# SPECTROSCOPY
world

Spectroscopy since 1975

Can YOU find life on Mars?
Sampling of hyper-heterogeneous lots
Four Generations of Quality: UV/vis

IMP**Open**
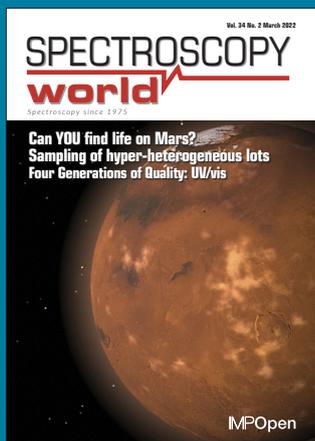
NASA has opened a competition to anyone to build a model to automatically analyse MS data potentially to discover life on Mars. Find out more on page 4.

ISSN: 2634-2405

CONTENTS

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

IMPOpen

EDITORIAL

Predatory publishing

Predation takes many forms, and in recent years has also come to refer to a type of Open Access journal that misleads authors both in the publishing services and expertise offered and in the fees that may be charged. According to a recent report from the InterAcademy Partnership (IAP), "Predatory academic journals and conferences are those that are motivated by profit rather than scholarship, soliciting articles and abstracts from researchers through actions that exploit the pressure on researchers to publish and present their work." I actually don't agree with this, the problem with predatory journals (and the report also discusses predatory conferences) is not just a profit motive. Most academic journals are published for profit, or at least with the hope of profit!

I do not think that there is anything wrong *per se* with publishing for profit; where the problem lies with predatory publishers is in their unprofessionalism—not providing proper copy editing (or none at all) and generally cutting the publishing process to the bone—and plain dishonesty.

How do you avoid predatory publishers? One initiative is Think. Check. Submit. (https://thinkcheck-submit.org), which is certainly worth looking at. However, I think most readers will find the suggestions worthy but obvious. Whilst anybody can be caught out, the big problem is for authors from countries where there may not be the same levels of experience and support for publishing in academic journals. Susan Veldsman, Study Co-Chair of the IAP report (https://www.interacademies.org/publication/predatory-practices-report-English) says "We estimate that over 1 million researchers are likely to have used predatory outlets (largely unknowingly) at a cost of billions of dollars of wasted research. This is largely due to a lack of awareness and not knowing how to recognise what is predatory and what is not. Training is both urgent and imperative."

Another Co-Chair of the study, Abdullah Shams Bin Tariq, says that "The author-pays model of open access is particularly open to abuse, allowing publishers to predate on researchers and driving many of them, especially in poorly resourced countries, into the arms of predatory outlets."

What they say is fine, but please don't throw the baby of Open Access publishing, with its multitude of benefits, out with the bathwater of predatory publishing. As so often, the answer is education (or "training") not over regulation.
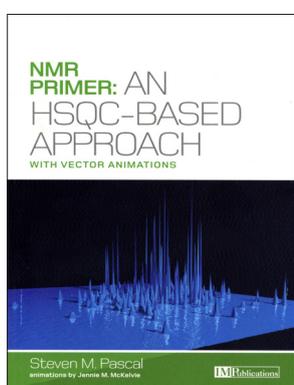
NMR PRIMER:
AN HSQC-BASED APPROACH
(with vector animations)

by Steven M. Pascal

This book has one aim: to explain the key two-dimensional protein NMR experiment, the $^1H,^{15}N$-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.
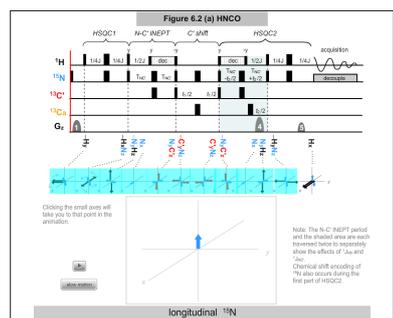
First, a brief introduction to spins, populations, the NMR experiment and relaxation is provided. Evolution due to J-coupling is next described and used to explain magnetisation transfer in the HSQC experiment and several variants. The extraction of structural, sequential and dynamic information is then illustrated via various extensions of the HSQC. Extensive footnotes and appendices introduce several more advanced concepts, such as sensitivity enhancement and the TROSY effect.

NMRPRIMER.IMPOPEN.COM

NEWS

Can YOU find life on Mars?

NASA has opened a competition to anyone to build a model to automatically analyse mass spectrometry data collected for Mars exploration. The model should detect the presence of certain families of chemical compounds in data collected from performing evolved gas analysis on a set of analogue samples. The winning techniques may be used to help analyse data from Mars, and potentially even inform future designs for planetary mission instruments performing *in situ* analysis.

Full details of the competition can be found at https://www.herox.com/MarsSpectrometry

Laser for LIBS on the Moon

The probability of finding volatiles such as water on the moon is highest in the polar regions, as they are frozen. These substances can be detected, for example, using laser-induced breakdown spectroscopy (LIBS). To this end, scientists in the Solid-State Lasers group of the Laser Zentrum Hannover (LZH) have designed and built a laser model. The Institute of Optical Sensor Systems of the German Aerospace Center (DLR-OS) incorporated the laser from the LZH into a demonstrator model of the actual "Volatiles Identification by Laser Ablation" (VOILA) measuring instrument. Then, they tested the functionality on regolith simulant, a substance that is very similar to Moon dust, and were able to use it to generate the desired measurement data.

The long-term goal is to integrate the VOILA laser system into a Moon rover. For a laser to be suitable for use on the Moon, it must meet specific requirements. It must function reliably in extremely cold areas with temperatures significantly lower than −100° C, which are extremely problematic for conventional laser systems. For transport on a Moon rocket, it must be small and compact, and also very robust so that it does not get damaged during the strong vibrations of the rocket launch.

The plan for real-world use on the Moon already exists, and the concept for a laser flight model design ensures that the planned laser will actually fit into the available volume on the Moon rover.

Deep learning with NIR and MRI can improve breast cancer imaging

Researchers have developed a new image reconstruction approach that could contribute to better breast cancer detection. The deep learning algorithm overcomes a major hurdle in multi-modality imaging by allowing images to be recovered in real time. The new algorithm, known as Z-Net, works with an imaging platform that combines optical spectral information with contrast-free magnetic resonance imaging (MRI) to improve detection of breast cancer.

"The near infrared spectral tomography (NIRST) and MRI imaging platform we developed

The laser developed by the LZH, which will enable the VOILA LIBS instrument to search for water on the Moon in the future. Photo: LZH

NEWS

has shown promise, but the time and effort involved in image reconstruction has prevented it from being translated into the day-to-day clinical workflow", said Keith Paulsen, who led the research team from Dartmouth College. "Thus, we designed a deep-learning algorithm that incorporates anatomical image data from MRI to guide NIRST image formation without requiring complex modelling of light propagation in tissue."

Paulsen and colleagues from the Beijing University of Technology and the University of Birmingham report that their new algorithm can distinguish between malignant and benign tumours using MRI-guided NIRST imaging data from patient breast examinations.

"Z-Net could allow NIRST to become an efficient and effective add-on to non-contrast MRI for breast cancer screening and diagnosis because it allows MRI-guided NIRST images to be recovered in nearly real time", said Paulsen. "It can also be readily adapted for use with other cancers and diseases for which multi-modality imaging data are available."

Today, dynamic contrast-enhanced (DCE) MRI is recognsed as the most sensitive breast cancer detection method. However, DCE MRI requires intravenous injection of a contrast agent and has a substantial false positive rate. Although non-contrast MRI-guided NIRST offers an alternative that does not require contrast injection or ionising radiation, reconstructing the combined images requires complicated light propagation models as well as time consuming MRI image analysis. The researchers used deep learning to make the image reconstruction process faster.

"The Z-Net algorithm reduces the time needed to generate a new image to a few seconds", said Jinchao Feng, the lead author of the study published in *Optica* ([doi.org/hj3p](doi.org/hj3p)). "Moreover, the machine learning network we developed can be trained with data generated by computer simulations rather than needing images from actual patient exams, which take a long time to collect and process into training information."

After training the algorithm, the researchers used simulated data to confirm that the quality of the reconstructed images was not degraded by eliminating diffuse light propagation modelling or by not segmenting MRI images. They then applied the new algorithm prospectively to MRI-guided NIRST data collected from two breast imaging examinations—one leading to a biopsy-confirmed cancer diagnosis, the other resulting in a benign abnormality. The new algorithm generated images that could tell the difference between the malignant and benign cases.

"In addition to showing the potential of our approach, the results also demonstrate that when *in vivo* data is insufficient or unavailable for training a deep learning algorithm, a large amount of simulation data may work", said Shudong Jiang, a study co-author and pioneer in developing simultaneous MRI and optical breast imaging technology.

The researchers are working to adapt the new image reconstruction method to work with 3D data and plan to test it in a larger clinical trial in the near future.

