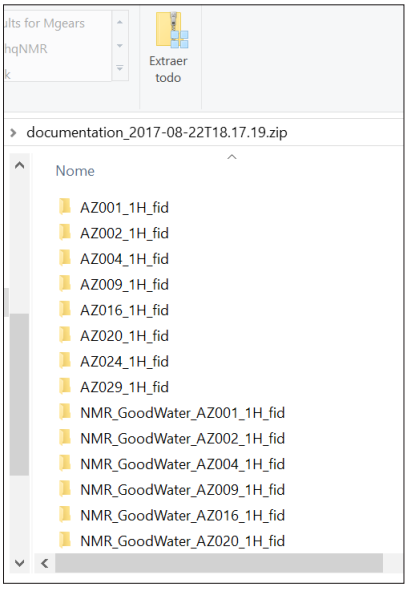

Figure 4. A zip file created as specified in the *Organic Letters* guidelines with separate directories for each figure in the publication.

It is also worth noting that the use of the vendor software to prepare the data is not a prerequisite for the review system to work. Authors can always submit data prepared with a different processing software, upload the original raw data acquired by the instrument and could manually prepare the processed and raw data to fulfil the publisher format expectations. In this case, the raw data can still be signed by the publisher, and the free version of the review software would still allow full review of the digitally signed data.

Conclusions

It is possible for publishers and software vendors to get together to provide tools for the spectroscopic community to take most of the pain out of submitting real spectra as supplementary data. Such a solution may also be of interest within less publicly open environments, such as inside companies, as presented by Steve Hollis of Amgen and co-authors at the ENC conference in 2016 where a solution combining a number of different third-party software vendors was presented for open access NMR inside his company.[8] Not all journals currently have such detailed requirements as the guidelines adopted by *Organic Letters*, but the solution does show that in an internet age it is possible to actually do less work whilst submitting all the full spectra supplementary data than you would need to carry out without the support of the current breed of spectroscopic data processing and reporting tools!

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Into the future (Part 2): changes to ISO 17025 and ISO Guide 34

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In Vol. 26 No. 5 (2014),[1] in the appropriately titled "Into the future: changes to ISO 17025 and ISO Guide 34", Peter Jenks and I discussed the status of these two important ISO documents, and considered the way forward.

We finished the article with a significant phrase, namely:

Part 1: *"John and I will continue to report on developments as they are revealed!"*

Given that ISO 17034:2016 was published on 1 November 2016, and the revision of ISO/IEC 17025 is approaching completion, and thereby publication, this article looks back at some of statements made in 2014, and reviews the outcome, and again the way forward.

However, before moving forward to this comparative review, there are significant changes to the 17xxx series of Standards in both the new ISO 17034 and revised ISO/IEC 17025, and these need to be explained first.

ISO 17xxx series Standards

This restructuring is based on the common structure adopted by other International Standards on conformity assessment (e.g. ISO/IEC 17020 Requirements for the operation of various types of bodies performing inspection) developed by the ISO Technical Committee on conformity assessment (ISO/CASCO), and in a significant change, includes the option to use ISO 9001 to meet the management requirements.

In addition, there is the requirement to include the obligatory and recommended requirements detailed in ISO/CASCO procedure QS-CAS-PROC 33:

- Impartiality
- Confidentiality
- Complaints and appeals
- Management system

The most significant change is in the structure of the Standard(s), which are completely revised, now distinguishing "resource" from "process" and acknowledging the possible role of an ISO 9001 based management system. So now, unlike the previous structural template, where "Section 4—Management requirements" preceded "Section 5—Technical requirements", these Standards sequentially follow and re-define the requirements in this order: "General"; "Structural"; "Resource"; "Process"; and "Management", effectively reversing the sequence.

There are two options available to fulfil the Management requirement, Option A and Option B.

Option A will require the laboratory to address the requirements of:

- Management system documentation;
- Control of management system documents;
- Control of records;
- Actions to address risks and opportunities;
- Improvement;
- Corrective action;
- Internal audits;
- Management reviews.

Alternatively, Option B allows a laboratory that has established and maintains a management system in accordance with ISO 9001 (which can support and demonstrate the consistent fulfilment of the "General", "Structural", "Resource" and "Process" requirements) to be recognised as fulfilling the intent of the management system requirements as outlined in Option A.

Also, clearly stated in the introduction to these Standards (for the first time) is the following clarification with respect to the terms used:

- "shall" indicates a requirement;
- "should" indicates a recommendation;
- "may" indicates a permission;
- "can" indicates a possibility or a capability.

ISO Guide 34 / ISO 17034

Part 1: *"Within ISO, it has been resolved that a joint Working Group between ISO/ REMCO and ISO/ CASCO (the technical committee responsible for issues relating to conformity assessment) should be established, for the conversion of ISO Guide 34 into ISO Standard 17034. It is expected that this conversion would follow a similar route to that of the ISO Guide 43 for Proficiency Testing to ISO Standard 17043."*

ISO/CASCO Joint Working Group (WG) 43 was duly formed, with significant membership from ISO/REMCO and convenorship of the group, and the resultant Standard ISO 17034 was published on 1 November 2016, after a series of discussion and review meetings held at ISO headquarters in Geneva, Switzerland.

This first edition of ISO 17034 cancels and replaces ISO Guide 34:2009, which has been technically revised, and incorporates the following major changes:

- inclusion of requirements for production of all types of reference materials, and additional specified requirements for certified reference materials;
- harmonisation with the revisions of ISO Guide 31 and ISO Guide 35;
- inclusion of more details on required reference material documentation;
- inclusion of risks and opportunities;
- restructuring based on the common structure adopted by other International Standards on conformity assessment developed by CASCO;
- incorporation of modifications based on ISO/CASCO PROC 33.

It outlines the general requirements for the producers of RMs, including certified reference materials (CRMs). It supersedes ISO Guide 34:2009 and is aligned with the relevant requirements of ISO/IEC 17025. Further guidance (e.g. concerning the content of certificates and the design of characterisation, homogeneity and stability studies) is provided in ISO Guide 31 and ISO Guide 35. While the approaches outlined in ISO Guide 31 and ISO Guide 35 meet the relevant requirements of ISO 17034, there might be alternative ways to achieve compliance to this International Standard.

RMPs that comply with this International Standard will also operate generally in accordance with the principles of ISO 9001. For tests performed in the medical field, ISO 15189 can be used as the reference instead of ISO/IEC 17025.

Part 1: *"This also has ramifications in respect to the normative references associated with ISO Guide 34/ISO 17034, in as far as these '30 series' guides, namely ISO Guide 30, ISO Guide 31 and ISO Guide 35, will now have a mandatory aspect when considered as normative references to ISO 17034."*

At the time of drafting Part 1, and as shown in the document, once the decision to convert ISO Guide 34 into ISO 17034 had been taken, the discussion was now centred on the associated ISO/REMCO Guides, and whether these supporting documents should be considered as normative references to ISO 17034. ISO Guide 35, which deals with the characterisation, and associated stability, homogeneity and uncertainty budget considerations was central to this debate, as it was also scheduled for review and update.

However, as required by any Standard development process, a clear and unambiguous statement is required, and therefore the agreed resolution is very clearly stated in the introduction to ISO 17034:

"This International Standard outlines the general requirements for the producers of RMs, including certified reference materials (CRMs). It supersedes ISO Guide 34:2009 and is aligned with the relevant requirements of ISO/IEC 17025. Further guidance (e.g. concerning the content of certificates and the design of characterization, homogeneity and stability studies) is provided in ISO Guide 31 and ISO Guide 35. While the approaches outlined in ISO Guide 31 and ISO Guide 35 meet the relevant requirements of this International Standard, there might be alternative ways to achieve compliance to this International Standard."

Implicit in the above statement, and clearly stated in Section 2, the only normative reference to ISO 17034 which is "indispensable for its application" is ISO/IEC 17025.

It is also significant that this reference is undated, because for dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies, and therefore ISO 17034 will require compliance with the new version of ISO/IEC 17025 once this becomes available—see below.

Therefore, "the wheel has turned full circle", and the ISO/REMCO Guides now essentially fulfil the purpose for which they were originally intended as stated in Part 1.

Part 1: *"As a technical committee of ISO, ISO/REMCO was formed in 1975, principally to address the lack of guidance with respect to the production, use and certification of reference materials. The output from this committee, resulted in the first versions of the ISO '30 series' of guides, (ISO Guide 30 to ISO Guide 35) which were produced purely as guidance documents, aimed to provide non-mandatory, technical assistance to reference material users, and producers."*

However, now there is the appropriate ISO 17034 Standard in place, and the significance of these documents in providing the essential, additional guidance to Reference Material producers in the required areas should not be under estimated. For this reason, they continue to be revised and developed further, as you will see when the recent ISO/REMCO meeting is discussed in a later article.

ISO/IEC 17025

Part 1: *"It is normal for ISO Standards to be reviewed every five years: on the last occasion (2010) it was felt that ISO/IEC 17025 met the needs of the users and no change was needed, so it is now ten years since the last full revision of the Standard in 2005. In 2013 it was agreed by ILAC to push for a full revision of the Standard, this process has started."*

The background to this decision is detailed in Part 1, but indeed ISO/CASCO did respond to the International Laboratory Accreditation Cooperation (ILAC) request, as this was formally submitted as a New Work Item Proposal (NWIP) jointly with the South African Bureau of Standards. Thereby, in October 2014 CASCO/WG 44 was formed and tasked with the three-year process to update and revise ISO/IEC 17025, due for completion in October 2017.

On publication, the mandated implementation period by the national accreditation bodies, is three years. If one considers, for example that there are approximately 1600 Calibration and Testing Laboratories accredited to ISO/IEC 17025 by the United Kingdom Accreditation Service (UKAS) in the UK, then the logistics of this process could surely be described as "challenging"?

ISO/REMCO

The recent 40th meeting of the Reference Material Committee of ISO, ISO/REMCO, was hosted by BAM on behalf of the German Institute for Standardization (DIN) in Berlin, Germany, from 26 to 29 June 2017, and in relation to this article one of the key topic discussed was the revision and publication of ISO Guide 35:2017. Other topics discussed will form the content of another article in the series.

Why revised ISO Guide 35:2006?

