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Sampling Column: "assay exchange"

John Hollerton: a life in industrial spectroscopy

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CONTENTS

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IMPOpen

EDITORIAL

A belated Happy New Year to all readers. I just wanted to reiterate my invitation from the last issue to complete a short survey about your views on what and how we publish. It really does help us, so please do take a couple of minutes and go to https://www.spectroscopyeurope.com/2023-survey. Thank you!

In the Tony Davies Column, we have the second half of the Interview Tony and Mohan Cashyup did with John Hollerton: more interesting insights from John's life in analytical science. The importance and value of apprenticeships and what John looked for from universities. I was also pleased to see that John is on the same wavelength as I am over the term "Human Resources", rather than the traditional "Personnel". HR is a horrible term!

Kim Esbensen and Aldwin Vogel consider "Unsubstantiated complacency re. the 'assay exchange' paradigm: sampling uncertainties with hidden economic consequences". Yet more examples of why the Theory of Sampling (ToS) is crucial in many business transactions as well as in analysis more generally.

The Product Focus in this issue is on Molecular Spectroscopy and can be found on page 40. Over 30 products from 13 companies are featured, and you can easily click through for more information.

Our update on applications can starts on page 37, covering topics from art to foods. There are a number of new products also and the first Diary of Future Events in 2023.

Intense fs light pulses in the mid-IR for spectroscopic and technical applications

A new light source generates ultrashort infrared pulses at wavelengths around 12 µm with previously unattained peak intensity and stability. First experiments in vibrational spectroscopy on water demonstrate the high potential of the system for applications.

Ultrashort light pulses represent an important tool in basic research and have also found their way into numerous optical technologies. The infrared spectral range with wavelengths longer than 1 µm plays a key role in optical communication, while pulses with wavelengths of up to 300 µm are required in optical measurement and analysis technology and in imaging techniques.

Extremely short pulses with only a few oscillation cycles of the light wave ("few cycle" pulse) are a particular technical challenge. Their generation requires precise control of the optical phase and their propagation conditions. Few-cycle pulses at wavelengths longer than 10 µm are important for fundamental studies of the non-equilibrium properties of condensed matter and exhibit a high application potential, for example in optical materials processing. As a result, the generation of such pulses is a cutting-edge research topic.

Researchers from the Max Born Institute in Berlin report in *Optica* (doi.org/gq9k8n) on a new light source that delivers ultrashort infrared pulses beyond 10 µm wavelength with record parameters. The extremely compact system is based on the concept of optical parametric chirped pulse amplification (OPCPA), in which a weak ultrashort infrared pulse is amplified by interaction with an intense pump pulse of shorter wavelength in a non-linear crystal. In the novel light source, pump pulses of about 3 ps duration at a wavelength of 2 µm drive a three-stage parametric amplifier with a pump energy of 6 mJ. The amplified pulses at a wavelength around 12 µm have an energy of 65 µJ and a duration of 185 fs, corresponding to a peak power around 0.4 GW within about five optical cycles of the light

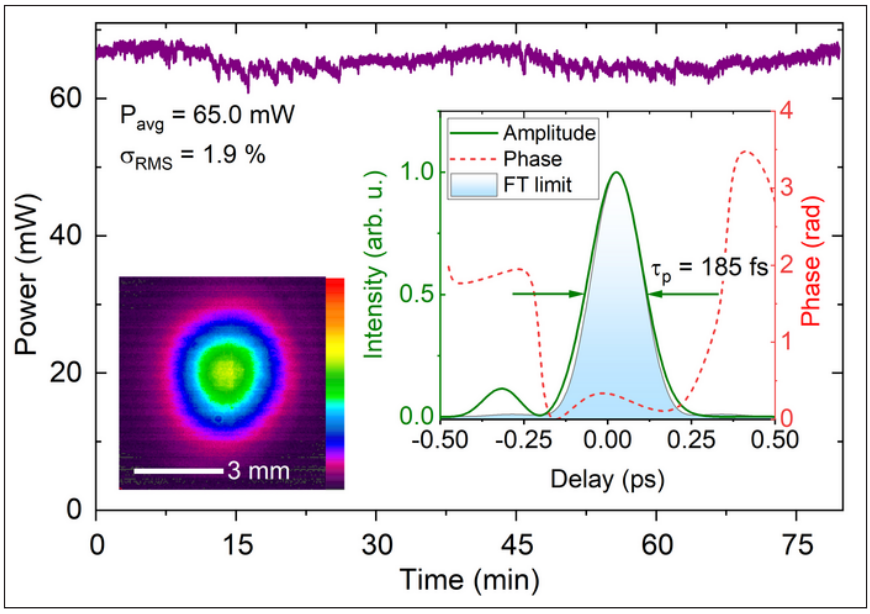

Figure 1. Characterisation of the OPCPA pulse performance at 11.4 µm. Long-term pulse stability measurement. The average power is 65 mW, the standard deviation σ_RMS = 1.9 %. Left inset: Far-field intensity distribution. Right inset: Retrieved temporal pulse shape of the few-cycle pulse. Credit: MBI

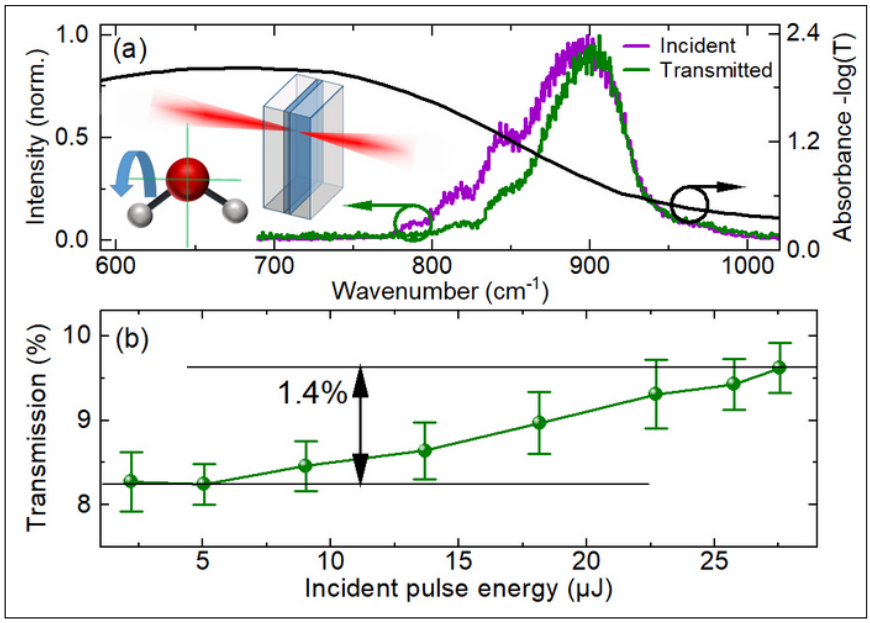

Figure 2. Non-linear transmission of liquid water (12 µm thick film held between two transparent windows) at the librational (L2) band (vibration indicated by the circular arrow). (a) L2 absorption of water (black line) and incident (magenta line) and transmitted (green line) spectra of the 11.4 µm pulses (energy: 25 µJ). (b) Transmission of the water sample as a function of incident pulse energy, showing a non-linear transmission increase. Credit: MBI

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wave (Figure 1). In the 1 kHz train the pulses are highly stable and of excellent optical beam quality (Figure 1). Output power and repetition rate of the system are scalable.

The potential of this unique source was demonstrated in experiments on liquid water. For the first time, hindered rotations, so-called librations, of water molecules were excited to such an extent that their optical absorption decreased significantly (Figure 2). From the analysis of this absorption saturation, a lifetime of the librational excitation of 20–30 fs is estimated.

πNIRS technique is a new way to monitor blood flow in the brain

The πNIRS technique could revolutionise medical diagnostics, including monitoring of strokes and Alzheimer's disease.

Monitoring the proper blood supply to the brain is crucial, not only to prevent neurological diseases but also to treat them. The parallel near infrared interferometric spectroscopy (πNIRS) technique could make life easier for doctors and patients worldwide.

Blood drives our entire body and is especially important for brain function. On average, about 50 mL min^{-1} 100 g^{-1} flows through brain tissue—about 80–90 mL min^{-1} 100 g^{-1} through the grey matter and 20–30 mL min^{-1} 100 g^{-1} through the white matter. When there is a lack of oxygen and, therefore, a lack of proper blood supply, the death of nerve cells occurs—then we speak of a stroke.

This is why it is essential to monitor cerebral blood flow in disease prevention and treatment. Neurology knows many effective methods for doing so, but many of them have their weaknesses. Now a team of neuroscientists led by ICTER researchers has developed a technique that can significantly improve the monitoring of cerebral blood flow *in vivo*.

Cerebral blood flow (CBF) uses about 15 % of cardiac output to deliver the essential substances (oxygen and glucose) to the brain and take away the unnecessary ones (products of metabolism). Any deviation from the norm can cause temporary brain dysfunction and irreversible trigger diseases, with Alzheimer's disease at the forefront. That is why non-invasive monitoring of CBF is so important—we have several practical tools for doing so.

The first that comes to mind is functional magnetic resonance imaging (fMRI), probably the most widely used diagnostic test in the world, which also works well here. It allows monitoring local changes in brain blood supply and associated fluctuations in neuronal activity *in vivo*. The technique offers high-resolution images but is quite expensive and difficult to use in young children, for example. This is where optical methods come to the rescue.

Brain oxygenation can be assessed using functional near infrared spectroscopy (fNIRS). This technique allows non-invasive measurement of regional cerebral oxygenation by using selective absorption of radiation of electromagnetic waves in the range of 660–940 nm by chromophores in the human body. It is often used as a tool to help monitor a patient's condition, including during neurosurgery.

On the other hand, blood flow can be continuously monitored by diffuse correlation spectroscopy (DCS). Their most advanced modifications are based on continuous-wave (CW) lasers, which prevent absolute measurements. Interferometric near infrared spectroscopy (iNIRS) can help here. Still, previous studies have shown that this method is too slow to detect

In experiments conducted at ICTER, a team of researchers (Saeed Samaei, Klaudia Nowacka) led by David Borycki used laser light along with an ultrafast camera to measure blood flow in the brain. The measurements showed that this novel technique (πNIRS) is sensitive enough to non-invasively analyse prefrontal cortex activation while reading unfamiliar text. Which contributes to the development of a non-invasive BCI. Credit: ICTER, Karol Karnowski, PhD

immediate changes in blood flow that translate into neuronal activity. This is because it is a single-channel system, which measures the intensity of only the single-mode of the light collected from the sample.

A team of researchers at ICTER decided to modify iNIRS, relying on πNIRS for multi-channel detection of cerebral blood flow (*Biomedical Optics Express*, doi.org/grmhg7). To achieve this, it was necessary to alter the iNIRS detection system. In πNIRS, the collected optical signals are recorded with a two-dimensional CMOS camera operating at an ultrafast frame rate (~1 MHz). Each pixel in the recorded image sequence effectively becomes an individual detection channel. With this approach, it is possible to obtain similar data as with iNIRS, but much faster—even by orders of magnitude!

Such an improvement, in turn, translates into greater sensitivity of the system and accuracy of detection itself. It is possible to detect rapid changes in blood flow related to the activation of neurons, for example, in response to an external stimulus or administered drug. The solution could be helpful for diagnosing CBF-related neuronal disorders and evaluating the effectiveness of therapeutic approaches, e.g. for neurodegenerative diseases.

This project will improve rapid, non-invasive systems for human cerebral blood monitoring *in vivo*. Continuous and non-invasive monitoring of blood flow could help treat significant brain diseases. In addition, quick detection of cerebral blood flow will bring us closer to developing a non-invasive brain–computer interface (BCI) that could help people with disabilities. Finally, our project will strengthen the tradition of Polish development in diffusion optics, says Dawid Borycki of ICTER.

Tests have confirmed that the technique used effectively monitors prefrontal cortex activity *in vivo*. Moreover, it can be further improved thanks to the development of LiDAR technology and ultrafast volumetric imaging of the eye, reducing the cost of CMOS cameras. Thus, the πNIRS technique can monitor cerebral blood flow and absorption changes from more than one spatial location.

The data obtained by the πNIRS technique can be applied to the diagnosis of cerebral circulatory disorders, which will facilitate the evaluation of the patient's condition and allow the prediction of early and long-term treatment results.

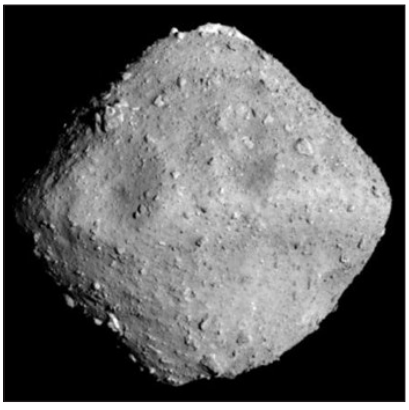
XANES analysis of ancient asteroid grains provide insight into the evolution of our solar system

The UK's national synchrotron facility, Diamond Light Source, was used by a large, international collaboration to study grains collected from a near-Earth asteroid, using XANES, to further our understanding of the evolution of our solar system.

Researchers from the University of Leicester brought a fragment of the Ryugu asteroid to Diamond's Nanoprobe beamline I14 where X-ray Absorption Near Edge Spectroscopy (XANES) was used to map out the chemical states of the elements within the asteroid material. The team also studied the asteroid grains using an electron microscope at Diamond's electron Physical Science Imaging Centre (ePSIC).

Julia Parker is the Principal Beamline Scientist for I14 at Diamond. She said: "The X-ray Nanoprobe allows scientists to examine the chemical structure of their samples at micron to nano length scales, which is complemented by the nano to atomic resolution of the imaging at ePSIC. It's very exciting to be able to contribute to the understanding of these unique samples, and to work with the team at Leicester to demonstrate how the techniques at the beamline, and correlatively at ePSIC, can benefit future sample return missions."

The data collected at Diamond contributed to a wider study of the space weathering signatures on the asteroid. The pristine asteroid samples enabled the collaborators to explore how space weathering can alter the physical and chemical composition of the surface of carbonaceous asteroids like Ryugu. The researchers discovered that the surface of Ryugu is dehydrated and that it is likely that space weathering is responsible. The findings of the study have led the authors to conclude that asteroids that appear dry on the surface may be water-rich, potentially requiring revision of our understanding of the abundances of asteroid types and the formation history of the asteroid belt.



Asteroid Ryugu. Image taken at 20 km on 26 June 2018, diameter 870 m. Credit: Hayabusa2/JAXA.

Ryugu is a near-Earth asteroid, around 900 m in diameter, first discovered in 1999 within the

asteroid belt between Mars and Jupiter. It is named after the undersea palace of the Dragon God in Japanese mythology. In 2014, the Japanese state space agency JAXA launched Hayabusa2, an asteroid sample-return mission, to rendezvous with the Ryugu asteroid and collect material samples from its surface and sub-surface. The spacecraft returned to Earth in 2020, releasing a capsule containing precious fragments of the asteroid. These small samples were distributed to labs around the world for scientific study, including the University of Leicester's School of Physics & Astronomy and Space Park where John Bridges, one of the authors on the paper in *Nature Astronomy* (doi.org/jt46), is a Professor of Planetary Science.

John said: "This unique mission to gather samples from the most primitive, carbonaceous, building blocks of the Solar System needs the world's most detailed microscopy, and that's why JAXA and the Fine Grained Mineralogy team wanted us to analyse samples at Diamond's X-ray nanoprobe beamline. We helped reveal the nature of space weathering on this asteroid with micrometeorite impacts and the solar wind creating dehydrated serpentine minerals, and an associated reduction from oxidised Fe^{3+} to more reduced Fe^{2+}. It's important to build up experience in studying samples returned from asteroids, as in the Hayabusa2 mission, because soon there will be new samples from other asteroid types, the Moon and within the next 10 years Mars, returned to Earth. The UK community will be able to perform some of the critical analyses due to our facilities at Diamond and the electron microscopes at ePSIC."

The building blocks of Ryugu are remnants of interactions between water, minerals and organics in the early Solar System prior to the formation of Earth. Understanding the composition of asteroids can help explain how the early solar system developed, and subsequently how the Earth formed. They may even help explain how life on Earth came about, with asteroids believed to have delivered much of the planet's water as well as organic compounds such as amino acids, which provide the fundamental building blocks from which all human life is constructed. The information that is being gleaned from these tiny asteroid samples will help us to better understand the origin not only of the planets and stars but also of life itself. Whether it's fragments of asteroids, ancient paintings or unknown virus structures, at the synchrotron, scientists can study their samples using a machine that is 10,000 times more powerful than a traditional microscope.

1.2 GHz NMR for University of Warwick

A consortium led by the University of Warwick has been awarded £17 M to procure the UK's most powerful NMR instrument at 1.2 GHz.

A consortium led by the University of Warwick has been awarded £17 M to procure the UK's most powerful Nuclear Magnetic Resonance (NMR) instrument at 1.2 GHz—one of only seven such spectrometers currently operating around the world. As well as Warwick, the consortium includes the universities of Lancaster, Liverpool, Nottingham, Southampton and St Andrews. The funding has come through the UK Research and Innovation's (UKRI) Infrastructure Fund, which is designed to support the facilities, equipment and resources that are essential for researchers and innovators to do ground-breaking work.

In the UK and at The University of Warwick, researchers are using NMR technology to improve green infrastructure. They are expanding their knowledge of how to make more efficient plant biofuels, to improve batteries and solar cells. The instrument will also be used in research on antimicrobial resistance and drug design and delivery.

Professor Steven Brown, from The University of Warwick's Solid State NMR Group, said: "It is exciting that Warwick has been selected as the site for this world-class NMR instrumentation. I look forward to working with the consortium partners and the UK community to deliver this world-class resource for UK science."

Professor Caroline Meyer, Pro-Vice Chancellor (Research) at The University of Warwick, said: "This instrument will provide the greatest resolution and sensitivity yet, allowing us to make scientific breakthroughs that will benefit us all as they improve our technology in a range of areas."

The 1.2 GHz NMR spectrometer will be housed in a new building and builds upon current capability at 1.0 GHz (https://www.spectroscopyeurope.com/news/1-ghz-nmr-uk) at the Warwick-hosted UK High-Field Solid-State NMR National Research Facility.

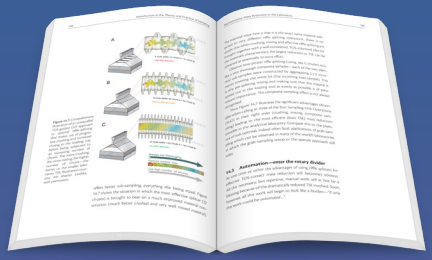
Introduction to the Theory and Practice of Sampling

Kim H. Esbensen

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

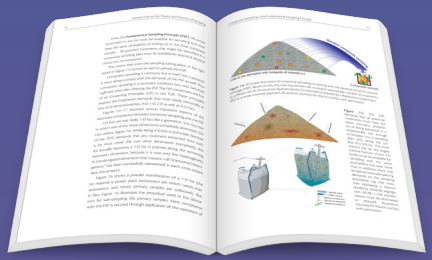
“Sampling is not gambling”. Analytical results forming the basis for decision making in science, technology, industry and society must be relevant, valid and reliable. However, analytical results cannot be detached from the specific conditions under which they originated. Sampling comes to the fore as 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”



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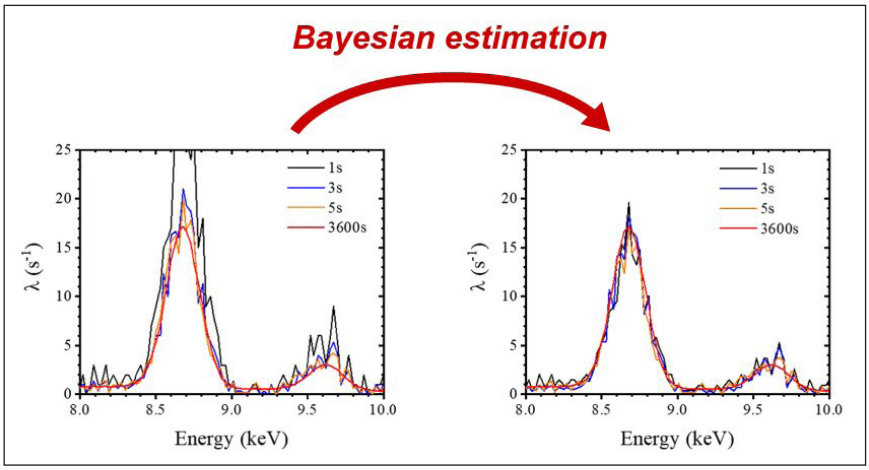
Bayesian inference massively cuts XRF analysis time

A new method by applying Bayesian estimation to X-ray fluorescence analysis can dramatically reduce the analysis time.

X-ray fluorescence (XRF) analysis can be used to identify an abundance of elements, e.g. to detect toxic heavy metals levels in soil. Current methods of XRF analysis take about 10 minutes to accurately identify elements, so new methods that can measure large quantities or take multiple measurements of unknown materials quickly are desired.

A joint research group, including Dr Tsugufumi Matsuyama, Professor Kouichi Tsuji and Masanori Nakae, a second-year master's student at the Osaka Metropolitan University Graduate School of Engineering, and researchers from the Japan Atomic Energy Agency, has developed a new method by applying Bayesian estimation to XRF analysis. The group succeeded in reducing the measurement time of an XRF spectrum per measurement point, from 7 s to 3 s—reducing the time needed by 4 s to obtain analysis results that were not significantly different to the spectra obtained from measuring a glass standard sample for one hour (*Spectrochimica Acta B*, doi.org/grk6zg). For example, when creating an elemental distribution, as many as 10,000 measurements may be taken, over a small area, depending on the sample. So, reducing the measurement time per point by 4 s can reduce the total measurement time by 40,000 seconds—about 11 hours—when creating an elemental distribution.



X-ray fluorescence spectra at 1, 3, 5 and 3600 seconds. The left graph shows measurements without Bayesian estimation, while the right graph shows measurements using Bayesian estimation, which tends to derive accurate values even at shorter measurement times.

Dr Matsuyama stated, "We have successfully integrated analytical chemistry and informatics, using applied Bayesian inference to XRF analysis. Further studies are needed to determine whether it is possible to use this method to detect trace amounts of elements. If we can perform rapid elemental analysis in a non-destructive manner without needing to contact the sample, this technique could be popular in many fields, such as analysis of industrial products or waste materials carried on conveyor belts, and monitoring of ongoing chemical reactions."

NIR spectroscopy: better than a hole in the head

A team from Carnegie Mellon University have developed methods using NIR and diffuse correlation spectroscopies to monitor intracranial pressure non-invasively.

Just as blood pressure informs heart health, intracranial pressure (ICP) helps indicate brain health. ICP sensing is the burgeoning focus of Jana Kainerstorfer's biomedical optics lab at Carnegie Mellon University. Her team is working to modernise ICP sensing approaches, which historically have been invasive and risky. Their non-invasive alternatives will ease risk of infection, pain and medical expenses, as well as present new monitoring capabilities for patients with an array of brain injuries and conditions, from stroke to hydrocephalus.

Investigating pressure levels in the brain is a laborious task for health professionals and hasn't progressed much since the 1960s. Current practice involves drilling a hole into a patient's skull and placing a probe inside for continuous monitoring of ICP levels. It comes with the risk of infection and damaging the brain itself, and while valuable data to have, ICP measurement is reserved only for the most critical of situations.

"At the core of it, what we've done is build a sensor alternative that doesn't require drilling a hole into the patient's head", said Kainerstorfer, associate professor of biomedical engineering. "We recently published two papers that explore the use of optical sensors on the forehead for non-invasive

ICP monitoring, using near infrared spectroscopy and diffuse correlation spectroscopy. Both approaches represent huge strides in improving the patient experience and providing better tools to monitor pressure levels in the brain, which can be a key variable in both diagnosis and treatment decisions."

The first body of work published in *Neurophotonics* (doi.org/gq4f54), in collaboration with Matthew Smith, an associate professor of biomedical engineering at CMU, demonstrates that non-invasive near infrared spectroscopy can be used for ICP monitoring. The process involves small, customised sensors that are placed on the head to measure light that has interacted with the brain. Every time the heart beats, it produces a pulse in the brain, and the sensors measure haemodynamic blood volume/blood flow changes. Then, a machine learning algorithm is applied to determine ICP.

"Our aim is to create a portable and user-friendly tool to measure pressure changes in the brain", explained Kainerstorfer. "We don't believe that fancy hardware is needed to measure blood flow or haemoglobin concentration, and right now, we don't have a good handle on how much brain pressure even fluctuates. There are other non-invasive methods that are out there, but what sets us apart is that we're using a sensor that can be made wearable and offers continuous monitoring."

Kainerstorfer's group also partnered with UPMC Children's Hospital of Pittsburgh, in collaboration with Dr Michael McDowell, to conduct a clinical study utilising more specialised sensors and hardware to measure ICP, via non-invasive diffuse correlation spectroscopy. Fifteen patients from UPMC's paediatric intensive care unit (ICU) participated, and the results were published in the *Journal of Neurosurgery* (doi.org/jpk4).

As part of the study, a probe with optic fibres was placed on the forehead of the paediatric patients who already had invasive ICP monitors to measure blood flow changes and quantify ICP and to compare the non-invasively acquired data to the invasively acquired data. The results of the non-invasive model were compared with those of invasive monitoring and found to be very similar.

"In this study, the patients had an invasive sensor placed in their brain, and it served as our ground truth", elaborated Kainerstorfer. "We worked alongside outstanding collaborators and were encouraged by the results we saw, which indicated that a non-invasive approach could yield accurate ICP measurement. It still requires very specialised hardware and expertise to interpret the data, but it's much better than drilling a hole in the head."

Miniature and durable spectrometer for wearable applications

A team led by P.C. Ku and Qing Qu has developed a miniature, paper-thin spectrometer measuring 0.16 mm^2 that can also withstand harsh environments.

Researchers have developed a wafer-thin chip-scale spectrometer that is suitable for wearable applications. The robust gallium nitride lab-on-a-chip device can also withstand harsh environments with severe radiation, such as space exploration, or those with high temperatures and can be adapted to do blood analysis by simply projecting light onto the skin. It measures 0.16 mm^2.

"As a wearable device, we'll be able to put our device on a flexible substrate, such as sheets or fabric—or maybe on skin", said doctoral researcher Tuba Sarwar.

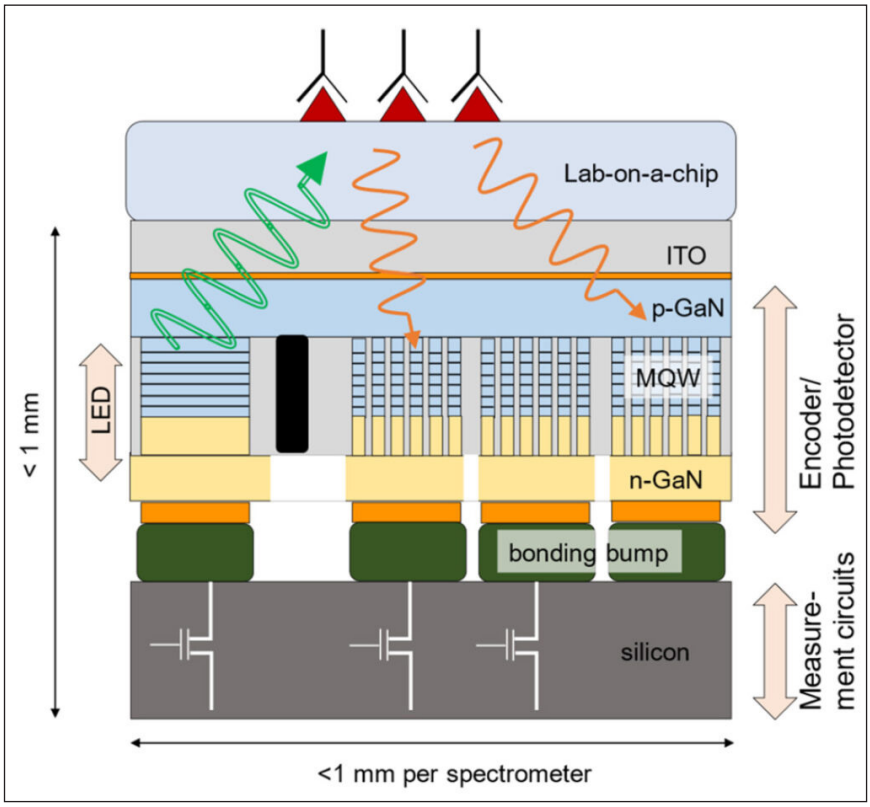
The prototype optical spectrometer created by Sarwar and other members of Prof. P.C. Ku's team was initially developed with a specific purpose: measuring an athlete's sweat in a device that could be worn as a skin patch. This application was determined by U-M's Exercise and Sport Science Initiative (ESSI). The device needn't last long; in fact, being disposable was a plus. Making such a device would require extreme miniaturisation of current devices available in the marketplace. It would also

require creating a device that can work in real time under changing conditions.

Ku, Qu and their team took on the challenge of creating a device that could achieve ESSI's goal, and created a miniaturised, low power, integrated device that works in over the wavelength range of 400–645 nm. The team's spectrometer includes only 16 photodetectors, each responsive to a unique spectrum of the light. This low number of photodetectors was made possible by two key techniques. First, the team used strain engineering on gallium nitride (GaN)-based spectral encoders. Strain engineering is a technique used, for example, in semiconductor manufacturing in which the material is stressed or deformed. Done correctly, it can lead to new material properties that are better suited to specific applications. GaN semiconductors were selected as the foundational material because of their excellent optical properties across the visible spectrum.

The desired result of a dramatically reduced dependence on the angle of the light was accomplished, which eliminated the need for precise positioning of the spectrometer and the associated optics. It also allowed the photodetectors to reside alongside the spectral encoders on the same chip.

Second, the team incorporated machine learning into the device's operation in order to decode the signal emitted from the detector. Doctoral researcher Can Yaras used a simple non-negative least-squares (NNLS) algorithm to enable an efficient computational algorithm to recover the spectral information from the detectors' signal. In terms of performance, the device was highly accurate in determining the peak wavelengths (with a standard deviation of 0.97%), but less accurate in measuring intensity ratio over different peak positions (with a standard deviation of 21.1%, or 10.4% after removing one outlier). The team expects that the reading of intensity ratios can be improved by increasing the number of photodetectors, and further developing the machine learning algorithm, such as by applying deep learning techniques. They are also working on several other enhancements to the prototype spectrometer reported in *Nano Letters* (doi.org/grchb9).



Conceptual illustration of the strategies used to achieve a miniature, ultra-thin spectrometer chip utilising an array of GaN-based spectral encoders and photodetectors on the same chip. A light source is also integrated into the device.

"Our goal was not to build the best spectrometer in the world in terms of the resolution", said Ku, "but to focus on other aspects that are just as exciting if not more: the size, the thickness, the power consumption and the ease of operation."

In terms of future applications, Sarwar says that this miniature spectrometer could be built into a skin patch for health monitoring and diagnosis. The advantage it would have over existing devices is the fact that the excitation light source can also be easily integrated. The radiation hardness of the GaN semiconductors also makes the device potentially suitable for space exploration.

Remote sensing provides a multifaceted view of land change

Work by a group of UConn researchers represents an effort to overcome communication challenges and provide a new framework in the emerging field of land change science.

Work by a team of UConn researchers from the Department of Natural Resources and the Environment (College of Agriculture, Health and Natural Resources) proposes a new framework that emphasises the multifaceted nature of land change through the lens of remote sensing (*Remote Sensing of Environment*, doi.org/grpf65). Many scientists are studying land change using remote sensing satellite data. But, given that land change science is still relatively new, there is often confusion about what language to use to describe what, exactly, people are observing.

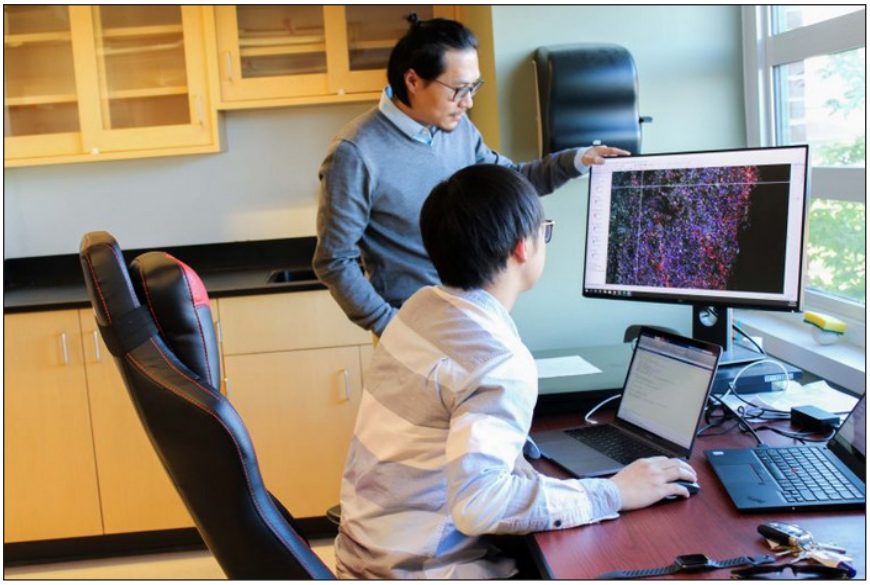
Zhe Zhu, assistant professor and director of the Global Environmental Remote Sensing Laboratory (GERS), is also editor for multiple remote sensing journals. In this capacity, he noticed many authors using terms that have different meanings interchangeably, something he noticed among his own lab members as well.

"I think the most important problem is that land change is an extremely complicated term", Zhu says.

Land change is not a binary process in which land either changes or does not. It is a multifaceted and dynamic process, meaning scientists need a consistent and systematic framework to accurately describe their observations.

"If you look at different facets of land change, you see different aspects of change", Zhu says.

There are five major aspects of land change the authors define: location, time, target, metric and agent. The location is where the change happens. The time is when the change happens. The target is what is changing; this can be factors like how the land is being used and what the land cover looks like. The metric describes how the land is changing; this aspect considers factors like if the change is abrupt or gradual, subtle or dramatic, and the duration of the change. The agent, or driver, explains why the land is changing; this can be something direct like a natural disaster, human construction or an insect infestation. There may also be distal drivers, which are less direct forces like changes in human population or land management policies.



Zhe Zhu and graduate student working in the lab. Credit: Carson Stifel/UConn Photo

Qiu's work is addressing this final aspect with a project that uses the group's previously developed algorithm to map land change location and time, and combines it with machine learning algorithms that can define the drivers of land change in the conterminous US. The work emphasises scientists publishing in this field should first clearly identify which change aspect they are talking about, then consider the multifaceted nature of land changes, and third, engage in multi-source data fusion. Incorporating data from multiple sources and even other fields is critical to creating an accurate picture of land change.

The researchers reviewed the current available global and North American remote sensing land change datasets. They found these datasets only capture one or two aspects of land change. Data from the social and environmental sciences can contribute important ancillary data. For example, data on human population density and poverty levels can provide insight into the drivers of land change not captured in satellite data.

Scientists can even use social media to capture near-real-time images of land conditions. For example, during a natural disaster, data from social media can be combined with satellite data to determine where an image was taken and gather important information about the conditions on the ground.

"This is a direction we think will be very important in the future", Zhu says.

Another problem they addressed is that when using satellite data, scientists have access to a tremendous wealth of information about

where and how the land is changing. But this data also includes noise that scientists need to untangle. Ye is developing a model that can isolate subtle land changes, which are often confused with noise.

"Usually, subtle change and data noise would be very easy to mix up, so we need some sample data to direct our models", Ye says.

Zhu says his research group plans to implement this framework moving forward to investigate all aspects of land change from this multifaceted perspective, a framework he says will be useful for others in the field as well.

New approaches to screen natural products to identify potential drugs

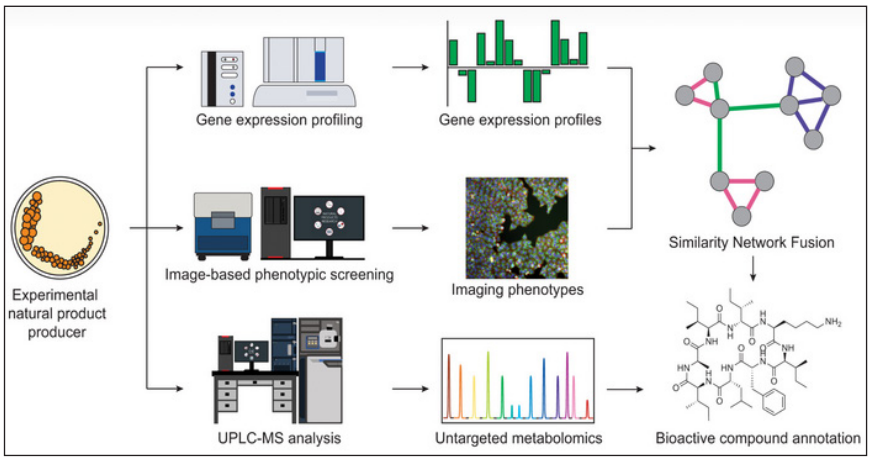
Researchers have developed a sample processing workflow using mass spectrometry and a modified Compound Activity Mapping platform.

Many successful drugs have their origins in natural sources such as plants, fungi and bacteria, but screening natural products to identify potential drugs remains a difficult undertaking. A new approach using molecular biology, analytical chemistry and bioinformatics to integrate information from different screening platforms addresses some of the biggest challenges in natural products drug discovery, according to a recent study published in *PNAS* (doi.org/grctp5).

A major challenge has been determining the mechanism of action and biological target of a novel bioactive compound. Another central challenge is identifying the molecule or molecules driving biological activity in a complex mixture from nature.

"These two big concepts have been at the heart of our collaborative programme, and this paper brings those two questions together in a fully integrated approach", said John MacMillan, professor of chemistry and biochemistry at UC Santa Cruz.

By integrating the results of two completely different screening platforms and combining this with next-generation metabolomics analysis of their natural products libraries, the researchers created a powerful framework for natural product biological characterisation. Using this approach to screen a small collection of randomly selected microbial natural product fractions, they were able to identify a known compound (trichostatin A) and confirm its mechanism of action; link a known compound (surugamide) with novel biological activity (cyclin-dependent kinase inhibition); and discover new compounds (parkamycins A and B) with complex biological activity.



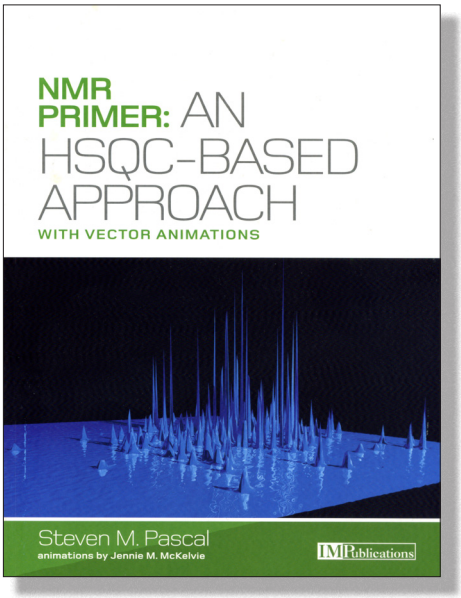
In an integrated approach for drug discovery, natural product fractions are isolated from marine bacteria, screened through two biological screening platforms and subjected to high-resolution mass spectrometry-based metabolomics profiling. Data are integrated using Similarity Network Fusion, which then provides biological annotation on individual metabolites identified. Credit: Hight *et al.*, *PNAS* 2022

"Finding a known compound that groups as expected tells us it's working, and then we were able to correlate a known compound with a new mechanism of action", MacMillan said. "Finally, we discovered a new chemical compound with a unique biological signature unlike any known compounds. That's an exciting finding we want to investigate further."

The researchers used a bioinformatic method called Similarity Network Fusion (SNF), developed for integrating complex datasets, to combine data from two natural product screening platforms their labs had developed. One platform (Functional Signature Ontology, or FUSION), developed by MacMillan's lab, uses gene expression signatures induced in cells by known and unknown compounds, coupled with pattern-matching tools to indicate mechanisms of action through "guilt by association".

"If we see similar effects to one of those known compounds, that suggests a similar mechanism of action. We have used this technology effectively to understand the biological activity of a number of unique small molecules", MacMillan said.

The other platform, a cytological profiling (CP) technology developed by Lokey's lab, involves high-content image analysis of cells exposed to the samples being screened and then stained with



NMR PRIMER: AN HSQC-BASED APPROACH

(with vector animations)

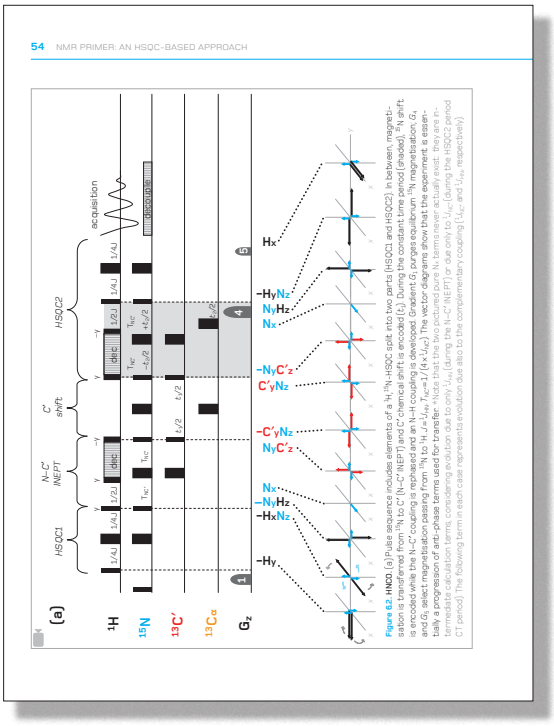
by Steven M. Pascal

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

a panel of fluorescent probes to highlight key cytological features. Automated fluorescence microscopy images yield a total of 251 unique cytological features for each sample.

The researchers used the CP and FUSION technologies to screen complex natural products libraries developed by MacMillan's and Linington's labs. These libraries were derived from marine bacteria isolated by the two labs. To search for bioactive natural products, the researchers grow the bacterial strains in the lab, make a crude extract of all the compounds produced by each strain, then use chromatography to separate each extract into a series of fractions, each containing two to 20 compounds.

Mass spectrometry methods are widely used for the large-scale study of small molecules ("metabolomics") and can help identify the chemical constituents of each fraction. An approach called Compound Activity Mapping developed by Linington and others combines mass spectrometry-based metabolomics with biological screening data to identify which compounds in a mixture are driving a particular biological signature. In the new study, the researchers developed a sample processing workflow using mass spectrometry and a modified version of their Compound Activity Mapping platform that incorporates the integrated results of their screening technologies obtained with Similarity Network Fusion.

"The question is, can we use all that to pull out the chemicals that are driving a particular signature and make more robust predictions of the mechanism of action? Our approach allowed us to accomplish that in a pretty substantial way", MacMillan said.

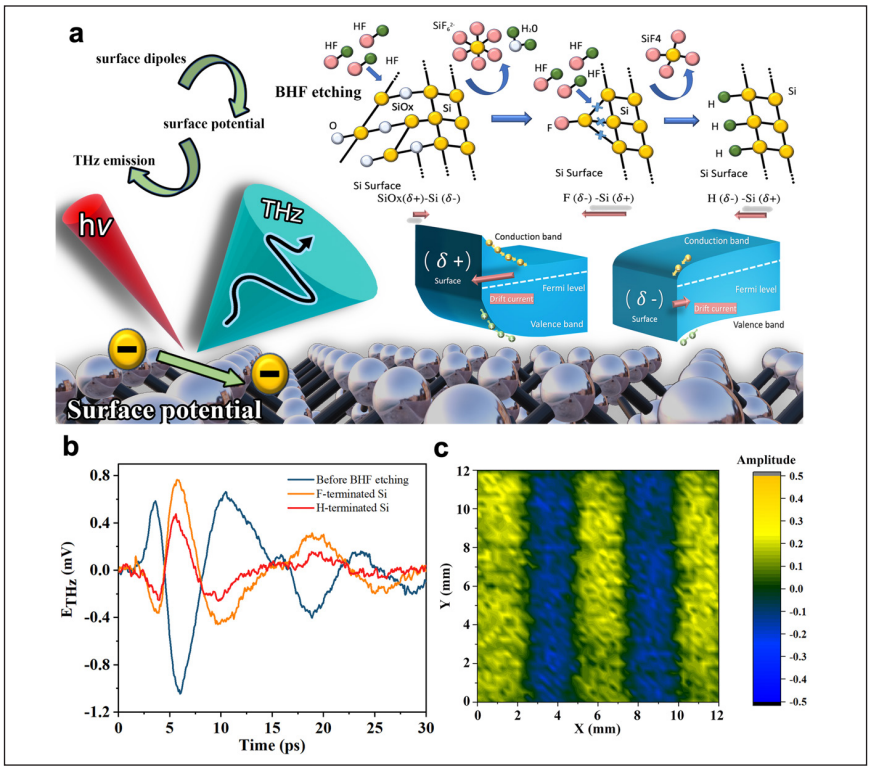
Silicon wafers inspection by terahertz emission spectroscopy

Methods for sensitive local surface evaluation and rapid surface property mapping of Si are still lacking and urgently needed, and now may be solved by THz spectroscopy.

Silicon (Si) has been the focus of the semiconductor industry and the modern electronic industry for the last half-century. However, its surface properties remain a mystery. The properties of the Si surface vary widely but are essential to fabricating Si-based devices. Hydrogen fluoride (HF) and its buffered (BHF) solutions are often used to treat the surface and remove the native oxide layer. After BHF etching, a hydrogen(H)-terminated surface forms, and the surface properties change significantly owing to the variation in the surface states and the generation of surface dipoles.

A team of scientists led by Professor Masayoshi Tonouchi from Osaka University have studied the terahertz (THz) emission properties of Si surfaces and have found an implied semiquantitative connection between the THz emission and the surface band bending with the surface dipoles (*Light Science & Applications*, doi.org/grd2f9).

Currently, various methods are used to characterise the defects at the wafer surface to confirm a better surface for the photolithography process in the semiconductor



a, Illustration of THz emission mechanism from Si surface with laser excitation and chemical process on Si surface with BHF etching and surface dipole moment resulting from different electronegativities of surface atoms. The native oxide layer is removed, F-terminated surface is generated as a mid-stage and the H-terminated surface is formed as the stable condition. b, THz emission waveforms of low-doped n-type Si surface before BHF etching, in F-terminated condition and H-terminated condition. c, LTEM images of the Si sample with a 2.5 mm interval line-space structure of photo resist on the surface after 1% dilute BHF etching for 300 s and removing the photo resist. Credit: Dongxun Yang, Abdul Mannan, Fumikazu Murakami, Masayoshi Tonouchi, Yang, D., Mannan, A., Murakami, F.

industry. The standard wafer inspection techniques include brightfield and darkfield inspection by using a laser beam and its reflection at a specific angle, the electron-beam inspection, and multi-beam inspection using an electron beam for higher resolution. Besides the defects at the surface of the Si wafer, the surface electric properties are also important to further fabrication and influence the device quality.

To improve the yield of products integrated into the Si wafer, it is essential to characterise the surface properties of the Si wafer rapidly, efficiently and quantitatively before and after the chemical treatment during the fabrication process. Several useful but complicated tools have been proposed to estimate the surface potential. These include X-ray photoelectron spectroscopy, surface photovoltage measurement and Kelvin force microscopy. Methods for sensitive local surface evaluation and rapid surface property mapping are still lacking and urgently needed.

The research team proposed laser-induced terahertz (THz) emission spectroscopy (TES) and laser-induced terahertz emission microscopy (LTEM) as the most promising candidate. These are performed as a sensitive and semi-quantitative non-contact, local characterisation method. It offers an additional mapping function that can efficiently evaluate surface properties, such as surface potential, a passivation layer and surface charge density.

Ultrafast laser excitation at the surface of a semiconductor generates THz radiation as a result of ultrafast charge transport. The mechanism can be classified mainly into two categories: photocarrier diffusion and the drift of photocarriers. The THz emission from the Si metal–oxide–semiconductor structure is considered to be the combined result of the drift current and diffusion in previous reports. The photo-Dember effect on the bare Si surface is relatively weak compared to the drift current resulting from the surface electric field.

The researchers observe the THz emission from the Si surface before and after removing the native oxide layer using a BHF solution. Meanwhile, the parameters of the doping types and doping concentration also indicate their impact on the observed THz emission waveforms in terms of both amplitude and polarity. The THz waveform's flipping reveals the THz emission's strong dependence on the surface band bending. It is dominated by the surface state energy and Fermi levels in bulk.

Furthermore, the researchers have looked at the parameters of the surface properties. They provided an LTEM image of the surface potential distribution on the Si surface with a line-space pattern after BHF etching as an example of the application. LTEM–TES is a promising tool for achieving rapid, non-contact and sensitive characterisation of Si surface properties and will benefit the modern Si industry.

Singapore research centre to advance molecular analysis with digital tools

Nanyang Technological University, Singapore (NTU Singapore) has launched the Institute for Digital Molecular Analytics and Science (IDMxS), which aims to advance the science behind analysing biomolecules through the use of information technology and data science. This could pave the way for instantaneous monitoring and analysis of health or environmental information, much like how we access real-time traffic information on our mobile phones.

IDMxS, NTU's newest national Research Centre of Excellence (RCE), is supported with a total investment of around S$160 million over 10 years, comprising S$94 million from the Singapore Ministry of Education, with the remainder from NTU and National University of Singapore.

At the heart of the work done at IDMxS is digital molecular analytics, a new field that drills down to the level of a single molecule to detect, identify and quantify biomolecules with unprecedented precision. Such a science will enable many branches of new discovery, including the development of diagnostic testing capabilities that could in turn lead to new technology development and spin-off commercial applications, such as blood testing kits that can produce immediate results using nothing more than a smartphone camera.

The IDMxS, hosted at NTU's Experimental Medicine Building, was officially launched by Singapore's Minister for Education, Mr Chan Chun Sing. Mr Chan said: "As the latest Research Centre of Excellence awarded by the Ministry of Education to NTU, IDMxS is a vital addition to the national Research, Innovation and Enterprise (RIE) efforts in supporting cutting-edge research that contribute to Singapore's long term developmental goals. The science done at the Centre will be instrumental in bridging the gap between biomedical sciences and information technology, and I look forward to IDMxS' future breakthroughs."

The Research, Innovation and Enterprise (RIE) plan lays the groundwork for Singapore's science and technology efforts every five years. RIE2025 was launched with a S$25 billion budget for 2021 to 2025.

NTU Acting President and Provost Professor Ling San said:

"The Institute for Digital Molecular Analytics and Science (IDMxS) is the third Research Centre of Excellence hosted by NTU and affirms the University's commitment to be at the forefront of cutting-edge research. IDMxS brings together world-class researchers and leading experts in the nascent field of digital molecular analytics, which will drive a paradigm shift in molecular detection and analysis and lay the groundwork for dramatic change in various fields such as biomedicine, biotechnology and clinical science. Another important objective of IDMxS is to nurture postgraduate students in interdisciplinary education across the molecular sciences and information technology, as well as to develop continuing education programmes to uplift the expertise of our healthcare workers in the area of digital diagnostics."

NTU Senior Vice President (Research) Professor Lam Khin Yong said: "The Institute for Digital and Molecular Analytics and Science (IDMxS) is an example of how world-leading researchers of diverse disciplines at NTU are coming together to pursue fundamental research and advance their disciplines to new boundaries. This is in line with RIE2025's aim to build up foundational research capabilities in Singapore to form a strong base of knowledge and capabilities for transformative innovations."

The research at IDMxS could pave the way for instantaneous monitoring and analysis of health or environmental information, much like how we access real-time traffic information on our mobile phones. Credit: NTU Singapore

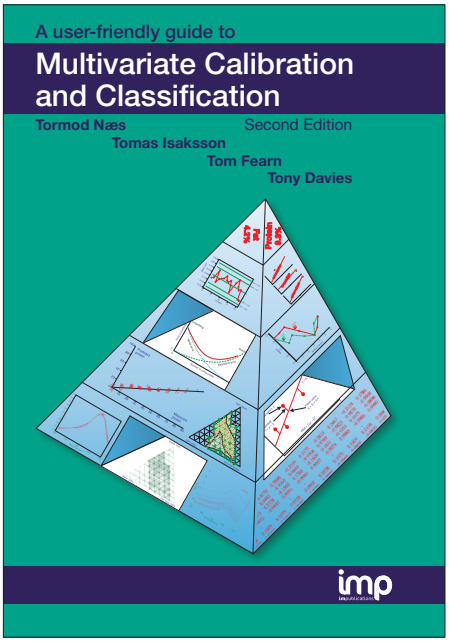
IDMxS is led by Founding Director Professor Jay T. Groves, President's Chair in Bioanalytical Sciences at the NTU School of Materials Science and Engineering. Joining him is Co-Director Professor Peter Török from the NTU School of Physical and Mathematical Sciences, who will oversee the centre's facilities and capabilities. The interdisciplinary centre is expected to bring together 100 full-time researchers and staff with expertise in areas spanning the gamut of science and engineering, from biology, medical technology and chemistry to optics, computer science and artificial intelligence (AI). The Centre will provide funding for more than 30 PhD students, four of whom have already started their studies.

Hyperspectral camera paves the way for *in vivo* detection of low-grade gliomas

A hyperspectral camera has been mounted on a standard OR-approved surgical microscope for *in vivo* detection of low-grade gliomas.

At this week's BiOS, the biomedical optics and biophotonics exhibition at SPIE Photonics West, imec are presenting a promising path to the *in vivo* detection of low-grade gliomas (a group of slow-growing brain tumours). The breakthrough was realised by mounting imec's snapscan VNIR 150 hyperspectral camera on a standard OR-approved surgical microscope. Intraoperative pilot tests were performed at the neurosurgical department of the University Hospital Leuven (KU Leuven). A milestone, imec researchers found the compact set-up to generate accurate clinical data, ready to be fed into a neural network that can convert those data into actable knowledge. In time, the approach could help surgeons detect intrinsic brain tumours' exact demarcations intraoperatively and label-free, which would make for a whole new way of providing medical care.

Low-grade gliomas are a diverse group of (slow-growing) brain tumours that often arise in young, otherwise healthy patients. While typically considered benign in origin, studies have shown that low-grade gliomas can expand at a rate of 4–5 mm annually and come with the risk of malignant transformation. The tumour's early surgical resection has thus become a much-favoured treatment option—although *in vivo* detection of low-grade gliomas and retrieving their exact demarcations is notoriously hard, even



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

What the experts say:

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"I recommend this text as an initiation in analysis of materials, processes, and systems, for engineers, chemists, biologists, and medical technologists seeking an entryway to modern analytical methods..."
Ewa S. Kirkor (Applied Spectroscopy)
"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.

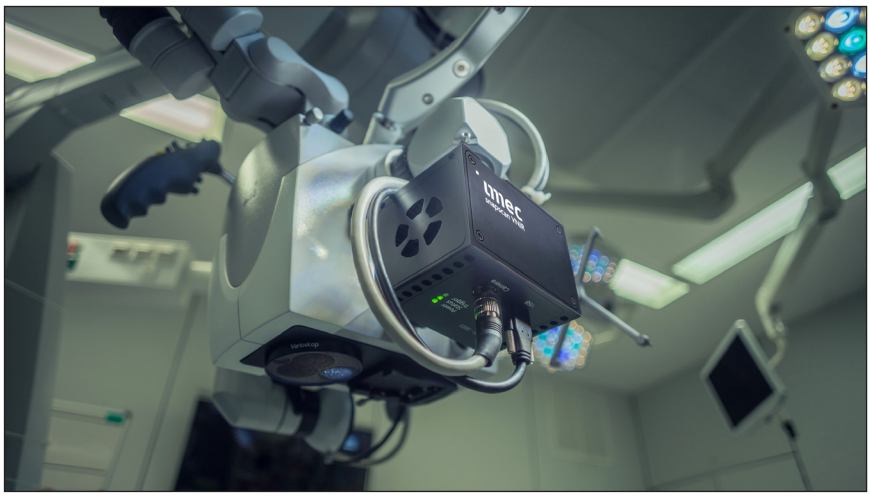
with the aid of surgical microscopes.

"Giving surgeons the proper tools to detect these tumours *in vivo* would make for an important breakthrough. Hyperspectral imaging (HSI) technology shows great potential to do just that", says Roeland Vandebriel, field application engineer at imec. "Using HSI, brain tissue is illuminated, after which its reflected light is captured in many narrow spectral bands—resulting in a different spectral signature for healthy and anomalous cells."

Bulky hardware and integration challenges have prevented HSI technology from being straightforwardly used in hospitals' operating theatres. Yet, two presentations at this year's BiOS now show a promising path forward.

Roeland Vandebriel: "It is a breakthrough we realised by mounting imec's snapscan VNIR 150 hyperspectral camera on a surgical microscope. We found this compact set-up to generate accurate clinical data that can then be fed into a deep-learning neural network to convert the data into actable knowledge, allowing surgeons to discriminate between healthy and anomalous tissue. Clearly, these learnings are an important first step to accommodating the *in vivo* detection of intrinsic brain tumours—such as low-grade gliomas."

Thanks to its small form factor (10 × 7 × 6.5 cm, and weighing 645 g), and its compatibility with standard C-mount optics, imec's snapscan VNIR can easily be mounted on a surgical microscope.



Imec's snapscan VNIR 150 camera mounted on a surgical microscope

It makes for a compact set-up that can be incorporated in hospitals' stringent clinical workflows, contrary to the bulky systems used in previous studies.

"Imec's contribution also focused on how to acquire accurate and relevant clinical data in a (sterile) intraoperative environment", comments Siri Luthman, imec's project lead. "It had us rethink HSI's existing spatial and spectral calibration methods, and necessitated us to interface imec's snapscan directly with the surgical microscope's optics and light source. As such, the first feasibility data set was generated—allowing us to evaluate HSI's potential for the *in vivo* detection of low-grade gliomas; an approach coming with minimal adaptations to both the system and our data pre-processing methods."

"Today's findings indicate which hyperspectral bands are critical when interfacing with high-end surgical microscopes for an *in vivo* classification of low-grade gliomas. While intraoperative use of our set-up is premature, the approach has so far been validated using a clinical dataset of six patients at Belgium's Leuven University Hospital. Going forward, we aim to further this project by integrating our snapshot technology, which accommodates video-rate hyperspectral imaging. This should allow us to explore the real-time detection of low-grade gliomas in surgical practice", Roeland Vandebriel concludes.

This study was conducted in collaboration with Carl Zeiss Meditec AG. The results are presented at SPIE BiOS 2023 in two papers: *Integrating Hyperspectral Imaging in an Existing Intra-Operative Environment for Detection of Intrinsic Brain Tumours*, R. Vandebriel (imec) and *Intra-Operative Brain Tumor Detection with Deep Learning-Optimized Hyperspectral Imaging*, X. Zhang (Carl Zeiss Meditec AG).

Hiden Analytical gains ISO 14001 accreditation

Hiden Analytical has gained the ISO 14001:2015 environmental accreditation. Hiden's green strategies have been integral to the development of an environmental management system (EMS) which provides a framework for improving resource efficiency as well as waste and cost reduction throughout the bespoke manufacturing of their systems.

Hiden now employ over 120 scientists, engineers, technicians and operations specialists at its UK headquarters. Recent company expansion incudes new clean room facilities for precision assembly, a new vacuum/mechanical assembly suite and new office space at Hiden's UK headquarters.

John Hollerton: a life in industrial analytical spectroscopy, part 2

Antony N. Davies,[a] Mohan Cashyap[b] and John Hollerton[c]

[a]SERC, Sustainable Environment Research Centre, Faculty of Computing, Engineering and Science, University of South Wales, UK
[b]MASS Informatics, Harpenden, UK
[c]Hollerton Scientific Software Consultancy, St Albans, UK

This is the second part of an interview with John Hollerton, the first part in is the last issue! John recently retired from a long career at GSK and we took this opportunity to have a chat with him, as Mohan Cashyap and our beloved editor Ian Michael both have had the opportunity to work with John on projects and on the LISMS conference (Linking and Interpreting Spectra through Molecular Structures). Here, we move the discussion on to technologies and innovation, the great, the over-hyped and the effectively lost to the modern analytical laboratory.

TD: So, looking at the time span of your career to date, we have seen enormous innovations in spectroscopy, completely different concepts of how to measure spectroscopic data, huge advances in precision and reproducibility of spectroscopic measurements. For you, what was the biggest innovation you have seen which advanced your science?

JH: 2D-nuclear magnetic resonance (NMR) as it has made a massive difference to the whole of NMR. It is hard to overestimate how much the 2D-NMR has changed the NMR technique. Which refers back to my answer in Part 1 of the interview about Ernst & Co. He was a lovely person by the way, I don't know if you ever got the chance to meet him, but he was the nicest, most self-effacing person that I think I have ever met. Sadly, he died a couple of years ago, but I had the opportunity to meet him and even had breakfast with him once, which was nice! He did a huge amount and he played it down: "Yeah… I did 2D-NMR…". That is probably the biggest innovation from my perspective. Of course, alongside that has to be powerful computing which enables it. Back in the day when he first did it, it was more an intellectual exercise as there were no computers that were really powerful enough to do 2D-NMR on a regular basis, so powerful computers were a key part to moving things forward.

TD: Of course, there is another side to that coin, which I have experienced with various organisations, and that is what was the biggest hyped innovation which failed to deliver as promised?

JH: In the liquid NMR world, I would say the hyperpolarisation of liquids. People are still working on it, but when it first came out it was considered to be the Holy Grail, because NMR is such an insensitive technique. Hyperpolarisation could give orders of magnitude increases in signal-to-noise, so it was a very laudable aim. However, whilst it has had limited application in liquids, it has turned out to be valuable for solid NMR, so the technique itself is valuable, it's just that it isn't great for liquids because of the stress you have to put your sample through in order to do the hyperpolarisation. You have to polarise it at very low temperatures and then suddenly convert it from a solid to a liquid with a rapid temperature cycle.

John Hollerton (left) and Tony Davies (right).

DOI: 10.1255/sew.2023.a1

Another issue can be transferring polarisation as it may not enhance uniformly across the molecule, so that integrals become meaningless. With all the negatives it's rarely appropriate in these cases, whereas it was pushed as the way that NMR would now be competing with Mass Spectrometry for sensitivity. Sadly, you don't always hit the thing that you've been going for—but for solids it's been great.

TD: and on the computing side?

JH: On the computing side? Well, there have just been so many of them! Almost everything goes through the hype curve, doesn't it? Everyone jumping on the bandwagon and then finally calming down and becoming more realistic. Cloud computing was originally very hyped up and then it declined as everyone became disenchanted with it, but now cloud computing is a big thing. So, sometimes hype is just things that are before their time. People tend to become too keen and try to ignore the difficulties. In computing there has been a lot of hype around Artificial Intelligence, but AI is now looking promising in many areas. So maybe the key in all these computing things is to use George Box's quote: "All models are wrong, but some are useful", so we need to remember that AI may not be reality, but it may be useful.

TD: Looking at instrument development, what were the go-to techniques from the start of your career that are now seldom used?

JH: Well certainly ultraviolet (UV) spectroscopy, as discussed in the first part of the interview. Infrared (IR) spectroscopy is also used far less, in fact, I can't remember the last time I saw a chemist run an IR spectrum on anything! Electron Ionisation MS (EI-MS) is much reduced, much work is using Electrospray these days because people want a molecular ion and they don't want fragmentation. Again, it was all originally EI or Chemical Ionisation and now it is probably >90% Electrospray in terms of volume (mass spec as an HPLC detector).

TD: What innovation would you have liked to have seen before your retirement which hasn't yet reached fruition?

JH: What I would really like to see is a true set of data standards for analytical data. As you well know with your involvement with JCAMP, it was a very, very powerful and useful thing, and still is—people are still using it today. But I think we have been extremely poor at pushing data standards despite numerous attempts like AniML and Allotrope. It always a chicken and egg situation, if people have it, they will use it. Allotrope have probably got the funding model right as they have a subscription model, so companies pay to belong to Allotrope and that money goes to fund work that is being done by different groups. I was on the Allotrope board for several years and I saw it heading in the right direction, but the trouble is everything takes such a very long time. Everyone has their day job, so it is quite hard to dedicate enough time to it. We also tend to get too fancy with it. One of the nice things about JCAMP was that it was very pragmatic. Often, we are not pragmatic enough and that can derail things in the end. That was probably one of the issues with AniML, as it seemed to get bogged down in the minutiae; maybe taking a step back would have moved things along a lot quicker. Again, it's just a model of the data, it's not the truth! So, you must accept that it is not the truth as that would make a huge difference. So, we have a £10 M NMR spectrometer and what we store at the end of the day is a PDF for long-term storage! Is that really the best we can do things in the 21st Century? We should be able to store data in a way that we know we can do something with it in 60 years' time. So yes, true data standards, I've spent quite a lot of time on it, and I hope that it will come… but I'm not confident.

TD: Looking back, did you see any fundamental differences between the various incarnations of GSK?

JH: That's a really good question! So, yes absolutely. When I joined Glaxo in Ware it was still known as Allen & Hanbury's and felt more like a family business. Over time, with the various mergers, it became more formal, more impersonal. One indicator of this was the change of title of the "Personnel" to "Human Resources" (HR) department. It says a lot to me about how companies saw their staff. "Human resources" is a very impersonal, "balance sheet", type of thing, whereas "Personnel" is talking about people. We have lost something important as a result. Some small companies still have it, but big companies generally don't and that is one of the big disadvantages of working for a big company as you might feel to be a plus or minus on the balance sheet.

TD: That is a very interesting observation about the different titles for the department handling people.

JH: Yes, I don't know where the term Human Resources came from—possibly out of the US, but it is such a hateful term, as if you're just running a farm, you talk about head counts… it's so impersonal.

TD: Was there any difference in access to capital funds?

JH: Well, no not really, access to capital is always tight. Except maybe in my early days at Glaxo when it was growing rapidly and if you wanted something you could probably get it. You just needed to convince somebody of the need. But, over time, there has been pressure to lower costs, because it is an expensive job getting a drug to

market. This is also true with operational costs. It is a cost-restrained business. This is what has driven a lot of what I have done. If you know you have limited equipment and limited numbers of people, what you have to try and do is get the most out of the equipment and minimise the time people spend doing things that a computer can do for them. One example is purification factories. Chemists spent a lot of time purifying what they had made. Why not simply automate that process so that they can go back to making more stuff and let someone else worry about purification and registering, as it doesn't take a chemist to do all that stuff?

TD: Does working in a tightly regulated industry strangle innovation or ensure consistent quality? Although having asked that, I seem to remember that years ago you were happy that you were working in Discovery where there was a much lighter touch if I remember rightly?

JH: Well, I spent time doing projects in Development, so I always had a reasonable understanding of what the compliance requirements were in the Development environment. But coming back to your original question about whether it strangles innovation or ensures consistent quality—the answer is it does both. Its why Discovery is less regulated than Development, because that is where you really want a lot of innovation. It does mean that people are very wary of moving things on, they are very risk averse and often will not take something on unless they can pretty much guarantee it will be a success. So, in that sense it does strangle innovation, and I see it coming more and more into Discovery, which I see with some horror as it will strangle innovation where it really has to happen. I think where regulation is appropriate, it is essential and I think anything that is going to go into humans absolutely has to be regulated, as you can't afford for there to be mistakes. Ironically if you spend a bit of money in the Development environments to make sure that data flows correctly, again going back to the data standards thing, you get a lot of this stuff for free; so, you need to be persuading people that are doing this fundamental data handling stuff that it will actually improve your compliance.When the regulator comes and says "tell me such and such…" you just press a button and you have your answer rather than "I'm going to go through all my records and going to get this out of this database and this out of this database and put it all together.." you can actually get a lot for free. But, it does require a lot of initial investment, so the question is do I spend the money getting the drugs out of the door or do I spend money so I can get drugs out of the door better in the future? It's the old story… I'm too busy mopping the floor to find time to turn off the taps!

TD: Now, although we have the habit of concentrating on technologies and software developments, none are effective without a good working environment, which means people. I think, as I have got older and further in different organisations, I concentrated far more on the people rather than the technology. Good people can do wonders with not the best technology, whereas average to poor people can be given the best equipment but still fail to deliver.

JH: Absolutely, I think it is a good point and I see the same as you do. I don't think companies spend enough time to get people to understand each other and understand their differences. There is a lot of talk about diversity, but it is quite often the wrong diversity—race, religion, gender identity—all aspects of which are important, but there are more fundamental issues around what makes people tick? I'm sure you've done the old Myers–Briggs, that was great because it doesn't matter whether you believe in their quadrants or not, you go through the process and you come out with what my preferences are. And when I was doing it, I was also thinking about people who work for me or work with me. How would they answer that question? And by the time you get to the end of the process you realise why you really do not get on with this person or that: it's because they are in this quadrant or that and we have very different outlooks on life.

TD: I'm astonished you picked that answer. I have worked in an international management team from quite different backgrounds and experiences that was often at loggerheads with each other. Really difficult to get agreement on anything. Until we undertook the Myers–Briggs training together. I think everyone was quite sceptical at the start. I think we split the workshops over a couple of days and came out of the process completely understanding why Person X found Person Y completely frustrating! So, instead of "why can't he understand", or "Why can't they see this…". Now I am against putting people in pigeon holes, but it was a great tool for putting people into Myers–Briggs pigeon holes to understand how they functioned and we all got along much better after it, as we now knew "why they couldn't understand it".

JH: Yes, in my example I was in charge of a registration team. Their job is to be absolutely focused on the details, so it attracts people who like to focus on the details. But they were turned-off by talk of the bigger picture, which I found very frustrating. So, after I had done the Myers–Briggs I asked them think about the questions as if they were me, and they got me down almost exactly as I had. At the end of it, the head registrar came up to me and said that he now understood that

when I said "that's just the details" it didn't mean I thought that the details were not important, but just that you were looking at the big picture. Once we understood that, we could see that we are both trying to end up at the same place but using our different skills. I have to say that it was never a bad relationship, but in terms of driving things forward it made a huge difference. People can be sceptical about Myers–Briggs but the key thing is that you understand your differences and you do something about it to use your strengths to get the best result. An ideas person is just that, but you need someone to actually make them work. Someone has to look at the details so you need both sets of people.

TD: If your younger self, just starting out on your career, was attending your retirement party in January, what words of wisdom or warnings would you like to give your younger self?

JH: I would say "Chill and don't take things personally" … because I used to get incredibly frustrated when people could not see what to me was obvious. I think my behaviour was not great when I started. I think I was arrogant, and I could be short tempered. And I've seen your follow-up question about would my younger self have followed that advice—probably not… the arrogance of youth! Persuading people is not about battering them with facts. Sometimes it takes time. My greatest thrill is if I have been banging on about something for a long time and not getting anywhere, to go to a meeting and someone uses my own words back at me as if they've just thought of it… Great, we've got there! One of the things I've learned is if you keep on going head-on against the barriers people put up, you will not achieve what you want but you just have to take a step back and approach things in a slightly different way. I don't think I would have listened as my younger self; I was far too sure of myself.

TD: From someone with one foot in the University world, I would love your views on whether we are teaching the correct skills to the people you would be recruiting?

JH: In terms of people coming in with degrees or PhDs, I'm not sure that people learn much from spending longer in academia. I think there comes a time when you got to come out and hit the real world. In my opinion the earlier you can hit the real world the better. While I was working at GSK we recruited a lot of apprentices. I think the apprentice approach in the UK is just superb in the right environment. People are brought in and they can do their degree part-time, somewhat going back to the days when you could do a part-time degree. The great thing is that while they are doing the theoretical side of things, they are actually carrying out real practical work and see how the two relate. Almost without fail, these apprentices are the best people that we recruit. By the time they finish their degrees, they are fully functional, very competent members of staff. Back in the day, Glaxo took on a lot of members of staff to do part-time degrees, HNCs or whatever. One day a week to do your academic work takes a lot longer of course, but especially these days you don't have a massive debt around your neck and businesses end up with the people who have the skills that they want. We should be trying to help Government encourage more of this as they will benefit from all these people getting degrees, whilst being productive for the economy.

TD: So, do you see this academic pairing as important for the skills base going forward?

JH: It tends to be only something we do on things like the apprentice. The standard academic institutions are generally not influenced by industry or if they are, it is very indirectly and particularly in the sciences there should be far more two-way communication about what the academic process is, what things are taught and what things are going to be useful going forward. I don't think that happens enough currently and it probably needs to happen more. There have been such instances in the past, GSK had a laboratory at Cambridge University in the chemistry department and that really helped cross-fertilise ideas. Unfortunately, that is no longer there, but I know other companies are doing this. Maybe there can be a formal way to engage without actually having to set up laboratories with regular communications between leading employers and academics just to see how relevant the education is. Of course, it doesn't all have to focused on business as there will always have to be purely academic topics in the curriculum.

TD: I must admit I have been horrified by how many academic institutions teaching chemistry don't actually let their students touch the analytical equipment. It would seem that the higher-ranking the institution, the more the funding has been funnelled into the research instrumentation, often purchased from research grants and the undergraduates are not even allowed in the room with them. Samples are handed over and spectra appear as if by magic. For me this is a massive mistake. You need to have instruments that people can make mistakes on.

JH: Yes, my example from my experience on the EM360 in the first part of the interview probably formed my thoughts on what my career would be going forward, what stuff I enjoyed doing. But if you don't get the chance to do this hands-on you will never know until you get into industry and then you might decide it isn't actually what you want. I think this is important for the sciences, maybe not for the

arts, but that's slightly different and I'm not sure how you would do that, but there are probably equivalent things in the arts. Having that link to the world outside academia is really good.

TD: What are your plans for the future? You've already mentioned you are doing some consulting?

JH: I am doing some consulting and I will continue as long as I find it interesting and am adding value. I do like to have time to do other things, which is fine. I would liked to have continued with Allotrope, but the way Allotrope is set up makes that almost impossible for an individual to contribute. This is something I may bring up with them at some point. I still see Allotrope as being the best chance we have at analytical data standards, but it has taken a long time. It always takes a long time for these things but it has taken a very long time so I would like to still have some influence on it.

TD: My worry about this and several other similar initiatives has been the fact that they wouldn't put anything out into the public domain. That made it almost impossible to help or critique or whatever. Often all you could get out of them was "we are working on it" to questions about how are you dealing with this? So, how's the documentation going... how far have you got... there is just no feedback. There was a lot of good, expensive marketing at a number of LIMS-type conferences, but in the end you couldn't get involved in any discussions of substance or try to align the work you yourself are doing.

*JH: I think Allotrope has changed as originally it was all about the funding model and I think the assumption was if you are going to pay money for it you need to get something out of it, so it was a closed shop. The reality is I think most companies would have joined even if they hadn't got exclusive rights on what was being produced. So, things like the ontologies are public domain, which I think is good and a step in the right direction. The simple data model they have got, which is a simple JSON representation of the data, will become public domain **de facto** as you can reverse engineer it. Where it was originally with the binary representations which required the libraries to do anything with it—well I was never a great fan. I understood why they did it, but it was too complex and you were required to have a very in-depth knowledge of how the data structure was set up and what the bits mean.*

TD: This reminds me of discussion in the ASTM AniML committee where the programmers said they would only store 8-bit numbers—we pointed out that many instruments were storing 16-bit natively, so they came back and said we will only store 16-bit numbers... so, we said what if the NMR instruments are storing 64-bit data? You simply cannot restrict the formats in these ways. You must be flexible enough to be able encode whatever the measuring system is providing.

JH: Yes, it's one of the areas where I have been in numerous discussions on the best way forward and the bottom line is it depends on what sort of data you have. The idea about Allotrope is that it is meant to be a data standard to cover all scientific data. Now, obviously that is a very big thing and its not going to happen straight away, and you need to concentrate on certain areas, but it should be capable of being extended to other things in the future. The first thing is to make sure you call the same things by the same names and that is the ontology. Next a lot of the data can be represented in ASCII, so you could put that in JSON, but very large data sets like TOF MS are too huge, so you have a companion file which is a binary representation of the original data which hooks into your JSON file. So, if you are only interested in the metadata, you can simply get that from the JSON ASCII file; but if you want to read the data you will need the binary file and some tools to do that. So, I pushed very hard while I was there for anyone with elementary programming skills to be able to say I've got an Allotrope JSON file and I know how to parse it; in fact I already have the framework to parse it. It should be democratised to that extent and that was the great thing about JCAMP—anyone could work out how to parse a JCAMP file. I know when JCAMP came out and I was working on vibrational spectroscopy I could parse the files and write my own peak picking algorithms as the ones on the instrument were a bit rubbish! So, I could properly identify shoulders and represent it all in a plot and all that stuff I could do because of JCAMP; otherwise it would have meant dealing with vendors' binary formats that they would not publish. So that was probably one of my experiences that made me so keen to get good analytical data standards and one of my biggest regrets that I didn't manage to do that. Maybe I left it in a slightly better place than when I arrived.

TD: So, on that positive note is there anything else you would like to discuss before we put a wrap on this interview?

JH: Well, I think it's been pretty extensive. It's brought back many memories of things I did when I was just starting out. I hope it will be interesting for people to read. Going back to the life lessons, I heard Digby Jones, once head of the Confederation of British Industry, say he used the phrase SUMO—Shut Up and Move On. He said that there are times when you've tried your best and you know that it's not getting anywhere. Shut up. Move on. There are other things to

do. He gave an interview about his history and that is one of the things that really stuck with me. It doesn't mean giving up on something it just means stop being so vocal about it, move on to something else because it will come around again. If it is important, it will come around again!

TD: So, it is definitely time to SUMO!" Thanks for your patience and I hope it wasn't too intrusive.

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SAMPLING COLUMN

Unsubstantiated complacency re. the "assay exchange" paradigm: sampling uncertainties with hidden economic consequences

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The Assay Exchange paradigm is an integral element in many contractual agreements stipulating how business transactions rely on comparison of two independent assay results for commercial trading purposes. It turns out that the current Assay Exchange vs splitting gap comparison paradigm incurs no less than two unrecognised sampling uncertainties, which leads to hidden adverse economic consequences at least for one—and sometimes for both contractual parties. The magnitude of this unnecessary uncertainty is never estimated, which leaves management without information about potential economic losses, a breach of due diligence. However, all that is needed to resolve this critical issue is stringent adherence to the Theory of Sampling (TOS) by mandatory contractual stipulations of only accepting representative sampling and sub-sampling principles.

Introduction: definitions

To appreciate the most general application of the findings described below, let's define a technical "black box" (BB) as an element in a business process. A BB connects product exchanges between a buyer and a seller, or the BB constitutes a comparison platform for analytical results from two or more analytical laboratories; a special manifestation of a BB would be as a depository for goods awaiting quality checks by one or both trading parties. The topic treated here is typically surfacing within the realm of, e.g., mining and metal refining, TIC company operations (Testing, Inspection, Certification), shipping agents, traders, regulating bodies, banks, financiers, investors etc.

In the treatment below a few definitions and synonyms are needed:

- Seller/depositor/supplier/laboratory 1
- Buyer/customer/laboratory 2
- Umpire (mutually agreed upon authoritative "third party" analytical laboratory)

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Reasons behind the "assay exchange" paradigm

For the present discussion, let the focus be on trading involving metal concentrates, or a depositor delivering a consignment to a refining facility with the aim of refining various precious metals. There is always a need for fast accounting in commercial trading, or, in the second example, since the physical–chemical refining process operates on a much longer time scale than the desired business closure; the speed and, of course, reliability of the business accounting is of the essence.

The seller's assay results recorded on the suppliers' waybills are the input documentation relied upon for capturing the physical movement of materials **into** the "black box" (documentation shall ideally reflect the depositors' materials type *in extenso*, i.e. content, weight and assays of the precious metals involved; sometimes also "deleterious metals" diluting the valuable metal grades).

However, the depositors' assays are generally **not** relied upon by contractual parties for the purposes of securing *reliable* output documentation accompanying the movement of processed metals out of the BB facility. In such cases, the sampling procedures used for providing the material for analysis is contractually the responsibility of *both* transaction parties *individually*. This means that all contractual documentation, comparison and/or reconciliation objectives

Black Box (BB)

Facility either processing incoming material ("active BB") or used as a passive facility recognised by both parties in a contractual trade relationship ("storage BB"). The objective of an active BB can, for example, be refining of precious metals, or it could be a mutually accepted secure depository holding a consignment until a later date, related to commodity trading (e.g. hedging). In general, a BB facilitates product exchanges between a buyer and a seller, or it can further split-sample exchanges between two analytical laboratories. Incoming material to a processing BB will be assayed either by the depositor (the seller), the BB facilitator or by a third-party agent appointed and approved by both contractual parties, producing "ingoing analytical information". When leaving the BB, processed, or end-of-storage material, will be independently assayed (outgoing analytical documentation), either by the opposing trading party (the buyer), or a third party (the "umpire"). The determining feature of a business transaction is the "assay exchange" paradigm, which is the standard agreement facility with which to close business.

MvG (Mismatch vs Gap) risk: Difference between assay values from two opposing parties, compared to the magnitude of a contractually agreed upon maximum "splitting gap". The absolute assay difference is compared to a mutually agreed splitting gap range, regardless of the general level of the average gap concentration level, which leaves analytical accuracy stranded as a victim of economic expediency—to be explained.

are exclusively based on the resulting analytical results from the two parties, each interested in optimising their own prospect in the commercial transaction. The assay exchange paradigm is designed to resolve the closing business settlement issues and interests on a fair and equal basis.

Function of the "assay exchange" paradigm

In commercial practice, an agreed assay is determined between a seller and its customer via a financial negotiation. The agreed assay is referred to as the "settlement assay" and the process of negotiation is referred to as an "assay exchange". The negotiation basis typically used is age-old and have remained effective and unchallenged for long. A short initiation is as follows:

- "A primary sample of the lot in question is split into three subsamples intended for i) buyer, ii) seller and iii) umpire".
- Both parties (seller and buyer) simultaneously advise the other of its assay result.
- Either party is obliged to use the assay determinations produced by their respective laboratories [the parties can in fact submit any assay result they may desire, but there is an in-built near certainty for a heavy punishment for a(ny) party wishing to tip the scales unilaterally hopefully in its own favour, see below re "payment to umpire"].
- If the two assays exchanged fall within a contractually specified range, "the splitting gap", the mean of the two assays becomes the settlement assay—end of business settlement: the accounting department makes the necessary multiplications of tonnages, concentrations × unit prices etc.
- But if the difference between the two assays is greater than the "splitting gap", an independent third-party umpire shall arbitrate, helping to determine a settlement assay in accordance with the contractually agreed procedure. Variants of the details of this latter part of the paradigm exist, but the basic principle of a splitting gap determinant remains. This process is referred to as "going to umpire".
- Details: The difference between the two reported assays is compared to the contractually agreed maximum "splitting gap". If the difference between the reported assays is lower than this threshold, the average of the two assays becomes the Settlement Assay. If the difference is greater, the business paradigm dictates that the third sub-sample of the primary sample is assayed by the Umpire laboratory (this sample has been kept in secure storage until it was decided whether to include it in the assay exchange scheme or not). In this case, the middle

Official definitions

The MINEHUB website describes the assay exchange process for the commodity concentrates (accessed 18 December 2022):

"Concentrates are finely ground materials (with waste rock removed) containing metals and minerals from mine sites such as copper, nickel, lead, zinc. The value of the concentrate is defined by the composition and prices of the individual elements that make up the concentrate. Every time the concentrate changes hands or custody, the buyer and seller rely on laboratory tests called assays to verify the metals composition. The assay exchange process is an iterative process in which the buyer and seller compare their respective assays and sometimes require umpire arbiters to ultimately agree on the chemical specification of the concentrate that is being transacted, and therefore the final price the buyer must pay the seller."

of the three assays becomes the Settlement Assay.

N.B. Whichever party is farthest away from the umpire's result pays the umpire's analysis fee, which is always (very) expensive (this is the potential punishment indicated above for trying to skew data without factual evidence). Following the conventional scheme, gains and losses to the buyer and seller will be the monetary value of the difference between the settlement assay and their respective own assays, adjusted for umpire fees for the "loosing party".

The fixed assay exchange *scheme* is designed to determine a settlement assay with ease, clarity and speed under the tacit *assumption* that the settlement assay will always lie close to a target lot's "true" metal content and that all analytical differences are *exclusively* a result of relative analytical ability. This assumption is incorporated in Figures 1 and 2; while Figures 5–9 portray the more realistic assay exchange setup, explicitly acknowledging a sampling-before-analysis variance that will always *also* be present. This case is explained in full detail below.

While in the real world the two-party setup has many manifestations, e.g. buyer vs seller, loading port vs discharge port sampling, analytical lab A vs analytical lab B (Figure 2) the principal issue is identical, a determining assay exchange. In the following, the example of sampling and certification at two ports (seller's loading port vs buyer's discharging port) is used.

The focusing issue is that non-representative sampling impacts *independently* at the two ports. Potential biased sampling, as well as other sampling deficiencies, if/when present, will unavoidably result in significant, increased uncertainties (blue: avr. ±2 std). The point here is that the magnitudes

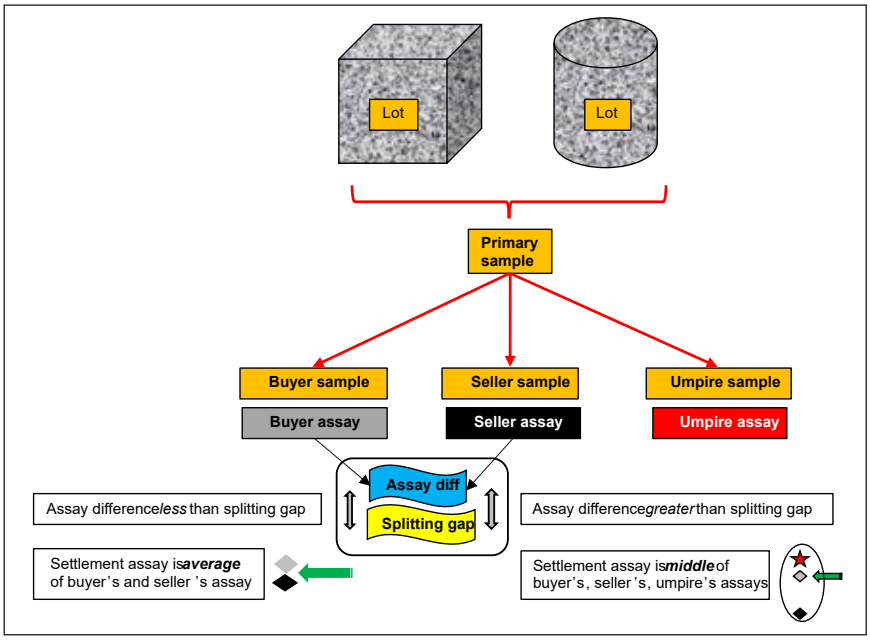


Figure 1. Conventional Assay Exchange Paradigm: focus is exclusively on relative analytical reliability.

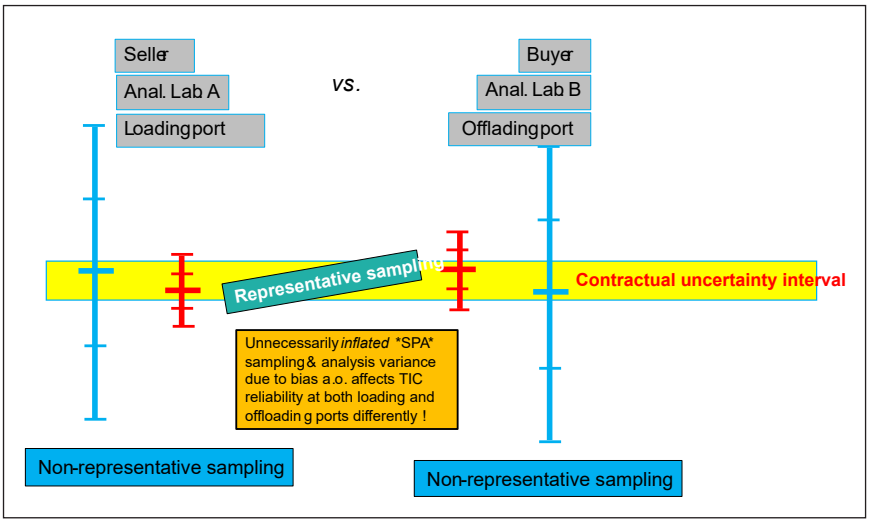


Figure 2. Two-party dilemma. Non-representative sampling compromises assay results independently at the loading and discharge ports. Compromised sampling performance will always result in larger-than-necessary uncertainties (blue: avr. ±2 std)

of these inflated sampling-plus-analysis variances are never known within the conventional paradigm—rather they are ignored.

An elephant in the room

Thus, the adverse impact from inferior sampling is not included in the conventional assay exchange paradigm; there are simply no sampling stipulations associated with the mandate: "the primary sample is divided into three subsamples" intended for the seller, the buyer and the umpire, Figure 1. Rather, since assay exchanges are financial *negotiations*, generally they are *business compromises*, under adverse sampling conditions this procedure *can* in fact produce a settlement assay significantly *different* from the actual

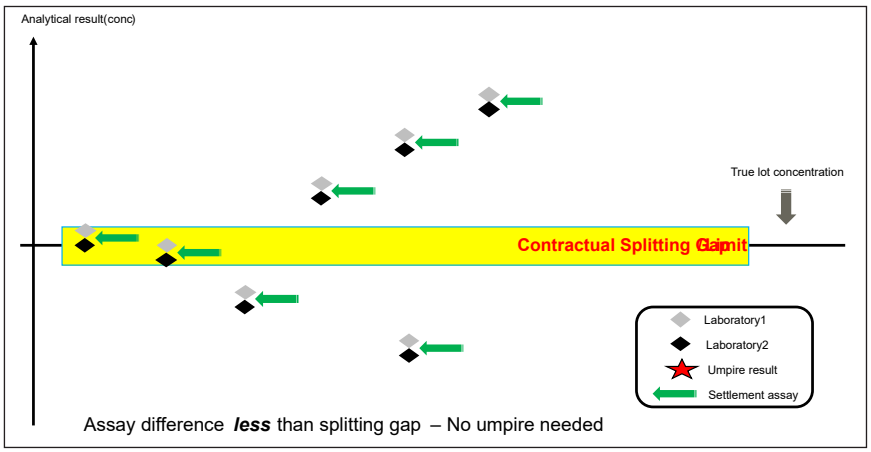


Figure 3. Functionality of assay exchange paradigm, the case of "no umpire needed". Note the tacit assumption that the splitting gap is centred on the "true lot concentration".

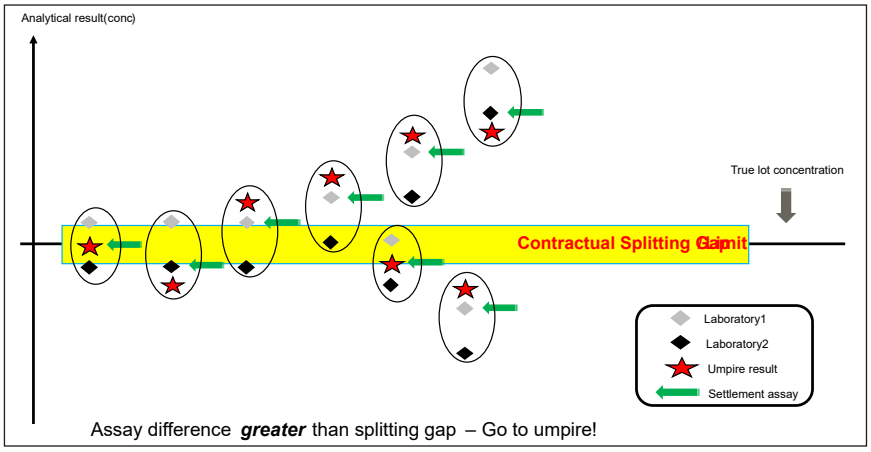


Figure 4. Functionality of assay exchange paradigm, the case of "go to umpire", after which the middle assay will be the settlement value. Note the tacit assumption that the splitting gap is centred on the "true lot concentration".

("true") metal content in the lot. This is here termed the *mismatch vs gap* error (MvG), to be exposed in full.

While the MvG is an acknowledged risk for/by both parties, in the interest of a quick business resolution, most parties are usually eager to get to the settlement assay, accepting the MvG (knowingly or unrecognised) without further ado, to get the payment for goods delivered effected as fast as possible. This *status quo* is presumably a reflection that both parties consider this a symmetrical risk, not worth elaborating much upon for every single transaction in view of the magnitude of day-to-day business economics: sometimes the seller (trader, depositor …) could perhaps be shown to be marginally over-paid (the BB facility pays a bit too much for a marginally overestimated material grade)—but in the long run this is considered levelled out by the opposite possibility in which the buyer (or the refined deposited allotment collector) is actually being paid marginally too little for material, the amount and concentration of which happened to be underestimated. *Status quo* for the, often hidden, MvG risk is that assessment hereof is only very rarely included in the commercial contract stipulations.

The current state of affairs is shown in Figures 3–4.

The **elephant in the room** is the tacit, unwarranted *assumption* that the contractual splitting gap is always centred on the true average lot concentration. Note for example in Figures 3 and 4 that an acceptable settlement assay is easily reached via the assay exchange scheme *regardless* of whichever general analytical level is bracketed by the interval spanning the three samples involved.

But this assumption is severely challenged by the fact that the crucial primary sample (which is immediately divided in three sub-samples) is in fact sampling a *heterogeneous lot/materials*.

But the reality is even more complex. The full scenario behind the assay exchange paradigm is shown in Figure 5, emphasising no less than two sampling operations, each with its own sampling/sub-sampling errors and uncertainties involved, all *before analysis*.

Following the TOS, when sampling heterogeneous materials (aggregate materials and mixtures, materials with significant grain-size contrasts …), there is every reason to take notice—and specially to take

The Theory of Sampling (TOS) interlude: **all** materials in the realm of technology, industry, processing, trading, commerce … for which Testing, Inspection and Certification (TIC) is on the agenda, are *heterogeneous*—it is only a matter of degree. The Theory of Sampling (TOS) has for over 70 years proved the severe danger involved in assuming that there is no sampling error involved in extracting the primary sample—but this is not the place to detail the TOS. There is ample background literature available, e.g. References 1–6.

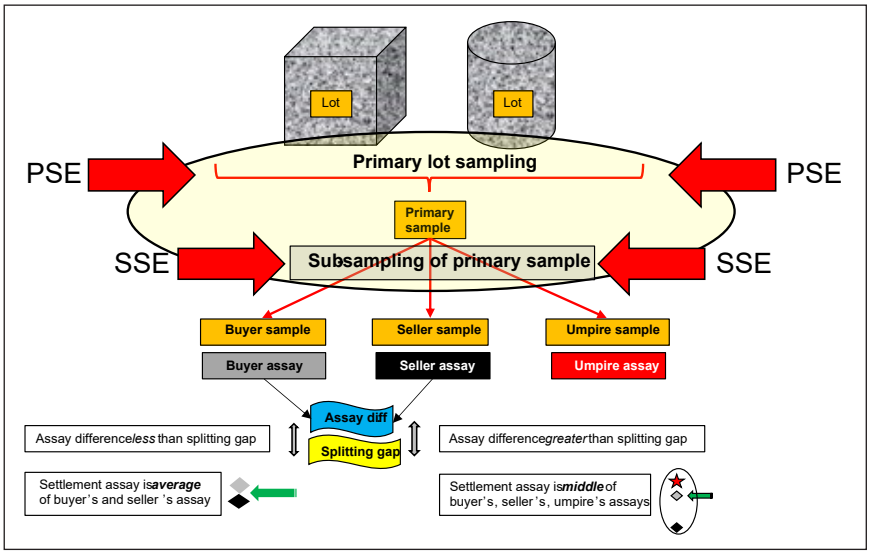


Figure 5. Assay Exchange reality—acknowledging two sampling stage uncertainty impacts: PSE, SSE (red arrows). PSE = Primary Sampling Error; SSE = Secondary Sub-sampling Error.

appropriate operational precautions—regarding the impact of the dominant primary lot sampling error (PSE).[1–6] And there are equally serious reasons to take appropriate precautions regarding the subsequent "sample division" producing the three tacitly "assumed equal" samples for the seller, the buyer and umpire, for which there will be a secondary sub-sampling error (SSE). The latter may perhaps typically be smaller than PSE, but never neglectable, especially if suitable practical facilities to be used for appropriate comminution and mixing are not mandated in the contractual stipulations.

Assay Exchange paradigm: the grim reality

The degree to which is has been possible to reduce PSE will determine the general analytical concentration level in the primary lot sample, which, therefore, *may* differ from the "true lot concentration" to some, generally unknown degree. Appropriate precautions first and foremost include the TOS' ability and success in eliminating the Incorrect Sampling Errors (ICS), which is the necessary condition for unbiased sampling.[1–6] Similarly, regarding the subsequent sample preparation and division, *ibid*. Of these the primary sampling error (variance) will usually contribute with a dominating uncertainty contribution, but accidental residual heterogeneity *within* the primary sample may also contribute significantly with appreciable uncertainty contributions regarding "sample division".

There is a logical order to these complementary influences, as follows. The degree of incomplete primary sampling bias elimination will lead to a random location of the splitting gap—which is manifested as a deviation from the *assumed* centring on the true lot concentration, as shown in Figure 6. This will be the situation regardless of whether the paradigm leads to "go to umpire" or not, Figures 6 and 7.

Mismatch vs Gap error (MvG)

A deviation between the settlement assay and the "true lot" concentration is termed the "Mismatch vs Gap" error, MvG. This uncertainty constitutes an economic risk, the MvG risk, which needs to be managed, which it manifestly is not a provision envisaged in the conventional assay exchange paradigm.

Adding in the sample division error (sub-sampling bias and/or variance), the relative disposition of the three analytical results cannot be ignored. The tripartite assay results from lab A, lab B and lab Umpire will depend on to which degree the primary within-sample heterogeneity has been successfully reduced/eliminated by appropriate TOS action before and during the practical sample division.

The full MvG risk can be illustrated with graphic clarity, Figures

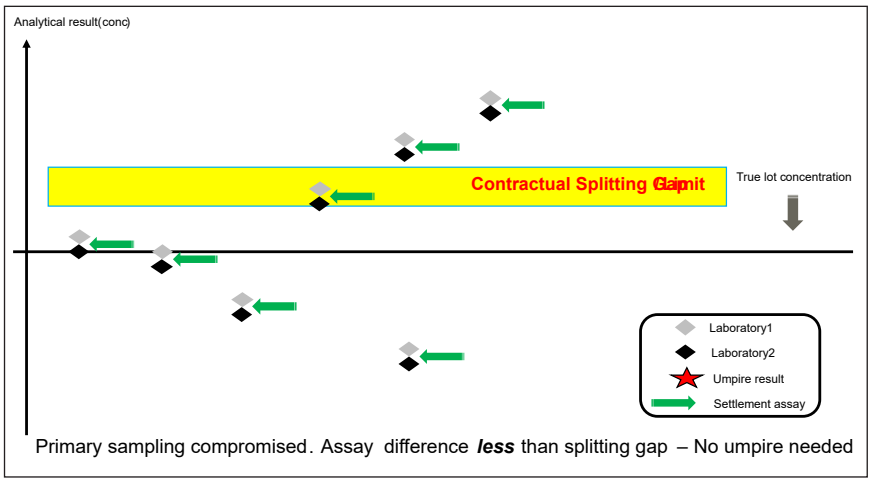


Figure 6. Same as Figure 3, now illustrating a realistic splitting gap location, which is random as a function of the degree of incomplete sampling bias elimination and other ISE deficiencies.

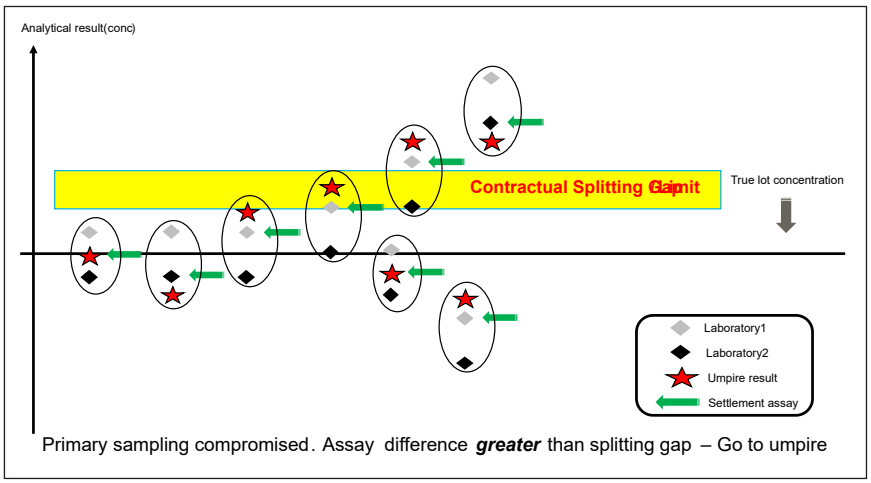


Figure 7. Same as Figure 4, now illustrating a realistic splitting gap location, which is random as a function of the degree of incomplete sampling bias elimination and other ICE deficiencies.

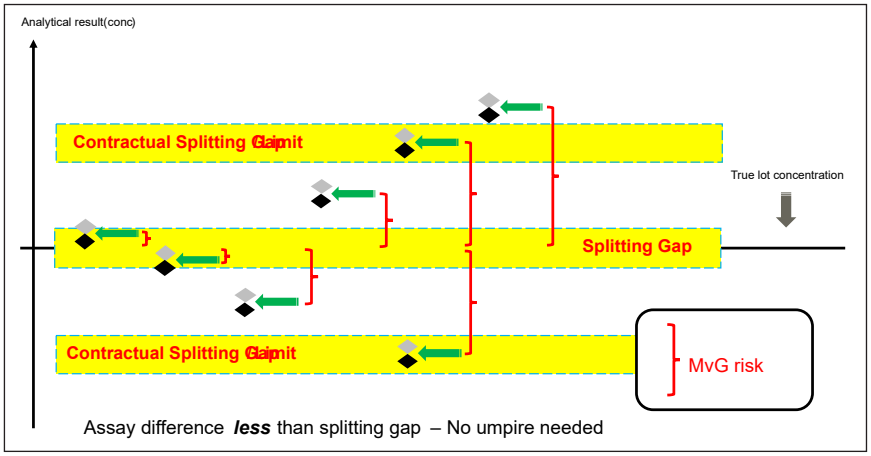


Figure 8. Illustrating the MvG risk; case of no umpire needed. The MvG error/risk is only (close to) zero in the case of vanishing primary sampling uncertainty.

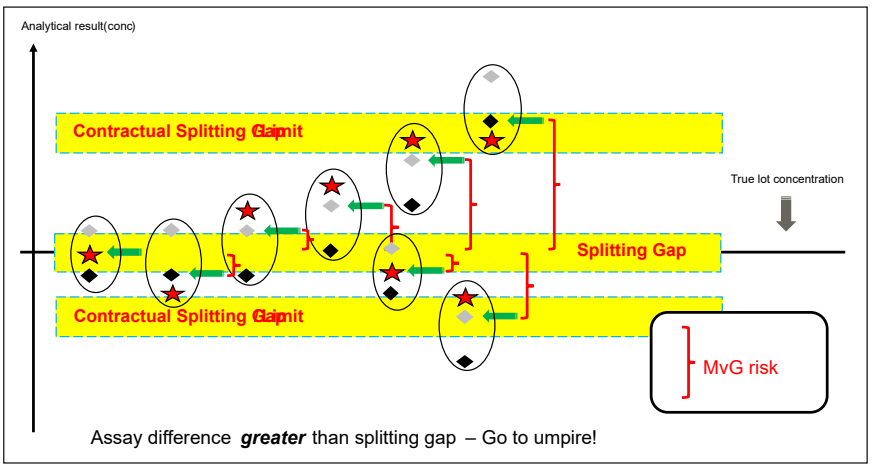


Figure 9. Illustrating the MvG risk; case of going to umpire. The MvG error/risk is only (close to) zero in the case of vanishing primary sampling uncertainty.

8 and 9. Note that within the conventional assay exchange paradigm, the MvG uncertainty is tacitly always assumed to be zero, and its risk management need is, therefore, never on the business horizon.

Figures 8 and 9 show that the location of the contractual splitting gap may be significantly *displaced* from the assumed closeness to the true lot concentration (location in the Y-axis direction), which is primarily caused by the degree of a primary sampling bias that has not been successfully mitigated. Note that the assay exchange scheme is followed *regardless* of this uncertainty, giving rise to potentially significant MvG errors—an uncertainty which is not acknowledged in the standard assay exchange paradigm. Is this deliberately overlooked? Ignored?

The point

The point to be made is that current assay exchange practices do not include mandatory means to deal with sampling influences in the splitting gap accounting scheme.

Thus, there will always be a real, non-vanishing risk of settling a business transaction based on the assay exchange paradigm at a level which may actually lie significantly distanced from the true metal lot content, a lot, Figures 8 and 9. The deviation, the MvG error/risk, *may* be small (low heterogeneity materials; acceptable sampling performance) or it *may* be large (significantly-to-excessively heterogeneous materials; non-representative sampling competence/equipment)—the point is that all this is studiously *unknown* to the contractual parties.

For many commodities, the economic risk involved *may* perhaps not constitute reasons for much worry (bulk commodities with relatively low unit value), but as tonnages go up, the sum-total economic effect may well still accrue to unacceptable amounts—while matters are always dramatically more serious for example

for the precious metals industry concerning, e.g. Gold, Silver, Platinum, some REE and *similar*, where even small amounts of misassigned concentration results between buyer and seller translate into highly significant economic consequences. As an example, a misappropriation of 1 kg Gold represent a value of ~USD62,000; 1 kg for Platinum, ~USD33,775. Readers can do their own maths.

There appears to be *some* awareness of the issues delineated in this feature, for example:

Dave Murray, Asahi Refining (excerpt from): *Deleterious Metals & Their Impact on Splitting Limits & Assay Exchanges for Gold Dore* (Presentation at LBMA Conference 2021). "The splitting limit is the percentage band in which when comparing a client's assay to the refiner's the average of the two assays will be used as the basis of settlement. When outside this percentage band, a third analysis is performed by an independent umpire laboratory. Most often the splitting limit is contractually 'negotiated'; almost becoming a commercial term. Maybe this is just based on historical contract traditions, or perceptions of risk with higher metal prices. Quite often there is very little consideration of 'process capability'. Not always is there a lot of consideration given to the nature of the material being sampled and assayed".[7]

Awareness is good, but advice, recommendation and practical "what-to-do-about-it" tools are often missing. A comprehensive analysis of the TOS as a determining element in risk assessment and risk management was presented recently in which all necessary-and-sufficient actions to remedy the critical issues delineated above were presented: "Framing TOS in Risk Assessment".[8]

Potential economic consequences

Because of omission of all sampling and sub-sampling variance influences in the assay exchange paradigm, there is a very big elephant in the room! Sampling errors and their effects (sampling bias and/or larger sampling variance than necessary) are overlooked in the conventional assay exchange accounting scheme. The economic consequences can be significant to severe, and always detrimental to at least one of the parties involved, but notably, **never** to the umpire institution or company—which is ok as the origin of the MvG risk is never with this entity anyway.

But the umpire costs can in fact be eliminated, see further below. Figures 8 and 9 shows with graphic clarity the principal non-zero magnitudes of the MvG risks under the ruling splitting gap assumptions. The magnitude of this unnecessary risk is never estimated, it is in fact rarely acknowledged and its economic consequences are, therefore, unknown, hidden from management.

The *status quo* is that the critical assay exchange paradigm ignores the MvG risk. It matters not that the economic value of this unmanaged risk *may* be small, because it *may* just as well be large—this is entirely a function of the managed, or unmanaged sampling errors, uncertainties and risks presented. Small effects may perhaps be wished-for in the *status quo*, but the real magnitude will forever be unknown, when studiously looking away…

However, there is a solution:

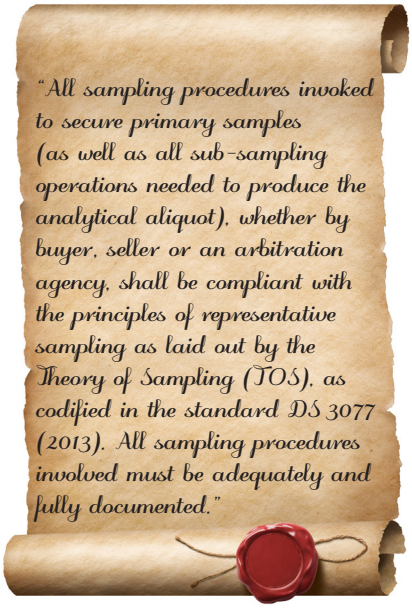
Universal resolution

One might perhaps worry that remedying the hidden MvG risk issues would entail a colossal effort—as checking for its magnitude at every commercial transaction would indeed be prohibitive.

However, all that is needed to resolve all these issues is remarkably much simpler!

The entire array of debilitating issues regarding the assay exchange *scheme* will conveniently go away if/when a mandatory statute is agreed upon by all parties **only** to use TOS-compliant representative sampling and sub-sampling procedures throughout the full lot-to-aliquot pathway. A one sentence mandate, to be included in every relevant trade contract going forward, will solve **all** problems:

"*All sampling and sub-sampling operations serving to provide the basis for the assay exchange accounting shall be in full compliance with the principles for representative sampling laid down in the Theory of Sampling (TOS)—sampling and sub-sampling operations shall be fully documented.*"



Parting shot

Various suggestions are often given in defence of the assay exchange paradigm, for example: "*Samples should regularly be sent for Round Robin (RR) assaying and comparison*".

To which: the findings of Round Robin comparisons, also called Proficiency Testing Programmes, are highly sensitive to whether the sample division process producing *assumed* "identical replicate samples" sent off to participating (and umpire laboratories) is indeed representative—or **not**. The Round Robin *scheme* is based on the premise that all primary samples are always divided into

a seller—buyer—umpire tripartite set of scrupulously identical subsamples (or into a series of individual Round Robin subsamples individually analysed by participating laboratories). If/when not enough, or no attention at all, is directed at the quality of the critical subsampling involved, the Round Robin scheme is subject to the exact same critique levelled above to the standard assay exchange paradigm. When no attention is directed to the sampling issues involved, the Round Robin facility is only able to compare the analytical performances alone, leaving the sub-sampling variance totally out of the comparison, effectively allowing a similar MvG risk.

Of course, good quality Round Robin organisers recognise that errors in subsampling may significantly influence the statistical study and the conclusions on performance of the participating laboratories in a certain testing programme. Therefore, Round Robin samples are often prepared to a much smaller particle size than what is the common for commercial settlement samples. The reasoning being that such final particle size will increase mixing efficiency and help reduce extraction errors, e.g. from smearing gold left behind on the pulverising instrument or by discarding oversize sample material that is too hard to crush. With Round Robin this "does not matter" as the aim is to compare analytical performances only. A Round Robin facility will sometimes perform homogeneity checks itself, to verify that each divided sample generates the same analytical result when analysed with its own in-house laboratory. Only after such vigorous measures have satisfied the Round Robin facility, will it send out the programme samples to participating laboratories. However, such proficiency testing samples have no longer a representativity relationship with the donor material they originated from; they have specifically been prepared to make the Round Robin exercise, or Proficiency Testing Programme, only focusing on the relative analytical performances; therefore, the Round Robin facility cannot validate the assay exchange paradigms. The Round Robin issues are identical to the assay exchange setup in that the accuracy w.r.t. the original lot composition will never be known. While this may be acceptable in the case in which one is really *only* interested in analytical performance comparison, this means that there is no saving grace w.r.t. the assay exchange paradigm: Round Robin checks will never be able to detect and to quantify the associated subsampling errors and their resulting uncertainties.

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SAMPLING COLUMN

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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Duncan Aldwin Vogel is a global expert in weighing, sampling and testing of traded commodities. Already during his study in business management at the International School of Economics, Rotterdam, Aldwin started building his pedigree in the renowned family inspection business Hoff & Co. Services BV that became part of Bureau Veritas in 2010. From 2011 to 2013 Aldwin was based in Houston, USA for BV as acting Director, Steel and Energy Products. From 2013 to 2022 he was responsible for BV Commodities Global Service Line as Director Technical Governance. In 2022 Aldwin changed from the large corporate multinational to return to an agile family-owned organisation, to earning trust and keeping his international client focus as Regional General Manager Europe for Alfred H. Knight. Most recently in 2023 launching a TOS compliant SamplingHub for circular commodity: Incinerator Bottom Ashes.

His expertise covers all aspects of inspection, sampling and analysis starting from green field prospect requirements to fully implemented turn-key projects. Embracing the Theory of Sampling (TOS) to the fullest, augmented inspection services through IoT and smart communication, Aldwin recently also came out as inventor and patent holder of several novel inspection solutions. He is highly experienced at all aspects of testing for Transportable Moisture Limit and was leader of the TML workgroup of the TIC Council. He is a delegate of the Netherlands on ISO Technical Committee 102 (Iron ore and direct reduced iron) and TC183 (Copper, lead, zinc and nickel ores and concentrates) where his focus is on sampling, sample preparation, moisture determination and TML.

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Hyperspectral imaging and art

Preservation of cultural heritage like paintings, manuscripts, maps and old photos through documenting and transforming to digital form for archives, research, conservation or for display is increasing remarkably. Museum laboratories and university researchers use a wider range of analytical instruments to study collections. There is a need to study, for example, materials like pigments, dyes and binding media. These are not only to observe possible degradation or changes due to ageing or environmental conditions but also to reveal the artist's painting technique and methods used in the work of art.

Hyperspectral imaging (HSI) is gaining wide acceptance as one of the most valuable optical tools for art archiving and restoration. As a non-invasive and non-destructive imaging technique, HSI is safe for even the most fragile samples. It is used remotely to scan all parts of the sample with a high spatial resolution (down to 15 µm pixel size). HSI records both spatial and spectral information, which can be used to classify the chemical, physical and/or biological properties of the object.

In the visible range, it gives improved precision in colour measurement for recording pigment colour-change, which is essential for conservation. In the near infrared, the information hidden behind the outer layer or written text that has deteriorated and faded under environmental conditions may be revealed. Besides, fluorescence investigation is prone to highlight different solvent and binders.

Quantum Design

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Trace detection of melamine in dairy products

The illicit addition of melamine to milk due to its apparent enhancement of protein content in foods attracted worldwide attention in 2008. It was discovered at this time that melamine was being deliberately added to raw milk at collecting stations in rural China. Thousands of young children and infants that consumed formula produced from melamine-tainted milk experienced kidney damage and death. As a result, both daily intake limits and increased monitoring of melamine in dairy products were established globally. Misa (Metrohm Instant SERS Analyzer) provides quick, easy and robust detection of melamine in a complex food matrix. As a direct test with no additional reagents, Misa's assay format requires minimal user training, in contrast to standard analytical tests for detecting melamine, including capillary electrophoresis, GC-MS, LC-MS and immune-based assays.

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Trace detection of potassium ferrocyanide in table salt

Potassium ferrocyanide (KFC) is an anti-caking compound added to table salt. Although KFC is a common non-toxic food additive, its spectroscopic response is representative of analogous cyanide compounds. Trace detection of other cyanides in food products is essential to the safety of consumers, as they can be toxic at

oral consumption levels as low as 20 µg g^{-1}. This application demonstrates rapid trace analysis of potassium ferrocyanide in table salt with Misa (Metrohm Instant SERS Analyzer), in a simple assay format with minimal use of laboratory reagents. Federal guidelines state that KFC levels may not exceed 13 µg g^{-1} as an additive to table salt.
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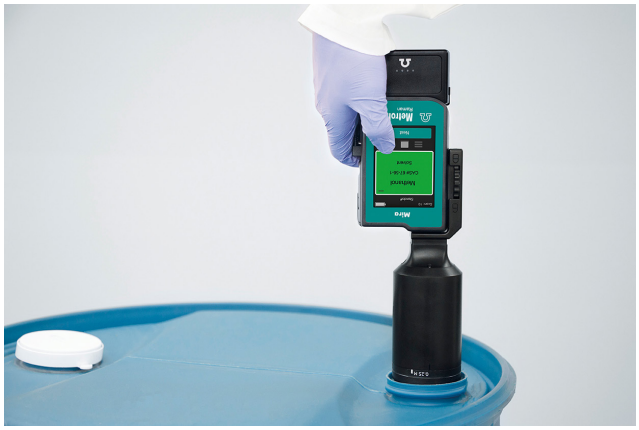

Analysis of highly fluorescent chemical materials: comparison between traditional and eXTRaction fluorescence-reducing Raman technologies

Use of handheld Raman analysers for industrial applications is limited by the fluorescent properties of the sample materials. Although fluorescence reduction is achieved with 1064 nm Raman, the higher laser power and longer integration time come with the risk of sample damage or ignition. The ideal Raman solution minimises measurement time and laser power while also providing a well-defined signal. Additionally, the ability to measure through containers and from a distance is required to reduce human interaction with hazardous samples.

This application note compares intelligent spectra eXTRaction Raman technology with conventional 785 nm and 1064 nm Raman devices for the analysis of chemicals that are difficult to measure due to their known fluorescent properties. Additional experiments were made to compare signal-to-noise ratios and to demonstrate analysis from a distance.
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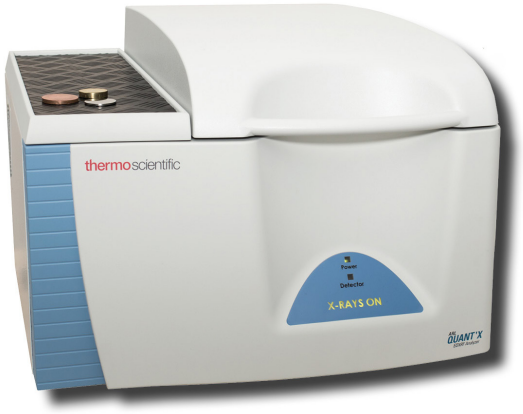

Studying the homogeneity of tourmalines with the ARL QUANT'X EDXRF spectrometer

Tourmalines are well-known, valuable gemstones available in a variety of colours. Chemically, tourmalines belong to the family of silicate minerals. The wide range of their potential chemical combinations explains how there are 37 generally accepted tourmaline species, with schorl as the most common, followed by dravite and elbaite. Each species can occur in several different colour varieties such as rubellite, indicolite and verdelite. Besides the major elements, tourmalines might contain a variety of trace elements such as Mn, Ni, Cu, Zn, Ga, Sr, Sn, Ba and Pb which can be used to identify the geographical origin of the stone.
Thermo Fisher Scientific

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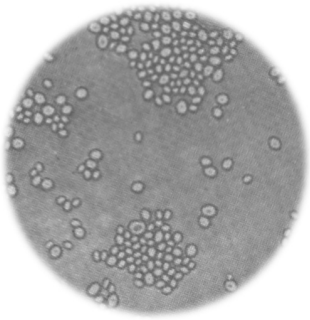

FT-IR analysis of biological yeast cells

Many biological samples are aqueous suspensions of large molecules and even whole organisms, such as bacteria. IR spectroscopy of aqueous samples can be challenging due to the strong absorbance of water. Horizontal multibounce ATR, often combined with temperature control, gives sufficient sensitivity to the biological components of a sample whilst also allowing for careful spectral subtraction of the water signal. This note looks at the analysis of yeasts and yeast protoplasts using the Gateway 6-reflection ATR. Spectra were

acquired from aqueous suspensions of yeast cells and a comparison was made between spectra of whole cells and of protoplasts, which are an important precursor for new genetic hybrids.
Specac

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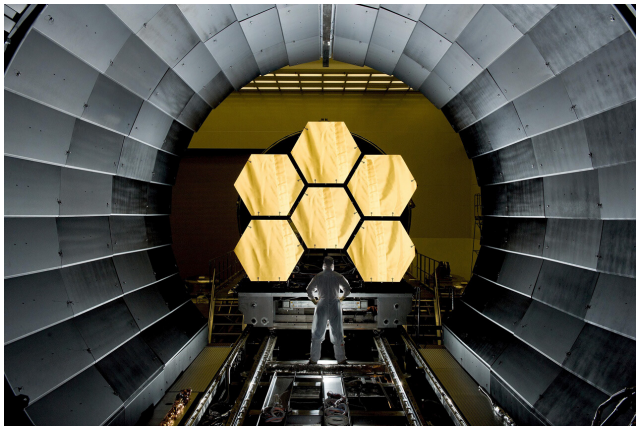

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Spectrum Two FT-IR Spectrometer
Easy to use, powerful, compact and robust, Spectrum Two™ is the FT-IR spectrometer of choice for everyone, everywhere. With fully integrated, robust universal sampling for trouble-free measurements and portability options, Spectrum Two is ideal for use in both laboratory and remote testing environments. Ideally suited to everyday analysis, you can confidently perform fast, accurate IR analysis and assure the quality of your materials across a wide range of applications. Choose the Spectrum Two + that combines a powerful industrial-grade touch screen with cloud connectivity to offer you maximum productivity.
MORE INFORMATION »

PIKE Technologies
Tel: 608.274.2721
info@piketech.com
https://www.piketech.com/

The IRIS Diamond ATR
The IRIS accessory is the go-to diamond ATR for every lab. You can expect high-quality spectra covering a wide range of samples from powders, gels, liquids, solids and more. It is ideal for research, QA/QC and sample identification. For most samples, data collection takes less than a minute.
MORE INFORMATION »

The Mid-IR IntegratIR
The Mid-IR IntegratIR is an integrating sphere that is often used when studying reflectance properties of solids, analysing light-scattering and/or highly absorbing samples and collecting spectra difficult to obtain with standard sampling techniques.
MORE INFORMATION »

The XY Autosampler
The XY Autosampler is designed around standard well microplate architectures—ideal for high-efficiency sample loading and FT-IR analysis in both transmission and reflection. Applications include high-throughput analysis of liquid residues and chemical reactions, and powdered samples.
MORE INFORMATION »

Thermo Fisher
Tel: 6082766100
info.spectroscopy@thermofisher.com
www.thermofisher.com

Thermo Scientific Nicolet RaptIR FTIR Microscope
In analytical labs where details matter most—when productivity is measured in microns and minutes—turn to the Thermo Scientific Nicolet RaptIR FTIR Microscope for answers. This research-grade microscope helps you 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. The Nicolet RaptIR FTIR Microscope provides answers quickly, regardless of industry or application.
See it fast. Identify it faster.
MORE INFORMATION »

TOPTICA

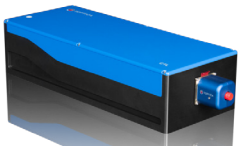
TOPTICA Photonics AG
Tel: +49 89858370
sales@toptica.com
https://www.toptica.com/

TOPO
Widely Tunable High-Power Continuous-Wave OPO Laser System for Mid-infrared Spectroscopy and Applications
TOPTICA has developed a continuous wave optical parametric oscillator 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.

MORE INFORMATION »

DLC pro—Digital Control
All-digital controller for tunable diode lasers. The DLC pro is a platform driving all tunable diode lasers of TOPTICA: One controller for all wavelengths. The performance of diode lasers is largely determined by its controller. The DLC pro is the first diode laser controller based on a digital foundation, which is essential to obtain the best performance on all key parameters: low current noise for narrow laser linewidths, excellent temperature control for stable operation and precise piezo control for frequency tuning. To unleash the full potential of this high-performance controller, intuitive user interfaces are available: with touch screen and knobs it is easy to adjust scans, zoom into observed features, activate frequency locks etc. The digital foundation also enables full remote control, including a GUI for Windows computer and a command interface. This interface is open to all programming languages; a Python SDK is provided.

MORE INFORMATION »

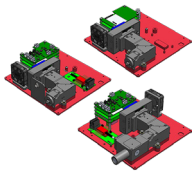


CTL—Continuously Tunable Laser
Wide mode-hop-free tuning (up to 120 nm), available at wavelengths between 880 nm and 1630 nm. The CTL is the ultimate choice when looking for a laser that is widely and continuously tunable without any mode-hops. It has high power, a narrow linewidth and low drift. Scans can be performed with highest resolution. Mode-hops are prevented by an innovative opto-mechanical design (patent US9960569B2) together with an active feedback loop called SMILE (Single Mode Intelligent Loop Engine) that keeps the laser on the same mode at all times. With the fully digital, low noise and drift DLC pro controller, the CTL laser is easy to use and operate via touch-screen and knobs as well as via remote PC GUI and command language (Python SDK). Since firmware 2.0.3 (free updates available), DLC CTL now includes a test system for characterising components or recording spectra.

MORE INFORMATION »

Wasatch Photonics

Wasatch Photonics
Tel: 1 919-544-7785
info@wasatchphotonics.com
wasatchphotonics.com



WP Raman XM Spectrometer Series for OEMs
Our XM-Series OEM Raman spectrometers are robust, compact and easy to integrate, with our signature high throughput. Available for 785 nm and 830 nm excitation, with choice of spectrometer only, with integrated laser, or fully integrated with sampling optics for max signal in the smallest footprint.

MORE INFORMATION »

OXFORD INSTRUMENTS | WITec

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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

PRODUCT FOCUS

- 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

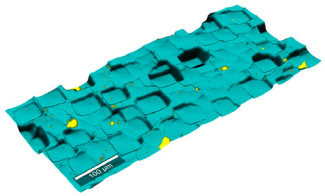
- Life sciences
- Biomedical research
- Living cell analysis
- Aqueous samples
- Inverted beam path for quick measurements of liquid samples
- Compatible with other microscopy techniques: fluorescence, DIC and phase-contrast
- No sample staining required

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

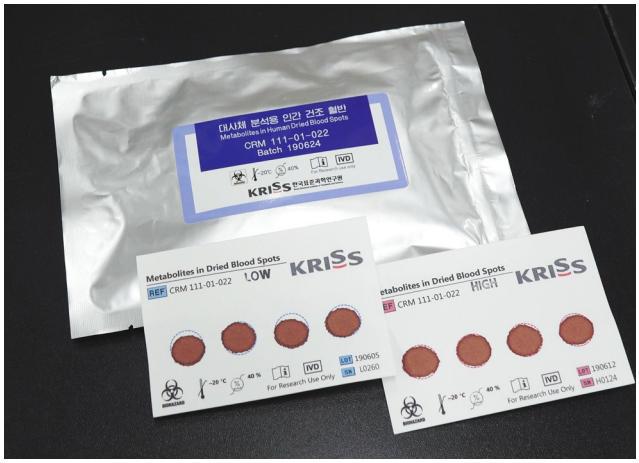
MORE INFORMATION »



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 »



CRMS

CRMs for dried blood spot testing for newborn screening

The Korea Research Institute of Standards and Science (KRISS) has developed Certified Reference Materials (CRMs) that can enhance the reliability of using dried blood spot testing for newborn screening. DBS is a sample obtained by drying a drop of blood from the finger or heel on a piece of filter paper. This approach is used for screening rather than actual diagnosis, as it is less accurate than venous blood sample tests. Its common applications include newborn screening for inherited metabolic disorders and doping control during Olympics.

The proposed CRM provides eight certified values and 10 reference values for amino acids, glucose, galactose and acylcarnitines, which are diagnostic markers of inherited metabolic disorders in newborns. This allows accurate measurement of the amount of target compounds in the DBS. The lack of reference values has made it difficult for DBS testing to be considered reliable for medical decisions. In addition, there has been a problem with measurement bias caused by the need to retrieve portions of blood spots using a paper puncher. The KRISS Biodiagnostics Analysis Team found that a 0.4 mm bias in diameter led to a 0.78 µL difference in sample volume. The research team controlled the sample volume to 50 µL during the CRM manufacturing stage, and proposed bias-free measurements as certified values, thereby successfully creating CRMs with complete measurement traceability to the International System of Units. This is the first-ever development of DBS CRMs.

KRISS plans to develop more CRMs for other diagnostic markers used in newborn screening.

KRISS

https://link.spectroscopyeurope.com/7154-P1-2023

DATA HANDLING

ACD/Labs Releases v2022 Software Update

ACD/Labs has announced the release of version 2022 software applications on the Spectrus® platform, and updates to the Percepta® platform software. The release of v2022 provides functionality for machine-readable structured output, which has the potential to assist stakeholders in R&D organisations with aspirations to digitalise laboratory workflows, reduce the degree of document-driven decision-making, and mitigate the risk of manual data transposition. Key highlights in this batch release include: NMR—a new optimised non-uniform sampling (NUS) data processing algorithm and

tools to help report the most accurate results; MS—introduction of tools for quantitative analysis and the ability to use the NIST MS search in spectral searching; Nomenclature—expansion of language support; Name now supports chemical nomenclature in 21 languages; Capabilities to export data in machine readable formats to support proliferation beyond the Spectrus environment (e.g., JSON and XML).

ACD/Labs

- https://link.spectroscopyeurope.com/660-P2-2022

IMAGING

Park NX-IR R300 infrared spectroscopy for semiconductor industry

Park Systems has introduced the Park NX-IR R300, a nanoscale infrared (IR) spectroscopy system for industrial applications. The Park NX-IR R300 is an infrared spectroscopy and atomic force microscopy integrated into one, for up to 300 mm semiconductor wafers. It provides chemical property information as well as mechanical and topographical data for semiconductor research, failure analysis and defect characterisation at an unprecedent high nano resolution.

The Park NX-IR R300 combines IR spectroscopy of photo-induced force microscopy (PIFM) onto the Park NX20 300 mm AFM platform. The PIFM spectroscopy provides chemical identification under 10 nm spatial resolution. It uses a non-contact technique that offers damage-free spectroscopy probing, highest resolution and accuracy throughout scans. Furthermore, the Park PIFM provides the user with spectroscopy information at varying depths, offering invaluable insight into sample composition.

Park Systems

- https://link.spectroscopyeurope.com/7167-P1-2023

Affordable multispectral drone

Spectral imaging has been growing rapidly and agriculture is an important market. However, the cost can be prohibitive for small farms (doi.org/jt8k). DJI have now introduced a multispectral version of their Mavic 3 drone, the Mavic 3 Multispectral, that should be affordable even for the smallest farm. The Mavic 3M has a four-lens multispectral camera in addition to the RGB camera. Each of the four multispectral cameras can capture 5 million pixels and scan for the following wavelengths: green (560 nm ± 16 nm), red (650 nm ± 20 nm), red edge (730 nm ± 20 nm) and near infrared (860 nm ± 26 nm). These wavelengths provide for a number of potential agricultural and forestry applications including the NDVI vegetation index. A built-in sunlight sensor captures solar irradiance and records

it in an image file, allowing for light compensation of image data during 2D reconstruction. This results in more accurate NDVI results, as well as improved accuracy and consistency of data acquired over time.
DJI

https://link.spectroscopyeurope.com/7128-P1-2022

INFRARED

ABB launches Sensi+™ for natural gas quality monitoring

ABB's Integrated Cavity Output Spectroscopy (ICOS) laser absorption technology has been used for over 15 years for reliable gas analysis. This spectroscopic method provides the highest accuracy, precision, sensitivity and reliability. The new Sensi+ is a single device for continuous, simultaneous measurements of H_2S, H_2O and CO_2 contaminants in natural gas streams for custody transfer, tariff compliance and process monitoring. Its fast response also enables quick reaction to process upsets, thus helping to reduce waste and methane emissions. ABB's proven laser-based technology virtually eliminates false readings and provides rapid response for reliable process control. The Sensi+ has been designed for remote and hazardous locations, and has a low cost of ownership.

Sensi+ requires about six times less sample flowrate for its measurement than other technologies, reducing the total carbon emission of the analyser and natural gas wastage in the atmosphere. Natural gas pipeline operators have the critical task of managing their installed base of analysers to ensure the necessary reliability, system integrity and performance. The Sensi+ is hazardous area compliant and needs only a simple wall mount installation and process tie-in without complex system purging. Following installation and validation, the analyser will deliver fast and reliable measurements in the field without calibration.

The Sensi+ analyser includes ABB's AnalyzerExpert™ features that provide experts with actions and insights directly from the device. Capabilities include built-in self-diagnostics, automated laser line-locking, real-time cross-interference compensation and health monitoring.
ABB

https://link.spectroscopyeurope.com/659-P1-2022

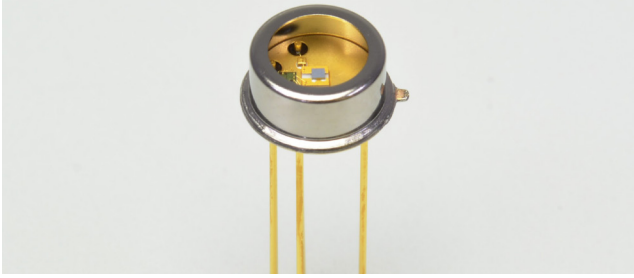
InAsSb photovoltaic detector

Hamamatsu have developed a new InAsSb photovoltaic detector (the P16702-011MN) with built-in preamplifier offering high sensitivity to mid-infrared light, up to 11 µm in wavelength. This combines an InAsSb (indium arsenide antimonide) mid-infrared detector with new circuit design technology. Compared to previous

detector modules with the same level of sensitivity, the P16702-011MN size and cost is drastically reduced, and it exhibits fast response time. This makes it an ideal choice for portable gas analysers able to immediately analyse exhaust gas components at measurement sites around factories.

Hamamatsu Photonics

https://link.spectroscopyeurope.com/1342-P1-2023



MASS SPEC

Waters introduces new PFAS quantitation workflow

Waters has announced a new Per-and Polyfluoroalkyl Substances (PFAS) quantitation workflow enabled by enhancements to its waters_connect™ for quantitation software. Through a combination of Waters instrumentation, sample prep chemistries and software, the end-to-end workflow simplifies and automates the measurement of PFAS in food, soil, air and water at parts-per-quadrillion levels that meet and exceed regulatory detection limits.

In addition to waters_connect for Quantitation Software, the new PFAS workflow consists of a Waters ACQUITY Premier UPLC System, a Xevo TQ Absolute tandem quadrupole mass spectrometer, ACQUITY Premier BEH Columns, Oasis WAX sample preparation cartridges, PFAS analysis kit and ERA PFAS Proficiency Testing and Certified Reference Materials.

A key component of the waters_connect for quantitation software is the MS Quan™ app which includes an Exception Focused Review feature allowing users to implement tailored rulesets to focus the review process on only those results that fall outside specified targets, cutting data review time by up to 50%.

Waters

https://link.spectroscopyeurope.com/103-P6-2022

NIR

High dynamic range UV/vis-NIR spectrometer

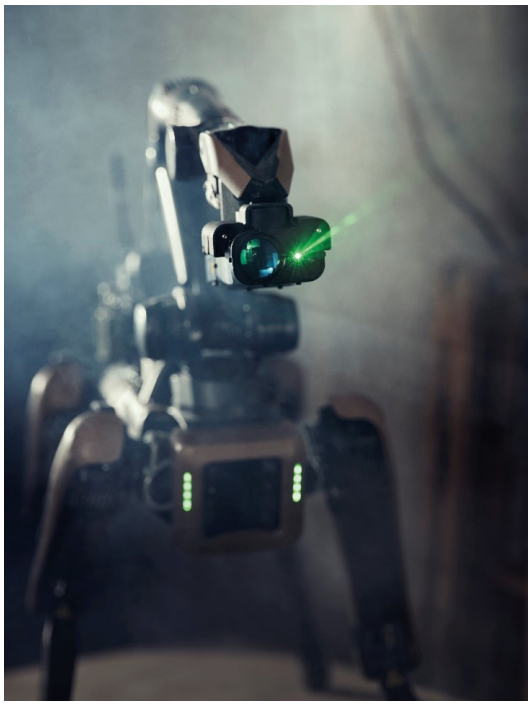
Hamamatsu has developed a new spectrometer with an extremely high dynamic range of 2,500,000:1 in the spectral range from 200 nm to 900 nm that allows simultaneous measurement of both strong and weak signals. The OPAL-Luxe C16736-01 is the top-end model from Hamamatsu. Incorporating the OPAL-Luxe into component analysers that utilise light absorption properties of substances in the ultraviolet to near infrared region, will allow simultaneous analysis of the various components within a sample. This includes components in large

quantities absorbing large amounts of light and components in small quantities absorbing small amounts of light. This increases component analysis efficiency in the quality control of chemicals by detecting the trace amounts of impurities in substances without having to repeat measurements. The OPAL-Luxe will also help make further progress in plasma application research since it can analyse plasma emissions with high accuracy.

Hamamatsu Photonics

https://link.spectroscopyeurope.com/1342-P2-2023

RAMAN



Raman and robot for remote detection of hazardous materials

The MIRA XTR DS handheld Raman spectrometer and Autofocus Standoff Attachment (AFSO) from Metrohm can be integrated into the IBEX CBRNE robot system equipped with environmental sensors. Operated remotely, IBEX can assess hazards, gather detailed intelligence and identify unknowns without ever placing a human in harm's way. The most powerful capability of IBEX is chemical identification. Using stand-off Raman technology, MIRA and the AFSO can identify unknowns from 2 m away. Point the laser sight at a suspicious substance and get a result seconds later. MIRA can identify more than 20,000 substances, including illicit drugs, explosives, precursors and other hazardous chemicals. IBEX transmits detailed information from the hot zone for instant assessment of human safety risks. The sensors include a Chemical Warfare Agent (CWA) Detector, Radiological/Nuclear Detectors and a PID Gas Monitor.

Metrohm

https://link.spectroscopyeurope.com/684-P1-2023

SPONSORED

Handheld Raman spectrometer

Toxic chemicals hit upon during Sensitive Site Explorations (SSEs), Improvised Explosive devices (IEDs) or powerful synthetic opioids (e.g., fentanyl) can be lethal treats to the lives of first responders and military personnel. Such threats can be reduced with MIRA XTR DS, the handheld Raman identification system from Metrohm. MIRA XTR DS can identify more than 20,000 of unknowns in the field and can deal with substances emitting fluorescence. The standard solution to deal with samples emitting fluorescence is a 1064 nm laser. MIRA XTR DS, on the other hand, combines the smaller size, higher resolution and lower power consumption of a 785 nm laser with machine learning to eXTRact a

NEW PRODUCTS

Raman signal even from fluorescent samples. The low power 785 nm laser allows interrogation of sensitive samples without the risk of igniting/destroying them; a compact, pocket-sized design enabling true single-handed operation; and lower power consumption than 1064 nm devices allows for longer battery life.

Fully automated, guided workflows make MIRA XTR DS easy to use from sampling unknowns to clear, coded results. MIRA XTR DS can be interfaced with the HazMaster G3 App to instantly provide actionable intelligence. First responders can calculate likely mixture outcomes on site giving them meaningful results and important chemical information about drugs, explosives and chemical warfare agents. With this information, they can take immediate action to protect themselves, their team and everyone else.

Metrohm

- https://link.spectroscopyeurope.com/684-P2-2023

Conferences

2023

16–18 February 2023, Lisbon, Portugal. **11th International Conference on Photonics, Optics and Laser Technology.** https://photoptics.scitevents.org/

8 March 2023, Hemel Hempstead, United Kingdom. **229th IRDG Meeting.** neil.everall@btinternet.com

16 March 2023, St Asaph, Wales, United Kingdom. **Dynamic Interferometry for Metrology Workshop.** angela@qd-uki.co.uk, https://qd-uki.co.uk/dynamic-interferometry-for-metrology-workshop/

18–22 March 2023, Philadelphia, PA, United States. **Pittcon 2023.** https://www.pittcon.org

26–30 March 2023, Indianapolis, United States. **266th American Chemical Society National Meeting.** natim-tgs@asc.org, https://www.acs.org/meetings/acs-meetings/spring-2023.html

27–30 March 2023, Leeds, United Kingdom. **The 56th Annual International Meeting of the ESR Spectroscopy Group.** https://www.rsc.org/events/detail/75495/the-56th-annual-international-meeting-of-the-esr-spectroscopy-group

30–31 March 2023, Cambridge, United Kingdom. **10th Analytical Biosciences Group Early Career Researcher Meeting 2023.** https://www.rsc.org/events/detail/75110/10th-analytical-biosciences-group-early-career-researcher-meeting-2023

3–5 April 2023, Ayia Napa, Cyprus. **Ninth International Conference on Remote Sensing and Geo-information of Environment.** http://www.cyprusremotesensing.com/rscy2023/

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

24–28 April 2023, 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 2023, San Jose, California, United States. **CLEO.** https://www.cleoconference.org/

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

10 May 2023, 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 2023, Kyoto, Japan. **25th International Symposium on Plasma Chemistry.** https://www.ispc25.com/

4–8 June 2023, Houston, Texas, United States. **71st ASMS Conference on Mass Spectrometry and Allied Topics.** https://www.asms.org/conferences/annual-conference/annual-conference-homepage

8 June 2023, 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 2023, 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

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

2–7 July 2023, Beijing, China. **12th International Symposium on EIS.** https://www.eis2022.com/

30 July–4 August 2023, Berlin, Germany. **The 15th Femtochemistry Conference (FEMTO 15).** https://femto15.mbi-berlin.de/conference

31 July–3 August 2023, Munich, Germany. **Optica Sensing Congress.** https://www.optica.org/en-us/events/congress/optical_sensors_and_sensing_congress/

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

25–30 August 2023, 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 2023, Krakow, Poland. **12th International Conference on Advanced Vibrational Spectroscopy (ICAVS12).** icavs2023@targi.krakow.pl, https://icavs.org/

3–7 September 2023, Vienna, Austria. **6th EuChemS Inorganic Chemistry Conference.** https://www.eicc6.at/

3–6 September 2023, Tokamachi, Niigata, Japan. **8th Asian Spectroscopy Conference (ASC2023).** http://www2.riken.jp/lab/spectroscopy/ASC2021/index.html

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

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

10–12 October 2023, Dresden, Germany. **3rd Food Chemistry Conference: Shaping a Healthy and Sustainable Food Chain through Knowledge.** https://www.elsevier.com/events/conferences/food-chemistry-conference

2024

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

Courses

2023

15–22 September 2023, Dresden, Germany. **6th Summer School Spectroelectrochemistry.** summer-school@ifw-dresden.de, https://www.ifw-dresden.de/de/news-events/scientific-events/summer-school-spectroelectrochemistry

17–22 September 2023, Cagliari, Sardinia, Italy. **6th International Mass Spectrometry School.** https://www.spettrometriadimassa.it/imss2023/

Exhibitions

2023

18–22 March 2023, Philadelphia, PA, United States. **Pittcon 2023.** https://www.pittcon.org

28–30 March 2023, Paris, France. **Forum LABO.** https://www.forumlabo.com/paris/en-gb.html

19–21 April 2023, Ho Chi Minh City, Vietnam. **Analytica Vietnam.** https://www.analyticavietnam.com/

2024

9–12 April 2024, Munich, Germany. **analytica.** https://analytica.de/

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www.thermofisher.com/elemental

Atomic Absorption

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www.perkinelmer.com

Atomic Emission

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