Fast and easy protein analysis with MS from trace amounts of cell samples

In recent years, proteomics research using mass spectrometry (MS) to comprehensively investigate the protein components of biological samples has become very popular. In order to detect proteins by MS, it is necessary to extract the protein components contained in the cells and digest them with proteases to a peptide size that is easy to analyse by MS. Protein digestion in this manner typically requires a long reaction time of 20 hours or more. Sodium dodecyl sulfate (SDS), a
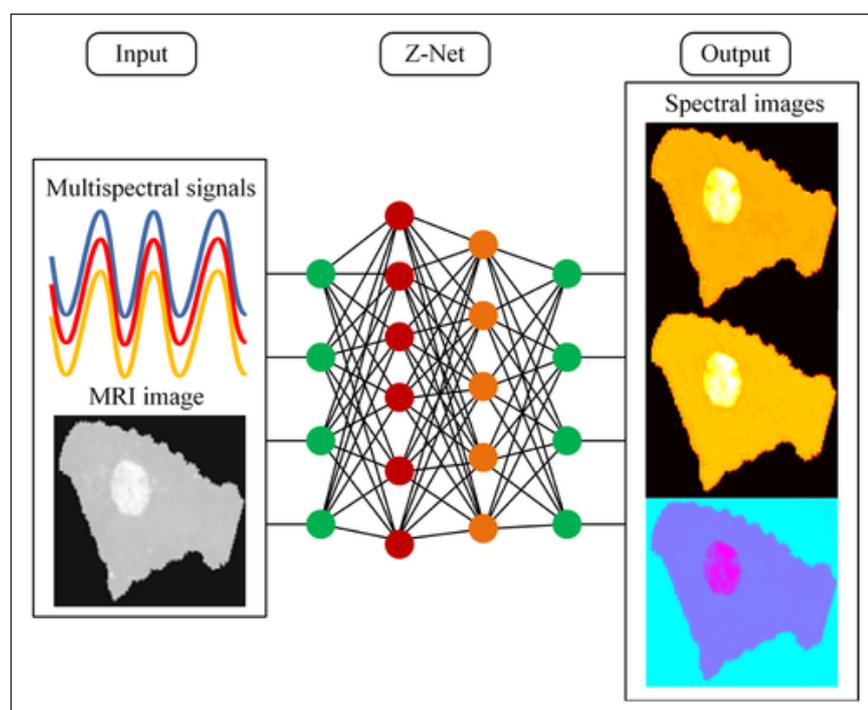
Researchers developed the Z-Net deep-learning algorithm for real-time reconstruction of images that combine spectral and MRI data. This could allow better breast cancer screening and diagnosis. Credit: Keith Paulsen, Dartmouth College

NEWS
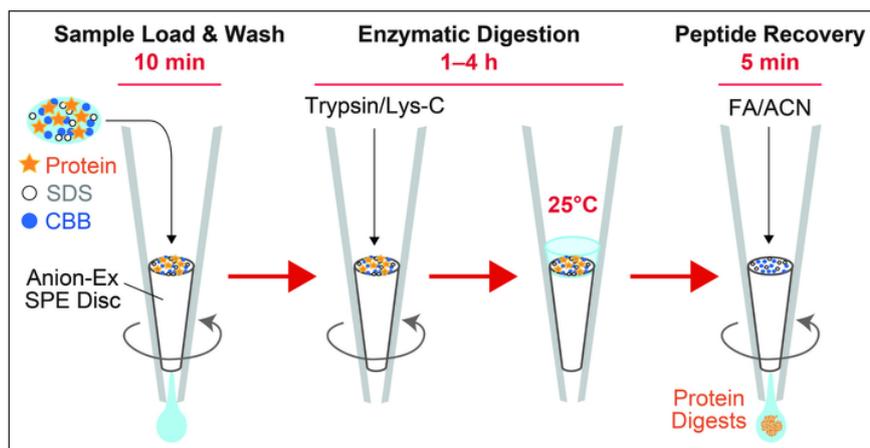
Sample preparation that used to take more than 20 hours with conventional methods can now be completed in less than 5 hours with AnExSP. Credit: Reprinted with permission from *Chemical Communications* © 2022 Royal Society of Chemistry (RSC)

surfactant often used in protein extraction processes, interferes with MS and protein digestion, and must be thoroughly removed prior to analysis. However, that process comes with a cost, namely sample loss. To overcome these challenges, the researchers from Ehime University, Japan, developed an innovative sample preparation method, AnExSP (anion-exchange disc-assisted sequential sample preparation), which uses a µL-sized spin column fitted with anion-exchange solid-phase extraction discs in a pipette tip called a StageTip as a tool for protein digestion.

They succeeded in completing the enzymatic digestion process in a minimum of 60 min by enriching the protein components on the disc surface. Furthermore, they established optimal conditions for eluting only the digested peptides from the discs while keeping the SDS contained in the sample on the discs, and achieved sample pretreatment with simple operation and minimal loss. By combining AnExSP with data-independent acquisition (DIA) analysis by Orbitrap mass spectrometry, they succeeded in detecting approximately 7000 different protein components in

1 µg of human cultured cell protein extract. By establishing sample pretreatment conditions using the reduced-size StageTip in the future, AnExSP pretreatment can be used for single-cell proteomics research, which has been growing in interest recently.

AnExSP can also be used for pretreatment of proteins separated by SDS-polyacrylamide gel electrophoresis (SDS-PAGE), which is commonly used in protein experiments. Compared to conventional pretreatment methods, AnExSP demonstrated superior performance, especially in the detection of long-chain digested peptides. In this study, they combined AnExSP and SDS-PAGE with a chemical cross-linking method for protein complexes, and succeeded in simple purification of target protein complexes and efficient detection of long-chain cross-linked peptides that are difficult to detect with conventional methods. Because of its far-reaching versatility, AnExSP is expected to be applied to highly sensitive structural analysis methods for trace protein complexes in biological samples.

This work was published in *Chemical Communications* ([doi.org/hj3r](doi.org/hj3r)).

FT-IR imaging used to investigate brain ageing

Dr Kendra Furber, Assistant Professor, UBC Northern Medical Program and the Division of Medical Sciences at the University of Northern British Columbia, is working to pinpoint the causes of brain ageing and how we can prevent or reverse the damage of time. Myelin degradation is one of the contributing factors to these lapses in memory and cognition. This fatty substance covers the neurons in your brain and spinal cord, helping to insulate the connections between cells and allowing lightning-fast information flow through the nervous system.

"Our brains continue to myelinate until midlife and then the volume and integrity of that myelin starts to decline. This often correlates with deficits in memory and cognitive processing speed", Furber said.

Furber and her team have been using FT-IR imaging at the Mid-IR beamline of the Canadian Light Source (CLS) at the University of Saskatchewan, to look at biochemical changes in the brain. Furber has focused her attention on specialised cells in the brain that form the myelin sheath. The myelin-producing cells look a little bit like an octopus with multiple "tentacles" that wrap around our neurons, providing them with the insulation they need. As they age, the "tentacles" wither, leaving cell connections unprotected. They hope to understand why the myelin starts to decline with age.

"At some point some of that myelin is lost and we get less and less efficient at repairing it", Furber said. "It's kind of this balance and it gets tipped to more myelin loss as we age—we're not making those new connections or wrapping up the nerve processes as well."

The brain likes to rewire pathways when we are learning new skills, what scientists refer to as neuroplasticity. As we age, the brain is not as flexible and rewiring

Introduction to the Theory and Practice of Sampling

Kim H. Esbensen

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

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

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

"I recommend this book to all newcomers to TOS"

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

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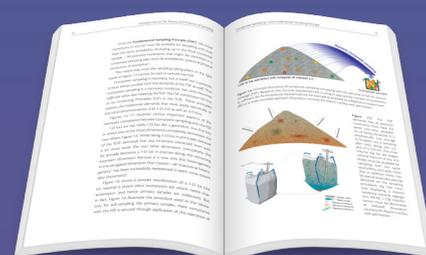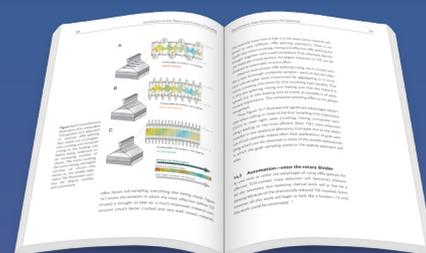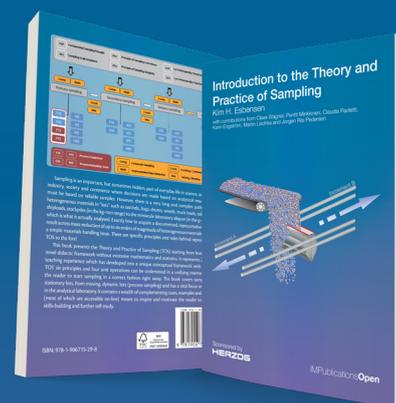
impopen.com/sampling

IMPublicationsOpen

NEWS
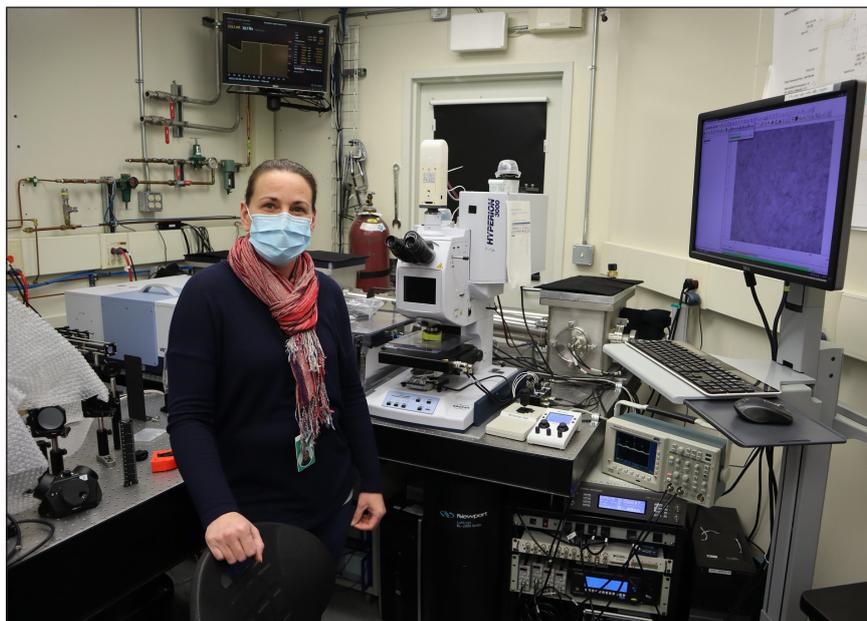
Dr Kendra Furber at the Mid-IR beamline of the Canadian Light Source.

pathways becomes more difficult, leading to changes in learning and memory. Furber and her team are currently looking at strategies to help make our brain cells more resilient to environmental stress. Data shows that simple things like exercise, sleep and a proper diet may help keep our myelin healthy.

"We started trying some really interesting stuff using the synchrotron light", Furber said. "The beamline scientists are the ones that are really pushing these new methods and now I get to think up all the fun questions that we can ask that we wouldn't be able to ask using our normal microscopes in our lab."

This work was published in *Neurochemical Research* (doi.org/hj3s).