In addition to the mandatory review process, the developments in RM production approaches, and the growing range of classes of RMs with advances in technology increased the need for more widely applicable technical guidance in RM production. In addition, increasing use of ISO/IEC 17025 and ISO 15189 by laboratories led to greater demand for clear statements of metrological traceability.

ISO Guide 35:2017 provides detailed guidance on a larger range of homogeneity study designs, and describes a wider range of stability management strategies than ISO Guide 35:2006. It also contains specific provisions concerning the establishment of metrological traceability in RM production.

The document explains concepts and provides approaches to the following aspects of the production of reference materials:

- the assessment of homogeneity;
- the assessment of stability and the management of the risks associated with possible stability issues related to the properties of interest;
- the characterisation and value assignment of properties of a reference material;
- the evaluation of uncertainty for certified values;
- the establishment of the metrological traceability of certified property values.

The guidance given supports the implementation of ISO 17034. As previously stated, other approaches may also be used if the requirements of the Standard are fulfilled.

Brief guidance on the need for commutability assessment is given in the document, but no technical details are provided. A brief introduction for the characterisation of qualitative properties (9.6 to 9.10) is provided together with brief guidance on sampling such materials for homogeneity tests (Clause 7). However, statistical methods for the assessment of the homogeneity and stability of reference materials for qualitative properties are not covered. The document is also not applicable to multivariate quantities, such as spectral data.

So, in summary, in 2017.

For reference material producers (RMPs), there is now an International Standard, (and one Normative Reference) and three ISO Guides that support the production and certification of RMs to ensure that the quality of the RMs meets the requirements of the end users;

- ISO 17034 outlines the general requirements to be met by an RMP to demonstrate competence.
- ISO/IEC 17025 provides the required Standard with relation to measurement.
- ISO Guide 35 provides more specific guidance on technical issues and explains the concepts for processes such as the assessment of homogeneity, stability and characterisation for the certification of RMs.
- ISO Guide 31 describes the contents of certificates for CRMs, and of accompanying documents for other RMs, respectively.
- ISO Guide 30 contains the terms and definitions related to reference materials.

Clarity at long last?

Once again, and with the aim of completing the trilogy, we will continue to report on developments as they are revealed!

Reference

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SAMPLING COLUMN

The variographic experiment

Kim H. Esbensen[a] and Claas Wagner[b]
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Pierre Gy, the inventor of the Theory of Sampling (TOS), pioneered applications of *variography* to understanding large-scale variability in process plants and process control from as early as the 1950s and devoted a major part of his TOS development period to this subject. The variogram allows one to identify *sources of variability* and provides valuable insight into correlations between successive samples. Neglect or poor understanding of the data analytical capabilities of the variogram means that it has not been widely applied in process control until now, except in industry sectors which have embraced TOS (mining, cement and certain parts of the process industries) because of the overwhelming consequences of making wrong decisions when treating vast tonnages—the consequences of wrong decisions are simply too great. Failure to address stream heterogeneity means that conventional statistics and Statistical Process Control (SPC) too often fail to identify and distinguish the true *sources of variability* in a process stream. For each type of heterogeneity, there is a matching variety of process variability. Although the method is powerful in terms of the insights one is able to gain in regard to plant performance and management, examples of the application of this particular method have been suspiciously little notable in the literature.

The variogram

Any process stream or similar that are to be sampled should always first be subjected to a "variographic experiment", the purpose of which is to tune in an optimised sampling frequency based on the increment size selected. The variographic experiment will also allow estimation of an optimal number of increments to be aggregated as composite samples. It is the responsibility of the sampler to come up with the best possible initial suggestion for the size of the increments to be used; obviously previous experience and knowledge regarding the specific process at hand are of premium value in this endeavour.

In order to characterise a process stream, it is necessary to extract a certain number of increments, N_U, to have these analysed in the laboratory and to conduct calculations based on the variographic master equation, Figures 1 and 2. The total number of analytical results (stemming from the N_U increments) *must* be between 60 and 100—it may well be larger (this is actually not such a harsh demand, when it is factored in that most of the variographic characterisations used extensively in science, technology and industry are usually realised based upon *automated sampling*). In general, it must *not* be smaller than 60, although

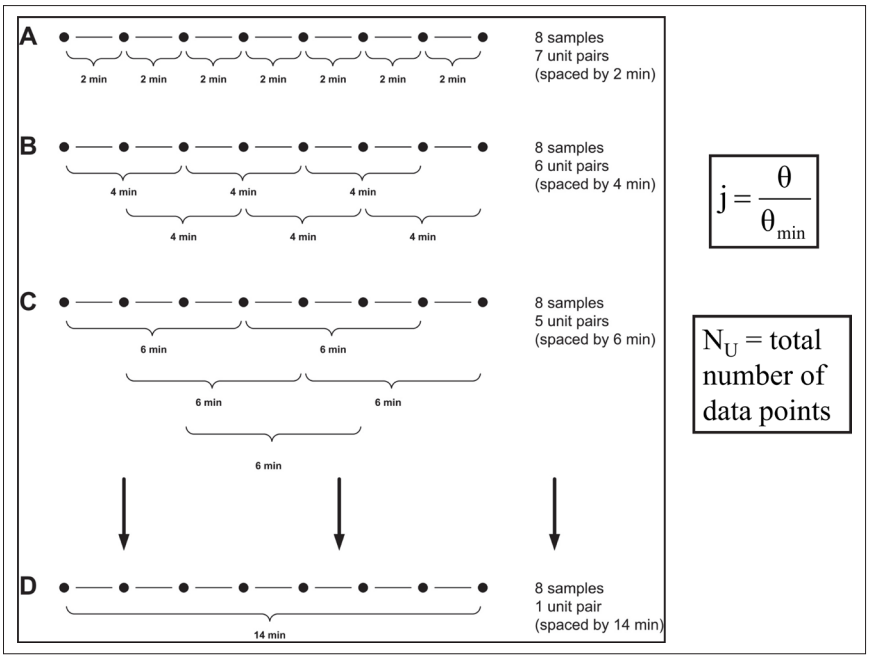

Figure 1. Based on a relevant problem-dependent sampling frequency, 60–100 increments need to be extracted (completely TOS-correct). In the specific example shown here the sampling frequency is 2 min.

very experienced operators occasionally cite the canonical number 42 (however, this is not recommended at large without considerable experience).

The sampling frequency used in the variographic experiment is either set by the process situation at hand (existing, proven knowledge), or it may be calculated as the total process interval under investigation divided by 60 (or 100). Often there are special circumstances that fix this issue, for example in the case where the variographic experiment is aimed at investigating a current situa-

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SAMPLING COLUMN

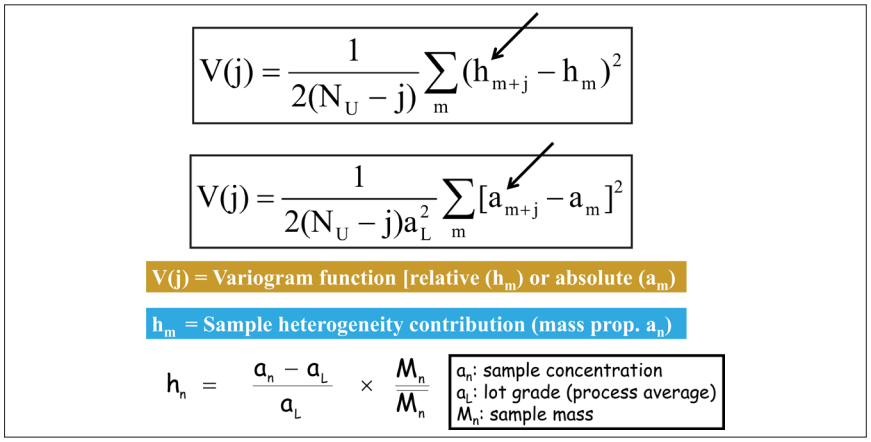

Figure 2. Variogram master equation, expressed both in terms of analytical results, a_m, or alternatively, in terms of the corresponding heterogeneity contributions h_m (the latter was defined in an earlier column, but repeated here for easy reference).

tion, which has an already set sampling frequency. This may be defensible, or it may not—a matter that will be revealed by proper interpretation of the variogram results (lots of examples to follow in subsequent columns).

There may, thus, be many objectives behind a variographic characterisation but all involve deciding upon the most relevant sampling frequency from which to gain a maximum of insight (more on these initiating issues after a first familiarity with the variographic experiment has been gained).

There is, thus, a minimum *resolution limit* associated with every variographic experiment; there can be no information gained at a scale *less* than the experimental sampling rate (2 minutes in the example in Figure 1).

The distance between two data points is called the lag, *j*. The minimum distance between any two data points is termed Θ_{min}. Any distance between pairs of data points, *j*, is always referred to the root Θ_{min}, and will therefore always be a *multiplum* of Θ_{min} [$j = 1, 2, 3, ..., N_{U-1}$]. This allows use of a general lag parameter, *j*, which is *independent* of the particular measurement unit used. This general lag parameter is a most welcome feature, allowing comparison between variograms of any process, type, material etc. As shall be shown this makes comparative variographic analysis indispensable in process technology and process sampling.

It is often recommended to oversample for the purpose of the variographic experiment, but we shall temporarily set aside these initiating issues until after an initial familiarity with the variographic experiment has been gained. Thus, in Figure 1 the current sampling frequency was actually ~8 min, but it was decided to over sample by a factor of ×4, because there was a suspicion that the current frequency was actually too high.

The primary job for variographic characterisation, Figures 3 and 4 is to express the variability of the set of N_U analytical results. Remember that due diligence (TOS correctness) must always be observed regarding extraction of all increments (see previous column). Indeed, the same adherence to TOS' principles is to be observed for all sub-sampling and sample preparation in the lab. On this basis, the only variability left is that between analytical results in the extension dimension (the process dimension). Thus, the variogram is a powerful characterisation of the *longitudinal heterogeneity* of the process interval under consideration (all *transverse* heterogeneity w.r.t. the process translation direction has been *covered*, i.e. *incorporated* in each increment extracted). N.B. Although in a variographic experiment it is *increments* which are extracted, they are at first treated as fully competent *samples* in their individual, own right. The result of a variographic experiment may subsequently result in a certain number of increments being aggregated, see further below. This minor apparent ambiguity need not lead to confusion, however, as soon as the full role and function of a variographic characterisation is comprehended.

The variogram principle is to calculate the *sum of all squared differences between all pairs of data points with in-between spacing equal to the lag, j, as j spans the entire interval of interest.* Thus, the fundamental calculation is repeated for all *j* lags, i.e. [$j = 1, 2, 3, ..., N_{U-1}$].

Figure 1 shows the spatial disposition of all possible pairs of data pairs as a function of the increasing lag [$j = 1, 2, 3, ..., N_{U-1}$].

The master equation returns one value, the variance *V* as a function of the lag, $V(j)$, i.e. there is calculated one variance measure *corresponding* to each lag. The variographic function thus characterises the set of data (in the present process, a time series) by the variance of a set of squared deviations, "one scale at the time" [$j = 1, 2, 3, ..., N_{U-1}$]. Plotting $V(j)$ [Y-axis] as a function of the lag *j* [X-axis] then produces the *variogram*, Figures 3 and 4.

There is an apparent ambiguity regarding whether to express the variogram based on absolute concentration values, or recalculated as heterogeneity contributions. Figure 2 shows both options, termed the absolute vs the relative variogram, respectively. This is a matter of no consequence, however, as the shape of the alternative variograms will be identical, with only the unit of measurements (and thus the unit on the Y-axis) differing. Every interpretation of both types of variograms will be identical. The advantage of using the relative variogram is significant, however, as it allows direct comparison of all variograms *inter alia*, including the levels and magnitudes of *ranges*, *sills* and *nugget effects*.

Based on the present and the preceding two columns, we are now ready for the promised bonanza of real-world examples and case histories from which to learn of the powerful capabilities of variographics.

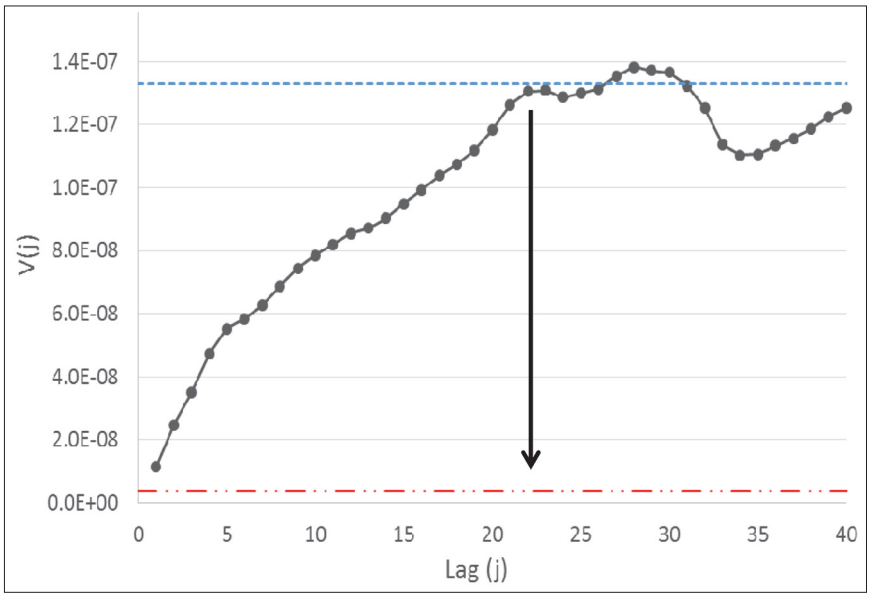

Figure 3. A generic variogram based on 80 increments. Real-world variogram. The lag axis of a variogram will always be of length $N_U/2$. This particular variogram shows a very small nugget effect (red horizontal line); the sill is marked with a blue line. The range is of the order of 22–23 lags. Note that it is also known from earlier studies of longer duration than the present, that the sill corresponds to the level shown here; this is an example of bringing in full domain-specific knowledge and experience in "reading a variogram".

Figure 4 is a real world variogram from a technological process, from which several general issues can be learned. The sill is always considered as a kind of *ceiling* for the total variability across the full lag spectrum—*technically*, however, the sill is defined as the average variance for all lags. In well-prepared variograms with a sufficient number of increments, the *range* will usually only constitute a small number of lags, the average variance will occupy exactly this ceiling disposition (note that the ceiling will not cap the variability from above, but from below, being lowered somewhat by the smaller variance levels below the range, made especially clear in Figure 3).

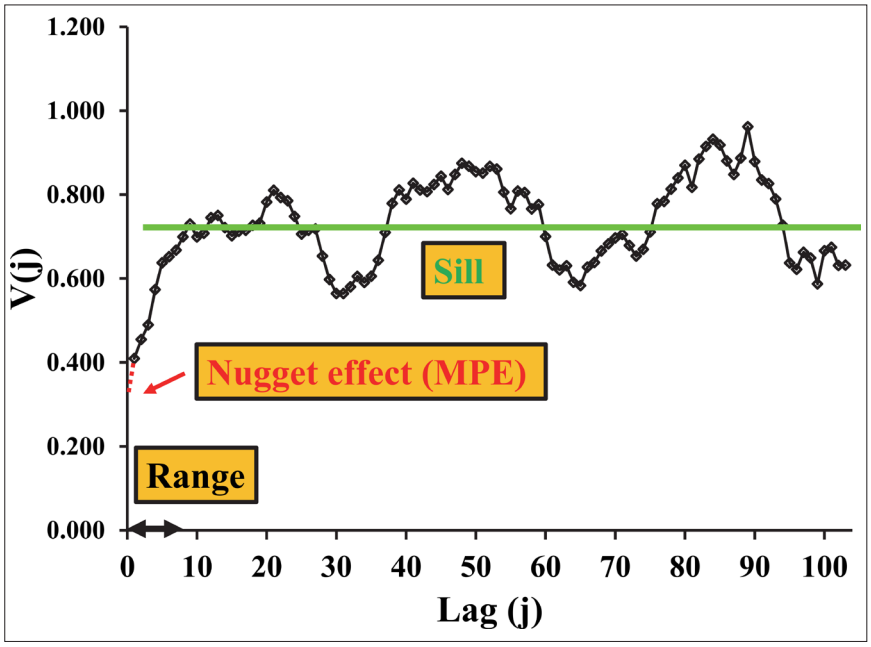

Figure 4. An experimental variogram from a process of great significance in technology and industry, mixing. Note that the original data series is larger than 200 increments.

As soon as the lag distance goes beyond the range, the particular variogram in Figure 4 shows a tell-tale periodic disposition with a period of ~30 lags, or slightly higher. The process being characterised is the output of a *mixing process* which is supposed to have been fully mixed at this stage. The empirical evidence in Figure 4 is interesting in this context as it shows beyond doubt that this objective has *not* been met—on the contrary there is solid evidence of a systematic compositional periodicity, which is an inheritance from inefficient mixing. This is a role model interpretation of a variogram. *Were* the mixing process fully efficient there would be no periodicity observable in the output variogram.

There are many other potential gains to be had from proper interpretation of variograms, for example regarding the specific sill level and the magnitude of the nugget effect w.r.t. the sill level, all to be explored in the next columns. Stay tuned—this is where sampling becomes immensely powerful.

As always, should the reader have become seriously impatient, we end with a set of in-depth publications exposing the features treated here more fully. Enjoy!

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Photoacoustic spectroscopy could help detect and diagnose metastatic melanomas

For years, melanoma researchers have studied samples that were considered uniform in size and colour, making them easier to examine by more conventional means. But melanomas are often irregular and dark, making them difficult to investigate. Researchers at the University of Missouri have devised a new technique to detect and analyse single melanoma cells that are more representative of the skin cancers developed by most patients. The study, recently reported in the *Analyst* (https://doi.org/10.1039/C6AN02662A), outlines the new techniques that could lead to better and faster diagnoses.

"Researchers often seek out the types of cancerous cells that are homogenous in nature and are easier to observe with traditional microscopic devices", said Luis Polo-Parada. "Yet, because the vast amount of research is conducted on one type of cell, it often can lead to misdiagnosis in a clinical setting."

The research team decided to supplement photoacoustic (PA) spectroscopy. They modified a microscope that was able to merge light sources at a range conducive to observing the details of single melanoma cells. Using the modified system, human melanoma and breast cancers as well as mouse melanoma cells were diagnosed with greater ease and efficiency. The team also noted that as the cancer cells divided, they grew paler in colour but the system was able to detect these newer, smaller cells as well.

"Overall, our studies show that by using modified techniques we will be able to observe non-uniform cancer cells, regardless of their origin", Polo-Parada said. "Additionally, as these melanoma cells divide and distribute themselves throughout the blood, they can cause melanomas to metastasise. We were able to observe those cancers as well. This method could help medical doctors and pathologists to detect cancers as they spread, becoming one of the tools in the fight against this fatal disease."

Raman imaging with Bessel beam enables deep-tissue imaging

The system, called stimulated Raman projection microscopy and tomography, makes possible "volumetric imaging" without using fluorescent dyes that might affect biological functions and hinder accuracy, said Ji-Xin Cheng, a professor at Purdue University. "Volumetric chemical imaging allows a better understanding of the chemical composition of three-dimensional complex biological systems such as cells", he added.

The technology uses a type of laser beam called a Bessel beam, which maintains focus for a longer distance than a traditional "Gaussian beam", making it possible to penetrate deep into tissue. Stimulated Raman spectroscopy eliminates the need for fluorescent dyes.

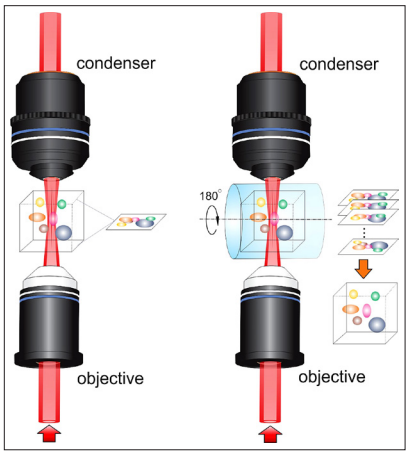
Because the Bessel beam makes possible deep-tissue imaging, it could lead to systems that eliminate the need to draw blood for analyses such as drug testing and detection of biomarkers for non-invasive early diagnosis of diseases, Cheng said. "This is a long-term goal", he said. "In the meantime, much more research is needed to improve the system."

The researchers proved the concept by imaging fat storage in living cells. Findings are detailed in a research paper published in *Nature Communications* (https://doi.org/10.1038/ncomms15117). The reported technology yields information about chemical composition, collecting a series of images while rotating the sample and reconstructing the 3-D structure through image reconstruction algorithms.

The Bessel beam is produced using a pair of cone-shaped "axicon" lenses and is combined with a microscope objective. Its use for volumetric fluorescence imaging was previously demonstrated by physicist Eric Betzig, who won the Nobel Prize in chemistry in 2014 for his pioneering contribution to super-resolution fluorescence microscopy. Super-resolution technology allows researchers to resolve structural features far smaller than the wavelength of visible light, sidestepping the "diffraction limit" that normally prevents imaging of features smaller than about 250 nm, which is large compared to certain biological molecules and structures in cells.

However, fluorescence microscopy usually requires the use of fluorescent tags, which may interfere with biological processes and hinder accuracy for determining chemical structure.

Future research will include work to increase the detection sensitivity of the system and improve the imaging quality and speed.



This schematic depicts an imaging system that uses a special type of laser beam called a Bessel beam that is produced using a pair of cone-shaped "axicon" lenses combined with a microscope objective. Purdue University researchers are using the system, which is able to penetrate deep into tissue and might lead to technologies that eliminate the need to draw blood for analyses including drug testing and early detection of diseases such as cancer and diabetes. (Purdue University photo/Ji-Xin Cheng)

"There is plenty of room for improvement," Cheng said. "The system is based on a bulky and relatively expensive femtosecond laser, which limits its potential for broad use and clinical translation. Nevertheless, we anticipate that this limitation can be circumvented through engineering innovations to reduce the cost and size of our technology. We also note that the Bessel beam can be produced using fibres, which could simplify the system and enable endoscopic applications."

NEWS

NMR may uncover secrets about male infertility

Scientists at the University of Sheffield have developed a new technique to examine human sperm without killing them; helping to improve the diagnosis of fertility problems. They used nuclear magnetic resonance (NMR) spectroscopy, and have shown that it could help to distinguish between populations of good or poor sperm. Unlike other more destructive examination methods, the RF pulses do not damage sperm, meaning they could potentially go on to be used in IVF treatment. The work was published in *Molecular Human Reproduction* (https://doi.org/10.1093/molehr/gax025).

Professor Martyn Paley, from the University's Department of Infection, Immunity and Cardiovascular Disease, said "The technique of magnetic resonance spectroscopy has been previously used to examine the molecular composition of many cells and tissues in other diseases such as cancer, but it has never previously been used to examine live sperm. As such, these results are a world first."

During the study, scientists examined fresh sperm samples from healthy volunteers and patients for just over an hour. From the data gathered, they were able to build up a profile of the molecules present in the sperm and how they differ between samples.

Professor Allan Pacey, fertility expert from the University of Sheffield, who was part of the study team, said: "Most of the advanced techniques we have available to examine the molecules in sperm end up destroying them in the process by either adding stains or by breaking open their membranes to look at the contents. To potentially have a technique which can examine the molecular structure of sperm without damaging them is really exciting."

One of the technical challenges that the team faced was how to detect the molecules that were present in sperm rather than those present in semen. To do this, the team examined a number of "sperm washing" techniques that are currently used to prepare sperm for IVF. They found that by spinning the samples very fast in a centrifuge several times they were able to reduce the background noise from molecules in semen to a point where they could reliably detect the ones from sperm.

The results of the study show that a number of molecules such as choline (a vitamin-like essential nutrient) and glycerophosphocholine (a natural choline compound found in the brain), lipids (common components of sperm cell membranes) and lactate (an end product of cellular energy usage) were significantly different between samples of sperm separated into "good" and "poor" populations.

Achema 2018 Congress inviting paper submissions

Achema is a huge exhibition and conference for all sectors of the process industry, offering an overview of current technology trends for chemistry, biotechnology and process engineering. Achema will be held next from 11 to 15 June 2018 at its usual home in Frankfurt am Main, Germany. The Achema Congress offers two different presentation options; the Congress Programme or the PRAXISforums. The Congress Programme comprises the complete spectrum of chemical and process engineering as well as biotechnology themes. The topics range from reaction technology, energy supply, analytics, process design and safety through to biotechnology. The lectures provide insights into current research activities and new scientific results. The Achema PRAXISforums focus on industrial applications, trends, new products and services in chemical engineering, biotechnology and the process industry. Market- and practice-oriented topics are presented in a concise format by experts associated with our exhibitor groups. The Achema PRAXISforums are held in the immediate vicinity of the respective exhibition group.

The deadline for submissions is 22 September 2017.

For detailed information and paper submission visit http://www.achema.de/congress

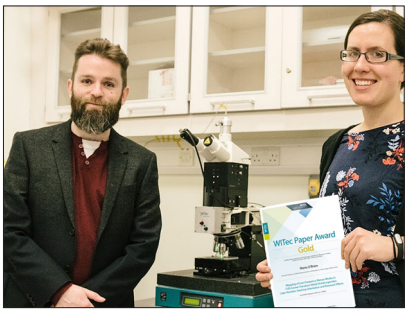
Agilent is acquiring Cobalt for £40 million in cash

Cobalt is privately held with 52 employees, most of whom are expected to join Agilent. Cobalt's CEO will remain with Agilent as the Director of Raman Spectroscopy. Oxford will become Agilent's global centre for Raman spectroscopy.

2017 WITec Paper Award for outstanding scientific publications

From nearly 60 submissions for the 2017 WITec Paper Award, the WITec jury selected the three best publications. They were written by scientists from Ireland, Portugal and Germany. These papers show how information on the chemical and structural composition of a material, obtained through this non-destructive technique, can lead to a more comprehensive understanding of a wide range of materials.

The **Gold Paper Award** is made to Maria O'Brien from Trinity College in Dublin (Ireland) for mapping low-frequency Raman modes of four transition metal dichalcogenides (TMDCs): MoS_2, $MoSe_2$, WS_2 and WSe_2. Together with Niall McEvoy, Damien Hanlon, Toby Hallam, Jonathan Coleman and Georg Duesberg, she used the Raman modes for in-plane and out-of-plane vibrations whose intensities depend on the thickness and the stacking order of the molecules' layers. The study has shown that the low-frequency Raman modes of these materials reveal additional information compared to conventional Raman



Maria O'Brien and Niall McEvoy with their workhorse, a WITec confocal Raman microscope.

modes. The scientists are convinced: "This study presents a major stepping stone in the fundamental understanding of layered materials as mapping the low-frequency modes allows the quality, symmetry, stacking configuration and layer number of 2D materials to be probed over large areas." They suggest using low-frequency Raman mapping for the analysis of TMDCs that show no significant changes correlated to layer numbers in the high-frequency regions of their Raman spectra. https://doi.org/10.1038/srep19476

The **Silver Paper Award** is given to Helena Nogueira from the University of Aveiro (Portugal). She and her co-authors Sara Fateixa, Manon Wilhelm and Tito Trindade used three-dimensional Raman imaging and surface enhanced Raman scattering (SERS) to monitor the dyeing process of linen textile fibres with methylene blue. This dye is most commonly used for blue colouring and was applied by various procedures. The scientists also visualised how the silver nanoparticles that give textiles antimicrobial properties are distributed along and within the linen fibres. The authors conclude that regarding textile production "…Raman imaging and SERS are valuable assets that complement or eventually provide unique characterisation data". https://doi.org/10.1002/jrs.4947

The **Bronze Paper Award** goes to Jonas Higl from the University of Ulm (Germany) for a Raman study on hydrating of cementitious materials. With his colleagues, Marcus Köhler and Mika Lindén, he used confocal Raman microscopy to document which structures and molecules are formed during the complex process of hydrating C_3S clinker. To the knowledge of the authors this study was the first published using Raman imaging to study hydrating of cement. https://doi.org/10.106/j.cemconres.2016.07.005

The annual awards recognise outstanding scientific work published the preceding year that employed a WITec device as part of its experimental setup. The evaluation criteria include the significance of the results for the scientific community and the originality of the techniques used.

Paper Award 2018

WITec have announced the 2018 WITec Paper Award competition for research articles published in 2017. Scientists from all fields of application in both academia and industry are invited to submit their publications featuring results acquired with a WITec instrument to papers@witec.de. The deadline for submissions is 31 January 2018.

Raman spectroscopy quality control of new 2D materials

Two-dimensional (2D) materials have attracted significant interest in recent years due to their unique electrical and mechanical properties, alongside atomically-thin dimensions. While graphene was the first 2D material to be studied in detail, there is now also a focus on other 2D materials with diverse properties and new applications. Among these, single-layer molybdenum disulphide (MoS_2), a semiconducting 2D material, is generating a lot of interest due to its technologically exploitable electronic and optical properties that could pave the way for the next generation of electronics and optoelectronics devices.

In order to commercialise electronic devices made of 2D materials, industry faces a challenge to carry out quality control checks without destroying or damaging the material. As a single-layer of a 2D material is only a single atom or molecule thick, assessing their quality so far has only been possible using destructive techniques. Defects are expected to critically impact the performance of MoS_2-based electronic devices,

so the ability to investigate and quantify the number of defects without causing damage is crucial for enabling large-scale manufacture of the material, device fabrication and material functionalisation.

Oxford Instruments were looking to develop a new deposition system and process that could produce MoS_2 in a more industrially-scalable manner. They turned to research from the National Graphene Metrology Centre (NGMC) at the National Physical Laboratory (NPL) published in *Physical Review B* (https://doi.org/10.1103/PhysRevB.91.195411).

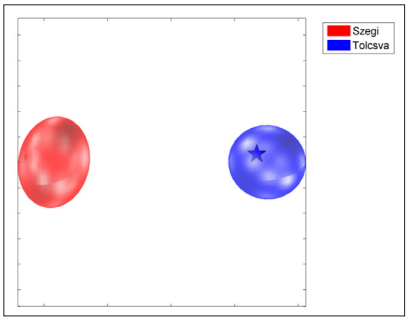
NPL's work on MoS_2 provided Oxford Instruments with the methodology they needed to develop their own quality control process, which characterises the 2D MoS_2 layers without having a destructive impact on the material's structure. This enables the team to efficiently characterise the MoS_2 produced via an industrially scalable technology, helping to accelerate the commercialisation of 2D materials.

Authentication and identification of Hungarian wines

The Hungarian Ministry of Agriculture has selected Bruker's collaboration partner Diagnosticum to implement a new programme to authenticate and identify Hungarian wines. Diagnosticum and Bruker will form the Hungarian Wine Consortium and develop a Hungarian wine model based on Bruker's NMR FoodScreener technology for rapid and comprehensive wine profiling. The model will be used to authenticate and identify Hungarian wines, including the famous Tokaji wines.

Hungarian wineries have two years to submit their samples and participation is required. The programme reflects a commitment to strengthening the authenticity of Hungarian wines and improving their position in a global market where consumers are becoming increasingly wary of food and wine adulteration and fraud.

Dr Ferenc Péterfy, President of Diagnosticum stated: "The lab is ready, instruments are installed, and we are excited to provide the technical expertise to support this national programme.



Feasibility study on Hungarian wines demonstrating the identification and differentiation of Hungarian sub-regions.

Building the model for Hungarian wines and validating their authenticity will increase consumer confidence and trust in these wines on a worldwide basis."

Wine profiling by NMR relies on the acquisition of the spectroscopic fingerprint specific of each individual sample. These metabolic profiles are compared to a large database of authentic wine samples using a multivariate statistical approach. This high-throughput technique provides a wide range of information that is both targeted (quantification of defined substances) and non-targeted (identifying deviations from reference spectra). The Hungarian model will extend the already existing database of Spanish, Italian, French, Chilean, Austrian and German wines.

Deep-UV probing method detects electron transfer in photovoltaics

Scientists from the Ecole Polytechnique Federale de Lausanne (EPFL) have developed a new method to efficiently measure electron transfer in dye-sensitised, transition-metal oxide photovoltaics. Sensitised solar cells consisting of a molecular or solid-state sensitiser that serves to collect light and inject an electron into a substrate that favours their migration are among the most studied photovoltaic systems at present. Despite its importance in determining the potential of a photovoltaic device, current methods for monitoring the interfacial electron transfer remain ambiguous. Now, using deep-ultraviolet continuum pulses, EPFL scientists have developed a substrate-specific method to detect electron transfer. The work is published in the *Journal of the American Chemical Society* (doi: https://doi.org/10.1021/jacs.7b06322).

The work was carried out by the lab of Majed Chergui at EPFL, which specialises in ultrafast spectroscopy. The group focused on two types of dye-sensitised solar conversion systems: one based on titanium dioxide, the other on zinc-oxide nanoparticles, both of which belong to the category of transition-metal oxide (TMO) substrates. These TMOs are characterised by specific absorption bands, which are fingerprints of the system and are due to neutral electron-hole pairs, called an exciton.

The EPFL team aimed to overcome the limitations of current methods of measuring electron transfer, which all use light in the visible-to-terahertz frequencies (wavelengths around 400–30,000 nm). However, this approach is sensitive to carriers that remain free in the TMO substrate. They are, therefore, unspecific to the type of substrate and cannot be extended to the new generation of solid-state-sensitised solar cells (such as those using perovskites as sensitisers). Instead, the researchers at EPFL used deep-ultraviolet (260–380 nm wavelength) continuum pulses to probe the TMO substrates in the region of their excitonic transitions and detect electron transfer, via their response. This opens a route to the study of solid-state sensitised cells, as there is hope that the response of the substrate will be distinguished from that of the sensitiser.

Compact accelerators generating terahertz light

Karlsruhe Institute of Technology are developing a new compact accelerator, the FLUTE accelerator, which will be used for the development of new accelerator technologies for compact and powerful terahertz sources that can serve as efficient research and application tools.

The FLUTE facility at Karlsruhe Institute of Technology (KIT) (this abbreviation is derived from its German name: Ferninfrarot Linac- und Test-Experiment) is a development platform for acceler-

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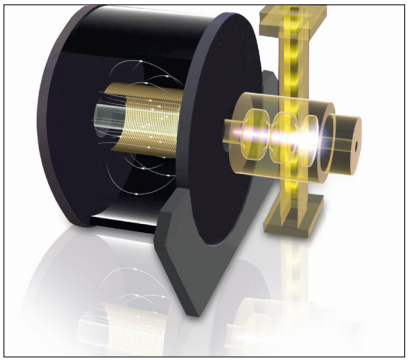


The FLUTE linear accelerator accelerates electron clouds in order to generate terahertz rays. (Illustration: KIT)

ator physics studies. It will serve as a test facility for methods that allow, in a first step, the better understanding, measurement and control of the complex dynamics of ultra-short electron bunches. Only very compact electron bunches can generate intensive, brilliant and coherent terahertz radiation. The special challenge faced when designing accelerators such as FLUTE is to keep the electron cloud so compact during the acceleration process that its expansion is smaller than the wavelength of the generated electromagnetic radiation. Only then, the waves overlap each other, forming pulses of high intensity with a duration of picoseconds or femtoseconds.

In the long run, control of the electron bunches must be improved in such a way that the terahertz radiation can be adapted perfectly to the intended application. Terahertz radiation could open up new domains of application for which the neighbouring visible light and radio waves are unsuitable. As a research infrastructure, FLUTE will also be used for the development of terahertz radiation measuring methods that can be employed in materials and life sciences. Protein oscillations can be examined just as well as the behaviour of superconductors or novel semiconductors.

Within the FLUTE accelerator, whose length is approximately 12 m, the electrons are accelerated to reach an energy of up to 50 MeV. The electron cloud is compressed to a few µm so that radiation with a frequency of 30 THz or more can be generated. Besides the Institute for Beam Physics and Technology at KIT, development partners from all over Europe, above all the Swiss Paul Scherrer Institute (PSI), are participating in the FLUTE project.

The potential for THz generation from FLUTE is described in a paper in *Rev. Sci. Instrum.* (https://doi.org/10.1063/1.4790431)

Infrared spectroscopy reveals relationships between fossil plants

A collaboration between researchers at Lund University, the Swedish Museum of Natural History in Stockholm and Vilnius University has established the relationships between 200-million-year-old plants using infrared spectroscopy and chemometric analysis [hierarchical cluster analysis (HCA)] of organic molecules in fossil leaves.

The researchers collected fossil leaves from rocks in Sweden, Australia, New Zealand and Greenland. Using FT-IR spectroscopy and chemical analysis, the fossil leaves were then compared with the chemical signatures from molecules in plant leaves picked at the Botanical Garden in Lund.

The use of genetic DNA analysis in modern research to determine relationships is not possible on fossil plants. The oldest DNA fragments ever found are scarcely one million-years-old. Therefore, the scientists searched for organic molecules to see what these could reveal about the plants' evolution and relationships.

The molecules were found in the waxy membrane, which covers the leaves and these showed to differ between various species. The membrane has been preserved in the fossil leaves, some of which are 200 million-years-old. Using infrared spectroscopy, the researchers carried out analyses in several stages. First, they examined leaves from living plants that have relatives preserved in the fossil archive. The analysis showed that the biomolecular signatures were similar among plant groups, much in the same way as shown by modern genetic DNA analysis.

When the method was shown to work on modern plants, the researchers went on to analyse their extinct fossil relatives. Among others, they examined fossil leaves from conifers and several species of Ginkgo. The only living species of Ginkgo alive today is *Ginkgo biloba*, but this genus was far more diverse during the Jurassic.

Fossil Ginkgo (photo: Stephen McLoughlin).

Finally, when the researchers had shown that the method gave consistent results, they analysed fossils of enigmatic extinct plants that have no living relatives to compare them with. Among others, they examined Bennettites and Nilssonia, plants that were common in the area that is now Sweden during the Triassic and Jurassic around 250–150 million years ago. The analysis showed that Bennettites and Nilssonia are closely related. On the other hand, they are not closely related to cycads, which many researchers had thought until now. Their results are published in *Nature Ecology & Evolution* (https://doi.org/10.1038/s41559-017-0224-5).

Per Uvdal, Professor of Chemical Physics at Lund University and one of the researchers who conducted the study, considers that the overall results are astounding. "The great thing about the biomolecules in the leaves' waxy membranes is that they are so much more stable than DNA. As they reflect, in an indirect way, a plants DNA they can preserve information about the DNA. Therefore, the biomolecules can tell us how one plant is related in evolutionary terms to other plants," he says.

The researchers are now going to extend their studies to more plant groups.

ATOMIC

PerkinElmer Launches Avio 500 ICP-OES

PerkinElmer has announced the launch of the Avio® 500 inductively coupled plasma optical emission spectrometer (ICP-OES). This spectrometer is designed for analytical laboratories running high throughput, multi-elemental, inorganic analyses for a wide variety of sample matrices. The Avio 500 is a simultaneous ICP-OES system, with simultaneous background correction for faster sample-to-sample time and improved data accuracy, matrix tolerance and low argon consumption. It is designed to meet the needs of customers requiring low and high concentration testing for a broad range of analytes. It will find application in areas including environmental, petrochemical (lubricants and used oils), geochemical, food, pharmaceutical and industrial (including batteries).

The Avio 500 has a vertical plasma with a quick-change torch that provides matrix flexibility and minimises sample preparation time. Flat Plate™ plasma technology generates a robust matrix-tolerant plasma using half the argon of other ICP systems. The Dual View optical system optimises axial and radial plasma viewing, measuring high and low concentrations in the same run, regardless of wavelength. Universal data acquisition enables simultaneous acquisition of all available wavelengths, helping to reduce or potentially eliminate the need to re-run samples. PlasmaShear™ argon-free interference removal technology eliminates interferences by removing the cool tail plume of the plasma, providing maintenance-free, argon-free interference removal. The PlasmaCam™ camera offers continuous colour viewing of the plasma, enabling remote diagnostic capabilities and simplifying method development.

PerkinElmer

link.spectroscopyeurope.com/29-W-039

The Avio 500 ICP-OES spectrometer from PerkinElmer.

ELLIPSOMETRY

Uvisel Plus reference ellipsometer for thin film measurements

Horiba Scientific has introduced the new Uvisel Plus, a modular ellipsometer for thin film samples. New acquisition technology, FastAcq, is based on a new electronic data processing and high speed monochromator, and enables a sample measurement from 190 nm to 2100 nm to be completed within 3 min at high resolution. The spectral resolution can be adjusted along the measurement range, enabling a sample to be scanned faster. The Uvisel Plus also introduces a new calibration procedure, delivering faster performance and accuracy. Features for thin film measurements include microspots for patterned samples down to 50 µm, variable angle from 40° to 90°, an automatic horizontal mapping stage and a variety of accessories. The spectral range from 190 nm to 2100 nm is covered by two configurations: 190–920 nm and a NIR extension up to 2100 nm.

Horiba Scientific

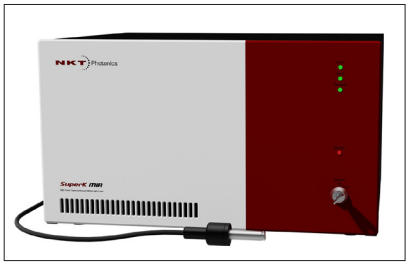
link.spectroscopyeurope.com/29-W-040

Horiba Scientific's Uvisel Plus, a modular ellipsometer for thin film samples.

INFRARED

SuperK MIR brings supercontinuum into the mid-IR

NKT Photonics' new SuperK MIR lasers are based on their existing supercontinuum platform, with the same benefits as the visible and near infrared sources with an output in the mid-infrared. The SuperK MIR laser delivers >450 mW of continuous light from 0.9 µm to 4.2 µm. The source features a monolithic all-fibre architecture, ensuring stability and maintenance-free operation over thousands of hours. The mid-infrared light is delivered through a broadband collimator, offering flexibility and easy use. Like other sources from NKT Photonics, the laser is ready as soon as you switch it on and is easy to operate through NKT Photonics unified laser control software, CONTROL. The new laser is compatible with FT-IR spectrometers for fast detection and short integration time across the entire spectrum. Applications of this source include component characterisation, mid-IR microscopy, gas and



The SuperK supercontinuum laser for the mid-infrared from NKT Photonics.

NEW PRODUCTS

combustion spectroscopy, environmental sensing and standoff detection.
NKT Photonics

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MASS SPEC

FDA approval for expanded pathogen identification by MALDI-TOF

bioMérieux has announced that VITEK® MS, its MALDI-TOF mass spectrometry system for rapid pathogen identification, has received 510(k) clearance from the US Food and Drug Administration (FDA) for the expanded identification of mycobacteria, *Nocardia* and moulds. This database includes more than 15,000 distinct strains to provide extremely high accuracy and, for the first time, enables the safe identification of the *Mycobacterium tuberculosis* (TB) group, the most frequent non-tuberculous mycobacteria (NTM), *Nocardia* and the most medically important moulds. The VITEK MS system's newly expanded database and *Mycobacterium*/*Nocardia* and moulds reagent kits are now commercially available in the US.

Mycobacteria, Nocardia and moulds are complex organisms to identify, requiring days or weeks of specific culture conditions for appropriate growth and subsequent advanced methods for reliable identification to the species level. With the newly expanded database, bioMérieux's VITEK MS system now offers simple, rapid, safe and reliable identification of these medically important pathogens, providing clinicians with actionable results to better manage these infections, such as tuberculosis, lung and bone infections, and other serious organ infections.

To gain new FDA clearance for these new species, bioMérieux submitted data from a multi-centre study consisting of 2695 clinical isolates for 47 moulds, 19 mycobacteria and 12 *Nocardia*. The FDA clearance of *Mycobacterium* species was from both solid and liquid growth media.
bioMérieux

link.spectroscopyeurope.com/29-W-045

LC-MS system for clinical diagnostics announced by SCIEX

SCIEX Diagnostics, the *in vitro* diagnostics division of SCIEX, has introduced their first fully integrated LC-MS system for clinical diagnostics, the SCIEX Topaz™ System. The heart of the system lies within the innovative ClearCore™ MD software, a platform which simplifies and streamlines workflows and method development and incorporates features that enhance usability to help new users build proficiency quickly. In addition, the first FDA-cleared (via the *de novo* pathway) LC-MS based Vitamin D assay kit, the SCIEX Vitamin D 200M Assay, is for use on the SCIEX Topaz System.

The Topaz System provides both an open system for lab-developed tests (LDTs) and a closed system for running locked, pre-validated assays. In addition, a turnkey, FDA-cleared Vitamin D solution is available for immediate implementation. The Topaz System enables clinical labs to rapidly expand their testing services and bring previously outsourced tests in-house.
SCIEX

link.spectroscopyeurope.com/29-W-043

The Topaz integrated LC-MS system for clinical diagnostics from SCIEX.

Collision/reaction cell, multi-collector ICP mass spectrometer

Nu Instruments has released Sapphire, a collision/reaction cell, multi-collector inductively coupled mass spectrometer (MC-ICP-MS). The instrument has a high-energy path that enables it to be used as a traditional multi-collector ICP-MS with no compromise in performance, as well as a low-energy path in which the ion beam is directed through a hexapole collision cell for the removal of the ICP-induced molecular species that interfere directly with the atomic ions of the same nominal mass of some non-traditional isotopes. Sapphire can analyse these systems in low-resolution mode by removing the molecular species, without compromising the ion transmission, significantly reducing sample size requirements and increasing the isotopic measurement precision and accuracy to the counting statistics level.
Nu Instruments

link.spectroscopyeurope.com/29-W-052

Nu Instruments' Sapphire multi-collector ICP-MS.

NIR

New tablet probe for handheld NIR spectrometer

Viavi Solutions has introduced the MicroNIR™ Tablet Probe, a handheld probe attachment for the analysis of pharmaceutical tablets and pills, small volume samples or single grain kernels.

Viavi's MicroNIR tablet probe.

The probe is compatible with the MicroNIR Onsite spectrometer system. The MicroNIR Tablet Probe provides users with an easy sample measurement interface without strict and specialised control of the sample and spectrometer. In addition, the probe seeks to eliminate the occurrence of random scatter effects, which often result in analysis error. Use of the Tablet Probe with the MicroNIR OnSite spectrometer allows field users to achieve repeatable, reliable and accurate results in difficult, uncontrolled field environments.

Viavi Solutions

link.spectroscopyeurope.com/29-W-048

PerkinElmer launches Spectrum Two™ N FT-NIR system

PerkinElmer has introduced the Spectrum Two N™ transportable FT-NIR system. This instrument is designed for laboratory technicians and staff using molecular spectroscopy to analyse a wide range of pharmaceutical, food and industrial samples. The Spectrum Two N has three sampling modules. A plug-and-play NIR reflectance module for fast, simple measurements for detection of raw materials; a heatable transmission module with three heating vials that is suitable for heating solid fraction oils such as coconut and palm oils; and a remote sampling module that provides a trigger-based probe for through-the-container analysis. Atmospheric vapour compensation is a digital filtering algorithm that automatically compensates for water absorption, and OpticsGuard provides a protective humidity barrier that allowing the instrument to be used in inhospitable working environments. A further feature, Absolute Virtual Instrument™, enables instruments to be accurately calibrated during standardisation using gas-phase spectra.

The Spectrum Two N FT-NIR spectrometer from PerkinElmer.

PerkinElmer

link.spectroscopyeurope.com/29-W-047

RAMAN

B&W Tek releases BWSpec software Version 4.10

B&W Tek has released updates to their BWSpec software, expanding the software supporting B&W Tek spectrometers, systems and accessories beyond spectral acquisition to a control and spectral analysis platform. These updates will provide improved support for the i-Raman series of portable instruments.

BWSpec Version 4.10 new features include a new application-based Raman workspace; a new file type (TXTR), which includes the relative intensity correction ratio spectra to ensure the integrity of spectral files; new experiment setup allowing users to configure data acquisition, spectral processing, analytics and timeline functions; a batch data processing function; a probe setup feature allows for the relative intensity correction of the fully configured instrument with the probe to be applied; and

NEW PRODUCTS

improved usability allowing spectral files to be opened by drag and drop.
B&W Tek
link.spectroscopyeurope.com/29-W-041

Deep-cooled high speed scientific spectroscopy camera

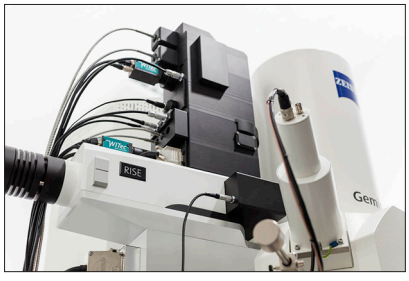
Horiba Scientific's new line of CCDs, the SynapsePlus, offers fast electronics with low noise and excellent signal linearity, all leading to sensitivity for low light and fast kinetics studies in applications such as Raman and photoluminescence. Available with multiple sensors, the Synapse CCDs are deep thermo-electric cooled to –80°C, and offer high spectral resolution. In addition, SynapsePlus comes with anti-fringing and quantum efficiency enhancement technology, and all are capable of acquiring data at thousands of spectra per second. The SynapsePlus is currently available in a range of sensor formats and sizes.
Horiba Scientific
link.spectroscopyeurope.com/29-W-050

WITec's RISE microscopy on Zeiss Sigma 300 SEM

WITec's solution for correlative Raman–SEM imaging is now available for the Zeiss Sigma 300, a field emission scanning electron microscope (FE-SEM). With this jointly-developed system, WITec and Zeiss are providing a fully-integrated instrument available as an OEM product through Zeiss that features a standard, unmodified vacuum chamber and SEM column along with a complete confocal Raman microscope and spectrometer.

RISE stands for Raman Imaging and Scanning Electron microscopy. The research-grade optical microscope capability integral to every WITec microscope also helps researchers survey their sample and quickly locate areas of interest. Both the objective and sample stage required for Raman microscopy are placed within the SEM's vacuum chamber and can therefore remain under vacuum for all measurements; the sample is simply transferred between the Raman and SEM measuring positions using the stage of the Zeiss Sigma 300. The configuration allows the Raman microscope to be attached through a standard port of the SEM. The correlation of data and control of Raman measurements are carried out through WITec's Suite Five software.

All the functions of the respective stand-alone SEM and Raman systems are preserved when combined. Switching between measurement modes is accomplished quickly and easily through the software, which also facilitates the transformation of Raman spectroscopic data into an image which can then be overlaid onto the SEM image to produce a RISE image. This correlative approach can greatly benefit researchers in nanotechnology, life sciences, geosciences, pharmaceutics, materials research and many other fields of application.
WITec
link.spectroscopyeurope.com/29-W-046



WITec's RISE system for correlative Raman/SEM imaging is now available on the Zeiss Sigma 300.

UV/VIS

Life science spectrophotometer

Cole-Parmer Ltd has announced that Jenway® has introduced the new Genova Bio life science spectrophotometer. The Genova Bio is a UV/visible spectrophotometer, and has been designed for fast and easy use in life science applications, whilst having a low-price point. It is suitable for molecular biology laboratories, biotechnology, biochemistry and cell biology applications.

The Genova Bio is compatible with a wide range of small volume cuvettes, allowing it to measure the purity and concentration of DNA, RNA and other biological samples. To optimise sample preparation, the Genova Bio is pre-programmed with methods for the quantification of nucleic acids and proteins. The instrument also has a pre-programmed method for measuring optical density of bacterial cell cultures such as *E. coli* and yeast cells, enabling scientists to measure cell growth before cell harvesting.

The Genova Bio life science spectrophotometer from Jenway.

The Genova Bio uses scanning diode array technology, with electrical scanning of the entire wavelength range (198–800 nm) simultaneously in under six seconds. This is useful where multiple wavelengths are required for purity ratios. The instrument features a large intuitive colour touchscreen interface for simple operation in the lab.
Jenway
link.spectroscopyeurope.com/29-W-051

X-RAY

Simultaneous WD XRF system for high-throughput analysis

Rigaku has introduced the latest version of their multi-channel simultaneous wavelength dispersive X-ray fluorescence (WD XRF) spectrometer system,

The Simultix 15 high-throughput WDXRF spectrometer from Rigaku.

the Simultix 15 high-throughput WDXRF spectrometer. For over 40 years, the Rigaku Simultix simultaneous WD XRF spectrometer system has been used for elemental analysis for process control in industries that require high throughput and precision, such as steel and cement. The new Simultix 15 system was developed to meet changing needs and customer requirements across a range of industrial applications, offering improved performance, functionality and usability.

The Simultix 15 analyser has a standard 30 fixed channel configuration that can be optionally upgraded to 40 channels. The Simultix 15 spectrometer has customisable, multiple discrete and optimised elemental channels and 4 kW of X-ray tube power. All channels measure simultaneously, with no moving parts and without time delay. The Simultix 15 system can be fitted with a 48-position automatic sample changer, as well as a scanning goniometer for analysis of other elements and an X-ray diffraction (XRD) channel for phase analysis, providing added flexibility.

Among the new features are the new "RX85" synthetic multi-layer crystal (producing approximately 30% greater intensity than existing multi-layers for Be-Kα and B-Kα), the XRD channel for quantitative analysis and improved software featuring a quantitative analysis flow-bar popular with users of Rigaku ZSX software.

Rigaku

link.spectroscopyeurope.com/29-W-049

Small-spot ED-XRF spectrometer for precious metals testing

Spectro Analytical Instruments have introduced the Spectro Midex MID05 spectrometer—a fifth-generation, small-spot energy-dispersive X-ray fluorescence (ED-XRF) analyser for precious metal testing. The new, compact Spectro Midex MID05 spectrometer delivers improved sensitivity and speed, and represents an alternative to fire assay testing. The new analyser offers users the choice of significantly increased precision, even for minor and trace element content, or substantially faster testing for higher sample throughput.

The Spectro Midex MID05 ED XRF spectrometer for precious metals.

Spectro

link.spectroscopyeurope.com/29-W-044

ZSX Primus 400 WDXRF spectrometer for large and heavy samples

Rigaku Corporation has introduced the new Rigaku ZSX Primus 400 sequential wavelength dispersive X-ray fluorescence (WDXRF) spectrometer. The new instrument has been designed specifically to handle very large and/or heavy samples and offers micro-mapping capabilities. The spectrometer accepts samples up to 400 mm diameter, 50 mm thick and 30 kg mass, making it suitable for analysing sputtering targets, magnetic disks, or for multilayer film metrology or elemental analysis of large samples. All the analytical capabilities of a traditional instrument are retained in this "large sample" variant, including measurement of beryllium (Be) through uranium (U) with high-resolution and precise WDXRF spectroscopic examination of samples from solids to liquids and powders to thin films.

A customised sample adapter system has a variable measurement spot (30–0.5 mm diameter with five-step automatic selection) and mapping capability with multi-point measurements to check for sample uniformity. A real-time camera allows the analysis point to be viewed on-screen, offering the operator complete certainty as to what is being measured.

Rigaku's ZSX Primus 400 sequential WDXRF spectrometer has been designed specifically to handle very large and/or heavy samples and offers micro-mapping capabilities.

The ZSX Primus 400 Windows-based software is user-friendly, yet powerful enough for the most complex analysis. Based on the Rigaku easy-to-use flow bar interface, the ZSX Guidance software walks the user through the steps required to set up an empirical or fundamental parameters application.

Rigaku

link.spectroscopyeurope.com/29-W-042

DIARY

Conferences 2017

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

18–20 September, Sopot, Poland. **5th European Optical Society Topical Meeting on Blue Photonics (Blue Photonics 5).** http://www.myeos.org/events/bluephotonics5.

18–21 September, Warsaw, Poland. **European Materials Research Society (E-MRS) 2017 Fall Meeting.** http://www.european-mrs.com/meetings/2017-fall-meeting.

18–22 September, Pula, Sardinia, Italy. **Sources, Interaction with Matter, Detection and Analysis of Low Energy Electrons 2017 (SIMDALEE2017).** http://www.iap.tuwien.ac.at/www/simdalee2017/index.

19–22 September, Boston, United States. **CASSS: 14th Symposium on Practical Application of Mass Spectrometry.** info@casss.org, http://www.casss.org/page/MS1701.

20 September, Dublin 9, Ireland. **Free Seminar: Raman and Infra-Red Microscopy Day.** Mark Croke, mark.croke@thermofisher.com, www.thermofisher.com/MeetTheExpert.

20 September, Nottingham, United Kingdom. **High-pressure XPS of Energy Materials 2.** https://www.eventbrite.co.uk/e/high-pressure-xps-of-energy-materials-2-tickets-34688996723.

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. lchelf@aoac.org, http://www.aoac.org.

24–29 September, Montpellier, France. **European Conference on Applications of Surface and Interface Analysis–ECASIA'17.** Mariem Blel, contact@ecasia2017.com, http://www.ecasia2017.com/.

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

25–27 September, Ulm, Germany. **14th Confocal Raman Imaging Symposium.** Dr Sonja Breuninger, Sonja.Breuninger@WITec.de, http://www.raman.net.

28–29 September, Vienna, Austria. **5th Workshop on Field-Flow Fractionation-Mass Spectrometry (FFF-MS).** Stephan Wagner, 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, info@centercongressi.

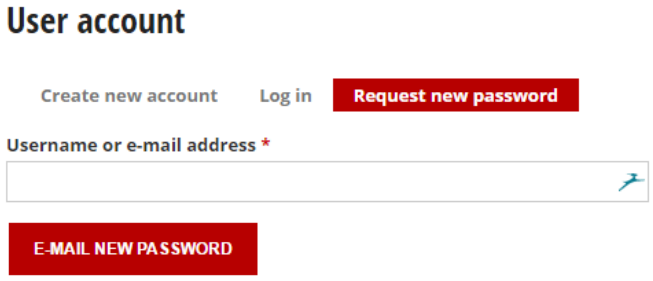
A New Website for *Spectroscopy Europe*

We have just launched a new website which works well on all devices from large screens to smartphones. The URL remains www.spectroscopyeurope.com.

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

1) Use the Lost Password facility

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

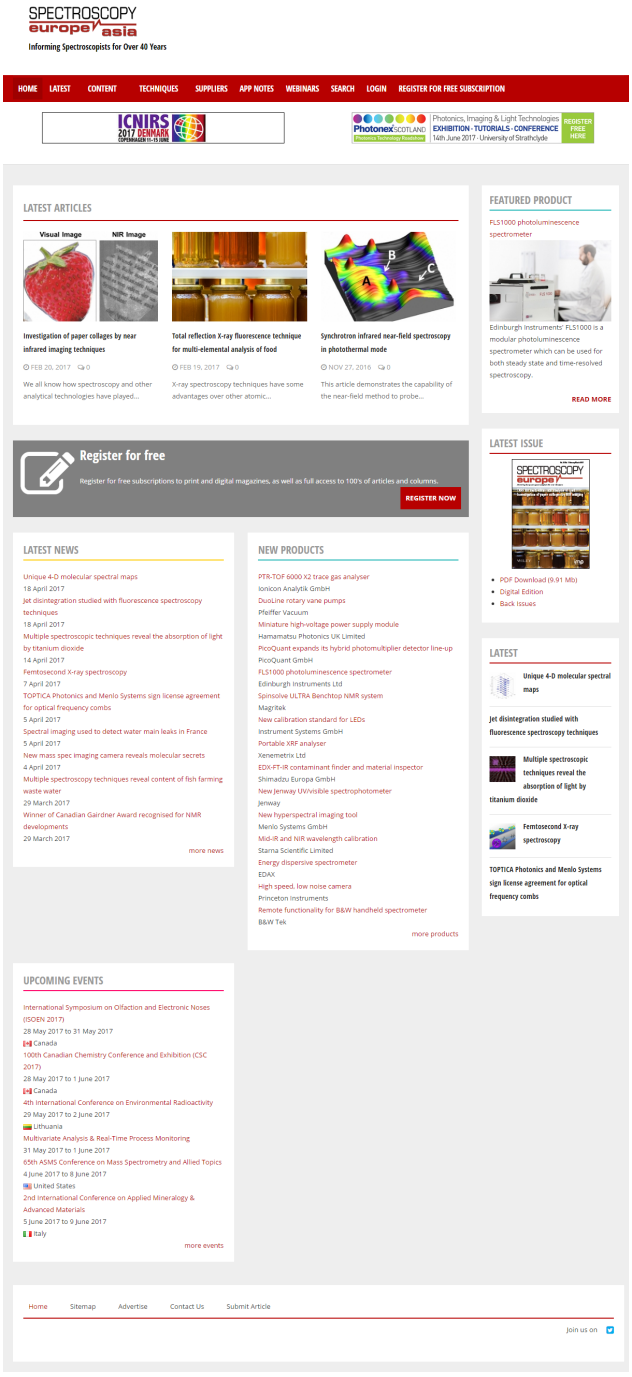


The e-mail usually arrives within seconds; if you do not see it, check your spam folder(s): these types of e-mails are often mistaken for spam.

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

2) Ask for help

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



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

www.spectroscopyeurope.com

DIARY

com, http://www.centercongressi.com/isbm10/.

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

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

4–6 October, Budapest, Hungary. **EuroFood Chem XIX Conference.** eurofoodchem2017@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.

8 October–13 August, Shanghai, China. **23rd International Conference on Ion Beam Analysis (IBA 2017).** http://iba2017.com/dct/page/1.

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

9–10 October, Mexico City, Mexico. **CASSS: CMC Strategy Forum Latin America.** info@casss.org, http://www.casss.org/page/CMCLAT1700/CMC-Strategy-Forum-Latin-America-2017.htm.

11–13 October, Berlin, Germany. **EXSA Workshop on Quantitative Methods in X-ray Spectrometry.** quant2017@exsa.hu, https://www.exsa.hu/quant2017/.

11–13 October, Bologna, Italy. **5th Mass Spectrometry (MS) Food Day.** Dr Davide Garbini, 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, yngvar.thomassen@stami.no, www.ipoims.com.

17–19 October, Calabar, Nigeria. **SETAC Africa 8th Biennial Conference.** SETAC North America, 229 S. Baylen Street, 2nd Floor, Pensacola, FL 32502, USA, seta-ceu@setac.org, https://saf2017.setac.org.

18–19 October, Osaka, Japan. **6th Global Conference on Mass Spectrometry (MASSSPECTRA2017).** massspectea@chemistryconference.org, www.massspectra.com/asia-pacific.

18–20 October, Barcelona, Spain. **Workshop in Environmental Omics, Integration and Modelling.** wenvomics2017@idaea.csic.es, wenvomics2017.info.

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

22–26 October, Tsukuba, Japan. **8th International Symposium on Surface Science (ISSS).** Nobuyuki Ishida, isss8@sssj.org, http://www.sssj.org/isss8/.

23–27 October, Nancy, France. **8th International Conference on Innovations in thin Film Processing and Characterization (ITFPC 17).** Mariem Blel, mariem.blel@vide.org, http://www.itfpc.com/.

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

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

30–31 October, Paris, France. **5th International Conference on Plasma Chemistry and Plasma Processing.** Christina Rebecca, plasmachemistry@alliedconferences.org, http://plasma-chemistry.alliedacademies.com/.

1–3 November, Barcelona, Spain. **Immunology–2017: International Conference on Immunology and Immunotechnology.** immunology@madridge.com, http://immunology.madridge.com/.

7–8 November, Birmingham, United Kingdom. **Metabolomics with the Q Exactive.** David Epps, d.epps@bham.ac.uk, http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/q-exactive.aspx.

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

8–10 November, Singapore, Singapore. **9th Electronic Structure and Processes at Molecular-Based Interfaces (ESPMI 9).** June Chan, junechan@nus.edu.sg, http://www.physics.nus.edu.sg/espmi9/.

9 November, Breda, Netherlands. **Free Seminar: An Introduction to Infra-Red, Raman Spectroscopy and Microscopy.** Dlangir Cordero, dlangir.cordero@thermofisher.com, www.thermofisher.com/MeetTheExpert.

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, aaps@aaps.org, http://www.aaps.org/annualmeeting/.

12–17 November, Matsue-City, Shimane, Japan. **7th Asia-Pacific Winter Conference on Plasma Spectrochemistry (APWC).** Takafumi Hirata, Koyto University, Kitashirakawa, Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan. hrt1@kueps.kyoto-u.ac.jp, http://www2.es.titech.ac.jp/okino/pdf/17APWCposter.pdf.

12–16 November, Minneapolis, MN, United States. **SETAC North America 38th Annual Meeting.** SETAC North America, setac@setac.org, https://msp.setac.org/.

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

26 November–1 December, Boston, MA, United States. **Materials Research Society 2017 Fall Meeting.** Materials Research Society, 506 Keystone Drive, Warrendale, PA 15086-7573, USA, info@mrs.org, http://www.mrs.org/fall2017.

10–13 December, Águas de Lindóia, Brazil. **5th Brazilian Meeting on Chemical Speciation (EspeQBrasil 2017).** espeqbrasil2017@rc.unesp.br, http://www.unesp.br/portal#!/cea/home/espeqbrasil2017/espeqen/the-meeting/.

11–15 December, New Orleans, Louisiana, United States. **American Geophysical Union AGU 2017 Fall Meeting.** meetinginfo@agu.org, http://www.agu.org/meetings.

2018

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

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.

22–23 March, London, United Kingdom. **11th Edition of International Conference on Proteomics.** proteomics@eurosciconmeetings.com, http://proteomics.euroscicon.com/.

26–29 March, Santa Fe, New Mexico, United States. **International High Power Laser Ablation Symposium (HPLA 2018).** Amy Walker, awalker@blue-52productions.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.

27–30 May, Lecce, Puglia, Italy. **CMA4CH Meeting 7th edition Multivariate Analysis and Chemometry: an essential support for Environment and Cultural Heritage.** infocma4ch@uniroma1.it, http://www.cma4ch.org/index2.html.

27–31 May, Edmonton, Canada. **101st Canadian Chemistry Conference.** www.csc2018.ca.

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

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

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

17–20 June, Seatlle, 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.

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

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

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, Sacramento, CA, United States. **SETAC North American 39th Annual Meeting.** setac@setac.org, www.setac.org/.

4–8 November, Indianapolis, Indiana, United States. **2018 Geological Society of America (GSA) Annual Meeting.** meetings@geosociety.org, www.geosociety.org/meetings/.

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

2019

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

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- ☐ Mass Spectrometry
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- ☐ Near Infrared
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- ☐ Photonics and Optics
- ☐ Raman
- ☐ Separation Science
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- ☐ X-Ray Diffraction
- ☐ X-Ray Spectrometry
- ☐ None

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- ☐ Hospital
- ☐ Government
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- ☐ Research Scientist
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www.icavs.org/contact/, http://www.icavs.org/2019-conference/.

15–20 September, Gold Coast, Australia. **NIR-2019.** www.nir2019.com.

2020

12–18 January, Tucson, Arizona, United States. **2020 Winter Conference on Plasma Spectrochemistry.** wc2020@chem.umass.edu, http://icpinformation.org.

Courses

2017

27–29 September, Oslo, Norway. **Multivariate Analysis of Spectroscopic Data (Oslo).** Jens Oestreich, http://camo.com/contact-form.html, http://camo.com/training/more/en/spectroscopy.html?id=795&tid=20&po=1.

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

9–11 October, Metzingen, Germany. **Multivariate Analysis of Spectroscopic Data (Metzingen).** Jens Oestreich, http://camo.com/contact-form.html, http://camo.com/de/training/multivariate-analyse-spektroskopie.html?id=785&tid=20&po=1.

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.

1–3 November, Frankfurt, Germany. **Process Analytical Technology (PAT) with Multivariate Analysis (MVA).** info@lsbh.de, http://camo.com/training/more/en/pat_with_mva.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/trfcourse.

7–8 November, London, United Kingdom. **Introduction to Multivariate Data Analysis (London).** Joseph McCurley, http://camo.com/contact-form.html, http://camo.com/training/more/en/mva.html?id=764&tid=7&po=1.

13–14 November, Berlin, Germany. **Introduction to Multivariate Data Analysis (Berlin).** Jens Oestreich, http://camo.com/contact-form.html, http://camo.com/de/training/multivariate-datenanalyse.html?id=778&tid=7&po=1.

22–24 November, Utrecht, Netherlands. **Multivariate Analysis of Spectroscopic Data (Utrecht).** Joseph McCurley, http://camo.com/contact-form.html, http://camo.com/training/more/en/spectroscopy.html?id=793&tid=20&po=1.

22–24 November, Norderstedt, Germany. **Chemometric Spectroscopy: Basics and Multivariate Analysis for Quantitative and Qualitative Applications.** info@sensologic.de, www.sensologic.de/download/SL-Training-Registration_Nov-2017.pdf.

6–8 December, Birmingham, United Kingdom. **Multiple Biofluid and Tissue Types, from Sample Preparation to Analysis Strategies for Metabolomics.** David Epps, d.epps@bham.ac.uk, http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/sample-analysis.aspx.

14–15 December, Birmingham, United Kingdom. **Metabolite Identification with the Q Exactive and LTQ Orbitrap.** David Epps, d.epps@bham.ac.uk, http://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/metabolite-identification.aspx.

Exhibitions

2018

25 February–1 March, Orlando, FL, United States. **68th Pittcon 2018.** pittconinfo@pittcon.org, http://pittcon.org.

10–13 April, Munich, Germany. **Analytica 2018.** info@analytica.de, http://www.analytica.de/.

11–15 June, Frankfurt on the Main, Germany. **ACHEMA 2018.** achema@dechema.de, http://www.achema.de

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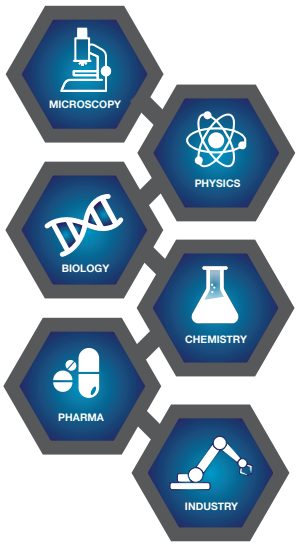

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