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Sampling Column: 800 years old PAT?

Tony Davies: Life and death of a data set

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Spectroscopy Europe is a digital magazine, published eight times a year and available free-of-charge to qualifying individuals in Europe and the Middle East.

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EDITORIAL

This issue starts with an enlarged News section, once again showing the breadth of application and value of spectroscopy to the world we live in. From the use of mass spectrometry for quality control of mRNA medications, through single-atom vibrational spectroscopy sensitive at the level of chemical bonds, a new technology for capturing hyperspectral images, a new Raman microscopy method with high-throughput hundreds of times faster than the traditional approach to new developments in proton transfer reaction mass spectrometry. I hope you find it interesting and inspiring.

In the Tony Davies Column, Tony considers the "Life and death of a data set: a forensic investigation". Over time, spectral data will become increasingly fragmented and lose important supporting information. Computer and software upgrades, and processing in chemometric programs can all cause this. Of course, the answer is to follow FAIR principles and ensure that they are implemented in the analytical laboratory. The recent publication of "FAIR principles for Scientific Software (FAIR4RS)" at the end of 2022 cites three software examples claiming to follow the FAIR4RS principles which could be worth following should you be interested.

Kim Esbensen's Sampling Column often uses interesting examples of the correct use of representative sampling. In this issue, you will also learn something of the history of Danish medieval stone churches in northern and western Jutland! "Danish geology icon Arne Noe-Nygaard picks up on an 800 years old sampling and invents the Replication Experiment: PAT in disguise" is firmly rooted in the Theory of Sampling but you will also learn some geology and history!

The issue concludes with Applications, a Product Focus on Imaging Spectroscopy, New Products, the Diary of future events and Directory of companies who are supporting our publication.

NEWS

Mass spectrometry for quality control of mRNA medications

A new analytical platform based on liquid chromatography, mass spectrometry and software analysis quantifies the structure of messenger RNA (mRNA) based medicines.

Researchers from Tokyo Metropolitan University and RIKEN CSRS have developed a new analytical platform based on liquid chromatography, mass spectrometry and software analysis that quantifies the structure of messenger RNA (mRNA) based medicines. They can elucidate mRNA sequences while quantifying "capping" at one end of the molecule and the integrity of the tail on the other, all vital in mRNA pharmaceuticals. The method is a crucial innovation for quality control in production lines.

Messenger RNA (mRNA) is a vital molecule responsible for transmitting the sequence information stored in our DNA to ribosomes, the protein-making machinery of our cells. However, the mRNA does not necessarily have to come from our DNA; by artificially designing mRNA molecules, we can use it as a drug which enables our cells to produce specific protein structures, like antigens which can trigger an immune response and act as a vaccine. mRNA medicines burst into the public consciousness as the primary component of the most effective COVID-19 vaccines. They have many advantages over competing technologies: they are considered much safer, as they do not integrate into the host cell genome; they are relatively easy to manufacture and scale up. Now, the technology is said to hold promise for treating a wide range of other illnesses, including cancer and metabolic diseases.
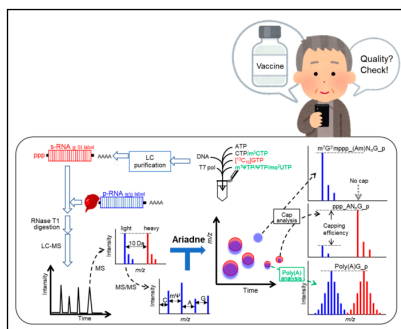
A mRNA molecule (p-RNA) is mixed with a standard (s-RNA) labelled with stable isotopes (SI) before being digested then characterised using a combination of liquid chromatography and mass spectrometry (LC-MS). The output is analysed using Ariadne software to yield information on the sequence, the state of the "cap" and the length of the tail. This yields vital information on the quality of the mRNA medicine. Credit: Tokyo Metropolitan University

But with the wide deployment of this new technology, methods are now needed to perform quality control in a more effective, efficient way. mRNA medicines have three key components: the sequence, which determines what proteins are synthesised; the 5'-capping, which ensures that the mRNA is read efficiently during protein translation; the poly(A) tail, which dampens the immune response against the foreign mRNA itself. All three need to be in good working order for the treatment to be effective. However, there is currently no method that can quantify the state of all three in one go.

Now, a team led by Drs Masato Taoka of Tokyo Metropolitan University and Hiroshi Nakayama of RIKEN CSRS have developed an analytical platform combining liquid chromatography, mass spectrometry and automated software analysis to quantitatively monitor the properties of mRNA molecules and published their work in *Analytical Chemistry* ([doi. org/grr376](doi.org/grr376)). The team's platform combines two important innovations. First, using liquid chromatography and mass spectrometry, they undertake a systematic comparison of different fragments of a mRNA molecule to be tested with a similarly fragmented reference mRNA labelled with a stable carbon isotope. Second, automated analysis using Ariadne software helps ascertain structures with the help of a sequence database. The team found that their analysis platform could successfully assign the primary structure of the reference, then rapidly identify even the most minute changes in the mRNA molecule being tested, all while yielding quantitative information on the capping and tail group.

The method is applicable to a wide range of mRNA lengths and sequences from completely different origins, allowing all three parts to be analysed in one go. It promises unparalleled efficiency in checking for the quality of mRNA medicines, both those in action now and yet to be developed.

NEWS

New MS technique detects protein–metabolite interactions

MIDAS helps improve the discovery and characterisation of elusive interactions between proteins and metabolites.

To help improve the discovery and characterisation of elusive interactions between proteins and metabolites, researchers have developed MIDAS (Mass spectrometry Integrated with equilibrium Dialysis for the discovery of Allostery Systematically). According to the authors of the paper in *Science* (https://www.science.org/doi/10.1126/science.abm3452), MIDAS represents a powerful new tool to "identify, understand and exploit previously unknown modes of metabolic regulation across the protein-metabolite interactome". The interactions between proteins and small-molecule metabolites

are among the most common and fundamental types of biological interaction and play vital roles in regulating protein functions and controlling diverse cellular processes. However, the discovery and characterisation of protein–metabolite interactions (PMIs) has been sporadic and challenging. To address this, Kevin Hicks and colleagues developed the MIDAS platform, which enables the systematic discovery of elusive PMIs. Using MIDAS, they analysed the interactions for 33 enzymes from human carbohydrate metabolism and 401 metabolites, which revealed 830 PMIs. Although

MIDAS identified PMIs with previously known regulators, substrates and products, the approach also allowed the authors to uncover many previously unknown PMIs from diverse metabolic pathways, including regulation of lactate dehydrogenase by ATP and long-chain acyl coenzyme A. According to the authors, this finding could be a mechanism underlying the unexpected physiological relationship between fat and carbohydrate metabolism in different tissues and could be exploited therapeutically to block aerobic glycolysis in cancers.

Upconversion time-stretch infrared spectroscopy

This ultrafast infrared spectroscopy method would fulfil many unmet needs in experimental molecular science, revealing various high-speed phenomena in detail.

Infrared spectroscopy is usually only applied for static samples because spectral data acquisition is a slow process. Detecting fast-changing phenomena requires multiple quick measurements. Thanks to Prof. Ideguchi and his team at the University of Tokyo, it is now possible to obtain high-speed and high-resolution spectral data. The team discovered upconversion time-stretch infrared spectroscopy (UC-TSIR) which can measure infrared spectra with 1000 spectral elements at a rate of 10 million spectra per second.

"With recent improvements in the capability of analysing spectra using machine learning and other techniques, it is essential for infrared spectroscopy methods to acquire a large amount of molecular vibration
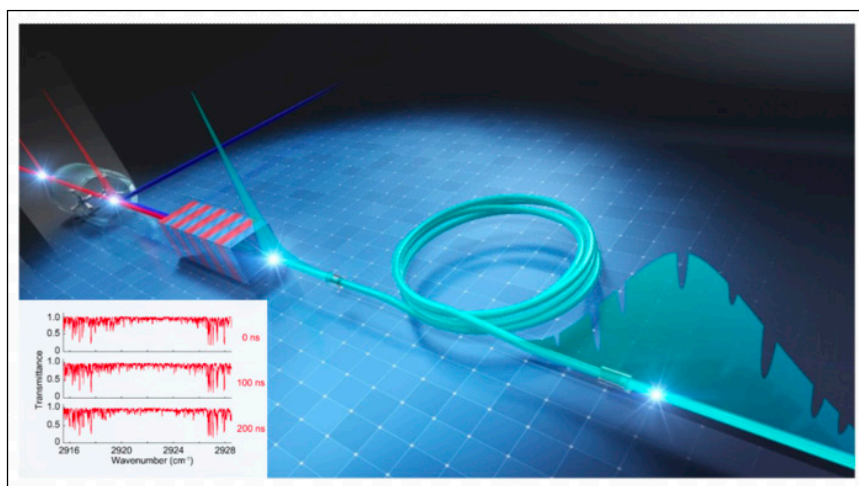
First, the sample is illuminated with infrared light. After the light interacts with the sample, the resulting wavelengths are "upconverted" from low-energy infrared to high-energy near infrared wavelength. The near infrared pulses then travel through an optical fibre which essentially "stretches" the pulse in time. A near infrared photodetector detects the pulses. The inset in the bottom-left corner shows the transmittance spectra of gaseous CH_4 molecules at three consecutive time points. Credit: Hashimoto *et al.* 2023

information rapidly. We wanted to develop the infrared spectroscopy method to achieve that", said Prof. Ideguchi, explaining the motivation of the research team.

Conventional time-stretch infrared spectroscopy data has fewer measurable spectral elements (~30) because the instruments work in the infrared region, where optical technology is currently limited. "UC-TSIR breaks the limit by converting infrared pulses containing molecular vibration information into near infrared pulses with wavelength conversion techniques (upconversion) and temporally

stretching and detecting the pulses in the near infrared region", said Dr Hashimoto. Compared to conventional methods, UC-TSIR provides over 30-fold more spectral elements and 400 times better spectral resolution. The UC-TSIR can trace high-speed phenomena such as the combustion of gaseous molecules and irreversible chemical reactions of biomolecules at a high temporal resolution. The work is published in *Light Science & Applications* ([doi.org/grv9fg](doi.org/grv9fg)).

In theory, the concept sounds simple and easy to implement; but it was far from that. "We carefully

selected optical elements and adjusted the parameters through trial and error. Even after building the setup, we dealt with various spectral distortions caused by unwanted non-linear optical effects and insufficient time stretching. We were overjoyed when we finally saw clear infrared absorption spectra after dealing with those issues", said Dr Hashimoto. "Nanosecond- or microsecond-scale ultra-fast continuous infrared spectral measurements by UC-TSIR can solve problems unresolved by conventional spectroscopy methods."

Chip-scale spectrometry using a photonic molecule

A new method overcomes the resolution-bandwidth limit in chip-scale spectrometry. The proposed scheme is based on a pair of identical tuneable micro-ring resonators.

Optical spectrometers play an indispensable role in many scientific and industrial applications, such as material analysis, biological sensing, optical tomography and hyperspectral imaging. Conventional benchtop spectrometers are susceptible to mechanical vibrations and are ill-suited for field deployment outside the laboratory. Integrated spectrometers, which are built with all-solid-state photonic integrated circuits, have advantages of small size, robustness to vibrations and potentially low cost. Nevertheless, most of the reported integrated spectrometers suffer from an inherent trade-off between spectral resolution and operation bandwidth. High spectral resolution requires long optical path length to
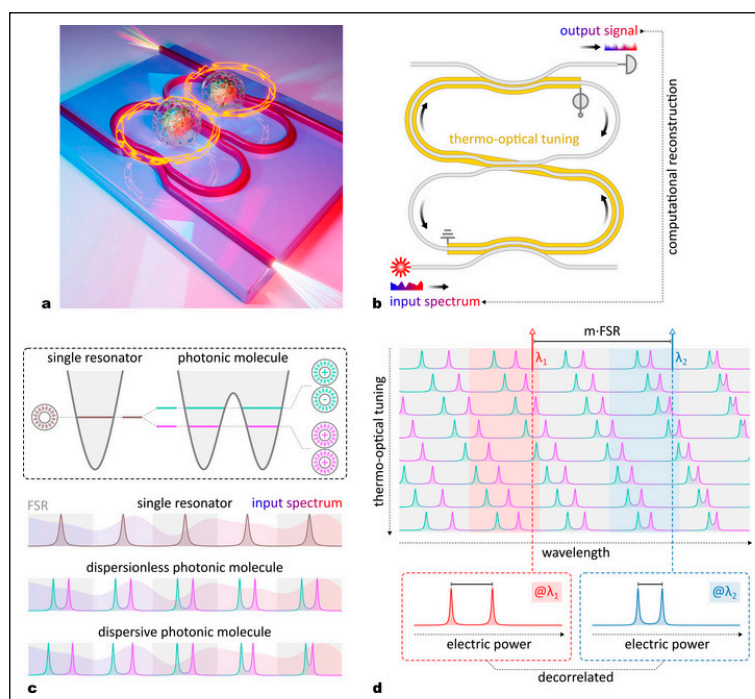
Concept of the photonic-molecule spectrometer. a Artist's view of the integrated spectrometer using a dispersion-engineered photonic molecule. b The structure consists of two identical tuneable micro-ring resonators. The unknown input spectrum is scanned via thermo-optical tuning to generate an output signal. The goal is to restore the spectral information from the signal with a calibrated transmission matrix. c For a single resonator, the information at different free-spectral ranges (FSR) are indistinguishable. If a pair of resonators are strongly coupled, then each resonance will split into a symmetric mode and an anti-symmetric mode, which resembles a two-level molecule. Furthermore, the splitting strength is proportional to the coupling strength between resonators. Consequently, by tailoring the dispersion, the splitting strength will vary over multiple FSRs. d For two wavelengths spaced by a integral multiple of FSRs ($\lambda_2 = \lambda_1 + m \cdot FSR$), their power scanning traces can be identified from the distinct peak spacing induced by the dispersive mode splitting. In this way, all wavelength channels are decorrelated, making it possible to reconstruct the spectrum beyond the FSR limit. Credit: Hongnan Xu, Yue Qin, Gaolei Hu and Hon Ki Tssang

Introduction to the Theory and Practice of Sampling

Kim H. Esbensen

with contributions from Claas Wagner, Pentti Minkkinen, Claudia Paoletti, Karin Engström, Martin Lischka and Jørgen Riis Pedersen

"Sampling is not gambling". Analytical results forming the basis for decision making in science, technology, industry and society must be relevant, valid and reliable. However, analytical results cannot be detached from the specific conditions under which they originated. Sampling comes to the fore as a critical success factor before analysis, which should only be made on documented representative samples. There is a complex and challenging pathway from heterogeneous materials in "lots" such as satchels, bags, drums, vessels, truck loads, railroad cars, shiploads, stockpiles (in the kg–ton range) to the miniscule laboratory aliquot (in the g–µg range), which is what is actually analysed.

This book presents the Theory and Practice of Sampling (TOS) starting from level zero in a novel didactic framework without excessive mathematics and statistics. The book covers sampling from stationary lots, from moving, dynamic lots (process sampling) and has a vital focus on sampling in the analytical laboratory.

"I recommend this book to all newcomers to TOS"

"This book may well end up being the standard introduction sourcebook for representative sampling."

"One of the book's major advantages is the lavish use of carefully designed didactic diagrams"
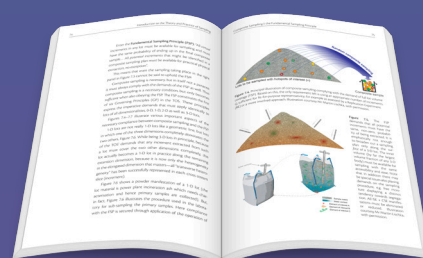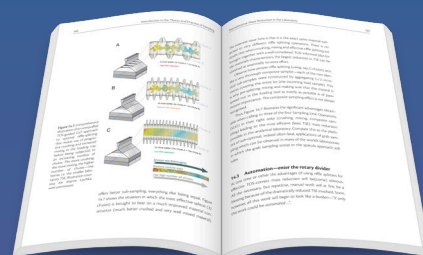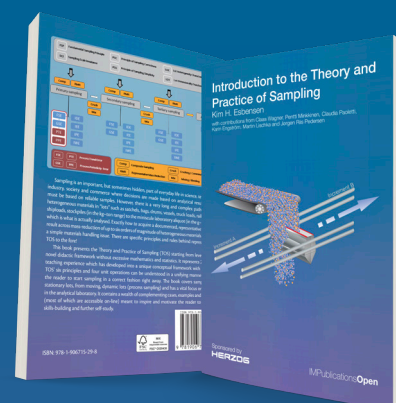
impopen.com/sampling

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support sufficient spectral decorrelation, which results in a smaller free-spectral range (FSR).

A team of scientists, led by Professor Hon Ki Tsang from the Department of Electronic Engineering, the Chinese University of Hong Kong, have developed a ground-breaking method that overcomes the resolution-bandwidth limit in chip-scale spectrometry; results are published in *Light Science & Applications* (doi.org/grwfg5). The proposed scheme is based on a pair of identical tuneable micro-ring resonators (MRR), in which the strong inter-cavity coupling splits each resonant mode into a symmetric mode and an anti-symmetric mode. This unique behaviour resembles the energy-level splitting in a two-level molecule that consists of two atoms.

Interestingly, the mode-splitting strength is proportional to the coupling strength. As such, by engineering the dispersion of the "photonic molecule", the splitting strength will vary throughout the whole bandwidth containing multiple FSRs. When simultaneously tuning two MRRs, each wavelength channel will produce a distinct scanning trace, making it possible to reconstruct any unknown input spectrum.

In the experiment, numerous test spectra with diverse complex features are retrieved using the photonic-molecule scheme. The demonstrated spectral resolution is 40 pm throughout a bandwidth of 100 nm. Remarkably, high reconstruction precision can be maintained even with the presence of thermal noises.

"Our spectrometer is a novel approach to capture a broadband spectrum with high spectral resolution. It relies solely on a pair of coupled resonators. The device has very low power consumption and is compatible with the mainstream nanophotonic fabrication technology."

"The spectrometer is based on the mode splitting in coupled resonators. This phenomenon is analogous to the energy level splitting in a molecule with two atoms. Our design features a simple configuration and a small size, so that it can be densely packed with other devices. We believe that this approach has the potential to be applied in future handheld or even wearable spectroscopic sensors."

SERS enhances arsenic detection in water, food and soil

A new sensor can identify the global content and form of arsenic-containing molecules at very low concentrations.

One of the main culprits for the pollution of potable and natural water sources is arsenic, an abundant and toxic element in the earth's crust. Arsenic is currently known as the cause of ground-water contamination in more than 100 countries—and can produce life-threatening diseases, especially for populations in developing countries. Such circumstances necessitate efficient and reliable arsenic detection methods for water, food and soil. A team of French scientists have used surface-enhanced Raman spectroscopy (SERS) to detect arsenic, even at very low concentrations; results are published in *Journal of Applied Physics* (doi.org/grtc3d).

"Arsenic exists in water in different forms, so it is important to be able to quantify the species, in addition to the global content", said author Dominique Vouagner.
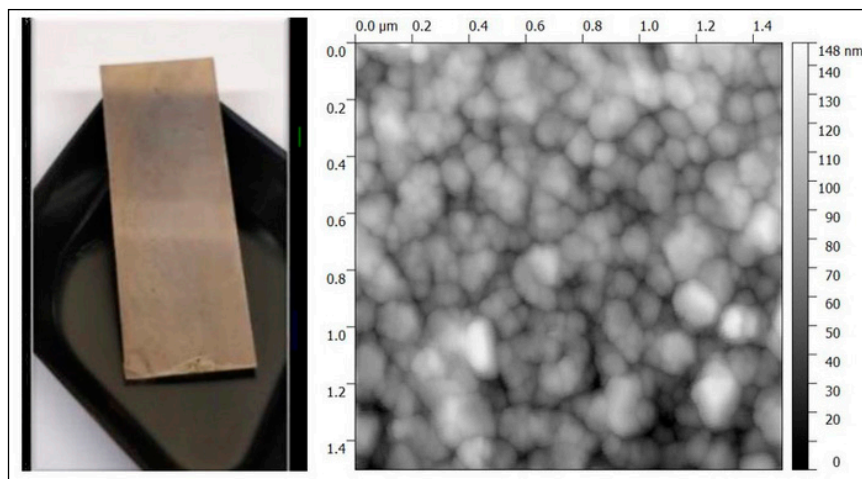
Left: a sample of a silver nanostructured film, deposited by the electroless technique on a glass plate with dimensions 2.5 × 7.5 cm. Right: a zoom in on the silver nanostructured electroless film at 1.5 μm × 1.5 μm by atomic force microscopy. Credit: Dominique Vouagner

"By using SERS, we can detect and speciate pollutants even at the lowest concentration. This includes arsenic, which should not exceed 10 ppb, as per the World Health Organization's recommendations."

The team compared the detection and speciation performances

of two SERS substrates. One was prepared by conventional thermal evaporation, where material is heated until it vaporises. The other was created with an electroless process, in which a coating is deposited on a material by submerging it in a liquid and instigating a chemical reaction. The latter was revealed to be much more sensitive and is relatively easy and safe to produce, according to Vouagner.

"Our technique for developing this SERS substrate makes it simple to manufacture because the electroless films can be easily deposited on various substrates", she said. "Plus, the starting compounds have low environmental toxicity, which is a benefit for detection measurements in natural as well as potable water."

The technique is a departure from existing reference methods for trace arsenic speciation, which are time-consuming and expensive. Conventional methods also require sample pre-treatment in a lab, so they are not ideally suited to on-site field assays. Additionally, the new method employs the use of a solid substrate, which enables optical interrogation.

"Because they're less 'noisy', optical detection systems are much more sensitive than electronic systems", said author Bernard Dussardier. "At the same time, they're less sensitive to parasitic electromagnetic fields. Also, the SERS technique allows direct physical-chemical property measurements, whereas electronic systems, and some other optical systems, are indirect." ⤴

Single-atom vibrational spectroscopy now sensitive at level of chemical bonds

Researchers have pushed the sensitivity of single-atom vibrational spectroscopy to the chemical-bonding-configuration extreme, which is critical for understanding the correlation of lattice vibrational properties with local atomic configurations in materials.

Researchers led by Professor ZHOU Wu from the University of Chinese Academy of Sciences (UCAS) and Professor Sokrates T. Pantelides of Vanderbilt University have pushed the sensitivity of single-atom vibrational spectroscopy to the chemical-bonding-configuration extreme, which is critical for understanding the correlation of lattice vibrational properties with local atomic configurations in materials.

Using a combination of experimental and theoretical approaches, the researchers demonstrated the effect of chemical-bonding configurations and the atomic mass of impurity atoms on local vibrational properties at the single-atom level.

In this study, published in *Nature Materials* (doi.org/grx8ng), the researchers investigated the atomic vibrations of two types of silicon (Si) point defects in monolayer graphene: the Si-C_3 defect, which arises from the substitution of one carbon (C) atom by a Si atom and forms an atomic defect with three bonds with nearest-neighbouring C atoms; and the Si-C_4 defect,
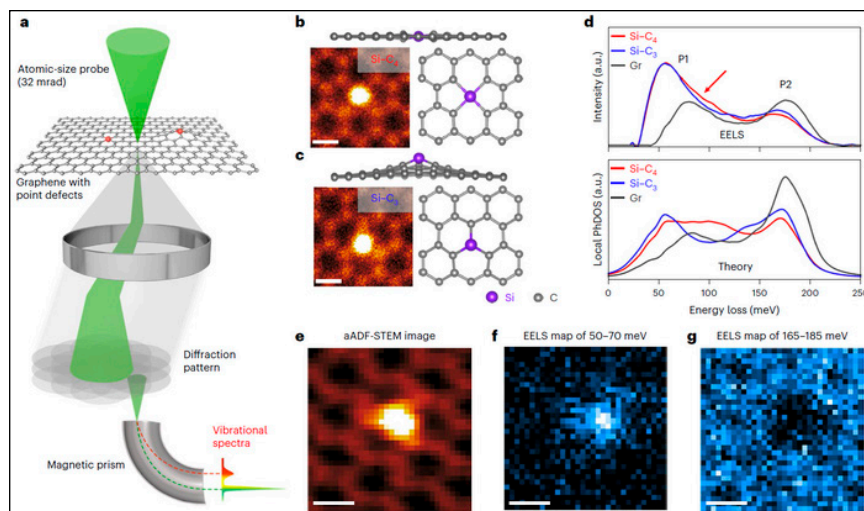
Vibrational spectroscopy of substitutional Si impurities in graphene with different bonding configurations. Credit: UCAS

which forms when two C atoms are substituted by one Si atom and results in a defect with four bonds.

The Si-C_4 defect produced stronger vibrational signals than the Si-C_3 defect in the energy-loss region around 100 meV, suggesting unique vibrational modes for the two defect configurations of the same impurity, according to the researchers. To examine the extended effect of the two defects, the researchers performed an atom-by-atom analysis focusing on the carbon atoms surrounding the impurities and found that the defects only have a pronounced effect on the nearest neighbouring carbon atoms. The next closest neighbouring carbon atoms behave

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almost like typical carbon atoms in graphene.

Remarkably, the researchers found different frequency shifts of the low-energy phonon peak for the nearest neighbouring carbon atoms in these two types of Si point defects with different bonding configurations. Complementing this discovery with density-functional-theory calculations, the researchers showed that the different vibrational signals of Si and the nearest neighbouring C atoms result from the unique vibrational modes of the two defects, which are primarily dominated by local configurational symmetry.

They also studied another defect with a much lower mass—nitrogen (N) in the form of $N-C_3$. In contrast to $Si-C_3$, the vibrational variation is mainly reflected in the high-frequency peak, which accounts for most of the optical phonon modes. The nearest neighbour extension persists.

This experimental progress was made possible by considerable efforts by the UCAS team to improve the stability of their monochromated scanning transmission electron microscope (STEM) and the sensitivity of the monochromated electron energy-loss spectroscopy (EELS) measurement. This work has pushed the sensitivity of single-atom vibrational spectroscopy in STEM to the level of chemical bonds and made precise measurements of the vibrational properties of point defects in graphene, providing insights into the defect-induced physics in two-dimensional materials. ⌇

New technology for capturing hyperspectral images patented

The new design uses dual-comb spectroscopy.

The Universidad Carlos III de Madrid (UC3M) has patented a new system for capturing hyperspectral images, which can operate in real time and provides a higher resolution than any other existing technology. This development could mean a breakthrough for scientific and industrial applications related to chemical analysis.

This system, patented by UC3M's Sensors and Instrumentation Techniques group, is made up of a light source that transforms a normal camera into a hyperspectral camera. This technology makes it possible to obtain complete characterisations of the chemical composition of the sample being analysed, by measuring the optical absorptions or molecular resonances that are characteristic of each compound. To do this, an advanced analytical technique known as dual-comb spectroscopy is used.

Dual-comb systems work by interfering light from two optical sources, called optical frequency combs. This mixing process generates an interferogram, at a speed that, until very recently, was too fast to be captured even by very high-speed cameras.
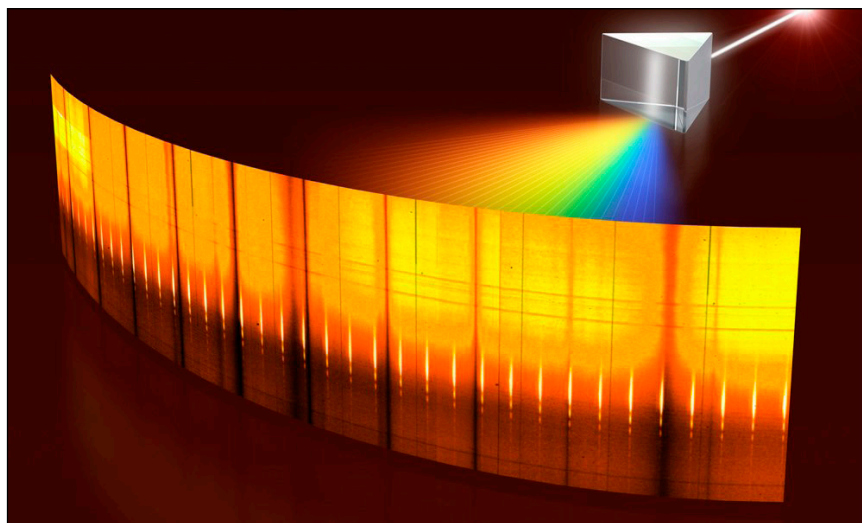
The research team for this patent has developed a system based on a dual-comb electro-optical source made with fibre optic components. The main part is a dual-comb illuminator capable of generating two frequency combs that interfere at much lower frequencies than can be obtained with other systems. This makes it possible to detect that signal with any camera that has sensitivity in the emission range of the dual-comb system used. In addition, it is capable of working in different frequency ranges (near infrared, mid-infrared and terahertz).

The technologies based on frequency combs used to date made it possible to analyse a single point of the sample, towards which the light source was sent. The system patented by the UC3M research team makes it possible to spectrally analyse the entire sample and is pioneering in terms of the measurement used because it uses a dual frequency comb instead of the spectral interrogators that current hyperspectral cameras are equipped with.

From this characterisation it can, in addition to identifying the compound, analyse other parameters such as its temperature, pressure and concentration. "The need arises from the shortcomings of current technologies, in which the measurements are very slow and optical absorptions are not identified precisely enough. The high optical resolution with which we can characterise the entire sample with our technology is essential when we work, for example, with gases", says Pedro Martín Mateos, lecturer in UC3M's Electronic Technology Department and project researcher.

This system makes it possible to analyse the chemical composition of a complete sample and can be used in many sectors. To date, it has been tested for the detection and analysis of gases, as well as for studying the characteristics of different foods and materials, such as plastic. "We have already demonstrated its usefulness for the study of gaseous samples. This would be useful for the development of more efficient burners or for safety issues. We have also used it for the analysis of certain foods and even for drying wood, and we are starting to develop a system that will allow us to monitor combustion processes with new fuels or alternative fuels, such as hydrogen", concludes the researcher.

Using a standard RGB camera and AI to obtain vegetation data

Pictures from a standard RGB camera combined with AI deep learning can provide equivalent crop prediction tools for a fraction of the cost.

Aerial imagery is a valuable component of precision agriculture, providing farmers with important information about crop health and yield. Images are typically obtained with a multispectral camera attached to a drone. But a new study from the University of Illinois and Mississippi State University (MSU) shows that pictures from a standard red-green-blue (RGB) camera combined with AI deep learning can provide equivalent crop prediction tools for a fraction of the cost.

Multispectral cameras provide colour maps that represent vegetation to help farmers monitor plant health and spot problem areas. Vegetation indices such as the Normalised Difference Vegetation Index (NDVI) and Normalised Difference Red Edge Index (NDRE) display healthy areas as green, while problem areas show up as red.

"Typically, to do this you would need to have a near infrared camera (NIR) that costs about $5000. But we have shown that we can train AI to generate NDVI-like images using an RGB camera attached to a low-cost drone, and that reduces the cost significantly", says Girish

A standard RGB camera attached to a drone, combined with AI deep learning, can provide crop health colour maps, a new study shows. Photo: Diane Godwi

Chowdhary, associate professor in the Department of Agricultural and Biological Engineering at U of I.

For this study, published in *Computers and Electronics in Agriculture* (doi.org/grww4k), the research team collected aerial images from corn, soybean and cotton fields at various growth stages with both a multispectral and an RGB camera. They used Pix2Pix, a neural network designed for image conversion, to translate the RGB images into NDVI and NDRE colour maps with red and green areas. After first training the network with a large number of both multispectral and regular pictures, they tested its ability to generate NDVI/NDRE

pictures from another set of regular images.

"There is a reflective greenness index in the photos that indicates photosynthetic efficiency. It reflects a little bit in the green channel, and a lot in the near infrared channel. But we have created a network that can extract it from the green channel by training it on the NIR channel. This means we only need the green channel, along with other contextual information such as red, blue and green pixels", Chowdhary explains.

To test the accuracy of the AI-generated images, the researchers asked a panel of crop specialists to view side-by-side images of the same areas, either generated by AI or taken with a multispectral camera. The specialists indicated if they could tell which one was the true multispectral image, and whether they noticed any differences that would affect their decision making.

The experts found no observable differences between the two sets of images, and they indicated they would make similar predictions from both. The research team also tested the comparison of images through statistical procedures, confirming there were virtually no measurable differences between them.

Joby Czarnecki, associate research professor at MSU, cautions that this doesn't mean the two sets of images are identical.

"While we can't say the images would provide the same information under all conditions, for this particular issue, they allow for similar decisions. Near infrared reflectance can be very critical for some plant decisions. However, in this particular case, it's exciting that our study shows you can replace an expensive technology with inexpensive artificial intelligence and still arrive at the same decision", she explains.

The aerial view can provide information that is difficult to obtain from the ground. For example, areas of storm damage or nutrient deficiencies may not be easily visible at eye level, but can be spotted easily from the air. Farmers with the appropriate authorisations may choose to fly their own drones, or they may contract a private company to do so. Either way, the colour maps provide important crop health information needed for management decisions.

The AI software and procedures used in the study are available for companies that want to implement it or expand the usage by training the network on additional datasets.

"There's a lot of potential in AI to help reduce costs, which is a key driver for many applications in agriculture. If you can make a $600 drone more useful, then everybody can access it. And the information would help farmers improve yield and be better stewards of their land", Chowdhary concludes. ⌁

Drought resistance traits in beans using hyperspectral remote sensing

A research team from the USA has used hand-held and tower-based equipment for phenotyping common and tepary beans.

Crops adapt to climatic and environmental changes by exhibiting certain modified biological traits. For instance, plants growing in deserts exhibit drought resistance. However, at times, plant breeding becomes necessary to ensure optimal crop yields, stress response and water utilisation. High-throughput phenotyping tools are then used for the cost-effective and rapid screening of desired biological traits. However, such monitoring becomes laborious and time-consuming. It can also lead to subjective interpretation and crop destruction. A research team in the USA has recently made an attempt to overcome this limitation using
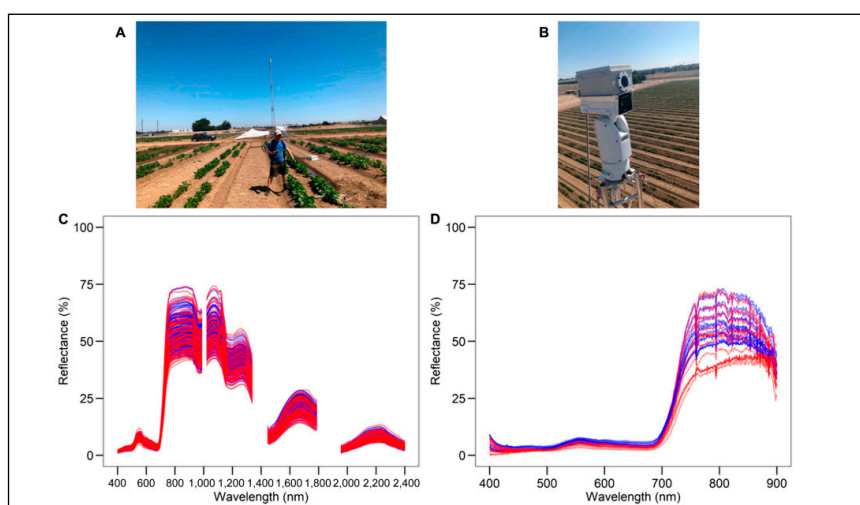
Hyperspectral reflectance of beans from ground-based (A and C) and tower-based instruments (B and D) for control (blue) and drought (red) treatments. Credit: Christopher YS Wong *et al.* from University of California, Davis

NMR PRIMER:

AN HSQC-BASED APPROACH

(with vector animations)

by Steven M. Pascal

This book has one aim: to explain the key two-dimensional protein NMR experiment, the ^{1}H,^{15}N-HSQC, along with variants and extensions, in a generally accessible manner. Vector diagrams of one-, two- and three-dimensional pulse sequences are provided, along with accompanying animated versions. The animations allow the evolution of net magnetisation during the course of the experiments to be visualised and directly compared with the corresponding spin operator terms.

First, a brief introduction to spins, populations, the NMR experiment and relaxation is provided. Evolution due to J-coupling is next described and used to explain magnetisation transfer in the HSQC experiment and several variants. The extraction of structural, sequential and dynamic information is then illustrated via various extensions of the HSQC. Extensive footnotes and appendices introduce several more advanced concepts, such as sensitivity enhancement and the TROSY effect.

ANIMATIONS

The animations were originally created in Flash, which is no more. The animations have been converted to animated GIFs which enable them to be viewed easily with any browser. Control of these animations works best in Google Chrome using the GIF SCRUBBER extension: this allows pause/restart/reverse/speed control/etc.

BUY THE BOOK

NMR Primer: An HSQC-Based Approach costs just £24.95, plus postage & packing. This includes online access to the vector animations via an access code and password provided in each copy.

NMRPRIMER.IMPOPEN.COM

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rapid hyperspectral remote sensing.

Says Christopher Y.S. Wong from the Department of Plant Sciences, University of California, Davis, "We assessed physiological (stomatal conductance and predawn and midday leaf water potential) and ground- and tower-based hyperspectral remote sensing (400–2400 nm and 400–900 nm, respectively) measurements to evaluate drought response in 12 common bean and 4 tepary bean genotypes across 3 field campaigns (1 predrought and 2 post-drought)."

The research team harnessed hyperspectral imaging with the help of a handheld device and tower-based equipment. The bean plantation was irrigated or left unirrigated to mimic normal and drought conditions respectively. The collected data were then analysed with the help of partial least squares regression (PLSR). Results were published in *Plant Phenomics* (doi.org/grwr7b).

PLSR modelling was able to specifically examine two physiological traits in common and tepary bean—stomatal conductance and leaf water potential (LWP). Both stomatal conductance and LWP are indicators of plant water status and often used for evaluating drought tolerance.

The research team also deployed unmanned aerial vehicles (drones) to further facilitate the remote measurements. A comparison was then made to assess the effectiveness of ground-based and tower-based methods. For instance, the team noticed that the ground-based method generally performed better than the tower-based method for all three traits—stomatal conductance, predawn LWP and midday LWP. The researchers then used heatmap clustering—primarily used to highlight drought response—to characterise the drought response phenotypes.

The hyperspectral data was able to successfully predict the bean traits under investigation. Moreover, there was good agreement between ground-based and physiological measurements, thus validating the technique. According to the researchers, this new remote-sensing-based modern agricultural technique can also be used for predicting crop traits in well-irrigated and drought-prone geographies.

"This study demonstrates applications of high-resolution hyperspectral remote sensing for predicting plant traits and phenotyping drought response across genotypes for vegetation monitoring and breeding population screenin", concludes Troy S. Magney, who serves as an Assistant Professor in the same department. ⅄

New device to measure electron spins with extreme sensitivity

The new technology integrates several important parts of the spectrometer into one device and is compatible with relatively large magnetic fields.

Associate Professor Jarryd Pla and his team from the University of New South Wales School of Electrical Engineering and Telecommunications, together with colleague Scientia Professor Andrea Morello, have described a new device that can measure the spins in materials with high precision.

"The spin of an electron—whether it points up or down—is a fundamental property of nature", says A/Prof. Pla. "It is used in magnetic hard disks to store information, MRI machines use the spins of water molecules to create images of the inside of our bodies, and spins are even being used to build quantum computers. Being able to detect the spins inside materials is therefore important for a whole range of applications, particularly in chemistry and biology where it can be used to understand the structure and purpose of materials, allowing us to design better chemicals, drugs and so on."

In fields of research such as chemistry, biology, physics and medicine, the tool that is used to measure spins is called a spin resonance spectrometer. Normally, commercially produced spectrometers require billions to trillions of spins to get an accurate reading, but A/Prof. Pla and his colleagues were able to measure spins of electrons in the order of thousands, meaning the new tool was about a million times more sensitive. Their work is published in *Science* *Advances* (https://www.science.org/doi/10.1126/sciadv.adg1593).

This is quite a feat, as there are a whole range of systems that cannot be measured with commercial tools, such as microscopic samples, two-dimensional materials and high-quality solar cells, which simply have too few spins to create a measurable signal.

The breakthrough came about almost by chance, as the team were developing a quantum memory element for a superconducting quantum computer. The objective of the memory element was to transfer quantum information from a superconducting electrical circuit to an ensemble of spins placed beneath the circuit.

"We noticed that while the device didn't quite work as planned as a memory element, it was extremely good at measuring the spin ensemble", says Wyatt Vine. "We found that by sending microwave power into the device as the spins emitted their signals, we could amplify the signals before they left the device. What's more, this amplification could be performed with very little added noise, almost reaching the limit set by quantum mechanics."

While other highly sensitive spectrometers using superconducting circuits had been developed in the past, they required multiple components, were incompatible with magnetic fields and had to be operated in very cold environments using expensive "dilution refrigerators", which reach temperatures down to 0.01 Kelvin. In this new development, A/Prof. Pla says he and the team managed to integrate the components on a single chip.

"Our new technology integrates several important parts of the spectrometer into one device and is compatible with relatively large magnetic fields. This is important, since measure the spins they need to be placed in a field of about 0.5 Tesla, which is ten thousand times stronger than the earth's magnetic field. Further, our device operated at a temperature more than 10 times higher than previous demonstrations, meaning we don't need to use a dilution refrigerator."

A/Prof. Pla says the UNSW team has patented the technology with a view to potentially commercialisation, but stresses that there is still work to be done.

"There is potential to package this thing up and commercialise it which will allow other researchers to plug it into their existing commercial systems to give them a sensitivity gain. If this new technology was properly developed, it could help chemists, biologists and medical researchers, who currently rely on tools made by these large tech companies that work, but which could do something orders of magnitude better."

A plutonium needle in a haystack

New results using could significantly improve resonance ionisation mass spectrometry ultra-trace analysis of plutonium isotopes.

Even tiny amounts of plutonium are harmful to human health and the environment. But plutonium also helps us study the universe: the isotope plutonium-244 hints at nucleosynthesis and neutron star mergers. Researchers, therefore, need ways to detect what they call "ultra-trace" plutonium. Ultra-trace refers to tiny amounts of a material—similar to the mass of a nucleotide of the DNA in a single human cell. Researchers have now used special lasers to study the fingerprints of plutonium's photoionisation. This is the absorption of enough energy from light to cause an electron to leave and create a positive ion. The technique allowed researchers to identify ultra-trace amounts of plutonium atoms at record levels of efficiency.

Detecting plutonium is important for many areas of scientific research. It is part of studies such as nuclear forensics and safeguards, environmental science, reactor safety and astrophysics. Among
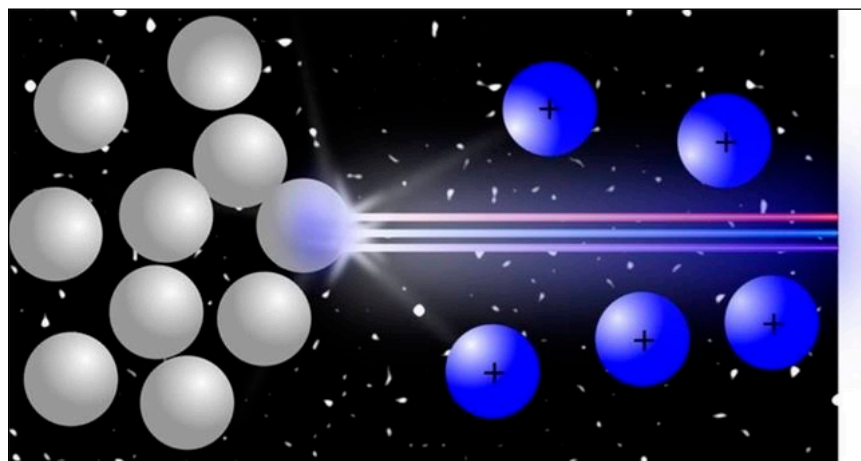
Resonance ionisation mass spectrometry is a highly selective and sensitive technique for analysing extremely small amounts of elements. It uses tuneable lasers to ionise atoms of the desired elements. Credit: Image courtesy of Elisa Romero-Romero

other variables, scientists study the concentration of plutonium and the ratios of its various isotopes in samples. However, these samples usually contain only tiny ultra-trace amounts of the element. With this new technique, nuclear physicists improved laser ionisation efficiency of plutonium tenfold. This frees more of this element for analysis by resonance ionisation mass spectrometry.

Investigators studied three-step resonance photoionisation spectra

of plutonium with titanium-sapphire lasers. The goal was to develop more efficient laser ionisation schemes for ultra-trace analysis of plutonium isotopes by resonance ionisation mass spectrometry. This technique can benefit a diverse range of applications. For example, plutonium-244 is the longest-lived plutonium isotope, with a half-life of about 80 million years, and its observation in deep-sea crusts and sediments tells scientists something about the nucleosynthesis of chemical elements in neutron star mergers. For these applications,

scientists need extremely sensitive analytical techniques to characterise plutonium isotopes and their abundances.

In this study, published in *Scientific Reports* (doi.org/j3rc), researchers from Oak Ridge National Laboratory and the University of Tennessee, Knoxville used three pulsed titanium-doped sapphire laser beams to examine spectra created from plutonium's photoionisation. The technique uses stepwise resonant excitation of the atoms with three photons to achieve extremely high element-selectivity. The ions

produced are mass-selectively detected. This leads to excellent isotope selectivity and background suppression from undesired species. The researchers observed thirteen new second-step energy levels, and they chose six to investigate a large number of third-step states. These efforts led to the identification of a highly efficient three-step scheme with an overall ionisation efficiency of more than 50 % for plutonium—a ten-fold improvement over its previously reported ionisation efficiency.

Diamonds as a source for THz radiation

Between 5 THz and 12 THz, stable, continuously tuneable, energetic fs pulses are challenging to come by but diamonds can be used to fill the gap.

The advent of intense ultrashort coherent light pulses has revolutionised the spectroscopy field. On the one hand, they allow easy observation of various non-linear optical effects and facilitate the characterisation of materials with non-linear optical spectroscopy. On the other hand, they provide means for strong selective excitation of materials and optical manipulation of material structure. It also enhances properties such as optical-field-induced ferroelectricity and superconductivity. They have also created the vibrant field of ultrafast dynamics of low-frequency excitations in materials.

Thanks to advances in laser technology over the past decades, intense femtosecond (fs) pulses from table-top setups are now available over the whole spectral range from ~10 THz to soft X-ray, even in ordinary laboratories. Below ~5 THz, high-intensity picosecond pulses exist, but between 5 THz and 12 THz, stable, continuously tuneable, energetic fs pulses are more challenging to come by. However, this is a spectral range of great importance for materials

studies. Phonons and vibrations of molecules and solids composed of heavier atoms are in this range, and so are the intermolecular vibrations of molecular systems in chemistry and biology. Various elementary excitations of solids also lie in this spectral region.

A team of scientists led by Professor Y. Ron Shen from the University of California Berkeley and Professor Chuanshan Tian from Fudan University have developed a novel technique for generating ultrashort tetrahertz pulses and published the results in *Light Science & Applications* (doi.org/grqq9n).

Currently, optical rectification (OR) or difference frequency generation (DFG) in second-order non-linear crystals is the standard technique to generate intense THz pulses. However, THz generation from crystals is limited because of phonon absorption. Organic non-linear crystals have been used for efficient THz generation, but they have only a few narrow transparent windows above 5 THz and suffer from low optical damage thresholds.
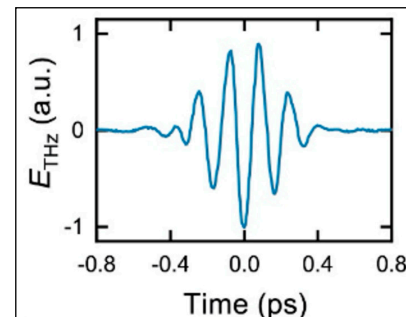
Temporal trace of a THz pulse with PM at 5 THz measured by EOS in GaP. Credit: Jiaming Le, Yudan Su, Chuanshan Tian, A.H. Kung, Y. Ron Shen

Laser-induced gas plasmas can generate energetic THz pulses. They are well suited as probes for linear THz spectroscopy over a wide spectral range. However, their complex spatial mode patterns make them less desired as pumps for strong resonant excitations. Free electron lasers and electron-driven THz sources can also produce fs pulses covering the entire THz spectral range, but they are not readily available for most researchers.
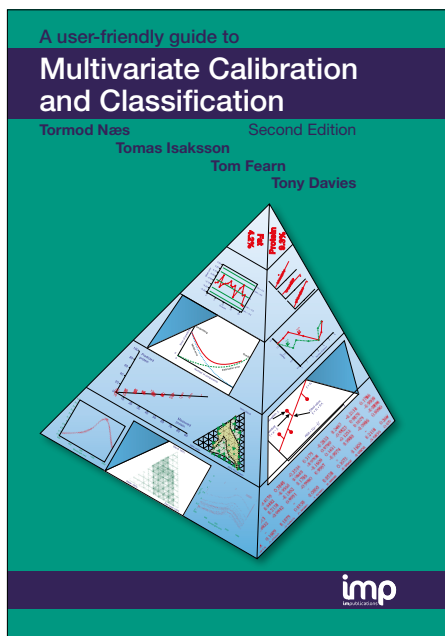
A User-Friendly Guide to Multivariate Calibration and Classification

by **Tormod Næs, Tomas Isaksson, Tom Fearn, Tony Davies**

This important book, which has been receiving excellent reviews, presents these topics in an accessible way, yet provides sufficient depth to be of real practical value

CONTENTS

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"Explanation of the differences between classical and inverse calibration, how to solve collinearity, and the problem of under-fitting or over-fitting are excellently described and illustrated with figures".
"Algorithms for locally weighted regression, scatter correction and other methods for coping with non-linearity in spectroscopy are described in three chapters"
"There is an extensive bibliography"
"In fact the whole book is particularly well produced by a small publisher who should be a model for larger competitors"
Prof D. Brynn Hibbert (Chemometrics and Intelligent Laboratory Systems)
"I am planning to use this text as a reference for some research projects I am planning to tackle in the near future"
"Clearly, the authors have done a reasonably thorough job on multivariate calibration"
"In conclusion I liked the text. The layout and the figures make it easy to read."
Barry Lavine (Journal of Chemometrics)
"I can recommend this book to all newcomers to the subject (and experts too …)"
Paul Geladi (NIR news)

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A User-Friendly Guide to Multivariate Calibration and Classification costs £65.00 plus postage & packing.

NEWS

Diamond has many attractive merits. Its high optical damage threshold allows input pump intensities to be so high as to induce third-order non-linear optical effects (e.g., four-wave mixing) that can compete with second-order effects (e.g., DFG) in other crystals. Transparency throughout the region from THz to UV leads to weak frequency dispersion of optical response coefficients that facilitates phase-matched THz pulse generation over an extensive spectral range. Moreover, the Raman phonon resonance is strong and has a long lifetime, greatly enhancing the third-order non-linearity of diamond on the fs time scale.

Resonant four-wave mixing (R-FWM) for fs THz pulse generation in a diamond can be considered a beating process between an fs IR pulse with a coherent phonon wave that is Raman-excited by two ps input pulses. The process down-converts the fs IR pulse by the phonon wave to the fs THz pulse. The energy conversion efficiency is given directly by the output THz pulse energy ratio to the input fs pulse energy.

The research team measured THz pulse generation with the centre frequency from 5 THz to 20 THz. This spectral range can be readily extended to >100 THz. Since the THz radiation efficiency increases with the square of the frequency, there is more pulse energy at a higher input frequency. The research team hypothesises that the output THz energy generated by R-FWM in a thicker diamond can reach a level comparable to that generated by DFG in GaSe or other crystalline compounds, especially at higher THz frequencies.

Their study has unequivocally established that R-FWM in a diamond can be made into a high-quality, powerful, fs THz generator over a wide spectral range without any gap. As a direct frequency down-conversion process via the Raman-excited phonon wave, R-FWM generates fs THz pulses that duplicate the input fs IR pulse except for a shift in frequency and some modification due to radiation efficiency. An input pulse of high quality generates a THz pulse of nearly equal high quality. Tuning the characteristics of the input pulse tunes the characteristics of the THz output pulse accordingly. In this respect, the researchers could amplitude- or polarisation-modulate the THz pulse simply by modulating the input pulse. ⌁

Size of X-ray beams successfully evaluated with mathematics

A new method to evaluate the diameter of X-ray microbeams, based on mathematical analysis, can be used to calculate beam diameters more accurately than the previously used conventional methods.

X-ray fluorescence analysis allows elemental analysis in a variety of environments without destroying the sample. The smaller diameter of the X-ray microbeam, the more accurate the elemental distribution can be. Because X-ray beams are not visible, an accurate method is needed to determine beam diameter.

A research group led by Professor Kouichi Tsuji and Specially Appointed Assistant Professor Tsugufumi Matsuyama of the Graduate School of Engineering, and Professor Hideyuki Ishi of the Graduate School of Science, at Osaka Metropolitan University, has developed a new method to evaluate the diameter of X-ray microbeams based on mathematical analysis and published it in *X-Ray Spectrometry* (doi.org/grq9fz). While validating the new method, it was
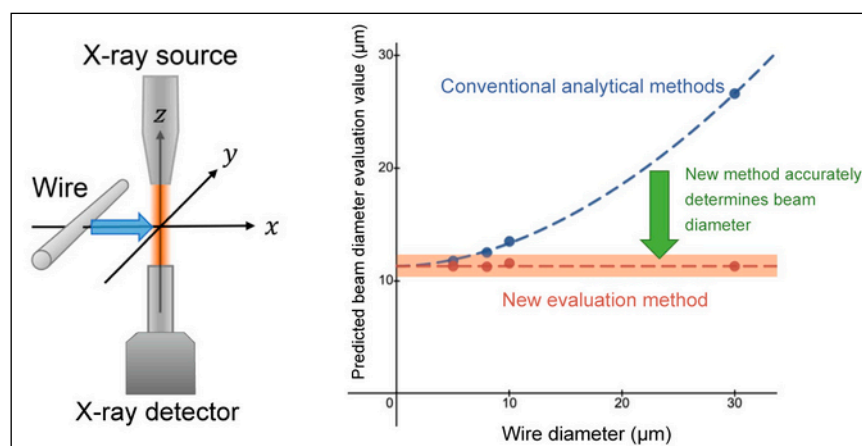
X-ray beam diameter can be calculated more accurately with the new evaluation method than with conventional methods used previously. The new method shows the same X-ray beam diameter, which remained consistent during this test, when using different wires with variable thickness. Credit: Kouichi Tsuji, Osaka Metropolitan University

found that it can be used to calculate beam diameters more accurately than the previously used conventional methods.

Currently, no uniform evaluation method for X-ray beam diameter has been established. Since this evaluation method was derived

using mathematical analysis, it is expected to be widely adopted as an international standard. Potential applications of X-ray fluorescence analysis include materials development, environmental analysis, forensic science, biological sample analysis and analysis of archaeological and culturally significant objects.

Professor Tsuji concluded, "We hope that this evaluation method will be widely used, and that the establishment of this method of evaluating spatial resolution in X-ray fluorescence will contribute to the development of a wide range of fields, including material development and bio-imaging."

Organosulfur content of vegetables quantified by mass spectrometry

Selective and sensitive measurement of reactive polysulfides in 22 different vegetables using mass spectrometry with a stable-isotope dilution method.

The health-promoting effects of sulfur-rich vegetables such as onions and garlic have been known for a long time. How food containing sulfur compounds promotes health has not been easy to explore, as the levels—and types—of reactive polysulfides found in different vegetables had not been accurately measured.

A research team, led by Assistant Professor Shingo Kasamatsu from the Osaka Metropolitan University Graduate School of Science, has established a method for selective and sensitive detection of reactive polysulfides—which can act as potent antioxidants. By using mass spectrometry with a stable-isotope dilution method, the team successfully quantified the total reactive polysulfide content of 22 vegetables, including onions and garlic and published the results in *Food Chemistry* (doi.org/grw7z6).

The team also measured the polysulfide content in vegetables to analyse the overall characteristics of the reactive polysulfide. As a result, they were the first to reveal that high levels of reactive polysulfides could be found, not only in vegetables of the leek genus (*Allium*), such as onions and garlic but also in cruciferous vegetables

Scientists quantified the reactive polysulfide content of 22 different types of vegetables. They revealed that reactive polysulfides are not only found in the leek genus (*Allium*), such as onions and garlic but also in the cruciferous family of vegetables (*Brassicaceae*), such as broccoli and cabbage. Credit: Osaka Metropolitan University

(*Brassicaceae*), such as broccoli and cabbage.

"The results of this study will provide a basis for research on reactive polysulfides in food, whose detailed properties and endogenous production mechanisms have not yet been clarified. This will significantly contribute to the development of the research field", stated Dr Kasamatsu. "In the future, we expect that this research will be helpful for developing foods and supplements rich in reactive polysulfide that exhibit superior antioxidant activity."

NEWS

# Studying negatively-charged chiral molecules

Researchers at the Fritz Haber Institute have integrated one of the new chiral optical methods with the study of gas-phase anions, which enable mass-selection and the use of a simple table-top laser for observation of the chiral effect.

The ability to distinguish two chiral enantiomers is an essential analytical capability for chemical industries including pharmaceutical companies, flavour/odour engineering and forensic science. A new wave of chiral optical methods have shown significant improvements in chiral sensitivity, compared to their predecessors, leading to potential analytical advantages for chiral discrimination. Researchers at the Fritz Haber Institute have integrated one of these modern methods with the study of gas-phase anions, which enable mass-selection and the use of a simple table-top laser for observation of the chiral effect. Results are published in *Angewandte Chemie International Edition* ([doi.org/grv8zw](doi.org/grv8zw)). Thus, taking another step closer to realising a robust analytical tool capable of chiral discrimination of dilute and complex, chiral mixtures.

From the difference in taste of spearmint and fennel, to the consequences of a drug, that either cures morning sickness or causes birth deformities, chirality and the properties of enantiomers, which trigger these differences, are known to be a crucial aspect of biological processes. Despite a pair of enantiomers' distinct biological behaviour, their similar chemical structures make them difficult to distinguish by analytical or spectroscopic methods. Much effort has gone into finding chiral discrimination techniques that can match nature's ability to differentiate between increasingly small samples of two enantiomers.

In the past two decades, a new wave of chiral discrimination techniques has emerged, which exhibit chiral sensitives that are magnitudes greater than their predecessors. This increased sensitivity allows for study of isolated chiral molecules in the gas-phase, at very low concentrations of initial sample. One of these contemporary techniques, which holds significant analytical promise, is known as photoelectron circular dichroism (PECD) spectroscopy. PECD is a chiral optical effect that emerges in the photoemission of electrons from a sample of chiral molecules, when illuminated with chiral light (ie. circularly polarised light). The effect is a difference in the average direction the electrons depart the molecular sample (either in the forward or backward direction). This direction is a function of the handedness of light and the enantiomer being probed. This effect is incredibly sensitive to many characteristics of a chiral molecule leading to an effect that is exceptionally perceptive to the chiral potential of a molecule.
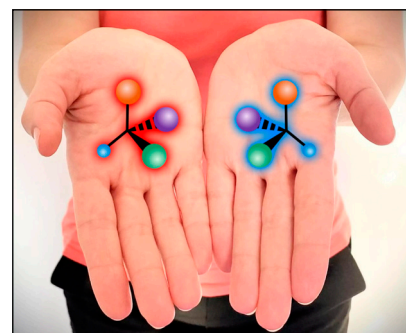
Chirality is defined as a pair of molecules, called enantiomers, which are non-superimposable mirror images of one another. Although these molecules look similar, they can have drastically different behaviour in nature. © FHI

Although studies of PECD have historically been carried out on neutral molecules, researchers at the Fritz Haber Institute have explored this effect in anions. The use of anions for PECD spectroscopy has a few important analytical
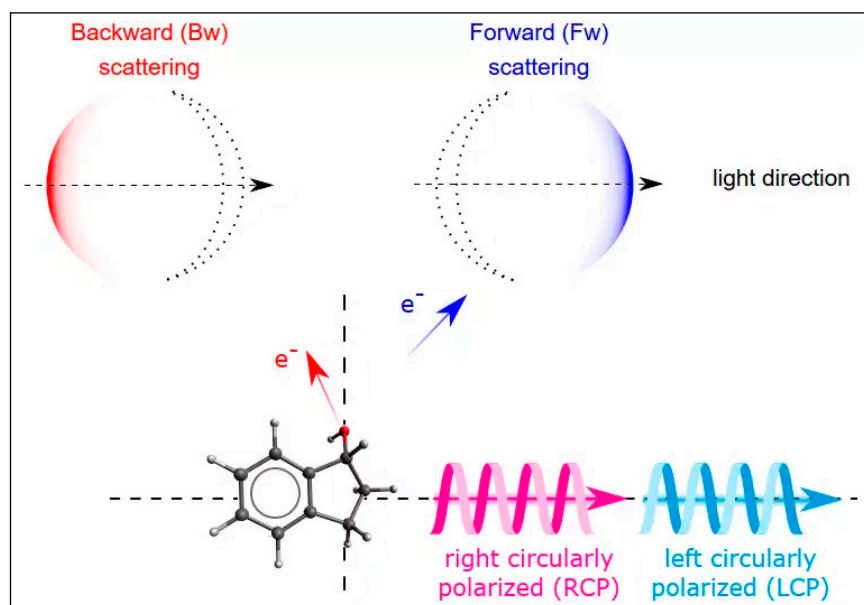
In PECD spectroscopy, switching the handedness of light or the enantiomer being probed leads to a reversal in the electron trajectory. © Jenny Triptow

advantages: first, as anions are charged particles, ion optics can be used for mass selection. Often, industrial chiral samples are known to be multi-component. The addition of mass selective capabilities would enable the isolation of target molecules before the photoemission process, thus simplifying final analysis. In addition, as this effect manifests through the removal of an electron from a chiral molecule, lower energies for electron detachment are preferential, as they allow for the use of commercially-available table-top lasers. Ionisation of an electron from a closed-shell neutral molecule requires either high energy synchrotron radiation or a multiphoton process

by visible or near-UV lasers. The smaller photon energies required for detachment of the extra electron in anions are accessible by common table-top lasers through single-photon detachment processes.

The research team in the Molecular Physics department has recorded a energy-resolved PECD signal for a mass-selected anion, for the first time. This is not only an important benchmark for the analytical possibilities of this technique, but also opens the door to understanding the differences in electron dynamics between photoionisation of neutrals and photodetachment of anions. As the observation of this effect in anions

has lagged two decades behind its observation in its neutral counterpart, comparisons of these photoemission processes could unlock comprehension of the universal dynamics that govern the PECD effect. In their initial findings, the research team has demonstrated a PECD effect surprisingly similar in magnitude to its neutral counterpart, and an effect that persists at much higher electron kinetic energies than was to be expected, when considering conventional theoretical descriptions of electron photodetachment. These results reveal a current gap in knowledge of this effect, which necessitates further investigation. 〰

Technology development could bring Raman microscopy to the clinic

New method offers high-throughput chemical imaging hundreds of times faster than traditional approach.

Researchers have developed a Raman microscope that can acquire information hundreds of times faster than a conventional Raman microscope. This technology development could help expand its usefulness in biomedical applications.

"Our high-throughput Raman spectral imaging can quickly image and analyse a large area without any sample pretreatment, which could make it useful for medical diagnoses and the tests used to screen for new drugs", said research team leader Katsumasa Fujita from Osaka University. "The label-free, high-throughput multiplex chemical imaging and analysis enabled by the technique could also be used to enable new applications or overcome limitations of current methods."

The new multiline illumination confocal Raman microscope works by detecting separate regions of the sample in parallel, enabling fast Raman hyperspectral imaging.
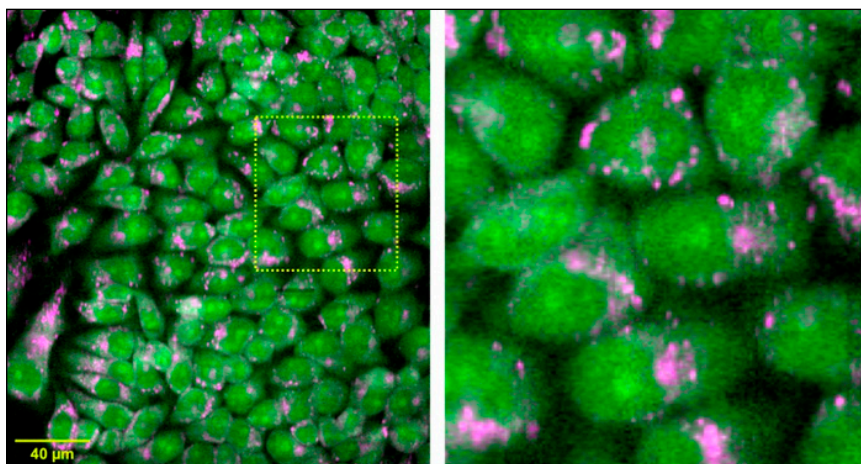
Researchers developed a Raman microscope that can acquire information hundreds of times faster than a conventional Raman microscope. This extra speed makes it possible to acquire large-area hyperspectral images of living cells, such as the ones seen here. Credit: Katsumasa Fujita, Osaka University

They show that the technique can acquire hyperspectral images of biological tissue with a field of view of 1380 × 800 pixels in about 11 minutes. This would require days to acquire with a traditional Raman microscope.

"We hope that high-throughput Raman imaging will eventually make it possible to perform medical diagnoses more efficiently and accurately while possibly enabling diagnoses that weren't possible before", said Fujita. "Label-free

molecular analysis with Raman imaging would also be useful for efficiently detecting drug response of cells, aiding in drug development."

The new multiline illumination approach builds upon a technique the research team previously developed known as line-illumination Raman microscopy. That approach was faster than conventional confocal Raman microscopy and enabled dynamic imaging of living cells but was still too slow for the large-area imaging often required for medical diagnosis and tissue analysis.

"To address this issue, we developed multiline illumination Raman microscopy, which acquires large-area images about 20 times faster than line-illumination Raman microscopy", said Fujita. "With our new technique, the spectral pixel number—or resolution—and imaging speed can be adjusted, depending on the application. In the future, even faster imaging speed might be possible as cameras continue to be developed with more pixels."

The team's new multiline-illumination Raman microscope irradiates about 20,000 points in a sample simultaneously with multiple line-shaped laser beams. The Raman scattering spectra generated from the irradiated positions are then recorded in a single exposure that contains the spatial information for the Raman spectra in the sample. Scanning the laser beams across the sample allows a two-dimensional hyperspectral Raman image to be reconstructed.

To accomplish this, the researchers use a cylindrical lens array—an optical element composed of periodically aligned multiple cylindrical lenses—to generate multiple line-shaped laser beams from a single laser beam. They combined this with a spectrophotometer capable of acquiring 20,000 spectra at the same time. Optical filters were also important for avoiding cross talk among the spectra at the spectrophotometer detector.

A high-sensitivity, low-noise CCD camera with a large number of pixels was also critical. "This CCD camera allowed 20,000 Raman spectra to be distributed on the CCD chip and detected simultaneously", said Fujita. "The custom-made spectrophotometer also played an important role by forming the 2D distribution of spectra on the camera without significant distortion."

The researchers used the new technique to acquire measurements from live cells and tissues to test its imaging performance and potential in biomedical applications. They showed that irradiating a mouse brain sample with 21 simultaneous illumination lines could be used to acquire 1,108,800 spectra in just 11.4 min. They also performed measurements on mouse kidney and liver tissue and conducted label-free live-cell molecular imaging. Results are published in *Biomedical Optics Express* (doi.org/grq6d3).

"Small-molecule imaging and super-multiplex imaging using Raman tags and probes could also benefit from this technique because they don't require a large number of pixels in a spectrum and can benefit from fast imaging", said Fujita.

For this technique to be applied for medical diagnoses, the researchers say it would be important to build a database of Raman images, something that can be accomplished efficiently with the new Raman microscope thanks to its speed and large imaging area. They are also working to increase the system's speed by a factor of about 10 and would like to reduce the cost of camera, laser and spectrophotometer to make commercialisation more practical. ⚡

Coherent Raman microscopy could be expanded through fusion of instruments and computers

A new paper has reviewed the combination of instrumentation and computational approaches to coherent Raman scattering.

Raman scattering is an inelastic scattering process that exchanges energies between photons and molecules to carry information on molecular vibrations. Raman microspectroscopy has become an indispensable analytical tool in biology and medical surgery mainly due to its two "frees": label-free and water background-free. These benefits enable us to study living samples without endogenous perturbation. In addition, Raman peaks have a much narrower spectral bandwidth than fluorescent dyes' emission spectrum, which enables the simultaneous study of various metabolic species in the same environment.

In a new paper, published in *eLight* (doi.org/grx6dk), Dr Haonan Lin and Professor Ji-Xin Cheng from Boston University reviewed the combination of instrumentation and computational approaches to coherent Raman scattering (CRS). Despite its significant advantages, one fundamental drawback of Raman scattering lies in its severely limited cross-sections. A typical Raman cross-section is $10–30\,cm^2$ per molecule, resulting in a very long signal integration time from seconds to minutes per focal

spot. Such limited speed makes it impractical to perform pixel-by-pixel imaging of dynamic systems. A non-linear optical process has been introduced to enhance the Raman signals coherently and to break the fundamental cross-section limits. With two synchronised ultrafast lasers, coherent Raman signals arose in coherent anti-Stokes Raman scattering (CARS) and stimulated Raman scattering (SRS). In CRS, two laser fields synchronously interact with the target molecule. When the beating frequency matches the Raman vibrational mode, a coherently amplified energy transfer process occurs. It annihilates the pump photon, converts it to the Stokes beam and generates photons at a new frequency.

CRS has enabled high-speed chemical imaging based on intrinsic Raman peaks on biological samples. However, biological samples are sophisticated microsystems that consist of various metabolites which often have spectral overlaps, especially in the strong yet crowded carbon–hydrogen (CH) region. It hinders the quantitation and identification of chemicals in cells and tissues using narrowband single-colour CRS. Over the past years, significant endeavours have been made to develop hyperspectral CRS that produces a Raman spectrum at each pixel.

Hyperspectral imaging offers the potential for deciphering the information on chemical compositions and abundance in a complex environment. However, due to the high dimensionality of the raw image, such information is not readily available. Algorithms are required to identify major pure components and decompose concentration maps. Parallel with instrumentation

developments in hyperspectral CRS, various hyperspectral image unmixing methods have been reported. Depending on whether prior information is given on the composition of pure components, we categorise them into either supervised or unsupervised methods.

Instrumentation innovations have pushed CRS imaging to the speed of up to 2 kHz frame rate, spectral coverage of up to 3500 cm^{-1}, and spectral acquisition speed of up to 5 µs per spectrum. However, these conditions cannot be realised simultaneously due to the physical limit determined by the sensitivity limit of CRS. For example, further increasing the speed will deteriorate the setup's signal-to-noise ratio (SNR), rendering it inapplicable to biomedical applications. Under the constraint of photodamage, this trade-off can be conveyed as a design space. It is a hyperplane intersecting with three axes representing speed, spectral bandwidth and SNR. Optimisation of instrumentation enables the system to reach an optimal condition point on the hyperplane, yet going beyond it remains challenging.

The research team introduced various computational methods used to push the boundary of CRS chemical microscopy. Attention must be paid to the applicable range of computational algorithms to avoid erroneous interpretations of the measurements. Evaluating whether the forward model can appropriately describe the underlying physical process is crucial. It involves the statistical distribution of measurement noise, the image convolution kernel of the imaging system and other techniques.

Rigorous experiments should be taken to characterise the

forward model and calibrate model parameters. When prior models/regularisations are used, a comprehensive understanding of the signal is necessary. Hyperparameter tuning for the prior models is crucial for yielding correct results and may require iterative updates and validations. For deep learning applications, although the task of sophisticated modelling on the inverse problem is alleviated, an appropriate selection of network structures and sufficiently large training and validation datasets are necessary.

Looking into the future, the research team expect instrumentation advances will continue to increase the data throughput on temporal, spatial and spectral dimensions. They should provide more features on data structures, such as sparsity and correlation. Meanwhile, new computational methods can be harnessed to break the design space trade-offs and provide enriched chemical compositions for biomedical research. With rapid advances in computational optical microscopy, we expect more ideas to infiltrate CRS.

Since most computational methods focus on wide-field implementations, the translation into CRS microscopy is non-trivial. Extensive modelling, system design and algorithm development need to be performed to ensure applicability to CRS imaging. In the future, computational methods will play an even more critical role as existing methods remain viable to boost the newly established design space. New methods may arise to achieve breakthroughs in aspects such as field of view, imaging depth and spatial resolution.

NEWS

Mapping molecular funnels with X-rays: precise timings of non-adiabatic excited state dynamics

Scientists at Stockholm University have proposed a non-linear spectroscopic technique to investigate the coupled nuclear electronic dynamics in a photo-excited molecule.

Time-resolved spectroscopy is a tool that provides access to the time-scale of chemical reactions as they happen. With the help of ultra-short light pulses, it is possible to observe conformal changes in molecules on the time-scale of the atomic motion and electronic motion. Photochemical reactions, such as the damage of DNA by means of sunlight or the key-step in the process of vision, can thus be observed in great detail. Observing a photochemical process with a time resolution corresponding to the molecular motion requires at least two pulses: a pump which triggers a reaction and a probe pulse that measure the result. Non-linear spectroscopy uses multiple pulses to explore excited state phenomena in molecules in even greater detail. Such non-linear schemes are well-established for optical laser pulses. However, in the X-ray regime, demonstrations of non-linear spectroscopy are more recent.

Scientists at Stockholm University have proposed a non-linear spectroscopic technique to investigate the coupled nuclear electronic dynamics in a photo-excited molecule. Non-adiabatic dynamics arise in molecules when the electronic motion slows down and approaches the same time-scale as the much heavier nuclei. This phenomenon may result in the formation of so-called conical intersections, which are "funnels" that connect different electronic states with each other. The energy of different electronic states becomes degenerate at the tip of the cone. Even though the existence of
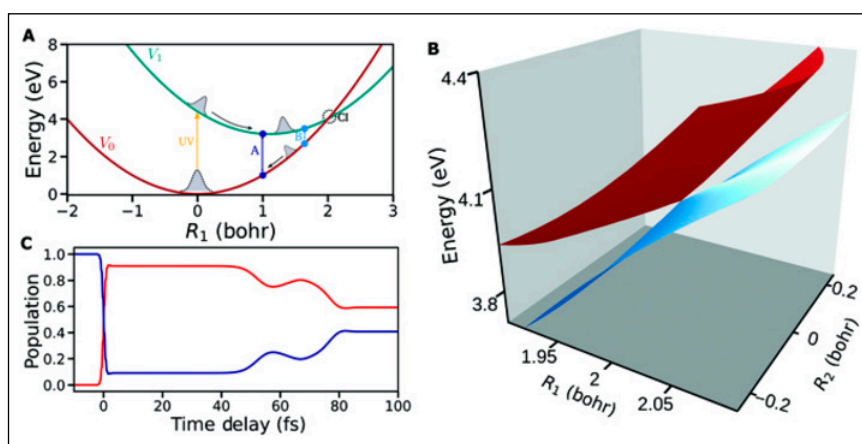
Overview of the model system. (A) One-dimensional slices of the PESs along the R_1 reaction coordinate are shown. The black dashed circle shows the point of degeneracy between the two electronic states. Vertical arrows indicate transitions between the electronic states. Transition A corresponds to an electronic state separation of ≈2.2 eV, and transition B corresponds to an electronic state separation of ≈0.8 eV. (B) Two-dimensional representation of the adiabatic PESs for the electronic states involved in the CI. (C) The population dynamics of the V0 state (blue) and V1 state (red). The time delay axis is referenced with respect to the pump–pulse interaction. Credit: *Ultrafast Science*

conical intersections in molecules was predicted in the late 1920s, their direct experimental observation is still challenging. The biggest obstacle is the femtosecond time-scale at which the conical intersections operate in a molecule.

In their theoretical study, published in *Ultrafast Science* (doi.org/grpf3q), Jadoun and Kowalewski propose an elaborate combination of three pulses to generate a spectroscopic signal that tracks conical intersections in a molecule. The photochemical reaction is initiated by an ultra-short ultraviolet laser pulse. After a short delay, a second pulse in the infrared regime creates a coherent superposition of electronic states. A third pulse in the X-ray regime

measures the quantum interference created by the second pulse. The observation relies on the information about the dynamic electronic state separation embedded in the quantum interference created by the second pulse. The time-varying energy difference between the two electronic states is visualised in spectra constructed by altering the time delays between the three pulses. The proposed method can also observe the lifetime of the quantum interference created by the visible/infrared pulse. The technique is capable of observing multiple indicators of a conical intersection in molecules, potentially giving deeper insight into the physical mechanism behind conical intersections.⚡

Improving confidence in measurement data from state-of-the-art PTR-MS

New calibration approach and new NPL reference materials will enable more widespread deployment of proton transfer reaction mass spectrometers (PTR-MS) for long-term atmospheric monitoring.

NPL and the University of Utrecht, Netherlands have collaborated to develop new SI-traceable gas reference materials and a fast calibration approach to improve the quantification and comparability of proton-transfer reaction mass spectrometry measurements.[1]

Proton transfer reaction mass spectrometers (PTR-MS) allow the simultaneous measurements of numerous volatile organic compounds (VOCs) in real-time at trace levels without any sample pre-treatment. As a result, it is utilised in a wide range of applications from atmospheric monitoring to disease diagnosis. The technology has matured over the last two decades and now with multiple instrument manufacturers and an explosion in datasets there is a growing need for accurate calibration and improved measurement comparability.

The large number of VOCs detectable with PTR-MS means it is impractical to have a calibration gas standard or standards for all observable compounds. However, it is possible to provide quantitative measurements for compounds without the need for specific calibration materials provided the mass dependent ion transmission rate is accurately known. This needs to be done experimentally because the transmission of PTR-MS instruments cannot be accurately predicted from theory as many use advanced ion optics to improve sensitivity that causes deviations at low masses and poor tuning and ageing of the ion detection system that result in deviations at high masses.

Chromatogram of PRM 0819 showing separation of compounds in the GC-FID/MS (red trace) and Cryo-GC-FID (blue trace). Reproduced from https://doi.org/10.5194/amt-16-1061-2023 under a CC BY licence.

Previous work in the field has established methods to calibrate and retrieve the mass dependent transmission. However, these are slow and labour intensive resulting in an inadequate calibration frequency limiting the application of PTR-MS to only short discrete deployments. Within the Aerosols, Clouds and Trace Gases Infrastructure (ACTRIS; www.actris.eu) project there is an interest to establish PTR-MS as a technique for long-term atmospheric monitoring. To enable this, colleagues at the University of Utrecht have developed a fast calibration approach to rapidly and accurately retrieve the mass dependent transmission when used in the conjunction with the new SI-traceable gas reference material developed by the Gas Metrology Group at NPL.

Dr David Worton, Principal Research Scientist in the Gas Metrology Group at NPL, states: "The implementation of this new SI traceable reference material with the fast calibration method described in Holzinger et al. (2019)[2] is the most pragmatic approach to directly addressing the accuracy and comparability of PTR-MS measurements and enabling the deployment of PTR-MS for long-term atmospheric monitoring."

Professor Rupert Holzinger at the University of Utrecht, Netherlands states: "This new SI traceable Gas Standard allows exploiting the full potential of the PTR-MS technique: semi-quantitative untargeted analysis of complex mixtures across long time scales and different platforms. I expect scientific advances from this technical improvement!"

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2. https://amt.copernicus.org/articles/12/6193/2019/amt-12-6193-2019.pdf
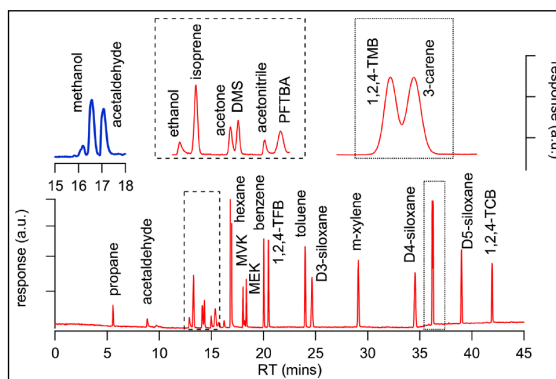
NEWS

PTR-MS of urinary acetone: a fast way to diagnose Type 2 diabetes

A new non-invasive screening method for T2D uses self-developed proton transfer reaction-mass spectrometry.

Type 2 diabetes (T2D) accounts for more than 90 % of confirmed diabetes cases. It has become a common metabolic disease and is expected to affect 380 million people worldwide by 2025. Currently, clinically used diagnostic tests are mainly based on fasting plasma glucose, oral glucose tolerance test and glycosylated hemoglobin A1c (HbA1c). Although these methods are highly accurate, they are all invasive tests based on blood sampling.

A research team led by Prof. SHEN Chengyin from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences (CAS) has been searching for a new non-invasive screening method for T2D. Using self-developed proton transfer reaction-mass spectrometry (PTR-MS), the researchers detected volatile organic compounds in the urine of T2D patients.
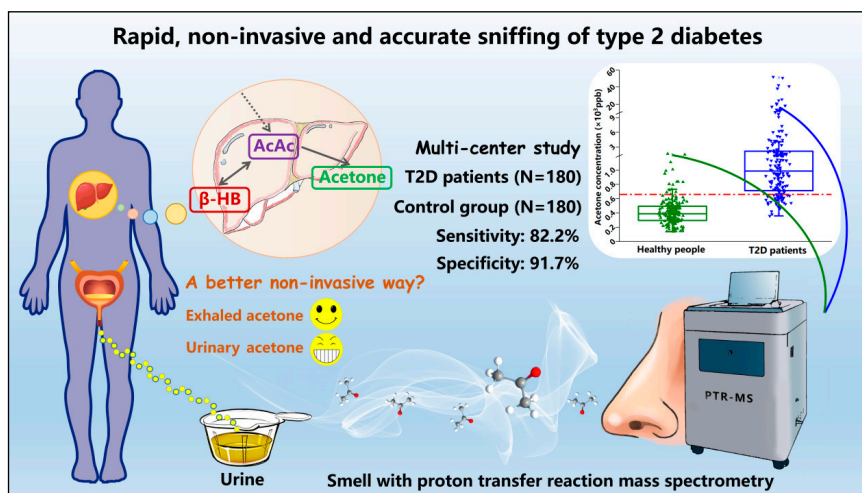
Urinary acetone is one of the ketones produced by fat metabolism. Due to insufficient utilisation and storage of glucose in the blood, T2D patients will accelerate

A brief schematic diagram of the detection principle and method. Credit: XU Wei

the metabolism of urinary acetone. The researchers recruited 180 T2D patients and 180 healthy volunteers for a multicentre study. The results are published in *Talanta* (doi. org/grwvvk).

A diagnostic model with an accuracy of 81.3 % and a threshold of 690.1 ppbv was established by using urinary acetone at centre one. The model was validated at two other centres with similar

results. Furthermore, the accuracy of this method was comparable to the diagnostic method used in clinical practice.

"Sniffing T2D by urinary acetone is safe, non-invasive, fast and accurate", said XU Wei. "We hope that the method can provide a reference for screening and diagnosis of T2D."

TOPTICA Photonics AG is to acquire Azurlight Systems

TOPTICA Photonics AG has entered into a definitive purchase agreement to acquire the majority of the shares of French fibre laser technology company Azurlight Systems SAS.

As of 22 December 2022, laser manufacturer TOPTICA Photonics AG has entered into a definitive purchase agreement to acquire the majority of the shares of French fibre laser technology company Azurlight Systems SAS. Azurlight will continue and further foster its fibre laser business under the new name TOPTICA Photonics SAS and form the French hub of the

Left to right: Dr Wilhelm Kaenders (Founder & Member of the executive board of TOPTICA Photonics AG), Dr Nicholas Traynor (Founder and President of Azurlight Systems who will become President of TOPTICA Photonics SAS) and Dr Juergen Stuhler (Vice President Quantum Technologies at TOPTICA Photonics AG who will become General Manager of TOPTICA Photonics SAS).

TOPTICA brand. The parties have agreed to maintain confidentiality regarding the purchase price. The transaction is subject to foreign direct investment (FDI) approval by French authorities.

Dr Nicholas Traynor (Azurlight Systems, Pessac, France): "We are proud to join the TOPTICA group and excited about the opportunities this offers for the next stage in our development. Putting together the proven technologies of narrow band and tuneable diode lasers with our lowest noise fibre amplifiers will be mutually beneficial for the product families of both companies. Together with the existing global sales and service network of TOPTICA, we will be able to serve customers' needs in quantum technology markets and beyond. We enthusiastically look forward to the years to come."

Dr Wilhelm Kaenders (TOPTICA Photonics, Germany) adds: "We are very pleased to welcome Azurlight Systems under the TOPTICA brand, adding best-in-class fibre lasers and amplifiers to our product portfolio. We envisage further strengthening of fibre laser development in France and strong common product development including our subsidiaries in the US and Germany. This will grow our offering for industry and scientific research, especially in the growing markets of quantum computing and biophotonics and industrial metrology."

Raman microscope at the forefront of battery research

WITec GmbH has delivered a new instrument to the Center for Solar Energy and Hydrogen Research (ZSW) Baden-Württemberg.

WITec GmbH has delivered a new instrument to the Center for Solar Energy and Hydrogen Research (ZSW) Baden-Württemberg. The Raman microscope will be used in the "Powder-Up!" pilot plant in Ulm, where cathode materials for lithium-ion batteries will be produced and the scalability of fabrication methods will be investigated.

Lithium-ion batteries are the primary enabling technology in the current shift toward electric mobility and their performance is almost exclusively determined by the materials used. ZSW is at the forefront of innovative energy storage development and is constructing a new building for the "Powder-Up!" pilot plant over the next twelve months. The new facility will focus on making improvements in the next
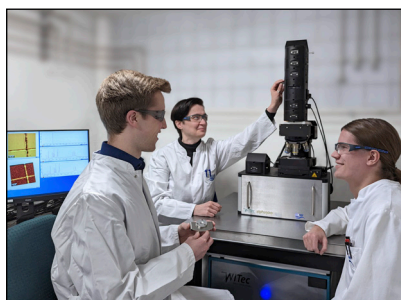
Florian Klein (left) and Leon Gläser (right) from the ZSW in Ulm together with WITec Application Scientist Dr Ievgeniia Iermak (middle) during training on the new Raman microscope.

generation of battery electrode materials, and on scaling up their manufacturing processes. This work is set to have far-reaching effects in terms of battery performance, resource use and unit costs.

According to Dr Margret Wohlfahrt-Mehrens, head of the Accumulators Materials Research department, "Raman microscopy is becoming a standard method in applied battery research. It quickly provides detailed information about how different electrode formulations function and degrade over charge cycles."

The "Powder-Up!" facility, funded by the Baden-Württemberg Ministry of Economic Affairs, Labor and Tourism and the German Federal Ministry of Education and Research (BMBF), is the first of its kind in Europe. Material batches of up to 100 kg can be produced in the new plant. Such quantities are required to produce large battery cells for electric cars or stationary energy storage units.

Agilent announces acquisition of e-MSion

Acquisition will make electron capture dissociation (ECD) technology available to more biopharma researchers and labs globally.

Agilent Technologies has announced the acquisition of e-MSion, an early-stage company behind innovative electron capture dissociation (ECD) technology known as the ExD cell. The ExD cell is a compact device for mass spectrometers that enables biological researchers to develop

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biotherapeutic products more quickly. This is done by more comprehensively and precisely breaking the chemical bonds of complex biomolecules, enabling more complete, accurate and detailed structural information to be obtained from them.

The ExD cell is compatible with instruments common in many labs, which will make this powerful characterisation technology—previously limited to only a few high-end mass spectrometers—more accessible to a larger share of labs and biopharma researchers worldwide. The ExD cell enables electron capture dissociation (ECD) and other modes of electron-induced fragmentation in benchtop mass spectrometers.

Because of its superior characterisation of larger proteins, protein fragments and their amino-acid modifications, ECD is preferred over other dissociation techniques including collision-induced dissociation (CID), which is the dominant methodology used today. ↗

Partnership to develop safety and materials database

ACD/Labs will combine their expertise in chemical information management with the knowledge and expertise of ELSIE consortium members to create a searchable knowledge repository of pre-competitive data.

ACD/Labs has announced a collaboration with the Extractables and Leachables Safety Information Exchange (ELSIE) consortium of bio/pharmaceutical and medical device companies. In further efforts to support member company scientists involved in extractables and leachables (E&L) research, ELSIE—with the help of ACD/Labs—will launch a database of E&L data. The resource, currently in development and testing, will be available to member companies as an educational and research tool in Q2-2023. It will be accessible through an intuitive web-based interface, which provides robust scientific search options and flexible reporting capabilities.

"ELSIE's guiding principle from the outset has been to have a forum to share safety data by reducing time and resources needed to gather this data, allowing our member companies to focus on developing safe and efficacious products", said Uma Bruen, ELSIE Chairperson. "The consortium is committed to expanding the knowledge-gathering and dissemination we currently offer through the ELSIE Safety Information Database beyond toxicological information to include extractable study results on raw materials, single-use products, drug product packaging and delivery systems and medical devices. ACD/Labs understands the science and informatics necessary to build a database that meets the needs of the E&L community. We're excited to take this leap forward to improve collaboration and data sharing in this area of research."

"Supporting scientific knowledge management and enabling collaborative research are two areas of focus for ACD/Labs", said Andrew Anderson, Vice President Innovation & Informatics Strategy, ACD/Labs. "In addition to creating a resource for pre-competitive intelligence, ACD/Labs will also make available to ELSIE members the ability to manage not only their own internal toxicological and extractable data but also leachable study results on their specific products in a similar system, capable of interacting with the ELSIE member system. Organisations need to move away from storing data in static reports and scattered data silos to power their R&D engine with the data they generate." ↗

Wiley and Digital Surf collaborate to accelerate surface analysis workflow

Extracted spectra from Mountains® spectroscopic images can be sent direct to Wiley's KnowItAll software for analysis.

Wiley has announced a new software integration between Digital Surf's Mountains® software for spectroscopic imaging and surface analysis and Wiley's KnowItAll software for spectral analysis and data management. Users of Mountains® will now have the option to send extracted spectra from spectroscopic images (Raman and IR: FT-IR, ATR, NIR) direct to Wiley's KnowItAll software to analyse components, taking advantage of its powerful search, prediction and mixture analysis algorithms and vast spectroscopic data collections. ↗

PiQuant wins CES 2023 Innovation Award for spectroscopy water analyser

PiQuant- Co., Ltd, a spectroscopy-based environmental IoT company, has won the CES 2023 Innovation Award from the Consumer Technology Association (CTA) of America.

CES (or the Consumer Electronics Show) is the world's largest international electronics fair that is held annually in Las Vegas, USA, with more than 2400 companies from 174 countries participating this year. It is a technological exhibition where companies and institutions from various industries showcase the latest IoT and ICT technologies.

At this year's event, PiQuant's water quality analyser "Water Scanner" won the award as the first portable spectrometer to do real-time analysis of the water components. It is an innovative device that can detect hazardous substances like bacteria, heavy metals and chemical compounds in liquid in real time.

The Water Scanner reduced the test time by 1/1440th compared to conventional PCR (Polymerase Chain Reaction). On top of that, the cost of testing was reduced to 1/50th. As a water bacteria scanner, the Water Scanner can monitor and manage data in real time whilst connected to a smart-phone. PiQuant is the first company in Korea supported by the Bill & Melinda Gates Foundation, as it specialises in the analysis of the drinking water environment in developing countries.

E. coli is the major cause of waterborne diseases associated with unsafe drinking water. Using PiQuant's portable bacteria water scanner, the detection of *E. coli* bacteria can be done within three minutes. PiQuant is introducing its products to several developing countries suffering from water pollution, including India and Vietnam.

TONY DAVIES COLUMN

Life and death of a data set: a forensic investigation

Antony N. Davies

SERC, Sustainable Environment Research Centre, Faculty of Computing, Engineering and Science, University of South Wales, UK

I recently reflected that life can be extremely unFAIR, especially if you are a spectrum. I had looked down on the body of this dead spectrometer and reflected how many keen enthusiastic young researchers had tussled with the complexities of what had once been a state-of-the-art scientific wonder which was now reduced to a problem of recycling, disposal and potential contamination risk.

How many now established scientists had benefitted from the children of this spectrometer, the excellent spectroscopic data sets that it was capable of generating in its heyday. They had crafted from these data sets—sometimes with a little help from their supervisors (and no doubt sometimes subtle data processing), their theses and early publications—the passports to their now established careers. But where is all that data now? (Figure 1).

Oddly enough we were lucky enough to attend a Rick Wakeman concert in London which included a very well received rendition of his famous "Six Wives of Henry the Eighth". This reminded me of my daughters' favourite mnemonic
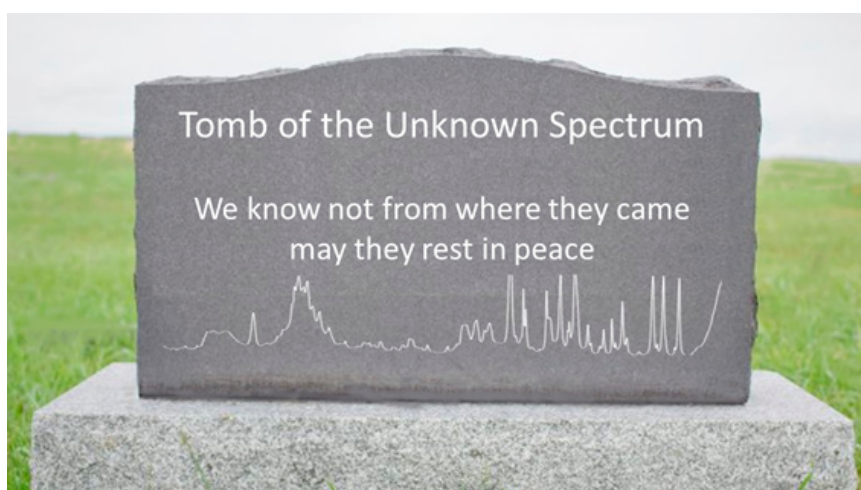
Figure 1. There are many ways a spectroscopic data set can "die".

chant of "*Divorced, Beheaded, Died, Divorced, Beheaded, Survived*" normally used to remember the fate of Henry VIII's six queens—Catherine of Aragon, Anne Boleyn, Jane Seymour, Anne of Cleves, Catherine Howard and Katherine Parr. But as you all know conversations sometimes take bizarre turns, this same mnemonic suddenly seemed very relevant to the various common fates of our spectrometer's data sets.

Birth of a spectroscopic data set

As originally delivered the spectrometer was capable of generating some of the best data sets we had ever been able to measure. Excellent signal-to-noise ratios and extremely stable calibrations. The associated computer hardware was

Figure 2. Does this remind you of your research supervisor? If so, look out! Photo 173782772 © Spiroview Inc. | Dreamstime.com

somewhat behind the state-of-the-art, but this was quite normal due to the long development times for the instrument hardware. And so, in the hands of many expert, and some less expert, scientists, this wonderful spectrometer gave birth to many spectroscopic data sets—reinforcing theories and dispelling some myths. Over its lifespan serving as an excellent measurement platform allowing many modifications to the original basic equipment. So, while our data was young there were no problems. All the measurement parameters were stored with the data set so we could check the instrument had been set up correctly. Where the appropriate comments had been written to the data file, we could even see how the background compensation had been carried out. However, life became more complicated when more advanced data processing was required which was not possible on the original spectrometer control computer.

Divorced

Early attempts to carry out more adventurous data processing required the data to be moved off the spectrometer computer. Where we were lucky, there was a data export function built into the spectrometer software and we were able to get at least the X-Y data points across on to the second computer. Even where there was a data exchange format deployed to the spectrometer such as the JCAMP-DX standard, we did not get all the information onto the new computer. Since the standard only required the minimum amount of information required for accurate data processing to be exported as a requirement to be compliant. All the additional metadata from the originating spectrometer system could be transferred in a defined compliant manner, but only if the vendors believed it was a good idea. In most cases this left the spectra data divorced from much of the metadata about how the spectra had been originally measured and with the death of the spectrometer any hope of recovery from this divorce was gone.

Beheaded

We were successful in setting up workflows to transfer the children off the birthing spectrometer and on to computer hardware capable of more advanced data processing. However, most of the commercial data processing packages were, and still are, not capable of maintaining the integrity of the spectroscopic data set during the import into, for example, a chemometrics data package. Even where the chemometrics software vendor has implemented file filters for direct import from the spectrometer's native file format the header information is very frequently left behind. So, the spectra are essentially beheaded of their supporting metadata.

Died

Often the divorced or beheaded children of the spectrometer were the lucky ones. Many precious spectra have died, not only when the instrument which measured them was retired, but also when the vendor enforced a systems upgrade—sometime completely replacing the control computer for one working on a completely different operating system. This meant the original native binary format files of the earlier work were no longer readable. On one instrument an early attempt to meet FDA guidelines on data integrity, we experienced original data files being embedded within another binary wrapper to provide electronic signatures capability proving no data manipulation had taken place. The only issue there was that the fully validated FDA-compliant ready data migration software for this spectrometer type knew nothing of the home-made additional wrappers and simply failed to read the spectra. In this specific case we were fortunate enough to still have access to some of the IT team who has dreamt up this "cost saving" one-off solution and could reanimate the "Dead" spectra with probably more effort than had been originally expended to measure them!

Divorced

Now looking further down the publication and exploitation pathway of the data, we can see that some journals are providing authors with the opportunity to supply the relevant spectroscopic data along with the submitted manuscripts. These ground-breaking publications have unfortunately little or no guidance on how the spectroscopic data is to be presented or uploaded. Indeed, Professor Robert Lancashire recently came across some guidance by one journal that limited the amount of data that could be deposited to a few MB.

During a recent meeting of the IUPAC FAIRSpec project team, they also suggested that the enforced limited upload of only a few selected example spectra (usually the best measured rather than "typical" for any given experiment) could also fall under the category of Divorced or even having suffered the medieval torture/execution category of Dismemberment of the complete experimental data set with the accompanying critical loss of context.[1]

Beheaded

In the second Beheaded category I have decided to mention an example of users or vendors carrying out what initially looks like a useful fix to a software issue which has unexpected consequences. Having worked in the spectrometer software industry I have experienced the pain of salespeople selling software features which only exist on paper or maybe have only been discussed in long-term planning meetings and haven't yet reached

TONY DAVIES COLUMN

the stage of being put down on paper. If the sales effort is successful these projects usually result in very rushed implementations of the absolute minimal number of feature improvements to meet the contract obligations. This is never a great way to develop robust software and often suffers from the law of unexpected consequences! Fortunately, this is not the norm.

One example, not from anyone I have worked for, involved an instrumentation engineer who was having difficulty fixing some relatively minor problems with an instrument at an important customer site. They decided to try using a version of the spectrometer software that they had been given to test and potentially glean customer feedback. However, the new version was never intended to get in the hands of real, live customers! Somewhat surprisingly this fixed the specific instrument problem the key account was having, and all were happy... for a while.

When the next regular update was due the key account customer obviously received the upgrade and were horrified to find that all the spectroscopic data they had measured in the last twelve months would no longer load. Unfortunately for the engineer and the important customer, the unreleased review copy of the software had also included an experimental, innovative new data storage concept which had failed at the pre-release testing phase and the vendor had reverted to the older tried and trusted storage file format. This truly beheaded the archived data and again cost a significant amount of money to recover from. I am not even going to attempt to discuss the compliance and data integrity issues this sort of mistake raises.

Survived

So how can the children of our spectrometer emulate Katherine Parr and survive all the potential pitfalls in their expected lifetimes? Well, many of the answers still lie in the FAIR principles and how to implement them in an analytical laboratory. One of the starting points would certainly be to assign all spectroscopic data sets a persistent unique identifier at birth [*FAIR Principle F1. (Meta)data are assigned a globally unique and persistent identifier and F3. Metadata clearly and explicitly include the identifier of the data they describe*]. This would make life much easier for researchers, supervisors, principal investigators, publishers and regulators alike. Even if, during the lifetime of the data set it, was separated from some of the critical metadata, so long as the unique identifier remained intact data archaeologists could always reinstate relevant metadata.

Now it may be wishful thinking at present, but if we look at many of the issues highlighted in the column above, keeping the metadata available would solve many of the problems commonly associated with the premature death of a data set—Accessibility Principal *A2. Metadata are accessible, even when the data are no longer available.* If correctly implemented would mean that it would always be possible to envisage metadata reinstatement as discussed above.

During a dataset's lifetime it will pass through many different software systems and rather than each stripping away metadata that it does not require for its specific operation—such as chemometric software only importing X-Y data pairs and ignoring the rest of the metadata—it should be possible that the original metadata is preserved with its own provenance and new processing should only add new metadata fully describing, maybe like a compliant audit trail, the actions that have been undertaken with the spectroscopic data. In this way the ability of subsequent researchers to reproduce a piece of scientific work published in the literature will be enhanced. We all need to stand on the shoulders of giants as Newton's famous metaphor confesses,[2] but there is still far too much published which belongs in the *Journal of Irreproducible Results*!

Finally, it is obvious that all we have discussed above, into the forensic investigation of the premature demise of spectroscopic data sets, revolves around misuse, mis-design, mis-deployment and mishandling of spectroscopic and general scientific data handling software. So, it was interesting to see the publication of FAIR principles for Scientific Software (FAIR4RS) at the end of 2022.[3] Unfortunately, there were no data sets or software code published with the paper although it does cite three software examples claiming to follow the FAIR4RS principles which could be worth following should you be interested.[3]

Where better to end than a quote purported to be from the great king himself, "*Of all losses, time is the most irrecuperable for it can never be redeemed*". So, let's not waste time generating spectra with artificially short lifetimes, let's get this FAIRification of scientific data done!

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TONY DAVIES COLUMN

Tony Davies is a long-standing *Spectroscopy Europe* column editor and recognised thought leader on standardisation and regulatory compliance with a foot in both industrial and academic camps. He spent most of his working life in Germany and the Netherlands, most recently as Lead Scientist, Strategic Research Group – Measurement and Analytical Science at AkzoNobel/Nouryon Chemicals BV in the Netherlands. A strong advocate of the correct use of Open Innovation.

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SAMPLING COLUMN

Danish geology icon Arne Noe-Nygaard picks up on an 800 years old sampling and invents the Replication Experiment: PAT in disguise

Kim H. Esbensen

Independent researcher, professor, owner KHE Consulting, Copenhagen, Denmark. www.kheconsult.com

This column showcases the extraordinarily versatile Replication Experiment (RE). Although presented and illustrated before within the professional sampling community, there are still many cases showing inspiring, didactic applications allowing a broader view on the types of "analysis" associated with sampling. Although so-called "economic geological processes" are of key importance within the traditional field(s) of sampling (TOS), i.e. mineralisations, ore exploration and mining, minerals processing, the column author and editor, here drags the reader into a realm very rarely visited in the sampling realm—academic geology. The present case could just as well have been termed "Danish medieval churches meet inspiring geologic icon inventing the RE independently of the TOS".

Arne Noe-Nygaard, Danish geologist (1908–1991)

Noe-Nygaard was a Nestor in Danish and Scandinavian geology through a long and very productive academic career. He was a professor for 40 years, also widely involved in popularising geology and was intimately involved in the founding of The Geological Survey of Greenland (GGU, now GEUS). His biography in Wikipedia is unfortunately only in Danish, but visit it anyway—lots of geology is communicated in pictures, images and maps, and his extensive oeuvre is liberally written in
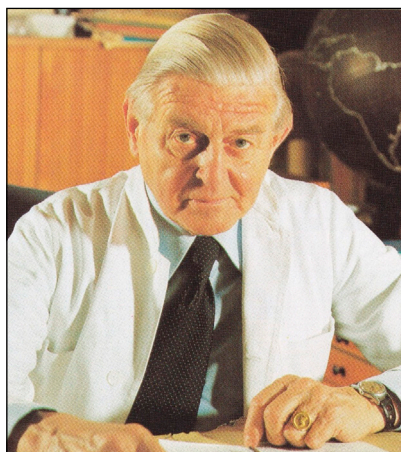
Figure 1a. Arne Noe-Nygaard at his desk at the Geological Museum, Copenhagen at the time of his retirement from a 40-year position as professor in dynamic geology at the University of Copenhagen. Photo: Preben Nielsen; reproduced with permission from GEUS.

English and German, scientifically spanning from the Pre-Cambrium era in Greenland and Denmark to

Figure 1b. Arne Noe-Nygaard. Photo: GEUS Archives; reproduced with permission.

the present (the Quaternary) with a focus on volcanology in Iceland, Greenland and the Faroe Islands, as well as many other topics, one of which is presented in the present column.

A most unusual sampling setting

The present exposé is based on what turned out to be

Noe-Nygaard's last book publication, titled *Larvikitter i Kvaderstenskirke* (DGU Publ. 1991) ISBN 87-88640-74-4 [*Larvikites in hewn stone churches*].[1]

Figure 2. Front page of *Larvikites in Hewn Stone Churches* published posthumously in 1991. Arne Noe-Nygaard died on 4 June 1991, but managed to edit the first proof of the book just before passing. An active geologist and scientist right up until the end.

Barely of book size (only 32 pages), it tells a fascinating geological detective story about the *provenance* of wall rocks in Danish medieval stone churches in northern and western Jutland. As the name implies, this type of church is built by square hewn rocks of local origin from the local landscape in medieval times. But their *ultimate* origin is much older—and this is the red line of this column.

The Romanesque hewn rock churches in Jutland were constructed in the period 1100–1200. There are still some 700 of them in a reasonably well-preserved state. In fact, this type of church is rather unique for the northern and western parts of Jutland, hardly found anywhere else in the world.[1,2] It is the professional historical view that the source for the rocks used for the original church building is *local*, i.e. they represent the surrounding

Figure 3. "Asp Kirke", Jutland, typical medieval Romanesque church illustrating the diverse assembly of hewn rock types. Note later improvement (enlargement) of windows, later lead roofing and addition of a bell tower.

landscape from where they were transported as short distances as possible before being hewn, probably at the church site. It is easy to compensate for later alterations and additions regarding improvements and modifications often with a distinct later architectural style, e.g. as seen in Figures 2 and 3 (enlargement of windows, lead roofing and addition of a bell tower). Compensating for this, the geologist Noe-Nygaard shared the belief that most of the original church walls in northern and western Jutland represent a well-preserved *sample* of the local rocks found on the surface at the time of building.

But why, and how did the medieval landscape come to be strewn with an abundance of boulders and rocks of a size that would suffice well for production of hewn rocks? This is where an underlying relationship between geology and religion has its origin. It is a fascinating story that involves "erratics"…

Erratics—composition, origin, glacial transportation

Of the use in everyday language (Meriam–Webster) has the following to say: "*Erratic* can refer to literal 'wandering'. A missile that loses its

guidance system may follow an erratic path, and a river with lots of twists and bends is said to have an erratic course. *Erratic* can also mean 'inconsistent' or 'irregular'. So, a stock market that often changes direction is said to be acting *erratically*; an erratic heartbeat can be cause for concern; and if your car idles erratically, it may mean that something's wrong with the spark-plug wiring".

In geology, however, this term is distinctly specific. Here *erratic* is used in one particular sense only, regarding composition, provenance and direction and distance travelled. Glacial *erratics* are stones and rocks that were *transported* by a glacier and were left behind after the glacier melted and retreated. Thus, glacial erratics were formed by erosion ("plucking") as a result from the flowing movement of ice over the local bedrock. Such erratics can range in size from pebbles to large boulders and can have been carried for hundreds of kilometres (800 km is an often quoted maximum). Scientists have a.o. used erratics to help determine ancient glacier movement(s), i.e. directions, distances and other local features. Particularly large erratics end up as marked landscape elements, Figure 4, sometimes associated
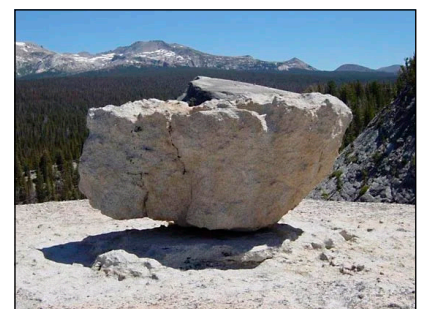

Figure 4. Archetypal "erratic". The composition of the conspicuous rock may be similar to the local rock types (short distance travelled only) but, much more often, is of markedly different habitus [travelled over long(er) distances]. Credlt: Daniel Mayer, Creative Commons Attribution-Share Alike 1.0 Generic, Encyclopædia Britannica

with much later local historical lore. **Of specific interest to the uninitiated reader, and directly related to the story in this column, is the fact that erratics** *differ* in composition and hence in appearance from the local bedrock upon which they are found; of course, mostly clear to the trained geologic eye. Erratics may be embedded in the fine-grained, ground up glacial deposits (called *till*), or, more often, occur as conspicuously independent "special" landscape elements on the bare ground surface.

Those transported over long distances generally consist of rock resistant to the shattering and grinding effects of glacial transport. Erratics composed of unusual and *distinctive rock types* can, by diligent and competent geologists, sometimes be traced to their source of origin and thereby serve as *indicators* of the direction of glacial movements. Studies making use of such *indicator erratics* have provided information on the flow paths of the major ice sheets in the ice age(s) of our planet (and indeed also on occasion the location of important mineral deposits). Erratics played an important part in the initial recognition of the most recent ice age(s) and their extent. Originally thought to be transported by gigantic floods or by ice rafting, erratics were first correctly explained in terms of glacial transport by the Swiss–American naturalist and geologist J.L.R. Agassiz in 1840.
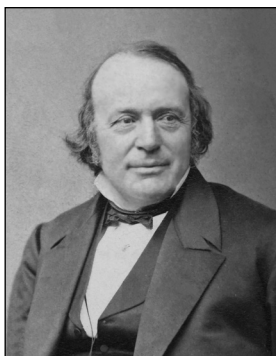
For more information, see the comprehensive entry on glacial erratics in Wikipedia: https://en.wikipedia.org/wiki/Glacial_erratic. In this widely covering entry on glacier-borne erratics, a wealth of examples are described, from Australia, Canada, Estonia, Finland, Germany, Republic of Ireland, Latvia, Lithuania, Poland the United Kingdom and the USA. Curiously, however, there is a distinct lacuna: Norway and Denmark are completely missing, which is a major affront to geologists from these two countries, something to be rectified with a friendly vengeance below!

Zooming in…

The reader is now in possession of the necessary subject-matter background for the *denouement* of this column. Here are the telling detective clues:

1) *Larvikite* is a distinct igneous rock formed by solidifying magma, not as a lava, but as a deep-seated intrusive magmatic body in the Earth's crust. Figure 8 below also shows the source area of known *larvikite* occurrences in Norway. Igneous rock types are named after the location of the occurrence of the type rock where and when it was first described scientifically.[a]

2) There are no occurrence of bedrocks of the larvikite type in Denmark—none!

3) But, very many hewn rock churches in the northern and western-most parts of the Jutland peninsula of Denmark contain a definite, identifiable proportion of larvikite rocks in their makeup. There are actually seven recognisable sub-types (varieties) of larvikite involved, which is for the professional geologists to keep track of, but no worries: Noe-Nygaard knew his larvikites!

4) So *how* come there were decidedly non-native, indeed "erratic" rock types to be found in the walls of medieval churches in Jutland? This was a major mystery at the time when the science of geology was developing in the 19th century. For example, it was suggested that major floods could have been responsible for such marked dislocations, but after the Agassiz breakthrough (1840), a modern understanding was quickly worked out: in earlier times large(r) parts of the continents in the northern hemisphere were covered (one, or several times) by thick sheets of ice, glaciers (really thick ice sheets, e.g. up to 3 km as in the present day inland ice sheet covering Greenland). Erratics were now envisaged as having been *transported* by the internal flow of ice masses during a specific (or possible recur-

Figure 5. J.L.R. Agassiz (1840). Photo: Wikipedia, Public Domain

[a]A few facts of interest:

1) Larvik (https://en.wikipedia.org/wiki/Larvik) is the birth town of the world renowned Norwegian explorer and historian **Thor Heyerdal** of Kontiki expedition fame.

2) The author of the present column also resided in Larvik for an extended period of time (1980–2000), from which grew a fascination with the particular rock type in question here. The city itself is immensely proud of its world renowned resources of dimension stone, in the form of polished façade rocks, a major export asset.

3) For a thorough description of the geology of larvikite, the comprehensive publication by Heldal *et al.* (2008) which, although written for professionals, can also be browsed with pleasure by interested parties: https://www.ngu.no/upload/Publikasjoner/Special%20publication/SP11_02_Heldal.pdf

rent) glacier event(s) during a specific *ice age*. An important part of this development is concerned with the evidence and the relics left by scouring *ice flows* interacting with the bedrocks over which it flows, plucking, plucking ...). There is an absolutely overpowering force at work at the bottom of thick ice flows.

5) So, it is no longer a mystery that, for example, larvikite erratics can now be found in Denmark several hundreds of km south of their point of origin; this picture is today well known and accepted. But the details of filling out this broad framework still leaves a lot of complex and highly fascinating questions, answers to which have been worked out by later generations of geologists, and this is where the legacy of Arne Noe-Nygaard's last book comes to the fore. Questions like from *which* of the three major ice ages that can be recognised in Denmark did this erratic complement of surface-found stones originate? (There are several other, intricate details involved here, which find their resolution at the end of Noe-Nygaard's account, but these can safely be left to the professional *connoisseurs* of Quaternary glacial geology). Here we leave such particulars and move fast forward to sampling and analysis in this fascinating context.

6) Noe-Nygaard's book gives readers a highly personal *tour de Jylland* in the form of numerical accounts of the assemblages of hewn rocks to be found in the makeup of the walls of the gamut of Roman churches, broadly constructed in the period 1100–1200. The final result of Noe-Nygaard's investigation is reproduced below as Figure 7, to be further commented upon.

In medias res: sampling and analysis

So, what kind of *sampling* was used in this story? And what kind of *analysis*?

One could perhaps imagine that church wall rocks were *sampled* in the traditional *field geological sense* with "field samples" brought to the laboratory for petrological, mineralogical and geochemical analysis with a view of identifying the different type of larvikite rocks and thus their proportions of the complete hewn rock church assembly. But no, the story is more interesting, and far more *personal* in a unique sense. In today's sampling and analysis terms as used in science, technology and industry, Noe-Nygaard unknowingly made use of what today is known as a "PAT-approach", although the concept of Process Analytical Technology was not to be established until years later than Noe-Nygaard's first field investigations.

A PAT aside

The key aspect of PAT is to perform sampling and analysis in one-and-the-same-operation. Within PAT the focus is nearly always on the many contending analytical modalities competing for attention and each claiming superiority, but there is also an underlying, unfortunately often unrecognised challenge, related to the role of the *sampling interface*.

The key characteristic of PAT is deployment of sensor technologies (physical probes, chemical sensors, other sensors) *intercepting* and *interacting* with a process stream. The key characteristic of PAT is that of performing sampling and analysis *simultaneously* as one unified process: probes and sensors interact analytically with an often small (sometimes minute) "effective volume" of the flux of matter which represents the support volume from which analytical signals are acquired. This is very often in the form of multi-channel spectroscopic

signals, which can be transformed into a predicted chemical or physical measurement, see, for example, the fundamental textbook by Katherine Bakeev, *Process Analytical Technology*,[3] in which *chemometrics* has made essential contributions by deploying the powerful multivariate calibration approach, e.g. Esbensen & Swarbrick.[4]

Methods and equipment of process sampling are front and centre in the realm of the Theory of Sampling (TOS). The TOS supplies a comprehensive, well-proven framework that derives all principles and implementation demands needed for **how to** extract representative *physical samples* from moving lots, i.e. from a conveyor belt or from ducted material streams. PAT aspires to take this situation over to the situation in which the task is **how to** extract representative *sensor signals* instead of physical samples.

For "sensor sampling", i.e. PAT, there is no similar foundational framework. Instead, a pronounced practical approach is evident in this realm, in which the question of **how to** achieve representative sensor signals is not so much related to the design and implementation of an appropriate sampling interface between the sensor and the streaming flux of matter. Rather, a survey of the gamut of sensor interfaces presented in industry and in the literature reveals a credo that appears to be: "Get good quality multivariate spectral data—and chemometrics will do the rest", exclusively relying on *multivariate calibration* of process sensor signals (multi-channel analytical instruments). There is a tacit misunderstanding that the admittedly powerful chemometric data modelling is able to take on and correct for any kind of sensor signal uncertainty—including "sampling errors". However, this leaves analytical representativity the victim of imperfect understanding of the nature of data

SAMPLING COLUMN

analytical errors (ε) vs sampling errors (TOS errors).

In the current PAT focus, representativity is wholly related to spectral and reference sample measurement uncertainty (MU) and to possible data modelling errors, which unfortunately ignores the geometric specifics of sensor signal acquisition in relation to the full cross-section of the streaming/ducted flux of matter even though this is the very domain where sampling errors occur in the exact same fashion as when extracting physical samples. The process sampling interface comes to the fore.

And this PAT framework relates to the rock assemblages in medieval Danish churches 800 years old—how?

Unknowingly, Arne Noe-Nygaard devised a quite similar *simultaneous* sampling and analysis approach, in his case in the form of field sampling and analysis all in one. But interesting, his field sampling was not the traditional geological sample collection for analysis in the laboratory.

Field rock identification: field sampling and analysis in one!

So here is how Noe-Nygaard went about his analysis, i.e. visual rock type identification (aka "rock classification"), based on decades of experience with this kind of rock in Scandinavia. Noe-Nygaard was a very experienced geologist able to recognise all the seven major kinds of syenitic rocks making up the family of larvikites.
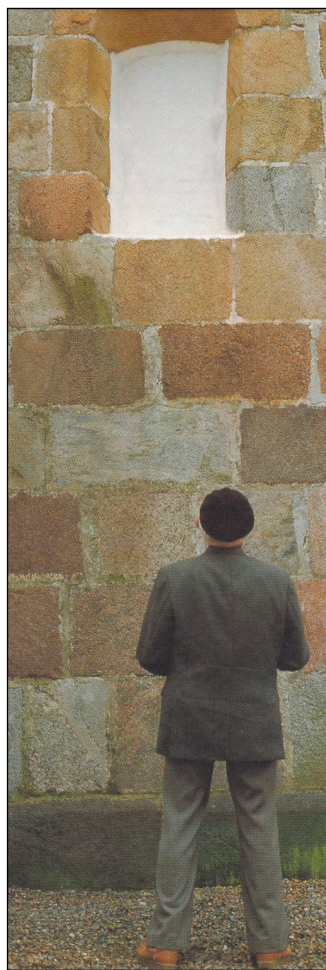
And now the story gets historical. The field sampling part (gathering the local surface rocks from the landscapes in Jutland) was undertaken by the original medieval church builders, who, with absolute certainty, were inspired and driven by *very different* motivations than science—masonry has it origin in the religious wish to build churches in which to worship. It was Arne Noe-Nygaard's inspired geological

brilliance to make explicit this hidden sampling aspect of medieval church building.[1,2] Sampling by religious proxy! Thus, each medieval church takes on the role as a (rather large) sample of local landscape boulders, the size of which amounts to the cumulative wall area of the lowermost 5–7(8) rock courses. In passing (a treat for TOS experts), one observes that samples of this type are comprised by very, very large "particles", making it imperative to be able to obtain a large enough square footage—the stated minimum of *ca* 500 rocks (see magazine front cover for a deliberate pointed focus).

Then, with a delay of some 800 years, fast forward to "analysis"—field rock identification, Figure 6.

"*As far as possible, I petrographically classified 500 rocks from each church involved in the investigation; this number could range between 300 and 800 depending on the local conditions (ambient light conditions, rock surface erosion, lichen overgrowth on north-facing walls). In churches with an appropriate number of available rocks, I usually restricted my work to the 4–5 lowermost rock courses. Identification of rock type up to eye-height must be considered as certain... Under less optimal conditions, classification uncertainty forced me to also observe a few courses higher up (to reach the stipulated 500 rocks). Classification certainty would in such cases have been less than normal, but still acceptable. Every year, at the start of the field campaign, I recounted ca 500 rocks in one or two of the churches visited previously without reminding myself of the earlier results.*

Deviations between two such counts larger than 10% were rare."

Figure 6. Geological maestro Arne Noe-Nygaard in the field, at work identifying (and counting) hewn rock types in a population of Romanesque medieval churches in Jutland.

From this field geological rock identification, the proportions of each larvikite rock (and, therefore, also their cumulative count) could easily be calculated as relative % w.r.t. all rocks counted for each church, which results were then plotted on a geographical map of Jutland, Figure 7.

To close the geological part of the story, Figure 8 shows the most recent ice age glacial flow direction patterns in southern Norway. For the reader not familiar with the geography and Quaternary geology of Scandinavia, Denmark is situated some 200 km south of the Norwegian glacial flow field shown. Herewith the connection between identifiable, diagnostic erratics from the area surrounding Larvik
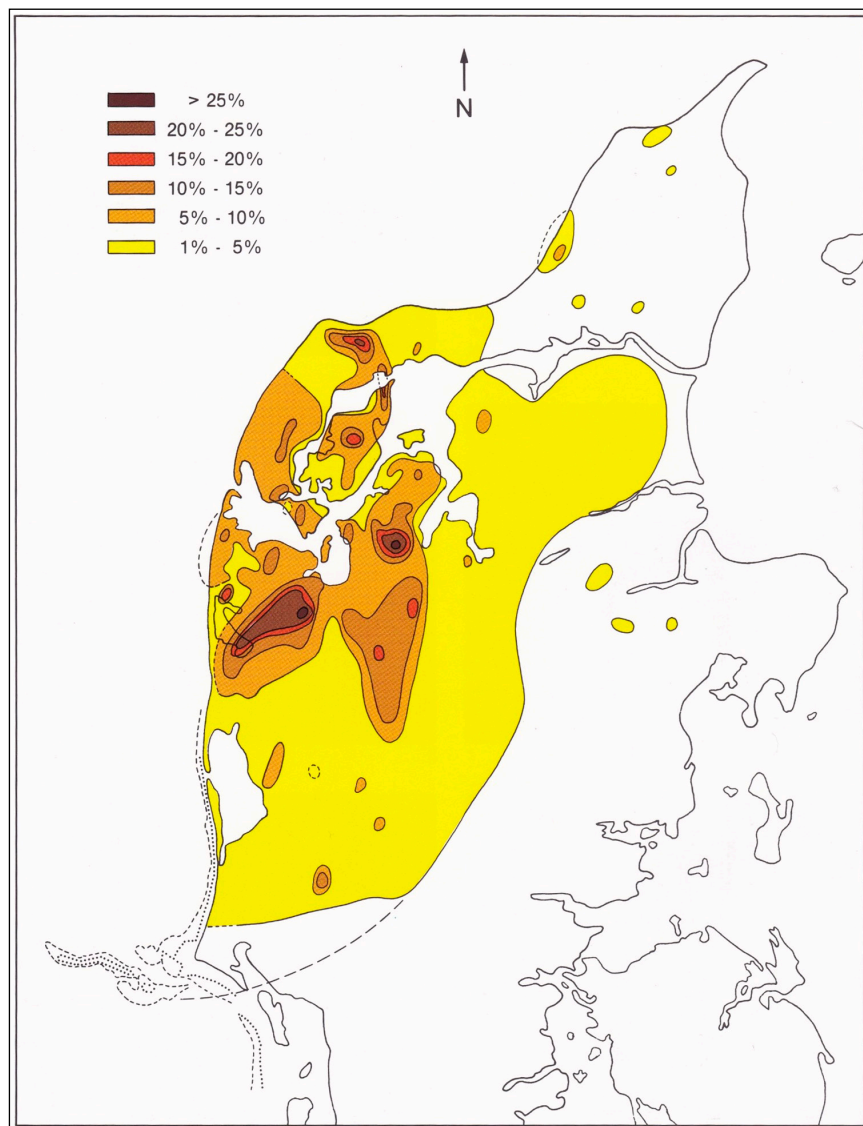
Figure 7. Relative % occurrence of larvikites (sum of all identifiable types) in Jutland hewn rock churches. The field work for this remarkable compilation was undertaken in a series of intermittent summer campaigns by Noe-Nygaard during his tenure as professor at University of Copenhagen, see Noe-Nygaard.[1,2]

Figure 8. Ice age glacial flow direction patterns in southern Norway, see Nesje *et al.* (1988).[5] Contours show the modelled surface of the glacier in late-Weichsel (*ca* 20,00 years ago). Illustration with permission from GEUS.

in southern Norway and medieval church rock assemblages in Jutland, Denmark, should be fully established and understandable for all, no specialised geological competence needed.

The TOS point: the RE
The point to this extensive geological introduction is the key theme of this sampling column, novel applications of the RE.

Noe-Nygaard was acutely aware that there was an inherent "analytical error" involved in his visual identifications (TAE in today's parlance of the TOS). Such was his awareness of his analytical performance that he devised his own RE. A translation (KHE) from the Danish in Noe-Nygaard (1991) is presented in Figure 6.

This is it! What a wonderful example of a conscientious scientist, aware that his professional classification performance (analytical performance) is associated with a significant non-zero uncertainty that must be considered. What is remarkable here is that,

for geologists, the ability to identify rock types (and mineral species) is a matter of intense *professional pride*—this is what distinguishes a competent field geologist. One does **not** question a geologist's rock identification competence!

And yet, in spite of his very impressive academic a.o. achievements, Arne Noe-Nygaard's example of professional self-awareness is a remarkable, humble reminder to all scientists, technologists and samplers of today!

But it is never an easy matter following the footsteps of a giant, Figure 9, not even for a geologist familiar with igneous rocks and who has lived 10 years in Larvik! A first foray comparison of performance uncertainty (RE%), performed during a summer 2019 vacation tour in Jutland taking in a number of beautiful medieval country churches, revealed just how good Arne Noe-Nygaard was to his *metier*. To be honest, and to Noe-Nygaard's legacy, his "<10%" RE uncertainty vastly outshined the score for the hopeful contemporary geologist in Figure 9 (IF the reader

SAMPLING COLUMN

Figure 9. "So how difficult can it be?" if one believes one is familiar with syenites from southern Norway, that is. The author of this column could not resist this temptation when driving past an especially inviting hewn rock church during a summer holiday in 2019. Not surprisingly, it turned out to be quite a challenge to even *try* to best the master geologist Noe-Nygaard, RE < 10 %.

must ask, the answer is "a considerable larger percentage").

Conclusion

The RE is a very versatile facility for evaluating the total uncertainty [TSE + TAE] of any measurement system in which sampling plays a role. While RE has a plethora of manifestations within traditional sectors in technology, industry, commerce, trading and society, this column treated an unusual application of *RE thinking* hidden away in a most unsuspected niche in academic geology. A famed Danish geologist devised his very own PAT-like sampling-analysis confluence spanning no less than 800 years. What's not to like?

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Kim H. Esbensen, PhD, Dr (hon), has been research professor in Geoscience Data Analysis and Sampling at GEUS, the National Geological Surveys of Denmark and Greenland (2010–2015), chemometrics & sampling professor at Aalborg University, Denmark (2001–2015), professor (Process Analytical Technologies) at Telemark Institute of Technology, Norway (1990–2000 and 2010–2015) and professeur associé, Université du Québec à Chicoutimi (2013–2016). From 2015 he phased out a more than 30-year academic career for a new quest as an independent researcher and consultant. But as he could not terminate his love for teaching, he is still very active as an international visiting, guest and affiliate professor. A geologist/geochemist/metallurgist/data analyst of training, he has been working 20+ years in the forefront of chemometrics, but since 2000 has devoted most of his scientific R&D to the theme of representative sampling of heterogeneous materials, processes and systems: Theory of Sampling (TOS), PAT (Process Analytical Technology) and chemometrics. He is a member of several scientific societies and has published over 250 peer-reviewed papers and is the author of a widely used textbook in Multivariate Data Analysis (35,000 copies), which was published in its 6th edition in 2018. He was chairman of the taskforce behind the world's first horizontal (matrix-independent) sampling standard DS 3077 (2013). He is editor of the science magazine *TOS forum* and this Sampling Column. In 2020 he published the textbook: *Introduction to the Theory and Practice of Sampling* (impopen.com/sampling).
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APPLICATIONS

Raman and SERS identification of a combination prescribed opioid

Handheld Raman spectrometers are valued for their ability to provide onsite material identification in seconds. A simple point-and-shoot analysis of bulk materials with the handheld MIRA DS results in chemical identification accompanied by both statistical support and relevant colour-coded warnings. In the case of combination pharmaceuticals, a single tablet contains more than one active ingredient in different proportions. MIRA DS can identify multiple compounds in such tablets by using Raman to identify the major component and SERS (surface-enhanced Raman spectroscopy) for the minor component.

This application describes quick, dual analysis of a prescription medication containing acetaminophen and hydrocodone. The application is easily extrapolated to the study of street drugs. With MIRA DS, forensic analysis of tablets reaches a whole new level of accuracy.
Metrohm

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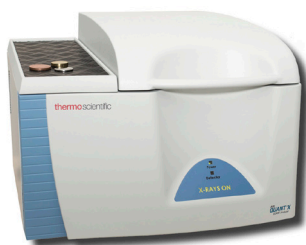
Analysis of nutrients in milk-based powders by EDXRF

A variety of analytical techniques are used in the food industry to determine the nutritional value of milk-based powders (e.g., infant formula), which consist of milk powder with added nutrients. Examples of nutrients found in these "fortified" milk powders include proteins, fats, carbohydrates, vitamins and minerals.

Energy-dispersive X-ray fluorescence (EDXRF) is used near the production line to control the elemental content of milk-based powders. A fast and straightforward sample preparation combined with short measurement times help to optimise production processes and minimise turn-around time. In this application note, the elements that are monitored with EDXRF include Na, Mg, P, Cl, K, Ca, Mn, Fe, Cu and Zn.

Na and Mg remain challenging elements for EDXRF due to their lower sensitivity. Here, we show that substantial improvement in their detection efficiency can be made when using a silicon drift detector (SDD) with a graphene window.
Thermo Fisher Scientific

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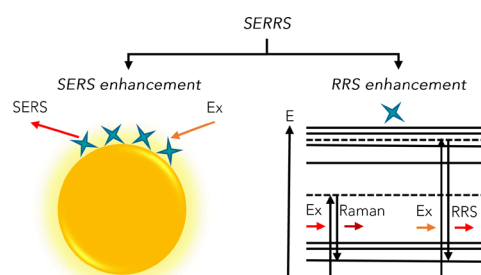
Characterisation of SERRS nanoparticles using UV-vis and Raman spectroscopy

Surface-enhanced resonance Raman scattering (SERRS) is a technique that offers unparalleled sensitivity and specificity in non-destructive spectroscopic detection. It is a combination of surface-enhanced Raman scattering (SERS) and resonance Raman spectroscopy (RRS), two techniques that are individually used to overcome the inherent weakness of Raman scattering. SERRS occurs when an analyte, with an electronic transition frequency matching that of the excitation laser, is adsorbed on or near a roughened metal surface, such as that of a noble metal nanoparticle (NP). The theoretical Raman signal enhancements achievable using SERRS are orders of magnitude greater than SERS and RRS alone, meaning that analytes of interest can be detected at very low concentrations. The technique is becoming increasingly popular in the fields of medical diagnostics and food science and is applied primarily via labelling methods that couple resonant Raman reporters with bioconjugation moieties using optically tuneable nanoparticles. Such labelling methods can be applied to the detection of biomarkers in immunoassays, microfluidic devices and lateral flow testing, and when coupled with Raman microscopy, they can be utilised in the tracking of novel drugs or biomarkers in mammalian cells.
Edinburgh Instruments

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APPLICATIONS
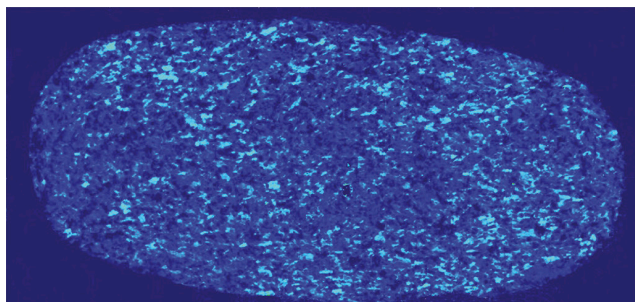
Content uniformity verification by IR laser imaging

The production of pharmaceutical tablets is a multi-stage process that includes powder processing, milling, granulating, mixing and compacting. Nevertheless, hundreds of thousands of tablets are produced per hour in modern, high-throughput production facilities. Variations in the process parameters, however, can strongly influence the composition of the tablets and thus their quality. It is not only the total content of active ingredients and excipients that is important, but also their granularity and distribution within the tablet.

Pharmaceutical products naturally require maximum product uniformity to ensure consumer safety for each individual tablet. Therefore, an analytical method is required that captures all relevant quality parameters in a short time enabling complete characterisation of a tablet's properties to optimise production processes and assure quality.

The application of (Fourier transform) infrared spectroscopy in pharmaceutical quality control is already well established. In this process, the unique spectral infrared absorption signature is used for unambiguous chemical identification.

Bruker Optics

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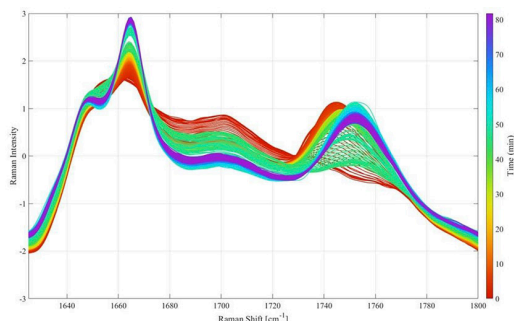
Enhancing pharmaceutical formulation development through the use of high performance Raman spectroscopy

Applying meaningful real-time analysis techniques to novel drug delivery systems can often be challenging. However, the ability to verify the physicochemical properties of these formulations both in the development phase and during production is critical. With a delivery system that involves drug inclusion in a carrier molecule, the verification of that inclusion is vital to the maintenance of the pharmacological integrity of the formulation. The work shown in this paper suggests that Raman-based spectrometers enabled by the High-Throughput Virtual Slit (HTVS) can be useful for *in situ* real-time verification of the inclusion complex formation. This makes it a potentially valuable PAT tool for the verification of the proper manufacture of these formulations.

Tornado Spectral Systems

⬇ **DOWNLOAD NOTE**

Pesticide detection on apple skin using SERS

Protecting food crops is vital to the world's food chain, and pesticides are a critical tool to kill, repel and control pests. Two million tonnes of pesticides are used annually worldwide, with this predicted to increase over time. However, pesticides can cause severe environmental issues to aquatic systems, wildlife (e.g., bees), air and soil. Additionally, the reported effects of pesticides on human health range from short-term, such as skin irritation and headaches, to chronic effects, such as asthma and cancer. There are also concerns about the consequences of consuming pesticides from the small, but repetitive, doses in our diet.

One method to reduce the dangers of pesticides is limiting the allowed concentration used on crops. This is controlled by analysing the crop and determining the level of pesticide present. Apples are one of the most pesticide-treated fruits and as such producers have a list of regulations they must abide by for sale to the public.

Phosmet is an organophosphate insecticide used on apple trees to control codling moths, the 2018 Code of Federal Regulations set the pesticide residue tolerance on apples of phosmet as 10 ppm. High-performance liquid chromatography, mass spectrometry and gas chromatography are currently the most used techniques for testing down to low concentrations. However, these are time-consuming and costly, and Raman spectroscopy offers several advantages such as rapid and non-destructive fingerprint-like identification with little to no sample preparation.

Surface enhanced Raman scattering (SERS) is an enhancement technique used with Raman spectroscopy

APPLICATIONS

to provide lower limits of detection. SERS offers a signal enhancement of up to 10^{10}–10^{15} and also advantageously quenches the fluorescence of analytes. Commercial SERS substrates are readily available, making SERS an accessible technique for low-concentration detection. In this application note, residual phosmet insecticide on apple skin is detected using SERS.
Edinburgh Instruments

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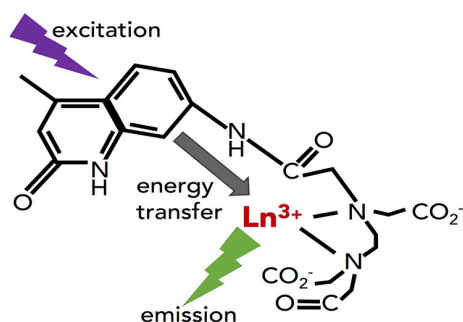
Photoluminescence of lanthanide-based optical probes

Luminescent optical probes based on lanthanide chelates have attracted particular attention over the last decades in the biomedical field due to their versatile magnetic and photoluminescent properties. Lanthanides exhibit large Stokes shifts and, therefore, reabsorption effects can be avoided. Their narrow emission bands allow for excellent spectral discrimination, they are resistant to photobleaching, and time-resolved detection can be facilitated thanks to their long photoluminescence lifetimes in the millisecond time regime. These characteristics make lanthanides useful for numerous applications. These include their broad employment in molecular imaging, such as in magnetic resonance imaging (MRI) as contrast agents. Lanthanide nanoparticles have been widely used in high-sensitivity immunoassays as well as in the detection and imaging of fingerprints.
Edinburgh Instruments

⬇ DOWNLOAD NOTE

Quality control of Bromobutyl rubber

Products made from either natural or synthetic rubber are a vital part of everyday living. Synthetic rubbers offer superior thermal stability and resistance to oxidising

agents and oils. One synthetic rubber uses Bromobutyl (BIIR), a copolymer of isobutylene and small amounts of brominated isoprene that provides unsaturated vulcanisation sites. Bromobutyl rubber is derived from halogenating butyl rubber with bromine in a continuous process. This elastomer has many of the attributes of butyl rubber, but the addition of bromine improves adhesion to other rubbers and metals, resulting in substantially faster cure rates (i.e., lower amounts of curative agents are required).

Usually, the determination of the bromine content and other quality parameters (e.g., Mooney viscosity, volatile content, calcium stearate content and functional bromide) requires various reagents and time-consuming analytical methods. However, near infrared spectroscopy offers rapid and reliable simultaneous quantification of those parameters in Bromobutyl rubber without the use of chemicals.
Metrohm

⬇ DOWNLOAD NOTE

Hiden Analytical launches new dissolved species applications catalogue

Hiden Analytical has published its new dissolved species applications catalogue. The catalogue showcases Hiden's solutions for analysing dissolved species in liquids, providing customers with a comprehensive guide to Hiden's dissolved species analysis technologies used in real-world applications.

The new catalogue features detailed information on Hiden's dissolved species analysis technologies, with highlighted applications being oceanic trace gas measurements, enzyme activity studies and environmental research. In-depth case studies of these applications demonstrate the performance and capabilities of Hiden's solutions in real-world applications.
Hiden Analytical

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APPLICATIONS
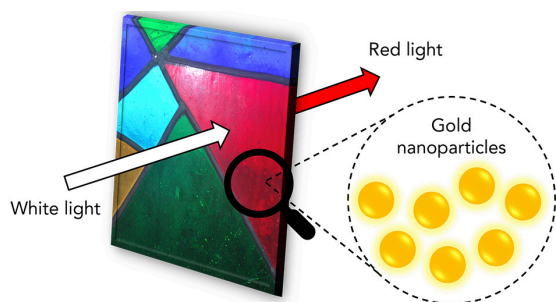
UV-vis spectroscopy for characterising the optical properties of gold nanoparticles

The use of gold nanoparticles (AuNPs) predates the scientific revolution and they have also been used frequently in stained glass windows. A nanoparticle (NP) is defined as a particle with at least one dimension between 1 nm and 100 nm in size. Metallic NPs have become abundant in scientific research because they exhibit interesting and tuneable physical, optical and chemical properties when compared with their bulk metal counterparts. This is true of AuNPs in particular, which have optical properties that are easily manipulated and related to their physical state and chemical environment. This means that they can be precisely engineered for a wide range of different applications.

Today, colloidal AuNPs are particularly useful for colourimetric and optical detection applications because they are efficient at absorbing and scattering light and can be tuned to exhibit optical activity at different wavelengths based on their physical and chemical characteristics. More specifically, they are capable of supporting a localised surface plasmon resonance (LSPR), caused by a displacement and coherent oscillation of the conduction electrons on the NP surface at a particular frequency when excited by incident light. The LSPR is an extremely useful parameter for optical sensing because its frequency depends strongly on several factors including NP size, NP morphology, interparticle distance and the refractive index of the surrounding dielectric medium, which can all be designed to change in response to an external variable in a detection assay. The optical properties of AuNPs are traditionally probed using UV-vis spectroscopy because it is an excellent technique for characterising a sample's response to light over a large wavelength range and the LSPR appears on the absorption spectrum of AuNPs as a distinct peak. Hence, in this application note, the optical properties of AuNPs are investigated using UV-vis spectroscopy. First, the LSPR of spherical colloidal AuNPs is investigated as a function of particle diameter. Then, the chemical sensing potential of AuNPs is demonstrated by tracking the LSPR during an induced aggregation experiment.
Edinburgh Instruments

⬇ DOWNLOAD NOTE

Choosing a portable Raman spectrometer

A good portable Raman spectrometer bridges the gap in performance, capability and size between handheld and benchtop Raman spectroscopy. It enables new point-of-use applications in medicine and industry by providing high sensitivity and dependable answers in a compact, cost-effective footprint. These qualities are important to both researchers and OEM instrument developers, particularly for applied research and commercialisation of new technologies. Medical diagnostics, environmental monitoring, and quality and process control in the food chain, energy industry and manufacturing are all beginning to harness the power of portable Raman spectrometers to provide sensitive and specific answers to difficult questions. Raman is also being used as a complementary diagnostic within other systems, from high-end research tools to machine inspection and surgical instruments.
Wasatch Photonics

⬇ DOWNLOAD NOTE

Photoluminescence Spectroscopy of Quantum Dots
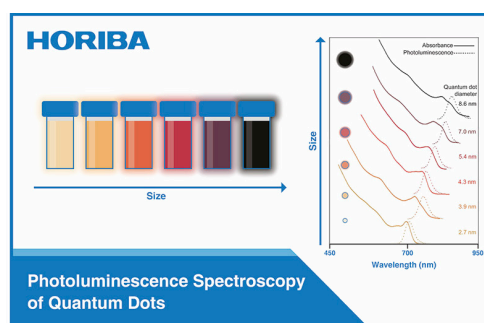
Photoluminescence spectroscopy of quantum dots

Quantum dots have potential applications in optoelectronics, biosensing, bioimaging, memory devices and light sources. In this application note featuring the FluoroMax Plus® spectrofluorometer, HORIBA shows that alloyed CdSeTe quantum dots have a non-linear change in their emission spectra, which is dependent on their size and composition. The QDs' emission can be as long as 850 nm, which could find application *in vivo* imaging, thanks to the greater penetration depth of NIR light.
HORIBA

⬇ DOWNLOAD NOTE

APPLICATIONS

New strategies for obtaining the SERS effect in organic solvents

The combination of electrochemistry (EC) and surface-enhanced Raman scattering (SERS) has received growing attention over the past several years due to the powerful features associated with the EC-SERS effect. In particular, the electrochemical activation of metal electrodes allows the generation of SERS substrates which in turn enhance the Raman intensity in a single experiment.

Many electrochemical methods have been developed but are traditionally limited to aqueous media. Raman spectroelectrochemistry in organic solutions is an interesting alternative, but developing new EC-SERS procedures is still required.

This application note demonstrates that the electrochemical activation of gold and silver electrodes enables the detection of dyes and pesticides in organic media.
Metrohm

⬇ DOWNLOAD NOTE

PRODUCT FOCUS

Product Focus on Imaging Spectroscopy

Bruker Optics GmbH & Co. KG
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info.bopt.de@bruker.com
www.bruker.com/optics

FT-IR Microscope LUMOS II
Applications:
- QA/QC
- Microspectroscopic failure analysis
- Microplastic analysis
- Plastic and polymer
- Particle & surface analysis
- Pharmaceuticals

Key features:
- Plug & play
- No dry-air purge
- Standard TE-MCT detector
- Optional FPA-imaging detector
- Fully motorised and automated hardware

MORE INFORMATION »

FT-IR and Laser Imaging Microscope HYPERION II
Applications:
- Materials research
- Tissue Imaging
- Forensics
- Chemicals
- Polymers
- Art & conservation

- Life science

Key features:
- FT-IR microscopy
- IR Laser and FT-IR imaging
- Sample flexibility
- UV/VIS
- NIR
- Binoculars

MORE INFORMATION »

DRS Daylight Solutions

Tel: +1-858-432-7643
taylor.stathopoulos@drs.com
https://daylightsolutions.com/

Spero QCL-IR Microscope
DRS Daylight Solutions, pioneers in QCL-IR technology, developed the first wide-field QCL-IR microscope to operate across the important spectral fingerprint region (5–11 µm). The Spero® QCL-IR microscope delivers high-throughput and high-sensitivity infrared microscopy. Spero microscopes have been field-tested in demanding applications, spanning tissue diagnostics and cancer research to characterising novel metamaterials and environmental microplastics.

MORE INFORMATION »

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

Headwall Hyperspectral Sensors from UV-VIS to SWIR
Headwall's Hyperspec® family of hyperspectral sensors and imaging systems are small, light, and rugged. The elegant all-concentric design uses precisely engineered master-quality holographic diffraction gratings made

in our own world-class cleanroom facilities to deliver outstanding signal-to-noise and spectral and spatial resolution, and a wide, aberration-corrected field of view.

Headwall® spectral instruments provide differentiated solutions for the remote sensing, advanced machine vision, medical/biotech and defence/security markets.

MORE INFORMATION »

Headwall Optical Components & Assemblies for OEM Instrumentation
Headwall has decades of experience taking a concept from idea to design, prototyping, validation, optimisation, verification and to mass production. We are with you all the way as a trusted hyperspectral imaging OEM partner with thousands of OEM products in the field and on the benchtop. Headwall-manufactured gratings, spectrographs and spectrometers maximize the quality of UV-VIS-NIR analysis. Each grating is an original piece. These master-quality gratings feature superior spectral and spatial resolution and extremely low scatter, meeting the demands of your high-performance instrument. We have more than 40 years of experience producing gratings and spectral engines for ourselves and for our OEM customers.

The addition of Holographix, industry leader in the replication process for a variety of products requiring the highest levels of quality adds a new capability. For over two decades, Holographix has focused on micro- and nano-structure replication of high-performance, custom-designed photonic solutions for the life sciences, semiconductor, aerospace & defense and metrology markets.

MORE INFORMATION »

Headwall Industrial Machine Vision Sensors & Systems

Introducing the newest member of the family of Headwall sensors, the Hyperspec MV.X. Hyperspectral systems have historically faced significant hurdles in industrial deployment due to the need to handle vast amounts of raw data as well as the complexity of model development. Headwall's award winning MV.X technology platform overcomes these obstacles by combining a high-performance spectrometer with powerful embedded computing to extract actionable results in real time.

The Hyperspec® MV.C combines exceptionally small size and light weight with high spatial and spectral resolution (342 spectral bands, 1024 spatial pixels). USB 3.1 connectivity is standard, with an SDK for your OEM application. Hyperspec® MV.C NIR brings reliable and intuitive operation to industrial inspection and detection. The MV.C NIR can be directly controlled using perClass Mira®, a powerful yet easy-to-use software package that dramatically simplifies interpretation of hyperspectral images collected. Spectral-classification models can be applied in real time, enabling fast and accurate inspection and detection along processing lines of all kinds.

MORE INFORMATION »

HORIBA

HORIBA UK

Tel: 01604 542500
enquiries.uk@horiba.com
https://www.horiba.com/gbr/

FLIMera—A New Concept in FLIM Imaging

The FLIMera camera is a new concept in FLIM technology: a wide-field imaging camera, rather than a confocal point scanning system, with the intrinsic benefit of acquiring FLIM dynamics at video rates, with time-correlated single photon counting measurements acquired independently in each pixel.

MORE INFORMATION »

PIKE Technologies

Tel: 608-274-2721
tdespins@piketech.com
https://www.piketech.com/

Refractive Objectives

PIKE Technologies' high NA, refractive microscope objectives uniquely target the near and mid-IR spectral region. For these multi-lens objectives, applications include imaging in the mid-IR fingerprint region and thermal imaging—all at micron-level resolution. Available in 5×, 10×, 20×, 25×.

MORE INFORMATION »

Reflective Objectives

PIKE Technologies' high NA, reflective microscope objectives deliver a high resolution with optimal brightness, targeting the full spectral range. These objectives are ideal for IR microsampling and imaging of micron-level spot sizes. Available in 15×, 20×, 25×, 40× and 100×.

MORE INFORMATION »

Diamond Pen Cutter

The Diamond Pen Cutter is a portable knife for sectioning both hard and soft biological and industrial materials. Its ultra-sharp blades are made of natural diamond, providing extraordinary sharpness and wear resistance for consistent and controlled cuts. Flat and angled (45°) blades are available.

MORE INFORMATION »

Quantum Design UK and Ireland

Tel: 01372 378822
info@qd-uki.co.uk
www.qd-uki.co.uk

Specim IQ Hyperspectral Imaging Camera

Specim IQ is a portable hyperspectral camera, where data capturing, data processing and result visualisation are integrated into a one ready-to-use package. The camera is able to screen the imaging target and show the results on the camera display in just seconds. The weight of the camera, 1.3 kg containing a chargeable battery and a memory card for data storing, allows true portability for imaging in locations, where it has not been possible before.

MORE INFORMATION »

Specim FX17 Hyperspectral Imaging Camera

The FX17 is a small footprint hyperspectral camera built around an InGaAs detector. It operates in the NIR spectral range (900–1700 nm). As with the FX10 camera, F/1.7 optics enables excellent light throughput, high sensitivity, short integration times and high signal-to-noise ratio. The FX17 operates with a frame rate of 670 fps (full frame) using 640 spatial pixels and 230 spectral bands. By reducing the number of spectral bands, the frame rate can be increased up to 15,000 fps. The camera is supplied with a high quality lens (38 deg FOV) and includes an integrated shutter. The camera is also IP52 rated, making it suitable for use in harsh environments.

MORE INFORMATION »

Specim FX10 Hyperspectral Imaging Camera

The FX10 is a compact, lightweight, cost-effective hyperspectral camera for the VNIR spectral range (400–1000 nm). F/1.7 optics enables excellent light throughput, high sensitivity, short integration times and high signal-to-noise ratio. The FX10 operates with an impressive frame rate of 330 fps (full frame) using 1024 spatial pixels and 220 spectral bands. By reducing the number of spectral bands, the frame rate can be increased up to 9900 fps. The camera is supplied with a high quality lens (38 deg FOV) and includes an integrated shutter and order sorting filter. The camera is also IP52 rated, making it suitable for use in harsh environments.

MORE INFORMATION »

PRODUCT FOCUS

Thermo Fisher

Tel: +1-608-276-6100
liz.steiner@thermofisher.com
thermofisher.com

Thermo Scientific Nicolet RaptIR FTIR Microscope

Rapidly locate and identify trace materials, inclusions, impurities, microparticles and the distribution of materials within a sample with incredible clarity and precision. Its clean, adaptive user interface provides increased flexibility and usability for all users, from specialists to novices.

See it fast. Identify it faster.

MORE INFORMATION »

Thermo Scientific Nicolet iN10 MX Infrared Imaging Microscope

The Nicolet iN10 MX Infrared Imaging Microscope is easy to use and provides the power required to rapidly acquire and analyse chemical images to enhance your understanding of the chemical distribution of materials in heterogeneous samples.

- Ultra-fast MX imaging detector
- Three detector options: DTGS, MCT-A and the 16-element MCT array

MORE INFORMATION »

Thermo Scientific DXR3xi Raman Imaging Microscope

Get a high-performance, high-spatial resolution Raman imaging system in a complete, integrated package. The DXR3xi Raman Imaging Microscope provides stunning chemical images and quick research-quality results for users of every experience level.

MORE INFORMATION »

TOPTICA Photonics AG

Tel: 08985837-0
sales@toptica.com
https://www.toptica.com/

TOPO: CW OPO Laser System for mid-infrared Spectroscopy

TOPO: State of the Art Mid IR Tuneable Laser Technology for Spectroscopy Mid-infrared tuneable lasers between 2 μm and 5 μm are necessary tools for applications like high-resolution molecular spectroscopy and gas sensing, mid-infrared integrated photonics, optical component characterisation and quantum optics. For this reason, TOPTICA has developed a continuous wave optical parametric oscillator (OPO) that delivers the widest coverage of any MIR laser in this wavelength range. This system, the TOPO, has high power and narrow linewidth, and is capable of fast phase and frequency modulation necessary for sensitive gas-phase MIR spectroscopy techniques.

The TOPO fills a critical gap in existing continuous wave laser technology. TOPTICA offers various tuneable diode laser platforms to provide wide wavelength coverage below 2 μm. Wavelengths longer than 4 μm can

be generated by quantum cascade lasers. Interband cascade lasers are the only laser diode technology with direct emission between 2 μm and 4 μm, and these lasers tend to have very small tuning ranges (few nm) and low output power (1 mW). The TOPO relies on TOPTICA's long experience with efficient non-linear frequency conversion of diode lasers to generate a high power MIR laser with wide tuning range.

Ideal tool for direct tuneable laser absorption spectroscopy

MORE INFORMATION »

TopMode: Powerful and Coherent Diode Lasers—from 375 nm to 515 nm

TOPTICA's TopMode lasers operate as easily as a HeNe, but also offer higher power and the choice of wavelength. The TopMode series sets records in terms of power, coherence and wavelength stability. The proprietary CoHerence-Advanced Regulation Method (CHARM) provides an active stabilisation of the lasers' coherence and ensures continuous single-frequency operation. TopMode and CHARM means nothing less than reliable 24/7 operation.

The short wavelengths provided by our TopMode lasers are particularly well-suited to Raman spectroscopy of inorganic materials, for which no fluorescence obscures the Raman signal. Raman intensity depends on the excitation wavelength by a factor $1/\lambda 4$. TopMode lasers allow strong Raman signals that remain detectable by Si-based detectors.

MORE INFORMATION »

PRODUCT FOCUS

TopWave 229: Industrial CW Laser for DUV Raman

The TopWave 229 is an exciting new choice for deep UV spectroscopists looking for an easy to use and reliable laser that enables the user to focus on their application rather than worrying about the light source. With its short wavelength and an ultra-narrow laser linewidth ($<1\,MHz$–$<4\times10^{-5}\,cm^{-1}$), the TopWave 229 provides the key features to take on an important role as excitation source in the field of deep UV Raman and deep UV fluorescence spectroscopy.

Excitation below 250 nm is crucial for fluorescence-free Raman, as this avoids the overlap between the spectral regions of the Raman signal and the native fluorescence. Compared to fluorescence, the Raman effect is orders of magnitude weaker, so that even minimal fluorescence is sufficient to mask Raman emission. Fluorescence spectroscopy also benefits from the 228.5 nm emission, because it allows the detection of molecules with fluorescence spectra in the range $\leq270\,nm$, which can only be excited with shorter wavelength light. As a CW laser system, the TopWave 229 offers another advantage: it avoids non-linear and saturations problems common with pulsed laser sources.

The compact footprint and low heat dissipation of the TopWave 229 laser head allow for easy integration in space restricted and temperature sensitive application environments. Comfortable, hands-off operation over the system lifetime (typ. 10,000 hrs) is ensured by fully automated optimisation routines for the internal opto-mechanics. In order to provide best reliability and consistent, diffraction limited beam quality ($M^2 < 1.3$), the complete UV beam path is enclosed in a specially sealed compartment.
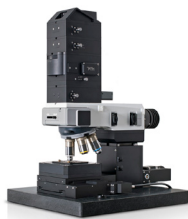
MORE INFORMATION »

WITec GmbH
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info@WITec.de
www.witec.de

alpha300 R – Confocal Raman Imaging Microscope
- Materials science
- Pharmaceutical research
- Life science
- Geosciences
- Battery research
- Particle analysis
- Unmatched speed, sensitivity & resolution—simultaneously
- Confocal setup for 3D image stacks and depth profiles
- Acquires a complete Raman spectrum at each image pixel
- Upgradeable to AFM/SNOM

MORE INFORMATION »

alpha300 apyron – Fully Automated Raman Imaging Microscope
- Materials research
- Pharmaceutics
- Forensics
- Life science
- Geoscience
- Unprecedented accessibility
- Easily configurable experimental workflow
- Polarisation rotation in excitation and detection available
- Capable of remote operation

MORE INFORMATION »

alpha300 Ri – Inverted Raman Imaging Microscope
- Life sciences
- Biomedical research
- Living cell analysis
- Aqueous samples
- Inverted beam path for quick measurements of liquid samples
- Compatible with other microscopy techniques: fluorescence, DIC and phase-contrast
- No sample staining required

MORE INFORMATION »

RISE Microscopy – Correlative Raman and SEM System
- Materials research
- Pharmaceutics
- Nanotechnology
- Life science
- Geoscience
- Correlative Raman-SEM imaging within a common vacuum chamber
- Automated switching between Raman and SEM measurements
- Quick correlation of results and image overlay

MORE INFORMATION »

PRODUCT FOCUS
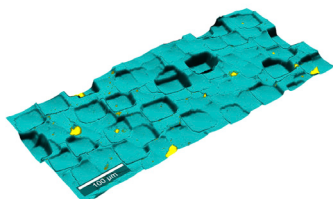
TrueSurface – Topographic Raman
Imaging Microscopy

- Large-area investigations
- Characterisation of roughly textured, curved & inclined surfaces
- Integrated optical profilometer
- Precise tracing of the sample surface while acquiring Raman imaging data
- Maintains focus during very long measurements

MORE INFORMATION »

NEW PRODUCTS

INFRARED

Edinburgh Instruments launches new IR5 FT-IR spectrometer

Edinburgh Instruments has released its new bench-top FT-IR spectrometer, the IR5, designed and manufactured at their global headquarters in Scotland. The IR5 is the first Fourier Transform Infrared (FT-IR) spectrometer from Edinburgh Instruments. The IR5 is a modern, high-performance benchtop FT-IR instrument which can be configured with a second detector or with Fourier Transform Photoluminescence (FT-PL) capability. The FT-PL option transforms the IR5 into a combined absorption and PL spectrometer in the MIR range, suitable for the most demanding research applications.

It has high sensitivity and spectral resolution, the Fourier Transform Photoluminescence upgrade with a choice of laser source and the option for a second detector giving higher sensitivity at selected spectral ranges. Simple operation makes it suitable for all user levels, from beginner to advanced, no maintenance is required with moisture control technology and it runs on modern, powerful and intuitive Miracle™ software designed specifically for the IR5.

Edinburgh Instruments

▶ https://link.spectroscopyeurope.com/670-P1-2023
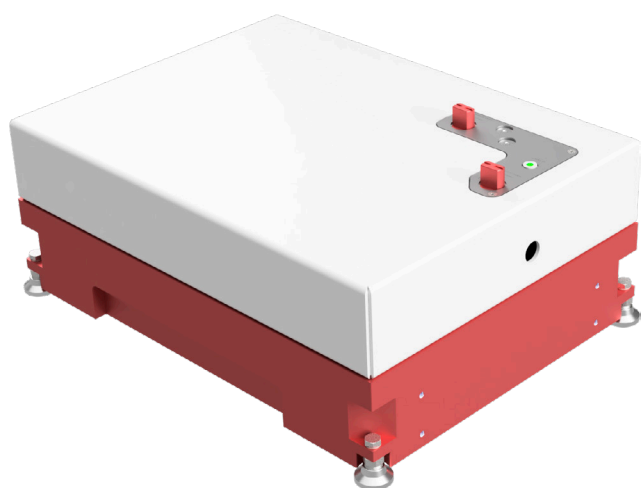
Cost-efficient mid-infrared dual-comb spectrometer

IRsweep has released release its latest spectrometer product, the IRis-C. It utilises dual-comb spectroscopy and quantum cascade laser frequency combs and is more compact, less complex and, with prices starting in the five-digit range (EUR/USD), significantly more cost-effective. Similar to IRsweep's previous dual-comb spectrometers, the IRis-C offers a unique combination of high speed, high signal-to-noise ratio per time, as well as optical power.

The new spectrometer is based on dual-comb spectroscopy—a Nobel-prize winning method that provides high-resolution, high-speed analysis of the molecular composition of samples. The light sources used in the spectrometer are quantum cascade laser frequency combs, which are known for their stability and high optical power in spectroscopy applications. The spectrometer's compact size and cost-effectiveness make it ideal for a variety of settings, including academic and industrial research. The modular approach of separating emission and detection unit further makes it suitable for integration into field applications ranging from stand-off detection to process monitoring.

IRsweep

▶ https://link.spectroscopyeurope.com/1836-P1-2023

NEW PRODUCTS

IMAGING

Infrared/Raman microscope enables acquisition of complementary molecular information

Shimadzu Scientific Instruments has introduced the AIRsight™ Infrared/Raman Microscope that provides a two-in-one solution for molecular analysis. This system is equipped with a Raman unit available on Shimadzu's AIMsight infrared microscope and compatible with the IRTracer-100, IRXross and IRAffinity-1 series Fourier transform infrared (FT-IR) spectrometers.

The AIRsight Infrared/Raman Microscope improves analytical efficiency by making it easy to perform all process steps, from sample observation to data analysis. The instrument also increases accuracy because users can obtain qualitative infrared and Raman spectra at the same position without moving samples on the same stage by simply switching lenses. The system incorporates Shimadzu's proprietary wide-view camera and microscope camera for infrared measurements and objective lens for Raman measurements. The wide-view camera shares positional information with the microscope camera and objective lenses.

AMsolution software includes measurement and analysis programs. The measurement software controls both infrared and Raman measurements via the same window so users can perform all processes, from image acquisition to measuring infrared and Raman spectra. The analysis software can also overlay and search infrared and Raman spectra. Operators can obtain information about both organic and inorganic substances from the same location, which can significantly improve the accuracy of qualitative analysis. In addition, this system saves valuable laboratory space because only one instrument is needed to perform infrared and Raman measurements.

The AIRsight Infrared/Raman Microscope is equipped with a standard extensive selection of libraries, including proprietary Shimadzu libraries and libraries for substances ranging from typical reagents to macromolecules. Optional software, accessories and libraries are also available.

Shimadzu Scientific Instruments
▸ https://link.spectroscopyeurope.com/6348-P1-2023

WITec releases Suite SIX software

WITec GmbH has introduced Suite SIX, its next stage in software for Raman and correlative measurement control, data acquisition and post-processing. Developed to enhance the configurability of the alpha300 microscope series, it offers multiple user profiles, regulatory compliance support and advanced sample navigation.

Suite SIX's multi-user management capability enables the site administrator to determine the instrument

NEW PRODUCTS

functionalities and data access rights associated with each system login. It also assists in efforts to comply with good practice (GxP) guidelines such as the US Food and Drug Administration's 21 CFR Part 11. This is especially important for pharmaceutical research and development. Additionally, the software allows users to develop a library of distinct hardware setups to further streamline recurring experiments.

TrueOrigin, Suite SIX's portable coordinate system, locates measurement areas in relation to markers on a sample holder or features on the sample itself. This expedites the correlation of data acquired by multiple techniques from the same position, even when the sample is moved between instruments. It can also import images of a sample made with an external camera to navigate to an area of interest and for convenient project documentation.

WITec

▸ https://link.spectroscopyeurope.com/702-P1-2023

MASS SPEC

Syft Technologies release next generation SIFT-MS

Syft Technologies has released its next generation Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) technology, Syft Tracer™. This real-time, direct injection mass spectrometry (MS) offers platform advancements such as greater sensitivity, performance stability and high reproducibility and repeatability. Analytical workflows that require fast time to data, high throughput and continuous operation will benefit significantly from the Syft Tracer's capabilities.

SIFT-MS is a form of direct mass spectrometry. It applies precisely controlled chemical ionisation reactions to detect and quantify trace amounts of volatile organic compounds (VOCs) and inorganic gases. SIFT-MS delivers real-time, chromatography-free direct analysis of compounds that traditionally require intensive sample preparation. No sample preparation is required for even complex matrices and high-humidity samples. It analyses compounds that cannot be easily targeted by traditional chromatographic methods such as formaldehyde, hydrogen sulfide, ammonia, ethylene oxide and nitrosamines. SIFT-MS is designed to be accessible to non-technical users and generates data that is easy to interpret.

Syft Technologies

▸ https://link.spectroscopyeurope.com/7238-P1-2023

NEW PRODUCTS

SAMPLE PREP

Markes International launches new sample preparation platform

Markes International is launching a new addition to its automated sample preparation platform, Centri®. Centri 90 is an automated sample preparation, extraction and concentration platform for the GC–MS analysis of VOCs/SVOCs in solids, liquids and gases. Centri-90 delivers sensitivity and enhanced productivity for routine headspace, SPME and SPME Arrow applications. The new Centri 90 is a smaller, modular, entry-level, instrument that complements the high-sensitivity and high-flexibility capabilities of the existing Centri platform. Markes' proprietary cryogen-free trapping technology maximises the sensitivity of these techniques and makes Markes' product unique. The Centri 90 platform can be upgraded, at any time, to add thermal desorption and high-capacity sorptive extraction capabilities.

Markes' Multi-Gas technology is in-built in Centri 90, enabling the instrument to be used with either helium, nitrogen or hydrogen as carrier gases. It's been independently certified for safe use with hydrogen, which delivers faster chromatographic speeds, and lowers the cost-of-ownership and maximising return-on-investment. The instrument also has automated system leak checks and innovative diagnostics and has an automated gas-phase internal standard addition—a requirement for compliance with some standard methods.

Markes International
▶ https://link.spectroscopyeurope.com/681-P1-2023

X-RAY

New micro-XRF analysers

HORIBA Scientific have expanded their XGT-9000 series product line with the release of the two new micro-XRF (X-ray fluorescence) analysers, the XGT-9000 Pro and XGT-9000 Expert. These have improved detection systems and a patented pulse processing algorithm to achieve higher-speed analysis. Additionally, the XGT-9000 Expert has light element analysis (down to boron) in a benchtop energy dispersive micro-XRF analyser. The ability to analyse supersensitive light elements, such as carbon (C), nitrogen (N) and oxygen (O) allows the analyses of oxides, nitrides, organic matter and other materials by a single micro-XRF analyser.

Further, with the increasing importance of quality control in manufacturing process, the detection of tens of microns-sized contaminants or foreign matter, which are difficult to visually recognise, has been a challenge. This is because even a microscopic contaminant can result in lower performance and other serious problems

NEW PRODUCTS

in products. That is why micro-XRF analysers are becoming more essential than ever before.

While micro-XRF analysers are powerful for the analysis of inorganic materials and metals, high-sensitivity analyses of light elements below sodium (Na) have generally been difficult for them up until now. The analysis of nitrides and organic matter had required a different type of analyser. The ability of the XGT-9000 Expert to achieve high-sensitivity analyses of light elements such as carbon (C), nitrogen (N) and oxygen (O), allows a single instrument to provide a way to analyse not only metals, but also oxides, nitrides and organic matter.
HORIBA Scientific
▶ https://link.spectroscopyeurope.com/673-P1-2023

DIARY

Conferences

2023

11–14 April, Vienna, Austria. **ANAKON 2023.** office@anakon2023.at, https://www.anakon2023.at

24–28 April, Nairobi, Kenya. **LC-MS—A Hands on Approach.** https://www.rsc.org/events/detail/75896/lc-ms-a-hands-on-approach-kenya-april-2023

7–12 May, San Jose, California, United States. **CLEO.** https://www.cleoconference.org/

7–12 May, Seattle, United States. **17th Annual Eigenvector University–EigenU 2023.** bmw@eigenvector.com, https://eigenvector.com/events/eigenvector-university-2023/

10 May, Sheffield, United Kingdom. **BMSS Imaging Special Interest Group Meeting 2023.** jillian.newton@shu.ac.uk, https://www.eventbrite.co.uk/e/bmss-sig-imaging-symposium-2023-tickets-518811959537?aff=erelexpmlt

21–26 May, Kyoto, Japan. **25th International Symposium on Plasma Chemistry.** secretariat@ispc25.com, https://www.ispc25.com/

4–8 June, Houston, Texas, United States. **71st ASMS Conference on Mass Spectrometry and Allied Topics.** https://www.asms.org/conferences/annual-conference/annual-conference-homepage

5–7 June, Berlin, Germany. **Workshop AK Chemometric with COST sensorFINT.** sensorfint-conference@go.gdch.de, https://www.gdch.de/sensorFINT

8 June, London, United Kingdom. **Analytical Research Forum 2023 (ARF 23).** https://www.rsc.org/events/detail/75380/analytical-research-forum-2023-arf-23

13–16 June, Snekkersten, Denmark. **3rd RSC Anglo-Nordic Medicinal Chemistry Symposium.** events@hg3.co.uk, https://www.rsc.org/events/detail/42807/3rd-rsc-anglo-nordic-medicinal-chemistry-symposium

18–23 June, Paris, France. **Vibrational and Electronic Spectroscopies Applied to the Study of Reaction Mechanisms.** mecareact@sciencesconf.org, https://mecareact.sciencesconf.org/

27–30 June, Padova, Italy. **11th Colloquium Chemiometricum Mediterraneum (CCM XI 2023).** https://ccm2023.gruppochemiometria.it/

2–7 July, Beijing, China. **12th International Symposium on EIS.** https://www.eis2022.com/

17–20 July, Newcastle upon Tyne, United Kingdom. **BSPR-EUPA 2023.** bspr.eupa2023@ncl.ac.uk, https://conferences.ncl.ac.uk/bspr-eupa2023/

23–26 July, Austin, United States. **Advancing Mass Spectrometry for Biophysics and Structural Biology–AMS 2023.** jbrodbelt@cm.utexas.edu, https://advancingms.org/

30 July–4 August, Berlin, Germany. **The 15th Femtochemistry Conference (FEMTO 15).** https://femto15.mbi-berlin.de/conference

31 July–3 August, Munich, Germany. **Optica Sensing Congress.** https://www.optica.org/en-us/events/congress/optical_sensors_and_sensing_congress/

13–17 August, San Francisco, United States. **267th American Chemical Society National Meeting.** natlmtgs@acs.org, https://www.acs.org/

20–24 August, Innsbruck, Austria. **NIR-2023.** nir23@cmi.at, https://www.nir2023.at/

25–30 August, Brighton, United Kingdom. **10th International Conference on Nuclear and Radiochemistry– NRC10.** https://www.rsc.org/events/detail/38385/10th-international-conference-on-nuclear-and-radiochemistry-nrc10#contacts

27 August–1 September, Krakow, Poland. **12th International Conference on Advanced Vibrational Spectroscopy (ICAVS12).** icavs2023@targi.krakow.pl, https://icavs.org/

3–7 September, Vienna, Austria. **6th EuChemS Inorganic Chemistry Conference.** https://www.eicc6.at/

3–6 September, Tokamachi, Niigata, Japan. **8th Asian Spectroscopy Conference (ASC2023).** http://www2.riken.jp/lab/spectroscopy/ASC2021/index.html

12–14 September, Manchester, United Kingdom. **43rd BMSS Annual Meeting.** admin@bmss.org.uk, https://www.bmss.org.uk/43rd-bmss-annual-meeting/

15–22 September, Dresden, Germany. **6th Summer School Spectroelectrochemistry.** summerschool@ifw-dresden.de, https://www.ifw-dresden.de/de/news-events/scientific-events/summer-school-spectroelectrochemistry

17–20 September, Baveno, Italy. **SMASH 2023— Small Molecule NMR Conference.** https://www.smashnmr.org/

17–22 September, Cagliari, Sardinia, Italy. **6th International Mass Spectrometry School.** https://www.spettrometriadimassa.it/imss2023/

8–13 October, Sparks, NV, United States. **SciX 2023.** https://www.scixconference.org/scix-future-conferences

10–12 October, Dresden, Germany. **3rd Food Chemistry Conference: Shaping a Healthy and**

Sustainable Food Chain through Knowledge. https://www.elsevier.com/events/conferences/food-chemistry-conference

6–8 November, Amsterdam, Netherlands. RME2023–15th Conference in the Rapid Methods Europe Series. https://www.rapidmethods.eu/

2024

15–21 January, Tucson, United States. **2024 Winter Conference on Plasma Spectrochemistry.** wc2024@chem.umass.edu, http://icpinformation.org

17–21 March, New Orleans, United States. **268th American Chemical Society National Spring Meeting.** natlmtgs@acs.org, https://www.acs.org/

24–28 March, San Diego, United States. **75th Pittcon 2024.** pittconinfo@pittcon.org, https://www.pittcon.org

2–6 June, Anaheim, United States. **72nd ASMS Conference on Mass Spectrometry.** office@asms.org, https://www.asms.org

18–22 August, Denver, United States. **269th American Chemical Society National Meeting.** natlmtgs@acs.org, https://www.acs.org

15–18 September, Burlington, United States. **SMASH 2024—Small Molecule NMR Conference.** https://www.smashnmr.org/

2025

2–7 March, Berlin, Germany. **20th European Winter Conference on Plasma Spectrochemistry.** https://ewcps2025.de/

1–5 June, Baltimore, United States. **73rd ASMS Conference on Mass Spectrometry.** office@asms.org, https://www.asms.org/

Exhibitions

2023

19–21 April, Ho Chi Minh City, Vietnam. **Analytica Vietnam.** https://www.analyticavietnam.com/

2024

9–12 April, Munich, Germany. **analytica.** https://analytica.de/

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