Hyperspectral sensing and AI for monitoring soil carbon at large spatial scales

Just how much carbon is in the soil? That is a difficult question to answer at large spatial scales, but understanding soil organic carbon at regional, national or global scales could help scientists predict overall soil health, crop productivity and even worldwide carbon cycles. In a recent study, University of Illinois researchers have shown that new machine-learning methods based on laboratory soil hyperspectral data could supply estimates of soil organic carbon with the same accuracy as lab-based methods. Their study provides a foundation to use airborne and satellite hyperspectral sensing to monitor surface soil organic carbon across large areas.

"Soil organic carbon is a very important component for soil health, as well as for cropland productivity", says lead study author Sheng Wang of the University of Illinois. "We did a comprehensive evaluation of machine learning algorithms with a very intensive national soil laboratory spectral database to quantify soil organic carbon."

Wang and his collaborators used a public soil spectral library from the USDA Natural Resources Conservation Service containing more than 37,500 field-collected records and representing all soil types around the US.

"Spectra are data-rich fingerprints of soil properties; we're talking thousands of points for each sample", says Andrew Margenot, assistant professor in the Department of Crop Sciences and co-author on the study. "You can get carbon content by scanning an unknown sample and applying a statistical method that's been used for decades, but here, we tried to screen across pretty much every potential modelling method", he adds. "We knew some of these models worked, but the novelty is

the scale and that we tried the full gamut of machine learning algorithms."

Kaiyu Guan says "this work established the foundation for using hyperspectral and multispectral remote sensing technology to measure soil carbon properties at the soil surface level. This could enable scaling to possibly everywhere."

After selecting the best algorithm based on the soil library, the researchers put it to the test with simulated airborne and spaceborne hyperspectral data. As expected, their model accounted for the "noise" inherent in surface spectral imagery, returning a highly accurate and large-scale view of soil organic carbon.

"NASA and other institutions have new or forthcoming hyperspectral satellite missions, and it's very exciting to know we will be ready to leverage new AI technology to predict important soil properties with spectral data coming back from these missions", Wang says. The work was published in *Remote Sensing of Environment* (doi. org/hj3t).

Young Fluorescence Investigator Award

HORIBA Scientific has presented Dr Ahmed Abdelfattah with the annual Young Fluorescence Investigator Award at the 2022 Biophysical Society event. Dr Abdelfattah is an Assistant Professor of Neuroscience at Brown University in Providence, RI, USA. The winner was selected by the Biological Fluorescence Subgroup of the Biophysical Society. Along with the recognition, HORIBA presented a $1000 check to Dr Abdelfattah and a crystal award.

Since April 2021, Dr Abdelfattah has been both an Assistant Professor of Neuroscience, and the Robert J. and Nancy D. Carney University Assistant Professor of Brain Science at Brown University. He worked in a post-doctoral fellow

Dr Ahmed Abdelfattah

position with Dr Eric Schreiter at Janelia Research Campus. During this time, he made a series of creative and highly impactful contributions in the high-profile area of developing innovative fluorescent probes for imaging of neural activity. One example of his postdoctoral work is the voltage probe designated as Voltron, which enabled recording membrane voltage from tens of cells in live animals. His PhD research was with Professor Robert Campbell and focused on the use of protein engineering to develop improved fluorescent genetically encoded indicators of neuronal activity.

HORIBA Scientific has been the sole sponsor of this award since 1997. The Young Fluorescence Investigator Award is presented to a researcher who has been nominated by their peers for significant advancements and/or contributions in or using fluorescence methodologies. The candidate must be a PhD, and a pre-tenured faculty member or a junior level investigator working in the field of fluorescence.

"HORIBA is very proud to sponsor this prestigious award again, and Dr Abdelfattah is a very deserving choice as this year's recipient", said Cary Davies, Director of the Fluorescence group at HORIBA Scientific. "Dr Abdelfattah is the 27th researcher to win the Young Investigator Award since 1997, and

joins a prestigious group of scientists who have had a tremendous impact in the biophysical research community."

Spectroscopy identifies and separates biexciton binding energy

A rare spectroscopy technique performed at Swinburne University of Technology, Australia, directly quantifies the energy required to bind two excitons together, providing for the first time a direct measurement of the biexciton binding energy in WS_2. As well as improving our fundamental understanding of biexciton dynamics and characteristic energy scales, these findings directly inform those working to realise biexciton-based devices such as more compact lasers and chemical-sensors. The study also brings closer exotic new quantum materials, and quantum phases, with novel properties.

Particles of opposite charge in close proximity will feel the "pull" of electrostatic forces, binding them together. The electrons of two hydrogen atoms are pulled in by opposing protons to form H_2, for example, while other compositions of such electrostatic (Coulomb-mediated) attraction can result in more exotic molecular states.

The optical properties of semiconductors are frequently dominated by the behaviour of "excitons". These compound quasi-particles can be created via the excitation of an electron from the valence to the
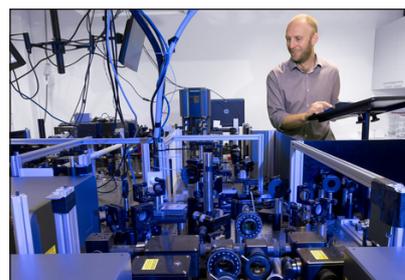
Professor Jeff Davis (Swinburne University of Technology) leads Swinburne's ultrafast spectroscopy lab. Credit: FLEET

NEWS

conduction band, with the negatively-charged conduction electron then electrostatically binding to the positively-charged vacancy (known as a hole) its excitation left in the valence band.

Understanding the interactions between excitons is crucial for realising many of the proposed device applications, and in bulk materials they are quite well understood. However, when things are reduced to two dimensions, the ways they can interact change, and important quantum effect can come into play. Monolayer semiconductors such as WS_2 are introducing a materials revolution due to the novel properties uncovered by research like this.

Due to the reduced dimensionality of two-dimensional materials, the binding energy of excitons and exciton complexes like biexcitons are greatly enhanced. This increased binding energy makes the biexcitons more accessible, even at room temperature, and introduces the possibility of using biexcitons flowing in novel materials as the basis for a range of low-energy future technologies. Atomically-thin transition metal dichalcogenides (TMDCs) like WS_2 are a family of semiconducting, insulating and semi-metallic materials that have gained a significant amount of attention from researchers in recent years for use in a future generation of "beyond CMOS" electronics.

"Before we can apply these two-dimensional materials to the next generation of low-energy electronic devices, we need to quantify the fundamental properties that drive their functionality", says Mitchell Conway, a PhD student from Swinburne University of Technology.

The need to understand the properties of biexcitons has driven significant conjecture and investigation in the semiconductor research community of their presence, binding energy and nature. Attempts have been made to investigate how much energy is required to separate
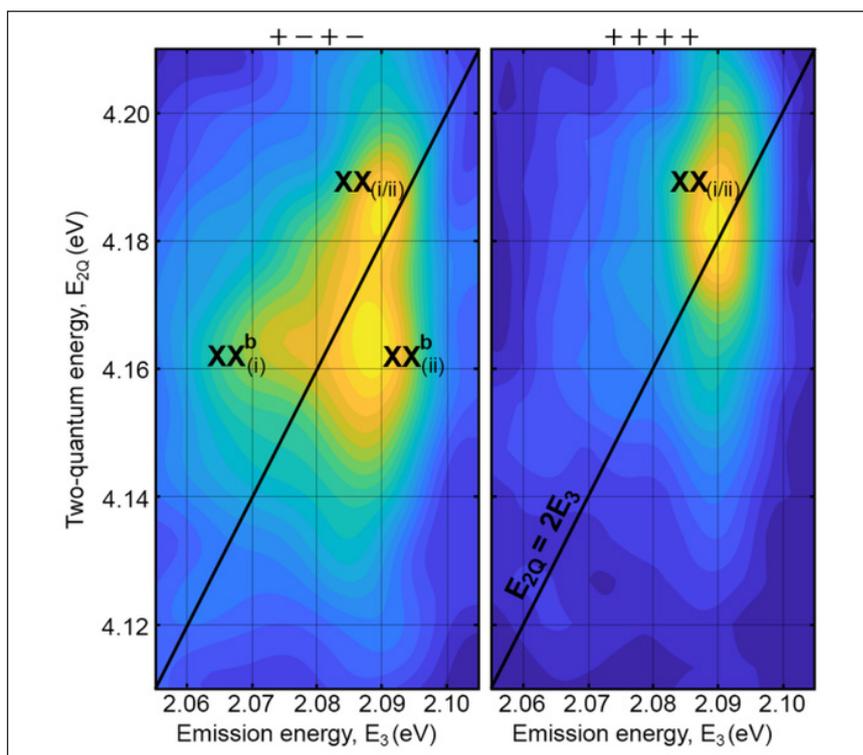
Spectroscopy identifies and separates biexciton binding energy. Credit: Mitch Conway

the two excitons in a biexciton, the obvious way being a comparison between the energy of the bound and unbound excitons. Yet, this is not what is typically done.

The Swinburne-led study has identified the optically-accessible biexciton in the atomically-thin TMDC tungsten disulphide (WS_2). To unambiguously measure biexcitonic signatures, the team of researchers employed a specific sequence of ultrashort optical pulses with a precisely controlled phase relation and well-defined wave-vectors.

"By using multiple pulses with a high degree of precision we can selectively and directly probe the doubly excited biexciton state, while eliminating any contributions from singly excited exciton states. This ability to directly excite the biexciton is inaccessible to more common techniques such as photoluminescence spectroscopy," says Professor Jeff Davis from Swinburne.

The technique the team used is known as "two-quantum multidimensional coherent spectroscopy" (2Q-MDCS), which enables a direct experimental measurement of the biexciton binding energy. When the biexciton is observed using 2Q-MDCS, a signal from an exciton pair that is interacting but unbound is also generated, referred to as "correlated excitons". Their work was published in *2D Materials* (doi.org/hj3n).

"The energy difference between the biexciton peak and the correlated two-exciton peak is the best means to measure biexciton binding energy", Mitchell explains. "This was an exciting observation, since other spectroscopic techniques don't observe these correlated excitons."

Techniques previously used to identify the biexciton are limited to measuring photons from the biexciton to exciton transition. These transitions may not reflect the precise energy of either relative

to the ground state. In addition, the study identified the nature of the biexciton in monolayer WS_2. The biexciton they observed was composed of two bright excitons with opposite spin, which in WS_2 is referred to as a "bright-bright intervalley" biexciton. In contrast, photoluminescence measurements reporting biexcitons in monolayer WS_2 are unable to identify the specific excitons involved, but are typically assumed to involve bright exciton and one "dark" exciton, due to the rapid relaxation into these lower energy exciton states that don't absorb or emit light.

The ability to accurately identify biexciton signatures in monolayer semiconductors may also play a key role in the development of quantum materials and quantum simulators. Higher-order electrostatic correlations provide a platform to construct coherent combinations of quantum states and potentially tune the interactions in order to realise quantum phases of matter that are still not well understood.

Canadian and Brazilian synchrotrons to cooperate in agricultural research

The Canadian Light Source (CLS) at the University of Saskatchewan and the Brazilian Center for Research in Energy and Materials (CNPEM) have signed a Memorandum of Understanding (MOU) for technical and scientific collaboration in synchrotron and accelerator science.

"We look forward to this new collaboration with our colleagues in Brazil", said Bill Matiko, Chief Operating Officer of the CLS. "Their world-leading expertise in the development of next-generation light sources will contribute enormously to our long-term planning. Together we will advance agricultural innovation in both our countries by expanding the applications of synchrotron technology in agricultural research—from soil and plants to foods and animals."

The Brazilian Synchrotron Light Laboratory is part of the CNPEM, a private non-profit organisation under the supervision of the Brazilian Ministry of Science, Technology and Innovations. The centre operates four national laboratories and is the home of the most complex project in Brazilian science, Sirius, one of the most advanced synchrotron light sources in the world.

The MOU will focus on two specific areas of collaboration. First, a new programme (the Maple Project) will create a rapid-access mail-in agriculture programme for Sirius users to access CLS's VLS-PGM beamline. Additionally, scientists from both institutions will work together to grow the applications of synchrotron science in the field of agriculture through workshops, presentations on proposal development and collaborative research projects.

Second, this agreement will enhance accelerator and machine development. The organisations will share best practices in maintenance, design and testing state-of-the-art technologies and equipment

as well as designing and building next-generation facilities.

"Studies in agriculture are essential to respond to the challenges that the future holds, and the use of synchrotron light as a research tool offers great potential in the search for scientific answers in this area", highlights José Roque, director-general of CNPEM. "The partnership between CNPEM and CLS will be able to foster research in agriculture, as both institutions have extensive experience in cutting-edge research with synchrotron light and may benefit from joint research and information exchange."

The MOU will be in effect for five years.

Laser spectroscopy reveals new states in 2D materials

Atomically thin two-dimensional (2D) materials can provide highly interesting excitonic properties, which render them an attractive platform to explore polaritonic physics. In the literature, a variety of inorganic exciton–polariton systems have been studied experimentally and described theoretically using the broadly accepted

Mark Boland, Lucia Zuin, Bill Matiko (seated), Chithra Karunakaran and Gianluigi Botton

NEWS
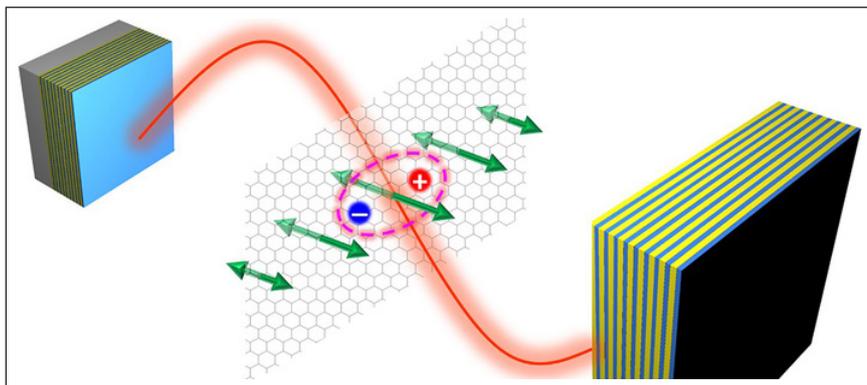
Coupling of phonon (green), exciton (pink), and photon of a microcavity (red) in a 2D material. Credit: Donghai Li / University of Wuerzburg

model of two coupled oscillators, where only the coupling between excitons and cavity photons is considered. Now, Donghai Li and a group of researchers from Julius-Maximilians-Universität (JMU) Würzburg in Bavaria, Germany, have found that placing 2D semiconductors in microcavities can lead to a strong interaction between not just excitons and cavity photons but also with phonons. The team believes that their results could shift the paradigm of exciton–polariton physics in 2D materials by highlighting and quantifying the role of phonons therein.

The team developed a novel method of coherent 2D microspectroscopy, which provides spectral resolution for both the excitation and detection steps in combination with microscopic spatial resolution and 20 fs temporal resolution. With this technique, a rich multipeak spectrum of excitations, which thus far remained inaccessible to linear photoluminescence experiments, is mapped. Comparison with a novel vibronic polariton model, which takes into account not only the degree of freedom of excitons and photons, but also that of phonons reveals multiple polariton branches induced by exciton–photon–phonon hybridisation.

This marks the discovery of previously unobserved bright states in microcavities with embedded 2D materials. The JMU researchers expect that the discovery will be of importance for the ongoing attempts of realising room-temperature Bose–Einstein condensation and polariton lasing in these systems. They published this research in *Physical Review Letters* (doi.org/hj3v).

Portable COVID breathalyser based on SERS

Breathalyser-type tests for COVID-19 have been developed, which rely on differences in concentrations of volatile organic compounds exhaled by those infected with the coronavirus, but most require bulky, non-portable instruments for analysis. Xing Yi Ling and colleagues from


A SERS-based breathalyser can distinguish volatile organic compounds in the breath of COVID-positive people in less than 5 minutes. Credit: Shi Xuan Leong and Yong Xiang Leong, Nanyang Technological University

Nanyang Technological University, Singapore, wanted to develop a quick, convenient and accurate breathalyser test that would be suitable for on-site screening of large numbers of people. They designed a handheld breathalyser that contains a chip with three surface-enhanced Raman scattering (SERS) sensors attached to silver nanocubes. When a person exhales into the device for 10 s, compounds in their breath chemically interact with the sensors. Then, the researchers load the breathalyser into a portable Raman spectrometer that characterises the bound compounds based on changes to the molecular vibrations of the SERS sensors.

The team found that Raman spectra from COVID-positive and -negative people were different in regions responsive to ketones, alcohols and aldehydes, which they used to develop a statistical model for COVID diagnosis. They tested the breathalyser on 501 people in hospitals and airports in Singapore, who were shown by RT-PCR to be negative (85.2 %), positive and symptomatic (8.6 %), or positive and asymptomatic (6.2 %) for the coronavirus. The method had a 3.8 % false-negative and 0.1 % false-positive rate, comparable to RT-PCR tests, but it could be completed on-site in less than 5 min. The breathalyser could someday be a new tool to reduce the silent spread of COVID-19 in communities, the researchers say. This work was published in *ACS Nano* (doi.org/gn6786).

Procedure to interpret x-ray emission spectra of liquid water

Water is an abundant and essential compound, found everywhere on Earth. Yet despite its familiarity and simple structure, water displays many unusual physical properties. For more than a century, scientists have turned their attention to the study of water, attempting to better interpret its structure. An
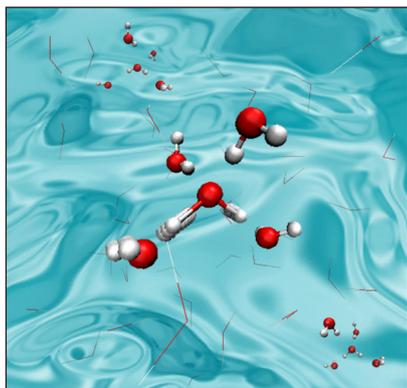
Water molecule in liquid phase accelerating dynamics by x-ray radiation. Image credit: Osamu Takahashi, Hiroshima University

international team of researchers, led by a researcher from Hiroshima University, has developed a procedure allowing them to reproduce the double peak feature of x-ray emission spectroscopy (XES) spectra in liquid water.

Through the years, as scientists have worked to better understand the structure of liquid water, some have studied water using a two-structure model. Other scientists, in a wide range of fields, have used a uniform, continuous liquid model. XES has proven to be a useful tool for researchers studying substances whose features are not homogeneous. For over a decade, scientists

have debated how to interpret XES spectra of liquid water. To solve this problem the research team performed molecular dynamics calculations to create the model structures of liquid water. Their next step was to estimate XES spectra for the liquid water, using first principles of quantum mechanical calculations.

The team was able to theoretically reproduce the double $1b_1$ feature, present in liquid water's x-ray emission spectra. They explored different effects, such as geometry and dynamics, to determine the shape of the XES spectra.

Adopting classical molecular dynamics simulations, the team was able to construct the water's structure in the liquid phase. In these simulations, the researchers worked at various temperature points with the bond length and water molecule angles fixed. In the spectra they calculated, the researchers were able to reproduce the features, such as the double peaks of the $1b_1$ state, that had been previously observed by other scientists in experimental XES spectra.

To better understand the features they were seeing, the research team classified the XES spectra they calculated based on the

different types of hydrogen bonds. They observed the double peak feature in the XES spectra in all the different types of hydrogen bonds they studied. After examining the spectra related to the hydrogen bonds, the team studied the effect of thermally excited vibrational modes on the XES spectra. They obtained nine independent vibrational modes and studied their effects on the spectra.

The researchers were able to successfully reproduce the XES spectra of liquid water by examining the effect of full vibrational modes, O–H stretching, bending and rotational modes. They explained both the temperature and isotope dependence by examining the hydrogen-bond configuration around the excited water molecule and core-hole induced dynamics. "Our procedure is general and can be applicable for various systems related to the phenomena including liquid water", Takahashi said.

The team is hopeful that their research, published in *Physical Review Letters* (doi.org/hj3w), may help to resolve some of the long-standing debates surrounding the interpretation of liquid water's structure. Looking to the future, the researchers see various potential applications for their procedure. "Development of new materials such as electrodes used in batteries, biomaterials such as artificial blood vessels and functional polymers such as water treatment membranes may be fascinating projects, which are related to the structure of liquid water", Takahashi said.

Proof-of-concept for COVID-19 detection via saliva screening

Researchers from the QIMR Berghofer Medical Research Institute in Brisbane, Australia, have collaborated with Agilent scientists on a proof-of-concept FT-IR-based saliva COVID-19 testing workflow using the Agilent Cary 630 FT-IR
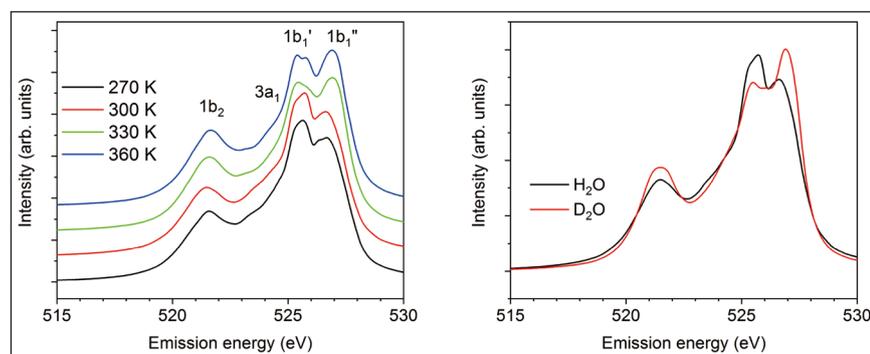
Left: theoretical XES spectra of water at different temperatures. Two $1b_1$ states are assigned as $1b_1'$ and $1b_1''$. Intensities of $1b_1''$ increase with temperature, whereas those of $1b_1'$ decrease, which is the same trend with the experiment. Right: isotope dependence of theoretical XES spectra of liquid water at 300 K. The same isotope effect can be seen in the experiment, with $1b_1'$ peak having much lower intensity than the $1b_1''$ for deuterium water D_2O, whereas for H_2O the situation is reversed. Image credit: Osamu Takahashi, Hiroshima University
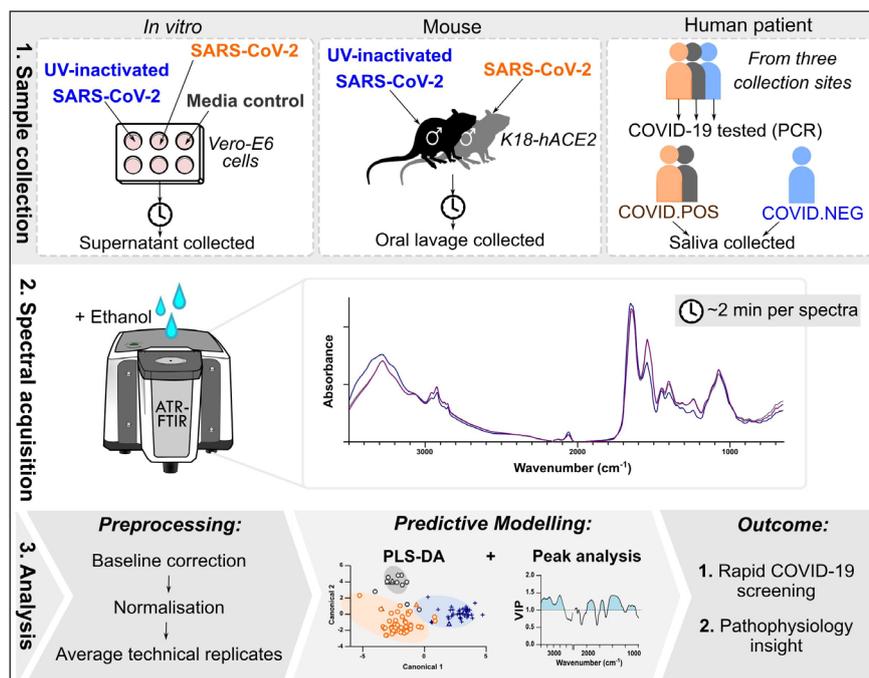
Reproduced from https://doi.org/10.3390/biomedicines10020351 under a CC BY licence.

spectrometer. The study, published in *Biomedicines* (doi.org/hj3x), investigated the pathophysiological response to a COVID-19 infection through ATR-FT-IR spectroscopy. The researchers acquired IR spectra of saliva samples following a quick and simple sample preparation requiring only ethanol and basic laboratory equipment.

Unlike other testing technologies such as PCR testing or rapid antigen test, the ATR-FT-IR method analyses the pathophysiological responses of the human body rather than detecting the pathogen/antigen itself, which is thought to make this method more robust against virus mutations.

"We applied a simple ethanol decontamination procedure for biosafe handling of self-collected saliva samples. A basic step of significant importance for any test that has the potential to be used in non-clinical environments such as in remote areas or in scenarios where large crowds require rapid testing, for example, in airports, or sports stadiums", explained associate professor Michelle Hill, head

of QIMR Berghofer's Precision and Systems Biomedicine Research Group.

"Earlier research studies on ATR-FT-IR for COVID-19 saliva testing were not conclusive on the biological basis for the saliva testing methodology. To shine a light on this aspect, we also conducted controlled infection experiments on cells and mice models and established the most characteristic COVID-19 positive spectral signature. We integrated our data from *in vitro* cell studies, *in vivo* mouse studies and independent human cohort studies, as well as data from recent publications to demonstrate the robustness of the methodology", Hill added.

Quantum processor beats the diffraction limit in spectroscopy

Several years ago, physicists from the Centre for Quantum Optical Technologies and the Faculty of Physics of the University of Warsaw designed and built the first quantum memory in Poland, which was further developed into

a quantum processor. "Our processor is based on a cloud of cold atoms. They can efficiently store and process information from light", describes Dr Michał Parniak, leader of the Quantum-Optical Devices Laboratory. They have used the device as part of a super-resolution spectrometer.

"Our device and algorithm allow us to not only gather information from light more efficiently, but it could also improve 'cramming' information into light", says Dr Parniak. He notes that this idea could be used in telecommunications as well, where more efficient data storage and processing in light is becoming essential. Although there have been efforts to circumvent the Rayleigh limit in spectroscopy, the researchers of the University of Warsaw have demonstrated how to do this in a completely unconventional way—with the use of solutions from quantum information science. Because where classical physics can't cope, quantum physics sometimes offers a whole spectrum of possibilities.

Physicists of the University of Warsaw have built a device that can achieve a resolution in spectroscopy of 15 kHz, or forty parts per trillion, by using a small amount of light from a particular object. "Our spectrometer beats the classical limit using 20 times less photons than the hypothetical traditional spectrometer", says Mateusz Mazelanik, "But this is a remarkable achievement because a classical device with a similar resolution doesn't actually exist."

The processor, which was built at the University of Warsaw, uses a cloud of several billion cooled rubidium atoms placed in a vacuum field, in order to carry out calculations. If the atoms are placed in a magnetic field and illuminated with a laser, they can be controlled to perform particular logic operations, such as process information on the spectrum of light that they are illuminated with. Quantum effects are
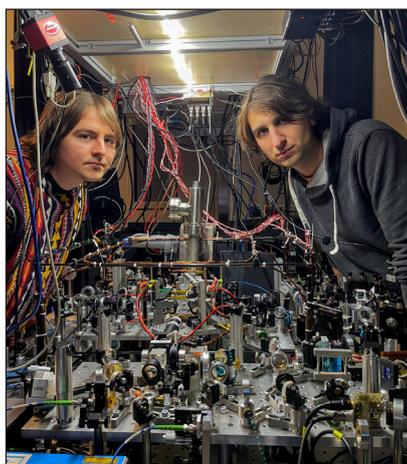
Left: Mateusz Mazelanik, the manager of the Quantum Optical Devices Laboratory, and Dr Michał Parniak next to the quantum-memory-based processor for light. Credit: Centre for Quantum Optical Technologies, University of Warsaw

Microscope image of the studied green algae *Chlamydomonas reinhardtii* and live-cell NMR detection of lipid conversion (upper graph) and fermentation products (lower graphs).

used in the calculations, so calculations in the "cold atomic cloud" don't substitute conventional binary calculations, but add a new level of quality.

"We came up with the idea of how a quantum processor could be used to solve particular problems in spectroscopy", says Dr Michał Parniak. And he emphasises that, up until this point, finding practical applications for quantum processors and designing devices like these with unique solutions in mind wasn't at all obvious. The work was published in *Nature Communications* (doi.org/hj3z).

Real-time solid-state NMR spectroscopy inside living cells

Solution-state nuclear magnetic resonance (NMR) spectroscopy becomes challenging for large structures, such as membrane proteins, polymers or lipid membranes. Magic Angle Spinning (MAS) NMR overcomes the size detection limit by rapid spinning of samples inside an NMR magnet and is typically applied to samples in the solid state. The Leiden University NMR facility houses a 750 MHz NMR spectrometer that recently has been upgraded to optimise micro-imaging and MAS NMR.

To gain selectivity, Anjali Pandit and her postdoc Faezeh Nami used NMR pulses with different "filters" that remove signals of either rigid or dynamic molecules. They used their approach to follow dynamic changes in heterogeneous, photosynthetic membranes extracted from a green microalga. When they proceeded to study intact microalgae, they made a discovery. The cells would still be alive inside the high-field magnet—but as they did not receive light and were deprived of oxygen due to their dense packing, they started to adjust their metabolism and switch to fermentation.

First author of the study published in *Angewandte Chemie International Edition* (doi.org/hj32), Faezeh Nami, could detect the accumulation of several fermentation products and distinguish lipids and carbohydrates. The cells were viable for up to ten hours during which fermentation and lipid metabolism processes were observed and a gradual loss of rigid structures, associated with the breakdown of starch and lipid membranes. Cultivated microalgae are often enzyme-pretreated before cell extraction of useful products, to disrupt the rigid cell walls. The NMR results show that concentrating microalgae creates anoxia conditions and subsequent loss of cell rigidity, which may facilitate product recovery.

A limitation of the method is the short viability inside an NMR rotor. Solutions for extending the cell lifetimes are being explored. Live-cell detection of small metabolites has found its applications in biology and medicine. With the power of MAS NMR, detection of macromolecular structures and assemblies in living cells may be within reach.

## THz–fingerprint vibrational spectroscopy at an ultrafast spectral rate

Raman spectroscopy offers a powerful approach to chemical measurement. By directly probing molecular vibrations, it obtains chemical specificity without the need for chemical labels. Thanks

NEWS

to these virtues, it has become an indispensable tool in a diverse range of fields, including materials science, biology, pharmaceuticals and food science.

Broadband Raman vibrational spectra are commonly segmented into three distinct spectral regions: terahertz (THz) or low-frequency ($<200\,cm^{-1}$; $<6\,THz$); "fingerprint" ($200–1800\,cm^{-1}$); and high-frequency ($2400–4000\,cm^{-1}$). While the fingerprint region derives its name from its target-specific intramolecular bond vibrations, the THz region can provide chemical structural information via intermolecular vibrations. The complementary nature of these two regions makes their marriage a powerful tool for chemical analysis.

Despite the rich information provided by broadband THz–fingerprint Raman spectra, existing methods to obtain them typically have low real-time spectral acquisition rates (generally, $<10\,spectra/s$), which manifests as coarse experimental temporal resolution. Although several research groups have pushed broadband Raman spectral acquisition rates to impressive levels (on the order of $10,000–100,000\,spectra/s$), the methods tend to be limited to detection of either the THz or fingerprint regions alone. These limitations pose a barrier to investigating short-lived irreversible phenomena at the molecular bond and structural level.

Researchers at the University of Tokyo recently overcame these limits, by developing a method for broadband THz–fingerprint Raman spectroscopy at an ultrafast spectral rate of 24,000 spectra/s. The new technique, named "dual-detection impulsive vibrational spectroscopy" (DIVS), enables synchronous measurement of two distinct types of vibrational signals, which provide dual-region sensitivity when detected in concert. More technically, DIVS blends optical longpass and shortpass
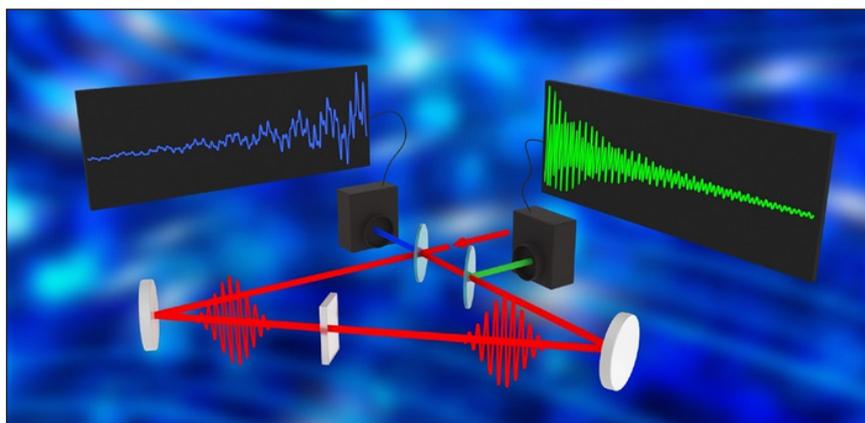
Sagnac interferometry and optical filtering come together to provide dual-region (THz–fingerprint) Raman spectral sensitivity at 24,000 spectra/s. Credit: Walker Peterson, University of Tokyo

filtering with common-path Sagnac interferometry to simultaneously detect frequency-shifted laser pulses ("FT-CARS", fingerprint-sensitive) and phase delay-shifted pulses ("SE-ISRS", THz-sensitive). Moreover, the DIVS setup is straightforward and requires only a single laser.

The researchers performed DIVS proof-of-concept measurements of several transparent liquid compounds over the Raman spectral range of $66\,cm^{-1}$ ($2.0\,THz$) to $1211\,cm^{-1}$. The strongest signature vibrational peaks in single Raman power spectra (acquired in $<42\,\mu s$) were demonstrated with high signal-to-noise ratios of >1000. At the current stage, DIVS is recommended for studying high-concentration transparent samples, though modifications of the design could possibly overcome these boundaries.

This work, published in *Advanced Photonics* (doi.org/hj6f), holds potential for interesting real-time broadband THz–fingerprint Raman measurements at sub-millisecond temporal resolutions. One promising direction for DIVS applications is in polymer science. In addition to signature molecular bond vibrations in the fingerprint region, polymers are known to exhibit rich structural information in the THz region.

Ultrafast DIVS could be well-suited to understanding rapid polymerisation systems at the molecular level.

Tiny, reusable sensing chip based on SEIRA

Nanostructures in optical sensing chips may contain nanostructures that are nearly as small as the biological and chemical molecules that are to be detected. These nanostructures improve the sensor's ability to detect the molecules, but their minute size make it difficult to guide the molecules to the correct area of the sensor.

Scientists at the Center for Integrated Nanotechnologies, Sandia National Laboratories, have created a new sensor for point-of-care applications based on surface-enhanced infrared absorption (SEIRA) spectroscopy that aims to address this size problem. The new sensor consists of several arrays of tiny rectangular strips of gold. Engineers dipped the strips in 1-octadecanethiol (ODT), which they chose to identify. They then added a drop of liquid metal (in this case, gallium) to serve as the sensor's base. Lastly, they placed a thin glass cover on top to form a sandwich-like structure.

The design of the sensor, with its layers and cavities, creates what is known as a "nanopatch
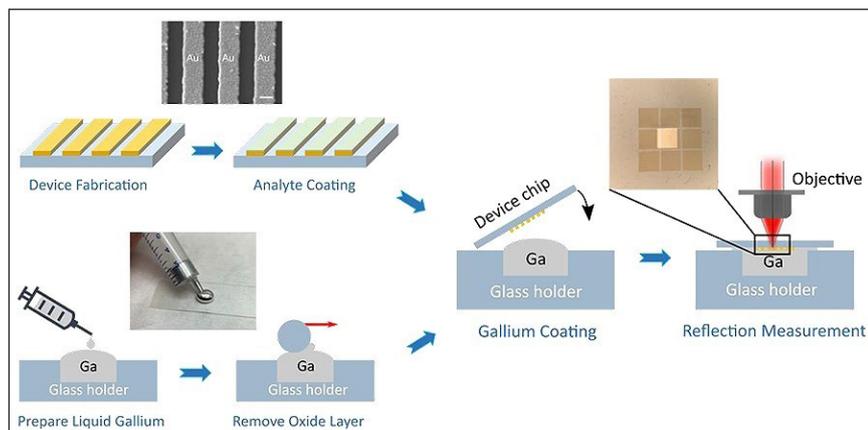
Illustration showing different phases of the sensor-building process. One image shows the gold nanostrips. Another shows ODT-coated gold nanostrips. Two others show the liquid gallium being deposited and then removed.

antenna". The antenna both funnels molecules into the cavities and absorbs enough infrared light to analyse biological and chemical samples.

"Even a single layer of molecule in our sensor can lead to a 10 % change in the amount of light reflected, whereas a typical sensor may only produce a 1 % change", says Liu, who adds that the team will continue to refine the sensor with the goal of using it for bioanalytical sensing and medical diagnostics applications, such as sensing biomarkers linked to certain diseases.

After measuring the ODT, the researchers removed the liquid gallium from the sensor chip surface with a swab. This process allows the sensor to be reused, which could make it more cost-effective than similar alternatives.

"The structure of our sensor makes it suitable for point-of-care applications that can be implemented by a nurse on a patient, or even outside the hospital in a patient's home", he says.

Waters acquires charge detection mass spectrometry technology

Waters Corporation has acquired the technology assets and intellectual property rights of Megadalton Solutions, Inc., a developer of Charge Detection Mass Spectrometry (CDMS) technology and services. Financial details of the transaction are not being disclosed.

Founded in 2018 by professors Martin Jarrold and David Clemmer at Indiana University, Megadalton Solutions has developed CDMS instrumentation that makes it possible to analyse extremely large proteins and protein complexes, such as those used in cell and gene therapies, that would otherwise be difficult to analyse with conventional mass spectrometry. Waters became a strategic investor in the company and in 2021 brought Megadalton's CDMS technology into the Waters Immerse™ Cambridge innovation and research lab for advanced testing and development.

"Large molecule mass spectrometry with CDMS offers an important tool for the characterisation, analysis and quantification of next-generation biologics, such as cell and gene therapies, which is an area of high interest among biopharmaceutical and biomedical research customers", said Dr Udit Batra, President and CEO, Waters Corporation. "Large molecules can be extremely challenging to characterise with conventional mass spectrometry because of their complexity. We are looking forward to further developing and commercialising the Megadalton CDMS technology to help customers analyse and quantify large molecules in applications such as cell and gene therapy drug development."

"We developed our CDMS detector to bring the precision of mass spectrometry to the analysis of complex biologics", said Dr Martin Jarrold, CEO of Megadalton Solutions, Inc. "It is an exciting milestone in our journey to have Waters carry forward and continue the development of CDMS for the analysis of large molecules such as gene-based therapies that represent the next generation of medicine."

ABB secures $30 million order for satellite imaging technology

ABB has been awarded a contract worth around $30 million by the Canadian data and analytics company EarthDaily Analytics Corp. (EDA) to develop and manufacture next-generation multispectral imaging systems to be placed on 10 satellites (including an in-orbit spare) that will circle the Earth. The EarthDaily Constellation network of satellites will be able to provide high-quality imagery in 22 spectral bands with resolution down to 5 m.

"We are proud to collaborate with ABB on the development of the ground-breaking EarthDaily Constellation, which will provide unprecedented daily global coverage of the Earth at ultra-high, scientific-grade image quality. Current Earth observation satellite systems provide either high image quality with low coverage or low image quality with high coverage. The EarthDaily Constellation brings high image quality and rich spectral band diversity together with daily

NEWS

Artistic impression of the EarthDaily Constellation satellite. Credit: Loft Orbital and Airbus

global coverage—something that has never been available before. ABB's long track record of success at the forefront of space sensors and Earth observation provides us with not only best-in-class technology, but also the confidence that comes from working closely with a leading technology company", said Don Osborne, CEO, EarthDaily Analytics.

Once deployed on the network of satellites, ABB's sensors will continuously capture images of the planet's land masses and large maritime areas as the satellites circle the Earth. EDA's artificial intelligence-based analytics system will then process the data gathered from these images based on any recorded changes and generate actionable insights that will include information on the state of Earth's ecosystems, as well as on the impact and progress of the changing climate.

The year of 2022 marks 100 combined years of reliable operations for all of ABB's optical equipment in orbit with core contributions to flagship missions of space agencies around the world. The space group within ABB's Measurement & Analytics Division specialises in advancing measurement capabilities from space, from enabling daily weather forecasts to precisely monitoring the rise of greenhouse gases or spotting strong emitters.

product range has further expanded to offer systems addressing the five main application areas of RGA, gas analysis, catalysis & thermal analysis, plasma characterisation and surface analysis. Hiden's bespoke design service continues to provide client interactive development of solutions to meet specific requirements.

In 1992, Hiden entered the field of microgravimetric gas sorption measurement in collaboration with the University of Birmingham, and a dedicated sister-company, Hiden Isochema, was established to manufacture these products. In 1996 Hiden Inc., was formed to provide sales and service support for the full Hiden product range in the USA, with offices established throughout the country. In 2019 Hiden Europe GmbH was created, providing a strong base of sales and application based technical support for Germany and Austria.

Further company expansion includes new clean room facilities for precision assembly, a new vacuum/mechanical assembly suite

Hiden Analytical 40 Year Anniversary

In 1982 in Warrington, UK, Hiden Analytical began life as a start-up company, initially focussed upon manufacturing quadrupole mass spectrometers for vacuum processing in the emerging semiconductor fabrication industry. Over time, application areas expanded and new products were developed. Early developments saw the design of real-time gas analysis systems followed by new products to address specific areas. Initially,

direct external ion measurement systems for plasma process diagnostics, then, secondary ion monitoring for surface characterisation (the SIMS technique). Recent developments have included systems for the direct analysis of dissolved species in environmental and electrochemical applications as well as improvements in system portability, with the pQA being a fully featured portable quadrupole analyser for environmental studies. Hiden's

and new office space at Hiden's UK headquarters, which will be completed this year. Hiden now employs over 120 scientists, engineers, technicians and operations specialists at its UK headquarters.

Hiden are offering readers a free 40 Year Anniversary Edition Hiden Wall Planner or Desk Calendar (https://bit.ly/hidenposter). Desk Calendars are available in International, UK, USA and German formats.

Newomics and Bruker announce collaborations on high-throughput bioanalysis

Newomics Inc. and Bruker Corporation have announced collaborations on a novel LC-MS platform for drug discovery in the pharma/biopharma industry as well as research institutions. The two companies agreed on co-marketing Newomics's Microflow-nanospray electrospray ionisation (MnESI) product line with Bruker's maxis II and timsTOF Pro 2 mass spectrometers.

"We are excited to expand our successful collaborations with Bruker", said Daojing Wang, Newomics Founder and CEO. "Our M3 emitter is the first commercial multinozzle emitter for mass spectrometry. The new MnESI source directly addresses several key pain points in mass spectrometry analysis of native proteins, protein complexes and oligonucleotides, and opens up new opportunities for biopharmaceutical and clinical research and development."

PerkinElmer and P1 Fuels team up to test fossil-free fuels

PerkinElmer has announced a long-term partnership with P1 Fuels, a specialist in fossil-free performance fuels for racing teams and the automotive industry. PerkinElmer will work with P1 Fuels to develop and test fully renewable fuels to be used in the upcoming series of the FIA World Rally Championship (WRC)—the highest level of rally global competition. The ultimate goal of this collaboration is to help the automotive sector, including motorsports, transition to climate-neutral, fossil-free fuels.

P1 Fuels will use PerkinElmer's GC and IR spectroscopy technology in its Berlin headquarters, as well as trackside, to perform quality-control checks. These two analytical techniques have a long history within the automotive space, but this is the first time that chromatography

and infrared spectroscopy will be used to test competitive, sustainable fuels. The aim is to show that fully sustainable fuels can deliver high performance without damaging the environment. PerkinElmer will provide P1 Fuels with a Spectrum^{TM} Two FT-IR spectrometer and a Clarus 590 gas chromatograph.

According to Gavin Aston, Director Strategic Initiatives EMEAI, PerkinElmer, "The partnership with P1 Fuels is yet another proof point of PerkinElmer's commitment to driving positive, lasting change by developing products to sustain the health and safety of people and the environment. This fantastic collaboration is empowering sustainability by enabling our valuable partner to perform all the analyses needed to continue to shape fossil-free mobility. "Our goal is to create better outcomes for everyone", Aston added. "Simple changes, such as switching from fossil fuel products to more sustainable alternatives can have a huge impact when done at scale. We can't wait to show the motorsport world how science and testing can support outstanding sporting performances whilst protecting the environment."

Martin Popilka, CEO, P1 Fuels, said: "We are thrilled to work with PerkinElmer, which can help the automotive industry, including motorsports and development teams, speed up the transition to climate-neutral mobility using fossil-free fuels. PerkinElmer's technology will support race

scrutineering and analysis of motorsports at global races and demonstrate how sustainable solutions do not have to come at the expense of sporting success. Fossil free fuels play an integral part of the future mobility mix, and motorsport plays a fundamental role in a broader adoption and testing of these fuels. We're excited that the FIA WRC is the first world championship to embrace completely fossil-free fuels and clearly demonstrates that their performance is on pair with their fossil counterparts."

Agilent acquires AI technology to enhance lab productivity

Agilent Technologies has acquired advanced artificial intelligence (AI) technology, known as ACIES, developed by Virtual Control, which Agilent will integrate the software into its gas chromatography and mass spectrometry (GS/MS) platforms to improve the productivity, efficiency and accuracy. With the acquisition, Agilent obtained the software and other assets associated with ACIES. As part of the transaction, core members of the ACIES team also became Agilent employees.

ACIES automates the labour-intensive task of GC/MS data analysis improving efficiency in the laboratory workflow, from sampling to reporting. Agilent will integrate the technology into its MassHunter software package for LC/MS and GC/MS instruments.

NEWS

Funding for hyperspectral imaging satellite company

Canadian hyperspectral imaging satellite company, Wyvern, has received a CAD $4M investment from Sustainable Development Technology Canada (SDTC), an foundation created by the Government of Canada to fund technologies with economic and environmental benefits. The investment is tied to a 3-year project that includes support from xarvio® Digital Farming Solutions, a brand of BASF Digital Farming GmbH.

"Wyvern's technology is addressing a major gap in the market", said Leah Lawrence, President and CEO of SDTC. "Their imaging products are going to help farmers use less fertiliser, pesticides and water and help produce bigger yields. SDTC is proud to support Wyvern in their mission to increase the productivity and sustainability of Canadian farmlands."

The funding from the SDTC will help Wyvern reach a significant milestone: the launch of their DragonEye satellite. Wyvern's proprietary deployable optics technology is key to their ability to deliver affordable high resolution
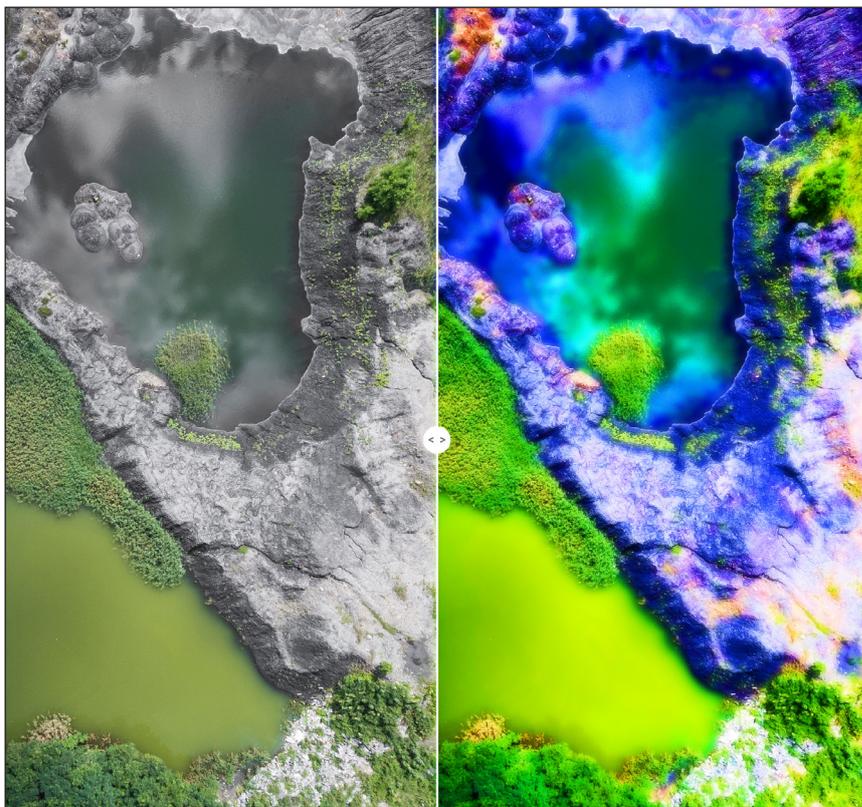
SWIR hyperspectral imagery. Courtesy: Wyvern

hyperspectral imagery, including 1 m VNIR and 5 m SWIR, in the coming years. DragonEye will be Wyvern's first satellite equipped with this innovative technology that unfolds a telescope in space, similar to the James Webb telescope launched in late 2021.

Process Insights acquires Guided Wave

Process Insights has acquired Guided Wave Inc. from Singapore-based Advanced Holdings Ltd. Guided Wave, based in Rancho Cordova, CA, USA will join Process Insights' existing broad portfolio of brands and technologies for process analytics, monitoring and control. Founded in 1983, Guided Wave designs and manufactures complete analytical systems utilising NIR and UV-vis spectroscopic technologies. Guided Wave's products and technologies are used in a wide range of applications across a multitude of markets and industries including chemicals, petrochemicals, semiconductor, pharmaceuticals, biotechnology and healthcare.

"For more than 35 years, Guided Wave has served a variety of customers and industries worldwide with leading spectroscopic process analyser solutions. With our acquisition by Process Insights, additional resources will propel Guided Wave into the next decade of innovation and industry leadership," said Susan Foulk, President of Guided Wave. "It's exciting to join the Process Insights team, and the team at Guided Wave looks forward to opening new pathways for growth as we continue to put our customers and their process analytical needs first," Foulk added.

"Guided Wave is a natural fit for Process Insights. We share many common customers, markets and applications. This is an exciting

opportunity for Process Insights to continue to expand our total differentiated solution offerings to our customers with the addition of Guided Wave's premium NIR and UV-vis technologies to our portfolio," said Monte Hammouri, CEO of Process Insights. "We have known Guided Wave, Susan and her team for many years through prior collaborations. Bringing them into the Process Insights family takes our collaboration to that next level where we can leverage Process Insights' global scale and operating footprints to further accelerate Guided Wave's growth and innovation," added Hammouri.

A History of European Mass Spectrometry

Edited by Keith R. Jennings

with contributions from Nico M.M. Nibbering, Andries Bruins, Michael Karas, Bob Bateman, Jochen Franzen, Michael C. ten Noever de Brauw, Peter Roepstorff, Károly Vékey, Jim Scrivens and Alison E. Ashcroft

The construction of Thompson's mass spectrograph in Cambridge followed by Aston's improved instruments and his pioneering work on non-radioactive isotopes is widely known. In the sixty years or so since then, European scientists and engineers have made many major contributions to the development of new instruments and techniques. Accounts of these contributions in the scientific literature necessarily give little idea of the contributors themselves or of the difficulties that had to be overcome before success was achieved.

Most newcomers to mass spectrometry in the last ten years will have little concept of the difficulties faced in obtaining the mass spectra of four solid samples during a working day before the invention of the vacuum lock probe. This was followed by several hours of counting spectra and trying to interpret them. Many will never have seen a magnetic deflection instrument and will be familiar only with mass spectrometers having both the operation of the instrument and the interpretation of the data under computer control.

This book aims to give an insight into how some of the more important developments came about, from the advent of the first commercial instruments to the present day. The various accounts, several of which contain personal reminiscences, both provide a human background to these developments and convey the excitement of being part of the European mass spectrometry community during this period.

impopen.com/mshistory

SAMPLING COLUMN

Inferential statistical sampling of hyper-heterogeneous lots with hidden structure: the importance of proper Decision Unit definition

Chuck Ramsey[a] and Kim H. Esbensen[b]
[a]President EnviroStat, Inc., http://www.envirostat.org, chuck@envirostat.org
[b]President KHE Consulting, Copenhagen, Denmark. https://kheconsult.com/, khe.consult@gmail.com

Sampling is nothing more than the practical application of statistics. If statistics were not available, then one would have to sample every portion of an entire population to determine one or more parameters of interest. There are many potential statistical tests that could be employed in sampling, but many statistical tests are useful only if certain assumptions about the population are valid. Prior to any sampling event, the operative Decision Unit (DU) must be established. The Decision Unit is the material object that an analytical result makes inference to. In many cases, there is more than one Decision Unit in a population. A lot is a collection (population) of individual Decision Units that will be treated as a whole (accepted or rejected), depending on the analytical results for individual Decision Units. The application of the Theory of Sampling (TOS) is critical for sampling the material within a Decision Unit. However, knowledge of the analytical concentration of interest within a Decision Unit may not provide information on unsampled Decision Units; especially for a hyper-heterogenous lot where a Decision Unit can be of a completely different characteristic than an adjacent Decision Unit. In cases where every Decision Unit cannot be sampled, application of non-parametric statistics can be used to make inference *from* sampled Decision Units *to* Decision Units that are not sampled. The combination of the TOS for sampling of individual Decision Units along with non-parametric statistics offers the best possible inference for situations where there are more Decision Units than can practically be sampled.

Introduction

There are heterogeneous materials and there are heterogeneous lots. Materials can be heterogeneous in the sense of dissimilarity between the fundamental constituent units of the material, e.g. particles (and fragments thereof), grains, minerals, cells biological units … (this is the definition of heterogeneity in the Theory of Sampling, TOS). Lots can be heterogeneous in the sense of dissimilarity between the characteristics of Decision Units (DU). Moreover, there are types of hyper-heterogeneous lots with significant internal complexity, which can be known or *hidden*. Below, lots of this latter type are in focus.

For many hyper-heterogeneous lots with complex internal structure(s), i.e. lots containing *groups* of more-or-less distinct DUs, complete sampling is, in practice, often impossible due to logistical, economical or other restrictions. Such lots cannot be sampled reliably on the basis of an assumed distribution, i.e. the distribution of the analyte(s) between the DUs does not follow any known distribution, making the archetype statistical inference based on a known distribution inadequate. Instead, the basis for the statistical inference of these types of lots is the *non-parametric one-sided tolerance limit*, which can be applied to all types of lots from uniform to hyper-heterogeneous, but which is especially relevant for the type of hyper-heterogeneous lots exemplified in this contribution.

This column shows the critical importance of the application of non-parametric statistical methods when there are more DUs present than can be sampled as an essential complement to the TOS. This situation in fact occurs in very many contexts, for very many sampling targets and materials and lots. What to do?

Different manifestations of heterogeneity

There is heterogeneity, and there is heterogeneity—there are heterogeneous materials *within* a DU and there is heterogeneity *between* DUs. Materials can be heterogeneous in the sense of the TOS reflecting dissimilarity between the constituent units of the material (particles and fragments thereof, grains, cells, other …) within a DU. Readers may be familiar with this type of sampling, see Reference 1 and further key references therein. There is a special focus on heterogeneity in this TOS sense in Reference 2.

Multiple DUs can be heterogeneous in the sense of differences *between* the characteristics of DUs, which can be defined more-or-less appropriately. An introduction to sampling of lots of this type is found in Reference 3.

Moreover, there are types of heterogeneous lots with even more internal complexity, which may be known or may be *hidden*.

This column presents a rationale for how to sample such hyper-heterogeneous lots, or more precisely how to sample in the presence of heterogeneity both within and between DUs.

A hyper-heterogeneous lot with hidden structure

An illustrative example of a hyper-heterogeneous lot shall be a legacy nuclear waste mega-lot (see Acknowledgements). Over a period of 50 years, extensive decommissioning of nuclear facilities and several temporary low-level nuclear waste storage facilities have been established, Figure 1, from which waste drums *can* be retrieved on demand in principle, but in practice associated with various degrees of logistical constraints. In total, there are today ~66,000 conditioned waste drums in temporary storage depots.

In 2021–2023 the time has come to start engaging in final end-storage of this legacy nuclear waste. Today there are much

stricter Waste Acceptance Criteria (WAC) in play than was the case in earlier decades, for which reason there is a critical need to pre-check "all" drums with the aim of reaching an operative classification into three categories: 1) Cleared for "Final storage"; 2) "Re-classification to intermediate/high-level storage"; or 3) "Needs further treatment". The sampling methodology needed for physical, chemical and radiological inspection of selected individual drums has been described by Tuerlinckx and Esbensen.[4]

The current Herculean task is **how to** inspect ~66,000 drums for a) physical characteristics; b) chemical characteristics; and c) radioactivity characteristics, which make use of very different types of analytes. With current economic budgets vs the prevailing practical conditions, complete inspection of all ~66,000 drums is likely not feasible, however desirable. In addition, the consequences of an incorrect decision are very serious.

Overview of hyper-heterogeneous (hidden) lot structure

There are reasons to assume that *some* similarities exist between Decision Units within resolved families—but this needs verification by empirical characterisation

There are other reasons to assume that the internal between-drum heterogeneity of many families can be significant or major. This also needs to be verified empirically.

Many "families" are small, and distinctly different from one-another. There is a broad spectrum of families in temporary storage depots.

The total of ~66,000 DU's cannot be assumed to correspond to a statistical i.i.d. population due to significant heterogeneities at all levels of drums, sub- and full families.

Figure 1. Illustration of a hyper-heterogeneous lot comprised by a hierarchy of units: drums – families – lot. For the discussions that follow, the operationally relevant DU is an individual drum.

SAMPLING COLUMN
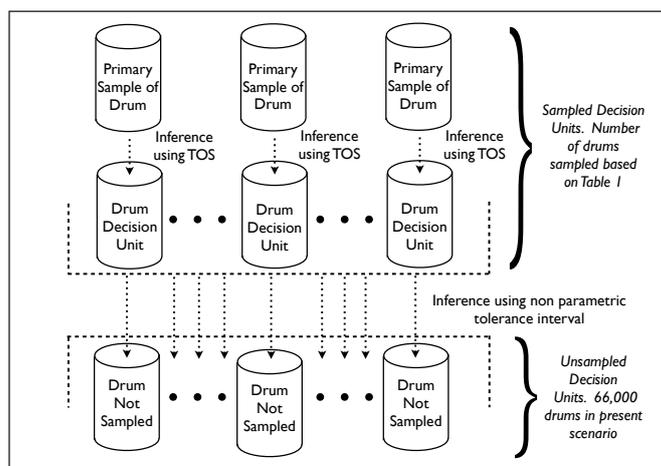
Figure 2. Illustration of inference from multiple sampled to unsampled DUs.

It would have been nice *if* the ~66,000 drums[a] could be viewed as one statistical population consisting of i.i.d. DUs with a known distribution between DUs. But because of the 50-year complex decommissioning history it is known that low-level nuclear waste drums not only *differ extremely* in compositional content(s), physical constitution and radioactivity profiles, but—horror-of-horrors from a statistical point of view—there are very good reasons to infer that there exist *groupings* within this population of 66,000 DUs. But the degree to which such groupings ("families" in the nuclear expert lingo) are well characterised and well discriminable *inter alia*, is markedly uncertain; some families are suspected to be clearly demarked, but certainly not all, or maybe not even most.

So far, diligent archival work has resulted in identification of some 40+ "families" or so, each with broadly similar radioactivity profiles. It is relatively easy to measure a radioactive profile fingerprint of an individual drum.[4] Due to the marked heterogeneity *hierarchy* (drums – families – meta-population), