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Research into climate change takes many directions, and storing carbon or understanding its release from stores is extremely important. Philippa Ascough, Michael Bird, Will Meredith and Colin Snape tell us about “Dates and fates of pyrogenic carbon: using spectroscopy to understand a “missing” global carbon sink”. Pyrogenic carbon comes from the incomplete burning of biomass, and can be natural, e.g. wild fires, or man-made, e.g. the production of charcoal. The authors describe the uses of a range of spectroscopy techniques to understand the molecular structure of pyrogenic carbon and its role in the global carbon cycle.

Much of the exterior surface of plants is covered by the cuticle. This plays a vital role in protecting the plant from water loss, attack by pests and pathogens and damage from UV radiation. Infrared spectroscopy is very useful in characterising cuticles, as we learn in “Infrared spectroscopy as a tool to study plant cuticles” by José Heredia-Guerrero, José Benítez, Eva Domínguez, Ilker Bayer, Roberto Cingolani, Athanassia Athanassiou and Antonio Heredia. The authors point out that, whilst still in its early stages, infrared spectroscopy has provided valuable information about the functional groups, chemical structure and arrangement and interactions of plant cuticle components.

In the Tony Davies Column, Tony is getting jealous of chromatographers in “Central spectroscopic data systems: why are chromatographers so much better equipped?”. Replicating the power of chromatography data systems for spectroscopic data is not that easy.

“Is your spectrometer in calibration?” ask Chris Burgess and John Hammond. The answer may not be as straightforward as you might think. However, Chris and John explain all.

Another side of ensuring that our results are valid is correct sampling. In the latest Sampling Column on “Sampling quality criteria (SQC)” Kim Esbensen and Claas Wagner continue our education in the use of the Theory of Sampling. The fundamental step in ensuring representative sampling is sampling quality criteria, and the authors describe why and how.

This issue each year is when we publish our report on new product introductions at the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon). This year it was held in Atlanta, GA. My report starts on page 21 and covers a wide variety of spectroscopic techniques.




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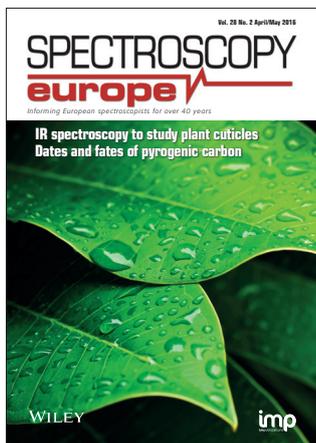
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Plant cuticles are an important barrier with a unique architectural design which confers multiple functions. Read how infrared spectroscopy is being used to investigate them in the article starting on page 6.

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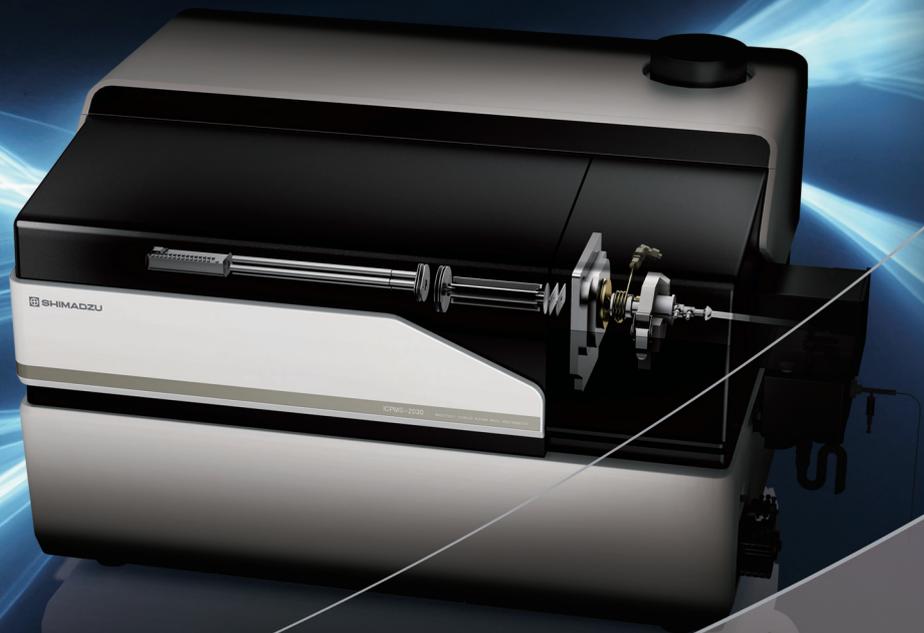
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Dates and fates of pyrogenic carbon: using spectroscopy to understand a “missing” global carbon sink

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Introduction: the many faces of pyrogenic carbon in the environment

Pyrogenic carbon is produced from the incomplete combustion of any type of biomass. The combustion process can be natural, such as wild fires, or controlled by humans, such as fossil fuel burning or domestic fires for heat and cooking. These processes have a very long history on Earth, with wildfires present from at least 400 million years ago,¹ and the use of fire possibly stretching back over almost the whole history of the human species.² During fires, a proportion of biomass is usually pyrolysed (exposed to high temperatures in conditions of restricted oxygen), and converted to pyrogenic carbon, which we also know as char, charcoal or soot. This process dramatically raises the carbon content of the material, and usually produces a highly polyaromatic structure, which is much more resistant to environmental degradation than the uncharred biomass. In recent years there has been a massive growth in interest surrounding how pyrogenic carbon behaves in the environment, as we have realised it can have some powerful negative effects. For example, we now know that pyrogenic carbon in the atmosphere is second only to CO₂ in terms of inducing global warm-

ing,³ and is a key factor in the retreat of Himalayan glaciers and Arctic sea ice through albedo feedbacks.^{4,5} Further, there are implications for global public health surrounding pyrogenic carbon emissions, which result in thousands of premature deaths through lowered air quality.

On the other hand, pyrogenic carbon is extremely useful for studies in archaeology and environmental science, as its aromatic structure means it remains in the environment for very long periods of time. As a result, it is one of the most common materials submitted for radiocarbon dating, and provides invaluable information on the activities of past societies and the chronology of past changes in environment. There is also intense interest in the possibility of using charcoal as a climate change mitigation tool; the idea underlying this is that carbon is “locked up” for millennia when biomass is converted to charcoal, also known in this context as “biochar”, which is then buried in soils.⁶ Despite this interest, however, we still know little about how pyrogenic carbon behaves in the environment, crucially, whether it forms a global sink of carbon and over how long this sink is stable. To address this knowledge gap, we need to know how much pyrogenic carbon exists in different global

carbon reservoirs and how rapidly it degrades, which is largely a function of its chemical structure. Because we presently have no definite answers to these questions, pyrogenic carbon could form a “missing” link in the global carbon cycle, explaining discrepancies in current carbon cycle models.⁷ One reason these questions remain open is that pyrogenic carbon is a difficult substance to isolate and study. There is a lack of consensus on what pyrogenic carbon actually is, and definitions cover a range of physical and chemical characteristics, as illustrated in the continuum of properties shown in Figure 1.

As a result, a range of analytical methods have been applied to try and extract pyrogenic carbon from environmental samples in order to better characterise it. A problem with many of these methods is that the pyrogenic carbon each technique isolates is operationally defined, and most techniques can result in a range of possible positive and negative artefacts. These problems result in variations of several orders of magnitude when a single method is applied to the same samples in different laboratories,⁹ and lead to large uncertainties over the actual amount of pyrogenic carbon in different carbon reservoirs; for example, uncertainty associated with published

pyrogenic carbon continuum			
	partly charred biomass	charcoal	black carbon
pyrogenic carbon content	lower		higher
chemical structure	'disorganized' low aromaticity		'organized' high aromaticity
common particle size	mm and larger	mm-cm	μm and smaller
common formation temperature	<350°C	>350°C	>500°C
material type	solid pyrolysis residue		gas phase condensation products
O/C and H/C		>0.5	<0.5
environmental alteration potential	higher		lower
transport potential	lower (surface)		higher (atmospheric)
porosity	lower		higher

Figure 1. The “pyrogenic carbon continuum” showing variability in physical and chemical characteristics of biomass that has been altered by fire. Note that the term “pyrogenic carbon” itself refers to a continuum of characteristics and not a single type of material. Reprinted from Reference 8 with permission from Elsevier.

estimates of atmospheric black carbon (the most resistant fraction of pyrogenic carbon) is a factor of two to five on regional scales and at least $\pm 50\%$ on global scales.¹⁰ A serious problem is the lack of understanding over BC (black carbon) degradation pathways and turn-over times in soils and sediments. While previous estimates of pyrogenic carbon indicated its extreme stability, leading to environmental half-lives of ~ 3000 years,¹¹ suspicions of decadal or even annual pyrogenic carbon degradation¹² are supported by new data showing degradation of charcoal over 67 days.¹³ There is therefore an urgent need to better characterise pyrogenic carbon, and understand its role in the global carbon cycle.

Novel methods to investigate pyrogenic carbon's molecular form

We have been using a new method to isolate a chemically well-defined pyrogenic carbon fraction from a range of environmental materials (e.g. soils, dissolved organic carbon from rivers and aerosols). The method uses high-pressure hydrogen to reductively remove

non-pyrogenic carbon from a sample, and is known as hydrolysis (HyPy). This technique isolates the pyrogenic carbon in a sample, which can then be quantified and characterised in more detail. In addition, the non-pyrogenic carbon fraction is trapped and can itself be investigated at the molecular level, for example by gas chromatography-mass spectrometry (GC-MS).¹⁴ During field trials HyPy has been used to track the fate of pyrogenic and non-pyrogenic carbon fractions in soils. HyPy is particularly sensitive to changes in these reservoirs and combining this with GC-MS analysis of extractable PAHs (polycyclic aromatic hydrocarbons) indicated that the latter decreased markedly with time over a two-year study. HyPy was

applied to 12 reference materials from a pyrogenic carbon ring trial,⁹ comprising five environmental matrices (two soils, aerosol, dissolved organic material and marine sediment), three laboratory-produced materials (two charcoals and soot), and four “blank” materials (melanoidin, lignite, shale and coal).¹⁵ This was to assess whether our method could accurately and precisely give us the pyrogenic carbon content in all of these types of materials. The method performs well for all materials apart from the coal, where HyPy cannot discriminate between pyrogenic carbon and the polyaromatic structure of the coal itself (which is not produced by biomass burning), and tests revealed that HyPy is the only method whereby the composition of the BC measured can be defined, atomic H/C < 0.5 corresponding to seven rings and larger with the non-BC fraction comprising up to and including six rings. In further tests, HyPy was effectively able to “clean up” ancient charcoals (ca 30,000–50,000 years old) for radiocarbon dating.¹⁶ Here, spectroscopy is an invaluable tool to track the removal of contaminants, with ¹³C-solid state nuclear magnetic resonance (¹³C SS-NMR) particularly useful in this regard. Pyrogenic carbon gives a distinctive peak in ¹³C SS-NMR spectra, centred on 130 ppm,¹⁷ so it is possible to track the removal of contaminants such as cellulose, with its characteristic peaks between ca 20–105 ppm, see, for example, Figure 2. Spectroscopy is also crucial in understanding the breakdown of pyrogenic carbon in the environment. Here, Fourier transform infrared (FT-IR) spectroscopy is very useful, providing information on the molecular structure of pyrogenic carbon itself, and on substances that can be extracted from this material after it has



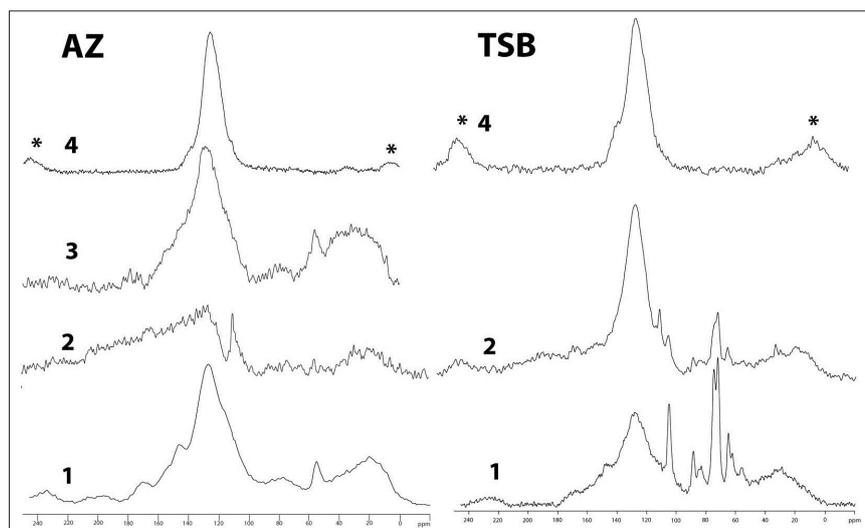


Figure 2. ^{13}C SS-NMR spectra of archaeological charcoals (raw charcoal is spectra 1) showing the incomplete removal of contaminants (e.g. cellulose) by acid-base treatment (spectra 2) and chemical oxidation (spectra 3), versus the complete removal of non-pyrogenic carbon by HyPy (spectra 4). (AZ: from the Faial Island, Azores; TSB: Toca do Serrote da Bastinia, Brazil). Reprinted from Reference 16 with permission.

been exposed to environmental conditions (i.e. the products of degradation). The C=C bonds of pyrogenic carbon are very distinct in FT-IR spectra, and can be readily separated from spectral contributions from other materials in the sample. FT-IR spectroscopy has also revealed that the process of pyrogenic carbon degradation involves carboxylation of the aromatic structure, again producing a very distinct IR spectral response. The application of FT-IR to these questions, using archaeological sample material, has revealed that after an extended time in soils or sediments, a portion of pyrogenic carbon is likely to be transformed into substances that are mobile in the soil, and could be leached away from the pyrogenic carbon structure, potentially then entering a faster-cycling pool of the global carbon cycle.¹⁸

Another application that gives ultra-high resolution insights into pyrogenic carbon dynamics in the environment is radiocarbon dating. This method applies accelerator mass spectrometry (AMS) to count individual atoms of the radioactive isotope of carbon, ^{14}C . Carbon-containing samples in the environment contain different levels of ^{14}C depending on the time of precursor death or moment of final formation, meaning that AMS allows us to identify how long a sample of pyro-

genic carbon has been in the environment, and how quickly it is turning over in the carbon cycle. AMS also allows us to discriminate between different sources of pyrogenic carbon in a sample, particularly one derived from fossil fuel burning versus biomass burning. This is helpful in understanding the sources of air pollution sources, for example, and is possible because biomass contains “modern” levels of ^{14}C , whereas fossil fuels do not contain measureable levels of ^{14}C , due to their great age.

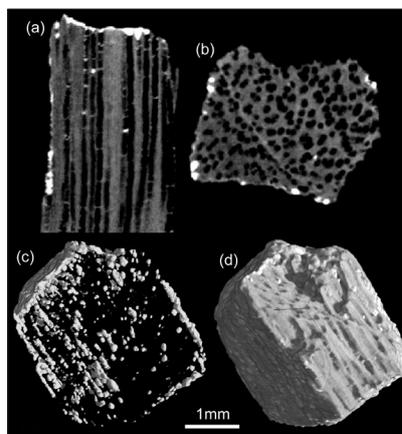


Figure 3. X-Ray microtomographic images of ancient charcoal. Image C shows the presence of mineral inclusions along micropores internal to the sample. Reprinted from Reference 19 with permission from Elsevier.

These methods of chemically characterising pyrogenic carbon can be backed up with methods of physically characterising its structure. An exciting development in this regard is the application of X-ray microtomography, which is a 3D scan of the surface and interior of pyrogenic carbon particles (Figure 3). This allows us to understand the surface area and porosity of samples, together with identifying mineral material that has become trapped inside the sample, and which may play a role in degradation of pyrogenic carbon in the environment.

Dates and fates: understanding the global cycling of pyrogenic carbon

Current understanding of pyrogenic carbon's role in the carbon cycle is evolving quickly, and reveals its importance as a form of carbon that has not yet effectively been incorporated into carbon cycle models. We now know that annual pyrogenic carbon production of 50–200 million tons per year²⁰ releases 7.5–17 million tons of pyrogenic carbon to the atmosphere,²¹ and contributes to storage of 54–109 billion tons pyrogenic carbon in soils.²² Inter-reservoir pyrogenic carbon fluxes are substantial, with an estimated transport of 19–80 million tons per year by rivers to the ocean²¹ and atmosphere-ocean transport of 7 million tons pyrogenic carbon per year, respectively.²² One concern is that climate change and human activity are currently playing a role in mobilising stocks of pyrogenic carbon that have been stored for periods of up to several thousand years. An example is enhanced melting of Arctic permafrost, which is a major repository of pyrogenic carbon as a result of boreal fires over millennia.²³ In addition, historical destruction of Brazil's Atlantic forest by humans since the time of the 15th–16th century explorer Christopher Columbus has generated massive stocks of pyrogenic carbon, that is being transported to the oceans at the rate of 50,000–70,000 tons each year.²⁴ We simply do not know how much of this pyrogenic carbon is released to the atmosphere as CO_2 , versus that being

stored in long-term sedimentary deposits, such as on the ocean floor.

Our work is starting to shed light on some of these questions, by monitoring the release of carbon from pyrogenic carbon in the environment. In the Daintree rainforest of Australia, we have observed loss of pyrogenic carbon on annual timescales, the rate of which appears linked to the chemistry of the soil in which the pyrogenic carbon is deposited. We have also observed the release of CO₂ derived from charcoal during laboratory soil incubation experiments on the order of months. This loss of pyrogenic carbon is strongly linked to the activity of soil microbes, which appear capable of breaking down pyrogenic carbon in order to obtain energy. The conditions that pyrogenic carbon is produced under also appear to play a role in its environmental fate; for example, fungi most readily colonise the surface of pyrogenic carbon produced at lower temperatures.²⁵

Summary

In summary, important questions remain surrounding the role of pyrogenic carbon in the global carbon cycle, and we are only just starting to address some of these questions. It seems as though the fate of pyrogenic carbon in the environment depends strongly upon, not only the specific chemistry of the material itself, but also the depositional environment in which it is emplaced. Spectroscopy is central to answering these questions, predominantly in the form of ¹³C-SS-NMR and FT-IR, although it is the integration of several methodologies that offers the most fruitful approach to understanding this missing link in the carbon cycle.

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Infrared spectroscopy as a tool to study plant cuticles

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Dedicated to the memory of José Heredia Romero

Introduction

Epidermal cells of fruits, petals, leaves and non-lignified stems are covered by a membrane called the cuticle.¹ This cuticle is an important plant barrier with a unique architectural design which confers multiple functions. Its main function is to avoid massive water loss from internal tissues. Additionally, the cuticle is involved in defending the plant against pests and pathogens, reflecting and filtering potentially harmful ultraviolet radiation, and establishing organ boundaries during plant development. Furthermore, the cuticle plays a key role in fruit quality and postharvest performance, agronomical traits of great economic importance.

The cuticle can be described as a heterogeneous and composite biopolymer,² as depicted in Figure 1. It is mainly composed of cutin, an amorphous and non-soluble polyester formed by condensed polyhydroxylated fatty acids, which act as a solid matrix for the deposition of the other components. Polysaccharides derived from the epidermal cell wall, chiefly cellulose, hemicelluloses and pectin, are another important cuticle component. Waxes can be located either covering the outer surface (epicuticular waxes) or embedded in the cutin matrix (intracuticular waxes). They are mixtures of C₂₀–C₄₀ *n*-alcohols, *n*-aldehydes, *n*-alkanes, fatty acids and esters. Cyclic compounds such as triterpenoids are also present in the wax fraction. Finally, a small fraction of phenolic compounds, mostly hydroxy-

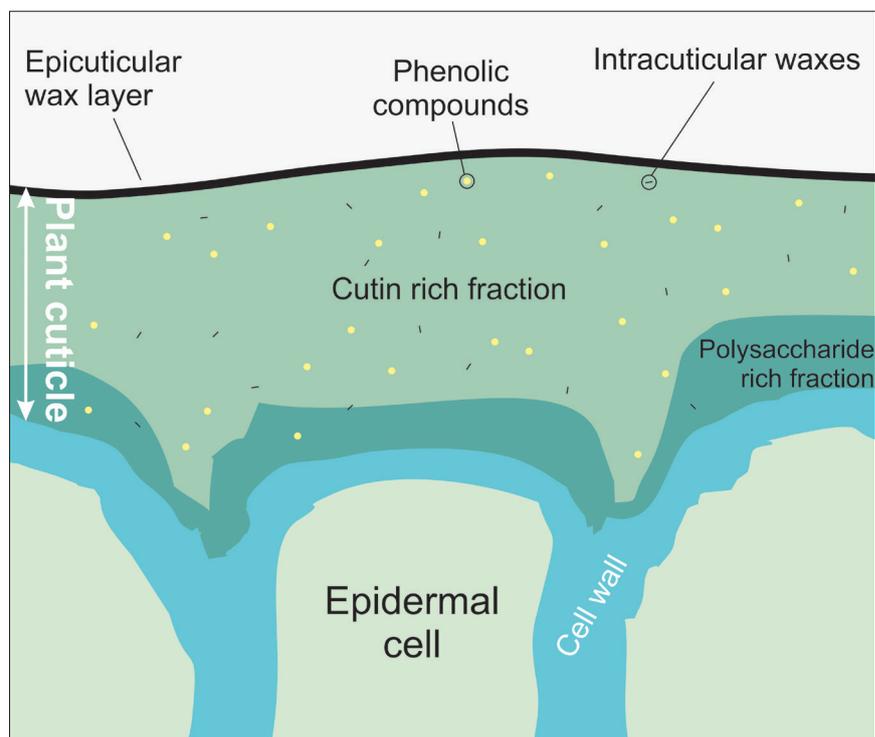


Figure 1. Scheme of the cross-section of a plant cuticle. The cuticle is located on the outermost region of the epidermal cell wall. From bottom to top, a polysaccharide-rich fraction in contact with the cell wall, a cutin fraction, that gives structural support to the cuticle and a thin layer of epicuticular waxes on the outer surface. Intracuticular waxes and phenolic compounds are distributed throughout the cuticle.

cinnamic acid derivatives and flavonoids, can be found within the cutin matrix.

The infrared spectrum of plant cuticles

Characterisation of plant cuticles by infrared (IR) spectroscopy has extensively provided valuable information about

their chemical composition and structure.³ Thus, IR spectroscopy has been used in the identification of functional groups and their molecular environments in isolated cuticles, in the analysis of the interaction, distribution and molecular arrangement of cuticle components, and also in the study of interactions between

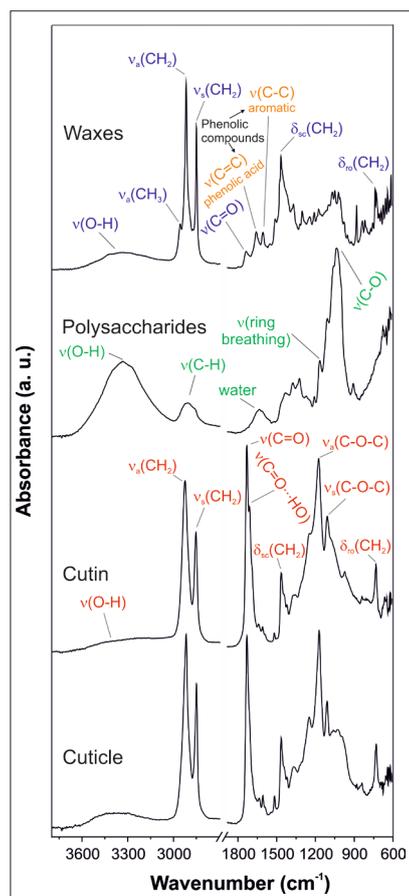


Figure 2. ATR/FT-IR spectra of isolated tomato fruit cuticle and its components. Main absorptions assigned to cutin (red), polysaccharides (green), waxes (blue) and phenolic compounds (orange) are indicated. [ν , stretch; ν_a , antisymmetric stretch; ν_s , symmetric stretch; δ , deformation; δ_{scf} , δ_{or} , scissors and rock deformation vibration motions, respectively.]

the cuticle and water or exogenous substances and in the remote sensing of plant cuticles.

Most plant cuticles show a similar IR spectroscopic profile. Figure 2 shows the attenuated total reflection Fourier transform infrared (ATR/FT-IR) spectra of an isolated tomato fruit cuticle. Five main spectral regions can be differentiated. The first region, ascribed to the stretching mode of hydroxyl groups interacting by hydrogen bonds, is located around 3400 cm^{-1} . Main contributors to this band are polysaccharides and the non-esterified hydroxyl groups of cutin. In the second region two strong absorptions at $ca\ 2920\text{ cm}^{-1}$ and 2850 cm^{-1} , associated

with the CH_2 antisymmetric and symmetric stretching vibrations, respectively, can be observed. These bands are usually accompanied by CH_2 bending vibrations at 1465 cm^{-1} , 1315 cm^{-1} and 725 cm^{-1} . They are mostly produced by fatty compounds of cuticle mainly present in cutin and waxes. In the third region, a strong peak at 1730 cm^{-1} ($\text{C}=\text{O}$ stretching mode of esters) together with three shoulders at 1715 cm^{-1} ($\text{C}=\text{O}$ stretching mode of esters interacting by hydrogen bonds), 1705 cm^{-1} ($\text{C}=\text{O}$ stretching mode of carboxylic acids interacting by weak hydrogen bonds) and 1685 cm^{-1} ($\text{C}=\text{O}$ stretching mode of carboxylic acids interacting by strong hydrogen bonds) are found. These bands can be attributed to the cutin matrix. In addition, other bands can be observed between 1650 cm^{-1} and 1500 cm^{-1} . They are assigned to different aromatic and $\text{C}=\text{C}$ chemical groups present in phenolic compounds. Aromatic molecules present in the cuticle are additionally characterised by two small bands at 816 cm^{-1} ($\text{C}-\text{H}$ out-of-plane bend) and 518 cm^{-1} ($\text{C}-\text{C}$ out-of-plane bend). Polysaccharides are featured by absorption at approximately 1030 cm^{-1} usually ascribed to the $\text{C}-\text{O}$ stretching mode. Significant differences can be observed in cuticle spectra of different plants, organs and stages of development, although they display an overall common chemical composition. Moreover, environmental conditions can directly affect the chemical composition of the cuticle and, hence, its spectroscopic characteristics. Figure 2 also shows the ATR/FT-IR spectra of cutin, polysaccharides, waxes and phenolic compounds. The weighted sum of the spectra of each cuticle component closely reproduces the cuticle spectrum.⁴

Applications

The main applications of IR spectroscopy in the study of plant cuticles are associated with different disciplines: from plant physiology to palaeobotany and biophysics. In this section, the interaction of cuticle components with water and exogenous molecules, the spectroscopic changes in plant cuticles during plant development and the deter-

mination of semi-quantitative IR band ratios in palaeobotany will be described. Considering the modern applications of remote sensing techniques to monitor plant development in agriculture and forestry, the role of the cuticle in light reflection and also in filtering the energy spectrum emitted by this process will also be addressed.

Interaction of plant cuticles with water and exogenous molecules

Since the cuticle is the outer barrier of the parts of plant organs exposed to air, the analysis of water–cuticle and exogenous molecule–cuticle interactions is of great importance. IR spectroscopy has provided very useful information about such interactions. In the case of water, two different configurations of H_2O molecules, *volatile* and *embedded*, were distinguished by FT-IR and near infrared (NIR) reflection spectroscopies,⁵ as illustrated in Figure 3. Some water molecules exhibited one weak hydrogen bond with the polysaccharide fraction of the cuticle. They were in equilibrium with the moisture and were designated as *volatile* H_2O molecules. On the other hand, other water molecules were involved in two strong or three weak hydrogen bonds with cutin and polysaccharides, and were designated as *embedded* H_2O molecules.

Sorption of some chemicals on plant cuticles has been also characterised by FT-IR spectroscopy.³ For instance, the analysis of isolated tomato fruit cuticles exposed to a flow of NO_2 showed significant changes in the region of phenolic compounds, indicating an irreversible interaction of the NO_2 with the aromatic fraction of the cuticle. Interestingly, the nitro functional group of the herbicides fenitrothion and parathion can interact with the polar functional groups of epicuticular waxes, significantly reducing their resistance to photodegradation. Sorption of dimethyl sulfoxide showed a reversible interaction between the sulfoxide ($\text{S}=\text{O}$) chemical groups and the ester groups of cutin, which was characterised by a shift to lower wavenumber of the $\text{S}=\text{O}$ stretching mode and an increase in intensity of the shoulder at 1715 cm^{-1} .

resonance and gas chromatography is recommended.

Furthermore, other typical IR techniques, commonly used for the analysis of thin films, could be employed in the study of plant cuticles. For example, the use of variable angle ATR/FT-IR could allow for the study of chemical depth profiles, while the control of the temperature would permit one to analyse the melting of waxes or the breaking of hydrogen bonds. Additionally, the polarisation of the infrared light would be useful in the detection of preferential orientations or crystalline domains of the different cuticle components. Additionally, ATR/FT-IR spectroscopy could be used for the determination of coefficients of diffusion of water or exogenous molecules through the cuticle. Another possibility to consider would be the use of IR spectroscopic analysis to carry out initial screenings of genetically modified plant cuticles.

Finally, it is important to emphasise that the number of plant cuticles of different species analysed is still low. Extrapolation of data and conclusions to other plants species could be erroneous. Thus, more studies by IR spectroscopy are necessary in the future for a better understanding of this

complex and important plant barrier membrane.

Acknowledgements

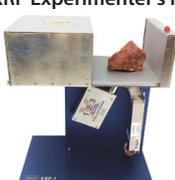
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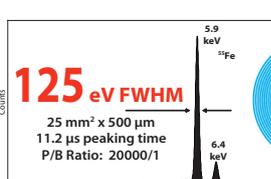
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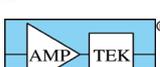


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Central spectroscopic data systems: why are chromatographers so much better equipped?

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I do not like being jealous, but looking at the systems our chromatographers have at their fingertips to control, program, monitor and analyse their experiments from a central Chromatography Data System makes me wish the spectroscopy community would catch up! The chromatographers are very fortunate in that their main vendors have a good offering of Chromatography Data Systems (CDS) which can run instruments from pretty much all of the various main chromatography instruments on the market. Why are we spectroscopists so poorly served?

Typical CDS

Depending on the size of your organisation, a central CDS can serve multiple laboratories in multiple locations, spread across different buildings, sites and even countries. In fact, it is possible to deploy these systems in a secure robust disaster recovery configuration which allows a fallback position of running the CDS from another continent. Essentially the only limiting factor is the availability of the network backbone infrastructure.

The enormous flexibility has been made possible by the exchange of instrument control specifications and tools between what would otherwise be competing vendors in the same instrument functionality space. This means that analysts are free to select the analyt-

ical system which they feel delivers the best performance for their particular area of work whilst selecting the control software which they feel best fits into their overall data analysis and reporting world. They have no need to compromise by being forced to buy a CDS from the same manufacturer as their instrument hardware.

The vendors must be applauded for having the strength to continue these collaborations, as you can well understand the pressure from the commercial side to try and gain a business advantage by not continuing this information exchange. In such deployments there must be serious discussion with the

users, management, compliance and IT support community if the addition of a Scientific Data Management System (SDMS) is actually to bring benefits. For laboratories working within a regulatory compliance framework, modern centralised CDS systems will normally be compliance-ready on installation and can operate alone (Figure 1). There may well be benefits arising in the area of long-term compliant archiving depending on the stability and granularity of the organisation. Where corporate policy may be able to dictate a centralised document archiving system across an organisation, this is significantly more

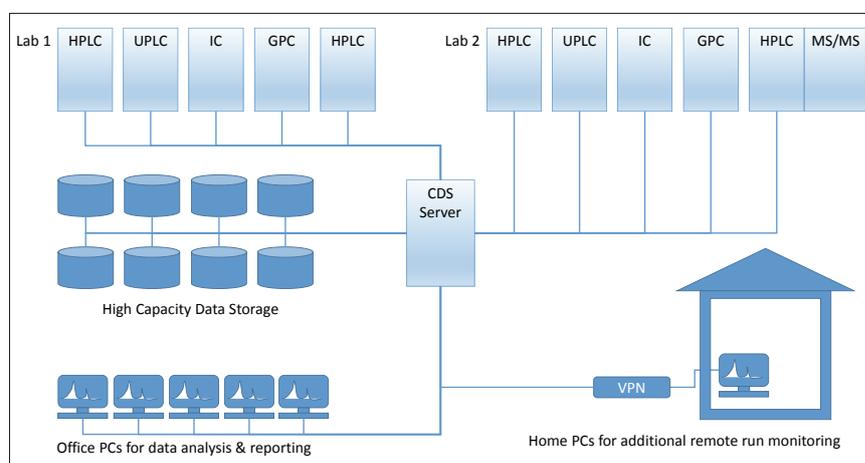


Figure 1. Potential modern CDS Deployment—now available with integrated mass spectrometry instrument control, data acquisition and analysis.

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difficult in the area of scientific data handling.

These systems have also made it possible for easy remote monitoring of the ongoing work which I have seen enhance the work–life balance amongst colleagues.

Adding spectroscopy

Recently, there have been updates to CDS systems which have started to include support for hyphenated instrumentation. Currently the instrumentation support has been limited to a selection of the instruments within the particular CDS vendor's own range of spectrometers. This integration has included complex mass spectrometry instrumentation control and data analysis with reference spectroscopic database integration. As a first step this is greatly to be welcomed—and we can only hope that the collaboration between vendors in exchanging instrument control information will extend in future to the spectroscopic detectors as well.

Unfortunately, we may well run into the old ideological battle which is always fun to watch between those who identify themselves as chromatographers—who see hyphenated systems such as an UPLC-MS/MS as just a top of the range chromatography system with an overly expensive detector; and spectroscopists who would just see the front end as a programmable sample preparation robot enhancement to the inlet of the spectrometer. I always try to promote the thought that they are all actually just analysts and they should be optimising all areas of their instrumentation to achieve the best results.

As we have seen in recent articles there is the potential for remote spectroscopic instrument control between different vendors,¹ but in this particular case I would think it necessary to add that I would guess the specific collaboration was eased by the long-standing good relationship between the parties involved and the lack of competition in the instrumentation market between them.

There have been many initiatives involving direct competitors, especially in the USA, to develop the “unified instrument control protocol” to allow central-

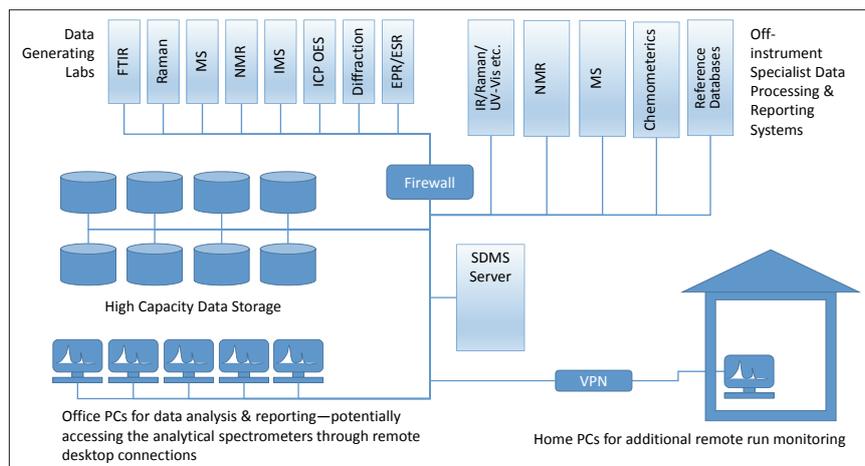


Figure 2. Potential for a Spectroscopic Data System—still a bit of a mess!

ised instrumental management systems to handle a multitude of different instruments. Some of the systems prototyped have been used by individual vendors, but I am unaware of any great impact in our deployed instrumentation park.

Can we rival the chromatographers' functionality?

Well the answer is not very inspiring and worryingly has not really changed much in the last ten years or so. Figure 2 shows one version of how an organisation may combine their available spectroscopic systems, data processing tools and an SDMS to get close to what the chromatographers' can boast is available out-of-the-box from several vendors in their space.

In a corporate environment one of the problems may well be incompatibilities between the laboratory PC infrastructure, due to the reliance on increasingly ageing spectrometer control systems and the demand to continually update to the latest operating systems. This is mainly driven by security reasons for all computers on the main corporate network. One workaround shown in Figure 2 is the introduction of segregation of the laboratory network from the corporate office network by a firewall. This adds another, although not insurmountable, level of complication to an integrated solution.

Although many spectrometer control packages now come with varying levels of complexity in the in-built data processing, many analysts have their own

personal preferences when it comes to advanced spectroscopic data processing, chemometric analysis or the use of particular reference database solutions. Maintenance update releases and security patches of these systems usually have no problems in remaining compliant with corporate IT policy so are usually found deployed on the normal corporate network.

If your organisation operates in a regulatory compliant space, there is probably little choice but to deploy an SDMS of some nature to meet the demands of the regulators around data integrity.

Conclusions

In conclusion it is possible for a spectroscopic environment to mimic the functionality available to our brother and sister chromatographers, but we are still required to deploy a highly fragmented—and therefore vulnerable solution if we are to get close to what they have at their fingertips. I suppose hope is on the horizon with the introduction of hyphenated instrument support to recent CDS releases... but do we really want to be told by chromatographers how we need to work?

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Is your spectrometer in calibration?

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A question that was easily answerable you might think, especially if you have used a certified reference material traceable to NIST, for example. After all it comes with a certified value with an expanded measurement uncertainty doesn't it?

So when you measure this CRM on your spectrometer, what are your acceptance limits? A good question because the expanded measurement uncertainty relates to the certified reference standard itself, not to the value measured on your spectrometer. So how do you establish acceptance limits for your spectrometer for your type of calibration?

The answer is somewhat buried in manufacturers' and NIST publications. You could carry out an uncertainty budget exercise. An example of this approach has been given recently.¹ Here an uncertainty budget calculation is used to show that the mean value of the measured value lies within the combined uncertainty. In other words, the difference between the certified value and the

measured value of 0.0042 absorbance units is within the combined uncertainty of 0.0058 absorbance units and hence within calibration.

However, as many laboratories would like to use simple acceptance limits, is there another way?

Some manufacturers and CRM suppliers use a simple acceptance limits statement contained in the NIST SRM 1930 Glass filters certificate:

“An acceptable level of agreement between the user's measurements and the certified value and its expanded uncertainty overlaps any part of the user's tolerance band defined by the measured mean and the user-defined level of acceptability”²

This has been interpreted as “Add the SRM expanded uncertainty to the manufacturer's tolerance and make those the acceptance limits for satisfactory calibration performance”. Let us see if this

works, as it is very easy to calculate and apply. Even QA will be able to understand it.

By way of an example consider an SRM absorbance value which has an expanded uncertainty (U) of ± 0.0049 absorbance units. The actual certified value does not matter as you will see. The instrument manufacturer's specification (A), at that absorbance value, is ± 0.005 absorbance units. Hence, simple addition gives Acceptance Limits of ± 0.0099 absorbance units from the certified value. Note that in the NIST statement it uses the term “measurement mean” implying that the user measures the standard more than once and takes the mean value. In other words, the difference between the measurement mean and the certified value must not exceed ± 0.0099 absorbance units for the instrument to be deemed in calibration.

We can test this approach by running a Monte Carlo Simulation (MCS) model,³ using Minitab Devize software and assuming that the SRM standard deviation is 0.00245 (i.e. half the expanded uncertainty) and that the manufacturer's specification has a uniform or rectangular distribution. When we run this simulation, the result is shown in Figure 2 for 50,000 iterations of the model and set the acceptance limits (specification limits) as ± 0.0099 .

As can be seen, more than 99.6% of the results would lie within the acceptance limits. So this would appear to be a reasonable approach.

Can this be applied to wavelength accuracy also? Yes indeed. This time let us assume that SRM has a standard devi-

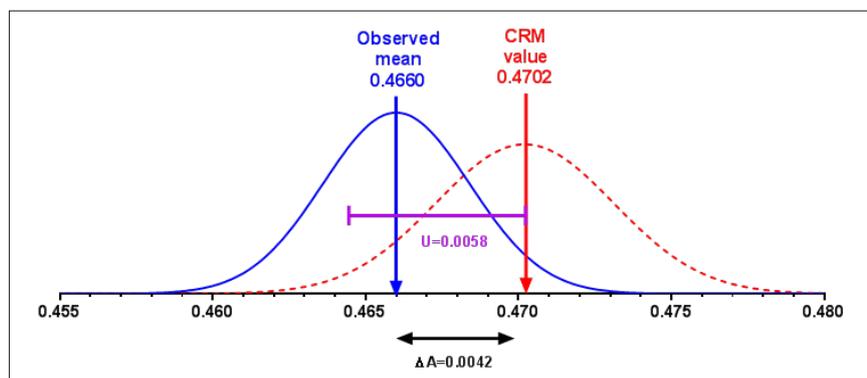


Figure 1. An example of a mean measured absorbance value lying inside the combined measurement uncertainty of the measurement and the CRM.¹

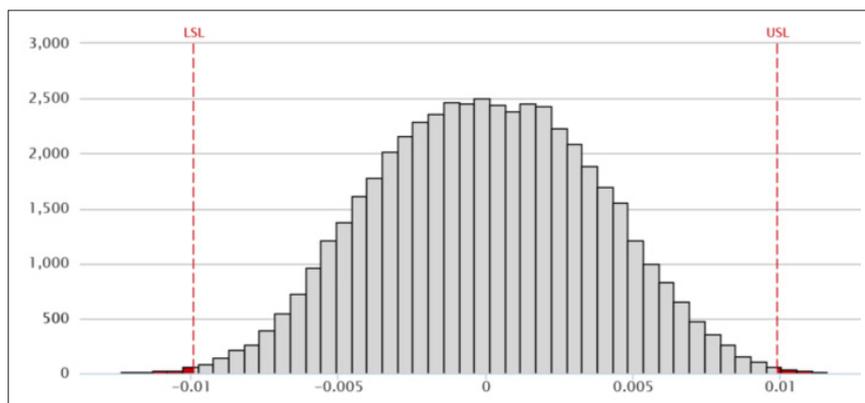


Figure 2. Minitab Devize MCS model output for absorbance accuracy acceptance limits of ± 0.0099 for $N = 50,000$.

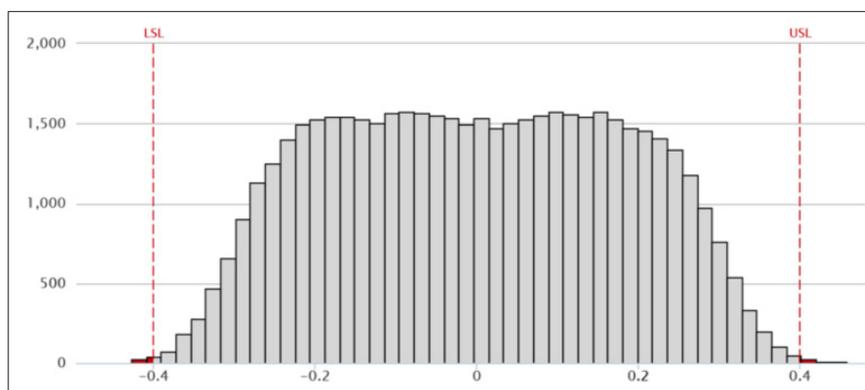


Figure 3. Minitab Devize MCS model output for wavelength accuracy acceptance limits of ± 0.4 nm for $N = 50,000$.

ation of 0.05 nm (expanded uncertainty is 0.10 nm) and the manufacturer's specification is ± 0.3 nm. In this instance, the acceptance limits would be $(0.1 + 0.3)$ i.e. 0.4 nm. The result of the MCS model is shown in Figure 3. This time more than 99.8% of the results would lie within the acceptance limits.

Does this simple acceptance limit method sound a bit too good to be true? Yes it is, because this method ignores the metrological uncertainty of the mean itself!

Careful reading of NIST Special Publication 829 reveals that, in section E3a, the statistically correct calculation for the acceptance limits (AL) required is given by:

$$AL = \pm t_{(0.05, n-1)} \frac{s}{\sqrt{n}} + (U + A)$$

These acceptance limits include the above mentioned approach for the acceptance limits ($U + A$) and, in addition, the standard error of the meas-

ured mean corrected for the number of determinations. These correct limits will be a little larger than the acceptance limits based on just ($U + A$) which are more conservative. From a compliance perspective the acceptance limits based on just ($U + A$) are "fail safe", so would be acceptable.

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Sampling quality criteria (SQC)

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Formulating proper Sampling Quality Criteria (SQC) is the initial step in a scientific approach to representative sampling: this activity can be characterised as “a framework for planning and managing sampling and analytical operations consistent with the overall project objectives”. It includes establishment of concise sampling objectives, precise outlining of the decision unit (DU) and deciding on the level of confidence wanted regarding the kind(s) of decisions to be made based on the analytical results. Once defined, these criteria serve as input to the Theory of Sampling for developing a representative sampling protocol.

Sampling quality criteria (SQC)

The first component in SQC is defining the *analyte(s)* to be involved, the concentration level of interest of the analyte(s) and how inference(s) will be made from the analytical data to the decision unit.

The second component of the SQC concerns definition and establishment of the physical *decision unit (DU)*, also known as the “lot” in the Theory of Sampling (TOS). The decision unit establishes the spatial and temporal boundary conditions of the sample collection process.

The third SQC component, the confidence level, establishes the desired probability that a correct inference (dec-

sion) can be made. The confidence level should typically correlate to the potential consequences of an incorrect decision, e.g. health, economic, societal consequences. The magnitude of the total combined errors in the sampling, sample processing and analytical protocols constitute the unavoidable basic risk level involved, and determines the likelihood of an incorrect decision. Thus, controlling errors to a greater extent increases the probability of a correct decision. The required confidence level also directly affects the sampling effort and quality control measures.

Establishing proper SQC is nothing but very carefully thinking through the *why*, *what* and *how* regarding the use of the final analytical results; surprisingly often

this prerequisite does not get the full attention it deserves.

First SQC component—definition of analyte(s)

The first SQC component addresses definition of the analyte(s), the expected concentration level of interest, as well as how the analytical data will be used; i.e. how *inference* is made with respect to the decision unit. This prerequisite sets the scope and limits the selection possibilities for sampling tools, sampling containers, sample handling procedures, sample preservation, laboratory preparation equipment, sample mass reduction procedures etc. For all sampling operations it is critical to secure analyte integrity from the primary sample all the way through to the final analysis.¹

Second SQC component—delineating the decision unit (DU)

The decision unit (*aka* the lot) defines the target (material, form, size, conditions) from which the primary sample is to be collected and importantly sets the *scale of decision-making*. This scale can be based on volume, mass, package size or any other definable criteria relevant for the project. As defined in a previous sampling column, a pre-requirement for the decision unit is physical accessibility (Fundamental Sampling Principle).² If a certain part of the decision unit is not accessible, the section either **must** be made accessible for the purpose of sampling or the (limited) target is

It so easy to do it **WRONG!** And so easy to do it **RIGHT!**



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disqualified from being a proper decision unit from which defensible and reliable decisions can be made. Sampling of a decision unit under limiting constraints, be these practical, logistical, economic etc., will unavoidably forfeit any chance of extracting representative samples; only worthless specimens will ensue.

Third SQC component— inference and confidence

Three basic types of inference can be applied from the final analytical data, i.e. from the concentration of the analytes of interest: *judgement*, *direct inference* and *statistical analysis*.

Judgement is never an acceptable methodology, irrespective of whatever personal experience is involved. Judgemental inference is not discussed further here.

Direct inference is the simplest proper inference approach in which the analytical result from a single primary (composite) sample is used as a reliable, and defensible, estimate of the average concentration of the analyte in the decision unit/lot. This approach requires no statistical analysis as long as the principles of the Theory of Sampling are obeyed. This is the tacitly assumed sampling situation in many “straightforward” situations.

In comparison to direct inference, *statistical analysis* involves multiple primary samples. In such case, the upper confidence limit of the mean is compared to a specification limit or a statistical comparison of one decision unit to another decision unit (e.g. reference decision unit). In “acceptance sampling”, e.g. in releasing a batch of drug dosages/tablets, it is the lower limit of the confidence interval that sets the operative threshold.

There is no rule for setting the confidence level. It is a function of the consequences of an undesired incorrect decision. Typically the larger the consequences of an incorrect decision the higher the desired confidence needs to be. It is **not** a good policy to always set the confidence at the same level (e.g., 95%) if it is not known *why* this level is actually used. Never mind that this “usually” is the level encountered; there

are enough “template statistics” governing complex problems, projects etc. that it may just be that careful consideration (proper SQC deliberations) reveal that some other level of confidence is more appropriate.

In order to calculate a confidence level for statistical analysis, an estimate of the global estimation error (*GEE*) is required, as defined in previous sampling columns:

$$GEE = Total\ Sampling\ Error + Total\ Analytical\ Error$$

For either case of direct inference or statistical analysis, the estimate of the *GEE* (all bias sampling errors need to have been eliminated first, TOS) can be determined from a properly conducted replication experiment, see previous *SE* column).³

If the sampling bias errors have not been properly eliminated, the estimate of *GEE* will forever be of varying magnitude, see previous sampling column,² with the consequence that the premise for a constant confidence level is broken.

Figure 1 graphically depicts the relationships between confidence, error and representativeness. Applying the Theory of Sampling, including the defined sampling quality criteria, to any sampling protocol ensures representativeness, because the primary goal of the Theory of Sampling is to minimise the total sampling error (*TSE*), which in turn increases the confidence of the inference made from the analytical data to the decision unit.

This column is but an introduction serving to raise the awareness of the need for proper SQC; the reader is

referred to more in-depth treatments in the references,^{4–9} with a natural starting point in Reference 1.

Perspectives

Industry is critically dependent on the highest data quality (data relevance, data reliability, data representativity). Representative data cannot be acquired without a *sampling process* initiating the full “lot-to-analysis-to-decision” pathway. In this endeavour the critical determinant is the potential *sampling bias*, an inconstant deviation between an analytical sampling result and the true average concentration of the lot, product or process, which must be *eliminated* from all sampling processes at all stages to ensure data validity. The sampling bias is fundamentally different from the well-known analytical bias, which can be eliminated by a statistical bias correction. However, this approach is impossible for the sampling bias, which, in addition, is orders of magnitude larger in most cases.

Sampling does not necessarily only refer to physical sample extraction, but also to on-line process and/or product measurements through the use of Process Analytical Technological (PAT) sensors. PAT is a framework originally developed by the US Food and Drug Administration to design, analyse and control pharmaceutical manufacturing processes through (continuous) measurement of critical process parameters, which is now being applied to many other manufacturing and processing industry sectors. In case the highly advanced measurement sensor technologies extract information from a wrongly defined decision unit or biased sample,

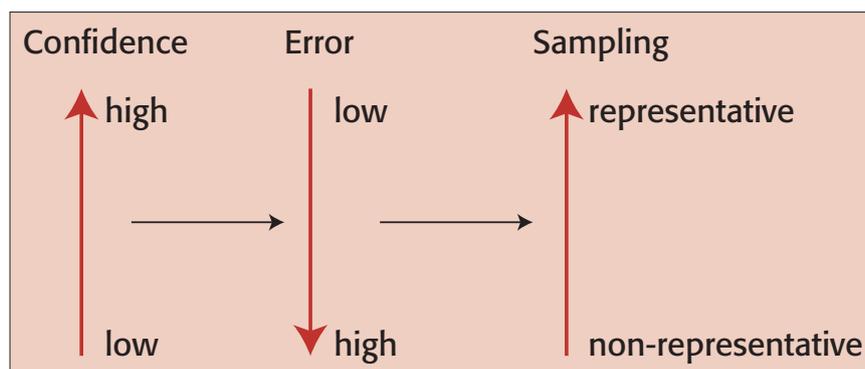


Figure 1. Relationship between confidence level, error magnitude and representativeness.

SAMPLING COLUMN

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the results of this advanced process control technique will unavoidably lead to biased results. The main challenge is therefore to ensure that highly precise measurements also reflect the true target value of the decision unit (requiring elimination of the sampling bias), which currently most of the times **remains unaddressed. A fully comprehensive SQC is a missing link in this context.**

In all sampling situations (whether sampled and analysed physically, or measured by the use of PAT), *representativeness* (of samples and signals) is the prime objective without which the derived analytical results and the decisions based on these data are invalid. Representativeness implies both elimination of the fatal sampling bias, as well as high reproducibility of the sampling process. Depending on the required use of data (used "as is" for monitoring or aggregate data for higher-level decision-making), there will always be a problem-dependent "decision unit" defining the target from which a sample is extracted or for which a signal is measured. **But critical DUs do not always conveniently suggest themselves; problem-based due diligence is required!**

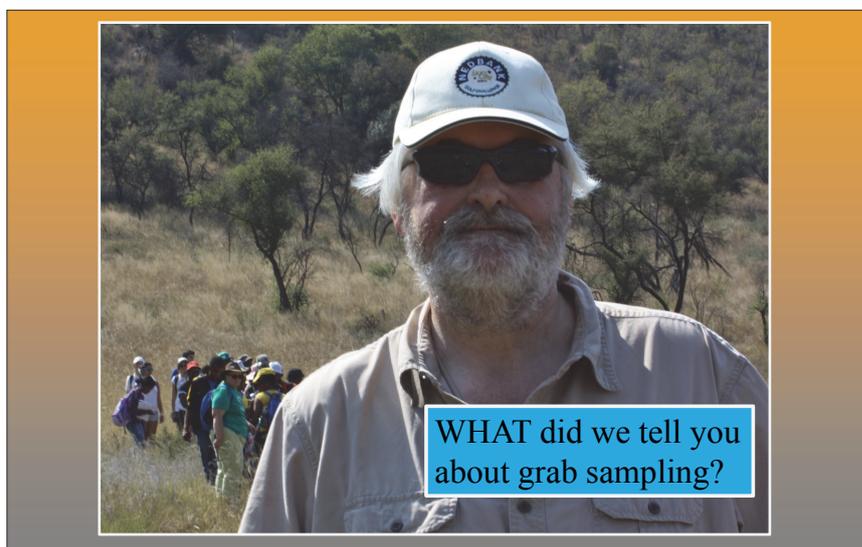
Conclusions

Defining sample quality criteria must be the initial step in the development of any sampling protocol. SQC defines the analytes, the decision unit and addresses the required inference and its

confidence level. The precise definition of the analyte(s) and the decision unit is currently one of the weaker elements, and not always sufficiently addressed in sampling protocols, with the potential consequence of using improper sampling protocols, ultimately with the end result of invalid inferences. Above all: never resort to using grab sampling!

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WHAT did we tell you about grab sampling?

Pittcon report 2016

Ian Michael

Over the (more than I wish to admit) years that I have been preparing reports on new product introductions at Pittcon for *Spectroscopy Europe* and its predecessors, we have tried various formats: both descriptive and tabular. For a change, this report combines the two. At the end you will find a table of new product introductions with links for more information. Before that, I have picked out some themes and instruments from the major spectroscopic techniques. As usual, this report does not cover instruments that may have been new at Pittcon but which we have already covered in previous issues. If I have missed anything, you are welcome to let me know and we will try and include it in a future issue.

New products in atomic spectroscopy covered a wide range of technologies, including ICP-OES, ICP-MS, LIBS and arc-spark instruments. Shimadzu's ICPMS-2030 has been designed to meet the requirements of the ICH Q3D guidelines for elemental impurities in pharmaceutical products. These specify allowable limits of daily intake of 24 elements of toxicological concern, which the ICPMS-2030 can detect with ppt sensitivity. This is achieved with a new collision cell and optimised internal structure, as well as new software and functionality. Thermo Scientific's iCAP RQ ICP-MS has been designed for maximum uptime and ease of use, with "intelligent" workflows, universal interference removal and automated sample handling accessories. It can run samples unattended 24/7. Arc/spark instruments were introduced by Spectro and Thermo Scientific. Spectro introduced a hybrid SpectroLab metal analyser combining analogue PMT detectors with digital CCD technology for simultaneous measurements, and an all-CCD SpectroLab for fast, accurate and flexible analysis. Thermo Scientific's ARL easySpark analyser is aimed at small to medium sized secondary metal manufacturers; it uses multi-grating/CCD-based optics, and is designed to be easy to use for non-experts. Portable LIBS analysers came from StellarNet (the case-based StellarCase-LIBS) and B&W Tek (handheld NanoLIBS).

Gas analysis featured amongst mid-infrared instruments. The Gasera One from Gasera is a portable instrument for sensitive, multi-gas analysis. It uses Gasera's cantilever-enhanced photoacoustic technology. The user interface has been carefully designed and can be worked via a single knob on the instrument or via your smart phone/tablet. Stability is another important point, with recalibration not needed for several months, even years. Bruker's Matrix-MG offers real-time monitoring of gas compounds, with the target gases analysed inside a cell with different optional optical path lengths to cover a broad range of applications. The identification and quantification of compounds is performed automatically by OPUS GA software with quantification of more than 400 compounds without the need for calibrations. As always, there a number of new sampling accessories including those from Czitek (ATR and microspectroscopy),



Shimadzu's ICPMS-2030



Thermo Scientific's ARL easySpark



The Gasera One from Gasera



Bruker's Matrix-MG

PITTCOON 2016

Harrick (diamond ATR), Pike (cylindrical ATR) and Specac's Pearl liquid cell that we have already covered.

Many of the larger new mass spectrometry instruments are now launched at ASMS, so software and add-ons were much in evidence. However, Shimadzu were showing the Nexera MX-DST multiplexed LC-MS system which provides continuous data acquisition by incorporating a special flow line structure and instrument control system. Instruments for gas analysis were introduced by JEOL (the InfiTOF which uses multi-turn ion optics) and Ionicon (PTR-TOF 1000 which increases sensitivity with Ion-Booster funnel technology. IonSense combined the DART ambient ionisation source with Waters' Acquity QDa detector for a small and potentially mobile instrument.

NIR spectroscopy saw a number of introductions. "Small" instruments ranged from portable bench instruments to very small MEMS-based. Thermo Scientific's iS5N is an NIR version of their FT-IR spectrometer, whilst Si-Ware Systems have started production of their NeoSpectra MEMS-based FT-NIR (Michelson interferometer including moving mirror fashioned from silicon). Ocean Optics had the matchbox-sized Flame-NIR, and StellarNet the case-based StellarCase-NIR. Viavi Solutions were showing three new instruments based on their linear variable filter technology. Another MEMS device came from Hamamatsu which combined a Fabry-Perot interferometer and a single element detector. Functional NIR spectroscopy (fNIRS) seems to be in the news often these days and Shimadzu were demonstrating their new system, LIGHTNIRS, which is both portable (battery-powered) and offers multi-brain imaging with synchronisation of up to four instruments.

Like mass spectrometry, the larger NMR spectroscopy systems tend to be launched at other events such as ENC. Nevertheless, there were benchtop NMR developments from Magritek (new 60 MHz versions of their Spinsolve spectrometers) and Nanalysis (NMReady-Flow interfaces for their NMReady spectrometers). Bruker introduced new modules for their NMR FoodScreener (honey and wine profiling), a toothpaste analyser based on the Minispec TD-NMR and InsightMR flow-tube online monitoring. Wiley Spectra Lab's NMR Collection of over 833,000 NMR spectra is powered by Bio-Rad's KnowItAll software.

Cobalt Light Systems caught the eye in Raman spectroscopy with their Resolve handheld SORS (spatially offset Raman spectroscopy) analyser for through-barrier Hazmat, explosives and narcotics identification. Analysis through containers and even boxes within courier packaging is possible, and the system's matching algorithm identifies individual chemicals as well as mixtures. Renishaw were showing their latest Raman microscope, the inVia Qontor which uses focus tracking technology to analyse samples with uneven, curved or rough surfaces. Focus is maintained during data collection and white light video viewing. Thermo Scientific had new versions of the DXR Raman microscope (DXR2 and DXR2xi). The former is a highly automated, push-button operated, dedicated macro-sampling Raman system. The latter is an improved version with new polarisation techniques and kinetic imaging.

Microvolume spectrophotometers were on offer from Thermo Scientific (NanoDrop One and One^C with cuvette option) and



The Shimadzu Nexera MX-DST



The LIGHTNIRS from Shimadzu



Ocean Optics' Flame-NIR



Magritek's 60 MHz Spinsolve



Cobalt Light Systems' Resolve handheld SORS



Renishaw's inVia Qontor

Pultton (P100 and P200). USP <857> becomes mandatory in May and CRM kits to enable you to comply are on offer from Starna Scientific and Hellma. The SpectroClick Kit for use in classroom teaching is now available for <\$100, and the new AAH-300a visible spectrophotometer will be available in the summer.

In X-ray spectrometry, the development of handheld instruments continued with new models from Thermo Scientific (Niton XL5) and Spectro (SpectroScout). There were also instruments aimed at specific markets: petroleum products (SLFA-6100/6800 from Horiba) and crude oil (Epsilon 3^{XL}E from PANalytical).

The Thermo Scientific NanoDrop One



Horiba SLFA-6800

Links for more information

To simplify your search for more information on products listed below, you can connect directly to the relevant product page for each product using the code number. If you are reading this in a printed copy, just put the number into your browser at the end of the URL string <http://link.spectroscopyeurope.com/28-02->. If you are reading this in a digital version, just click the links! Where a page is not currently available, we have provided a link to the company's home page or the most relevant page.

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PRODUCT FOCUS

Product Focus on Luminescence

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APPLICATIONS: Materials science ■ Energy industry ■ Flat panel displays ■ Semiconductors
KEY FEATURES: UV-visible-NIR spectral range ■ Transmission and reflectance ■ Raman ■ Luminescence

PRODUCT: 508 PV Microscope Spectrometer
APPLICATIONS: Materials science ■ Energy industry ■ Flat panel displays ■ Semiconductors
KEY FEATURES: UV-visible-NIR spectral range ■ Transmission and reflectance ■ Luminescence

Edinburgh Instruments

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PRODUCT: FS5 Spectrofluorometer
APPLICATIONS: Material research ■ Photochemistry ■ Biophysics ■ Quantum yields ■ Rare earth minerals
KEY FEATURES: Time resolved and steady state fluorescence measurements ■ Single photon counting for the highest sensitivity ■ Two emission ports as standard ■ NIR upgradeability ■ Ultrafast data acquisition

PRODUCT: FLS980 Fluorescence Spectrometer
APPLICATIONS: Material research ■ Photochemistry ■ Biophysics ■ Quantum yields ■ Rare earth minerals
KEY FEATURES: Time resolved and steady state fluorescence measurements ■ 25,000:1 water Raman SNR ■ Large sample chamber with 6-axis access to your sample ■ High performance monochromators with high straylight rejection

PRODUCT: LP980 Transient Absorption Spectrometer
APPLICATIONS: Singlet transient absorption ■ Triplet transient absorption ■ Structural analysis ■ Photochemistry ■ Solar cells
KEY FEATURES: All-in-one spectrometer for transient absorption, Laser-induced fluorescence, Raman and laser-induced breakdown spectroscopy (LIBS), Kinetic and Spectral data acquisition ■ Transients measured up to 2.55 μm ■ Integrated ICCD allows transient spectra to be measured within one laser flash

Energetiq Technology, Inc.

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info@energetiq.com
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PRODUCT: EQ-99X Laser-Driven Light Source
APPLICATIONS: UV-Vis-NIR spectroscopy ■ Monochromator source ■ Thin-film measurements ■ Optical component testing ■ Materials characterisation
KEY FEATURES: CW laser plasma discharge 100–200 μm plasma size ■ Very high brightness across spectrum UV-Vis-NIR (170–2100 nm) ■ Excellent spatial and power stability repeatable measurements ■ Electrodeless operation for long life, reduce cost of ownership ■ Ultra-clean construction—Improved stability & extended life



PRODUCT: EQ-99X-FC Fibre Coupled Laser-Driven Light Source
APPLICATIONS: UV-Vis-NIR Spectroscopy ■ Monochromator source ■ Thin-film measurements ■ Fibre optics testing ■ Advanced imaging
KEY FEATURES: FC fibre output for precision coupling ■ Very high brightness across spectrum—UV-Vis-NIR (190–2100 nm) ■ Superior spatial and power stability—Repeatable measurements ■ Efficient, high performance elliptical collection optics ■ Eliminates need for multiple lamps—Replaces D₂/Tungsten/Xenon arc



Technospex Pte Ltd

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PRODUCT: uSight-X
APPLICATIONS: Photo-luminescence ■ Raman and/or fluorescence measurement and mapping
KEY FEATURES: Empowers an upright microscope with laser induced luminescence micro-spectroscopy functionalities ■ Mapping at high spatial resolution down to (less than) 1 μm measuring spot ■ Allows user concurrent imaging such as fluorescence, DIC, polarisation dark field and bright field without moving the samples

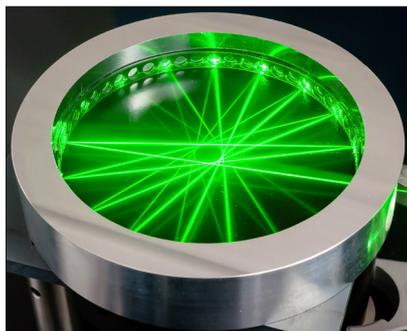


NEW PRODUCTS

INFRARED

New multipass gas cell design

IRsweep's IRcell is a multipass cell for optical trace gas sensing. It consists of a single, circular mirror on the wall of the cell, which makes the cell less affected



The optical path in IRsweep's IRcell multipass gas cell.

by mechanical stresses such as vibration or temperature changes. It also enables a compact setup: a 4 m pathlength can be achieved in a volume of 30 mL. The IRcell is targeted at applications requiring an optical pathlength between 1 m and 5 m.

IRsweep

▶ link.spectroscopyeurope.com/28-02-150

IMAGING

Data processing for airborne imaging

The Hypercore has been designed for UAV airborne applications and weighs 0.64 kg, measures about 89 × 76 × 76 mm and stores 500 GB of data. It has two Gigabit Ethernet connections, one base CameraLink connection and a multipurpose I/O port to handle GPS/INS, sensor commands etc. Depending on the instruments being connected, the necessary Hyperspec III software modules are included to provide an operational platform. It has been designed to work with Headwall's Hyperspec family of sensors, as well as other vendors.

Headwall Photonics

▶ link.spectroscopyeurope.com/28-02-151

MASS SPEC

Proteins and peptides analysis system

Advion have introduced the 'Tides Express proteins and peptides analysis system. It combines Advion's HPLC system and the extended mass range ExpressionL compact mass spectrometer. It will help chemists performing peptide synthesis and needing fast mass analysis of each reaction step and final product. It will also find use in solid-phase peptide synthesis, which allows for rapid, parallel synthesis of peptides of various amino acid lengths. Rapid analysis of each reaction step can prevent a sub-optimal synthesis cycle from causing re-runs. Additional fragmentation analysis and charge deconvolution tools enhance its use for protein characterisation.

Advion

▶ link.spectroscopyeurope.com/28-02-152

PHOTONICS

Single frequency laser diode for oxygen detection

The RWS-760 single frequency laser diode from Eagleyard is suited to gas spectroscopy detection of oxygen. It is available in 760 nm or 764 nm wavelengths and has an output power up to 40 mW. Linewidth is <0.1 ppm and it is available in a 5.6-mm and 9-mm TO housings.

Eagleyard Photonics

▶ link.spectroscopyeurope.com/28-02-153

MISCELLANEOUS

New family of high vacuum systems

Oerlikon Leybold Vacuum has introduced the Turbolab family of plug-and-play high vacuum pump systems. They are based

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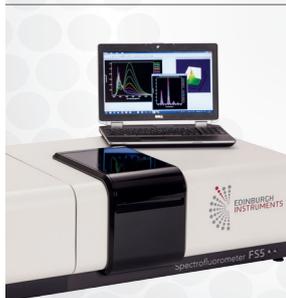


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on one basic design platform which can be supplied in several different variants covering the vacuum demands of applications throughout the R&D and analytical markets. Hydrocarbon-free pump operation is provided by the oil-free hybrid bearing design of the Turbovac i/iX turbo pumps and by using different dry compressing backing pump combinations.

Oerlikon Leybold Vacuum

▶ link.spectroscopyeurope.com/28-02-154

Ease, replacing the previous Design of Experiments (DOE) module. New methods include Moving Block Methods and Statistical Process Control for trending of process data, Piecewise Direct Standardisation for calibration transfer, improved plotting tools, a number of changes to PCA/PCR/PLSR analysis dialogues and more flexible usage of outlier statistics.

Camo

▶ link.spectroscopyeurope.com/28-02-155

spectrometer with improved functionality and performance. It includes "ZSX Guidance" software and error prevention functionality to help novice users. The tube-above configuration enables samples to be analysed without the use of protective film, due to spills not affecting the optical system, avoiding intensity reduction from the film. Light element sensitivity is boosted by the system's auto pressure control, which regulates and stabilises the vacuum conditions. During analysis, regions of interest can be located in enlarged images of the sample taken with a high-resolution camera. The r-θ sample stage can be accurately positioned to facilitate measurements with uniform sensitivity on these small areas.

Rigaku

▶ link.spectroscopyeurope.com/28-02-156

SOFTWARE

New version of Unscrambler X

Version 10.4 of the Unscrambler X now includes Design-Expert from Stat-

X-RAY

Tube-above sequential WD XRF spectrometer

Rigaku's ZSX Primus IV is a tube-above, wavelength dispersive X-ray fluorescence

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Conferences 2016

2–6 May, Lille, France. **European Materials Research Society (E-MRS) 2016 Spring Meeting.** ✉ <http://www.european-mrs.com/meetings/2016-spring-meeting>.

8–11 May, Bagnols-sur-Cèze, France. **EMAS 2016. 12th Regional Workshop on Electron Probe Microanalysis of Materials Today—Practical Aspects.** ✉ luc.vantdack@uantwerpen.be, ✉ <http://www.microbeamanalysis.eu/events>.

9–13 May, Mendoza, Argentina. **International Meeting on Photodynamics and Related Aspects.** ✉ <http://photodynamics9.wix.com/phd9#program/cfcg>.

10–11 May, Monheim, Germany. **Young Investigators in Lipid Science meeting.** ✉ <http://www.dgfett.de/meetings/aktuell/duesseldorf2016/#ort>.

13–14 May, Tokyo, Japan. **16th Symposium on Molecular Spectroscopy.** ✉ <http://regulus.mtr1.info.hiroshima-cu.ac.jp/~sms2016/en/e-index.html>.

14–17 May, Zlatni Pyasatsi, Bulgaria. **Developments and Applications of Solid State NMR to Materials Science, Chemistry and Engineering.** ✉ <http://www.zingconferences.com/conferences/solid-state-nmr>.

18–20 May, Lisbon, Portugal. **CEM 2016.** ✉ <http://www.cem.uk.com>.

19–20 May, Berlin, Germany. **4th International Conference on Advanced Applied Raman Spectroscopy (RamanFest 2016).** ✉ <http://ramanfest.org>.

23–25 May, Ormylia, Chalkidiki, Greece. **12th Biennial International Conference of the Infrared and Raman Users Group (IRUG12).** ✉ s.sotiropoulou@artdiagnosis.gr, ✉ <http://www.irug.org>.

25–28 May, Antalya, Turkey. **3rd International Conference on New Trends in Chemometrics and Applications (NTCA 2016).** Dr. Remziye Güzel, ✉ chemometrics@ankara.edu.tr, ✉ <http://ntca.ankara.edu.tr>.

5–9 June, San Antonio, Texas, USA. **64th ASMS Conference on Mass Spectrometry.** ✉ office@asms.org, ✉ <http://www.asms.org>.

5–8 June, Loen, Norway. **8th Nordic Conference on Plasma Spectrochemistry.** ✉ yngvar.thomassen@starni.no, ✉ <http://www.nordicplasma.com>.

6–10 June, Berlin, Germany. **7th International Conference on Spectroscopic Ellipsometry (ICSE-7).** ✉ <http://www.icse-7.de>.

6–10 June, Barcelona, Spain. **XVI Chemometrics in Analytical Chemistry.** ✉ rtagam@idaea.csic.es, ✉ <http://www.cacbarcelona.com>.

7–10 June, Karlsruhe, Germany. **13th International Conference on the Applications of Magnetic Resonance in**

Food Science. Leo Nick, Conference Bureau, Forschungs-Gesellschaft Verfahrens-Technik e.V. Theodor-Heuss-Allee 25, D-60486 Frankfurt am Main, Germany, ✉ mrfood@gvt.org, ✉ <https://mrfood2016.gvt.org>.

8 June, Edinburgh, UK. **Photonex Scotland Photonics Technology Roadshow.** ✉ <http://www.photonex.org/scotland/16/index.html>.

9–15 June, Novosibirsk, Russia. **12th International GeoRaman Conference.** ✉ georaman2016@gmail.com, ✉ <http://georaman2016.igm.nsc.ru>.

12–15 June, Todi, Italy. **Use of Multivariate Analysis and Chemometrics in Cultural Heritage and Environment (CMA4CH).** ✉ <http://www.cma4ch.org/index2.html>.

15–16 June, Graz, Austria. **chii2016: Conference on Hyperspectral Imaging in Industry.** ✉ <http://www.chii2016.com>.

19–24 June, Andover, New Hampshire, USA. **Gordon Research Conference on Multiphoton Processes.** ✉ <http://www.grc.org/programs.aspx?id=11703>.

19–24 June, Gothenburg, Sweden. **European Conference on X-Ray Spectrometry (EXRS2016).** EXRS2016, Sweden MEETX AB, SE-412 94 Gothenburg, Sweden, ✉ exrs2016@meetx.se, ✉ <http://www.exrs2016.se>.

19–24 June, Ludwigsburg, Germany. **Spectroscopies in Novel Superconductors (SNS 2016).** ✉ <http://www.fkf.mpg.de/SNS2016>.

19–24 June, Torun, Poland. **23rd International Conference on Spectral Line Shapes.** ✉ icls23@fizyka.umk.pl, ✉ <http://icls23.fizyka.umk.pl>.

20–24 June, Champaign-Urbana, Illinois, USA. **71st International Symposium on Molecular Spectroscopy.** Birgit D. McCall, International Symposium on Molecular Spectroscopy, University of Illinois, 306B Noyes Laboratory, 505 South Mathews Avenue, Urbana, IL 61801, USA. ✉ birgit@isms.illinois.edu, ✉ <http://isms.illinois.edu>.

26–30 June, Montreal, Canada. **SPEC 2016.** ✉ <http://www.spec2016.com>.

26–29 June, Inuyama, Japan. **7th International Workshop on Plasma Spectroscopy, IPS 2016.** ✉ ips2016@plasma.engg.nagoya-u.ac.jp, ✉ <http://www.ips2016inuyama.com>.

29 June–1 July, Groningen, The Netherlands. **8th International Conference on Coherent Multidimensional Spectroscopy (CMDS 2016).** ✉ <http://www.cmids2016.org>.

3–7 July, Aarhus, Denmark. **EUROMAR 2016.** Prof. Thomas Vosegaard, Interdisciplinary Nanoscience Center and Department of Chemistry, Aarhus University, Denmark, ✉ tv@chem.au.dk, ✉ <http://euromar2016.org>.

3–6 July, Chamonix Mont-Blanc, France. **6th International Conference of the**

International Association for Spectral Imaging (IASIM 2016). ✉ <http://iasim16.sciencesconf.org>.

3–9 July, Dubrovnik, Croatia. **Mass Spectrometry in Biotechnology and Medicine (MSBM) Summer School.** ✉ msbm.dubrovnik@gmail.com, ✉ <http://www.msbm.org>.

4–6 July, Liverpool, UK. **18th Biennial National Atomic Spectroscopy Symposium (18th BNASS).** ✉ <http://www.rsc.org/events/detail/19910>.

10–14 July, Stony Brook, New York, USA. **14th International Conference on Surface X-ray and Neutron Scattering (SXNS14).** Gretchen Cisco, ✉ sxns14@bnl.gov, ✉ <http://www.bnl.gov/sxns14>.

16–17 July, Biddeford, Maine, USA. **Gordon Research Seminar on Vibrational Spectroscopy.** ✉ <http://www.grc.org/programs.aspx?id=16690>.

17–22 July, Biddeford, Maine, USA. **Gordon Research Conference on Vibrational Spectroscopy.** ✉ <http://www.grc.org/programs.aspx?id=12221>.

17–22 July, Breckenridge, Colorado, USA. **58th Annual Rocky Mountain Conference on Magnetic Resonance.** ✉ <http://www.rockychem.com>.

17–22 July, Santa Fe, New Mexico, USA. **OSA Topical Meeting: International Conference on Ultrafast Phenomena.** ✉ http://www.osa.org/en-us/meetings/topical_meetings/international_conference_on_ultrafast_phenomena.

18–22 July, Mauritius. **International Conference on Pure and Applied Chemistry (ICPAC 2016).** ✉ icpacmru@gmail.com, ✉ <http://sites.uom.ac.mu/icpac2016>.

19–21 July, Hamburg, Germany. **9th International Symposium on Environmental Analytical Chemistry (ISEAC39).** Prof. Dr. Jose Broekaert, University of Hamburg, Institut für Anorganische und Angewandte Chemie, Lehrstuhl für Analytische Chemie heterogener Systeme, Martin-Luther-King Platz 6, 20146 Hamburg, Germany. ✉ jose.broekaert@chemie.uni8hamburg.de, ✉ <http://www.iaec.com>.

24–27 July, Heidelberg, Germany. **28th International Symposium on Chiral Discrimination (Chirality 2016).** Prof. Dr. Oliver Trapp, Heidelberg University, Im Neuenheimer Feld 270, 69120 Heidelberg, Germany, ✉ info@chirality2016.com, ✉ <http://www.chirality2016.com>.

25–27 July, Glasgow, UK. **BSPR 2016: Proteomic Approaches to Health and Disease.** Karl Burgess, ✉ karl.burgess@glasgow.ac.uk, ✉ <http://www.bspr.org/node/527>.

25–28 July, Heidelberg, Germany. **OSA Optics and Photonics Congress: Imaging and Applied Optics.** ✉ http://www.osa.org/en-us/meetings/optics_and_photonics_congresses/imaging_and_applied_optics.

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30 July–4 August, Szeged, Hungary. **33rd European Congress on Molecular Spectroscopy**. EUCMOS 2016 Secretariat, c/o Hungarian Chemical Society, Panna Korispataky, H-1015 Budapest, Hattyú u. 16. II/8, Hungary, ✉ eucomos2016@mke.org.hu, ☞ <http://eucomos2016.mke.org.hu>.

30 July–5 August, Chambersburg, Pennsylvania, USA. **18th International Diffuse Reflectance Conference (IDRC 2016)**. ☞ <http://www.idrc-chambersburg.org>.

1–5 August, Rosemont, Illinois, USA. **65th Annual Denver X-ray Conference (2016 DXC)**. ☞ <http://www.dxcicdd.com>.

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

14–19 August, Fortaleza, Brazil. **25th International Conference on Raman Spectroscopy (ICORS 2016)**. ☞ <http://www.icors2016.org>.

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

20–26 August, Toronto, Canada. **21st International Mass Spectrometry Conference**. ✉ contact@imsc2016.ca, ☞ <http://www.imsc2016.ca>.

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

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

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

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

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

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

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

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

31 August–2 September, Edinburgh, UK. **Ultra Fast Imaging of Photochemical Dynamics**. ☞ <http://www.rsc.org/events/detail/19765>.

4–8 September, Torino, Italy. **10th Conference of the European Federation of EPR Groups (EFEPR)**. ✉ efep2016@unito.it, ☞ <http://www.efep2016.unito.it>.

4–9 September, Bayreuth, Germany. **54th European High Pressure Research Group International Meeting (EHPRG 2016)**. ☞ <http://www.ehprg2016.org>.

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

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

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

11–14 September, Dresden, Germany. **20th European Symposium on Polymer Spectroscopy**. ☞ <http://www.ipfdd.de/ESOPS20>.

11–14 September, La Jolla, California, USA. **SMASH 2016: Small Molecule NMR Conference**. ☞ <http://www.smashnmr.org>.

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

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

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

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

18–23 September, Santa Fe, New Mexico, USA. **2016 SciX Conference (formerly FACSS)**. ✉ facss@facss.org, ☞ <http://www.facss.org>.

18–21 September, Dallas, Texas, USA. **130th AOAC International Meeting and Exposition**. ☞ <http://www.aoac.org>.

19–22 September, Warsaw, Poland. **European Materials Research Society (E-MRS) 2016 Fall Meeting**. Marek Godlewski, Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46 02-668, Warszawa, Poland, ✉ godlew@ifpan.edu.pl, ☞ <http://www.european-mrs.com/meetings/2016-fall>.

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

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

Courses 2016

13–16 June, Todi, Italy. **Multivariate Analysis Course, School for Novices**. ☞ <http://www.cma4ch.org/frames-cou.html>.

13–17 June, Warwick, UK. **Interpretation of Infrared and Raman Spectra**. James A. de Haseth, IR Courses, Inc. 165 Sunnybrook Drive, Athens, Georgia 30605-3347, USA, ✉ dehaseth@ircourses.org, ☞ <http://www.ircourses.org/schedUK.html>.

16–17 June, Milton Keynes, UK. **2-day The GC & GC-MS Clinic**. ☞ <http://www.anthias.co.uk/training-courses/GC-clinic>.

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

Exhibitions 2016

10–13 May, Munich, Germany. **Analytica 2016**. ☞ <http://www.analytica.de>.

1–2 June, Basel, Switzerland. **Chemspec Europe 2016**. ☞ <http://www.chemspec-europe.com>.

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

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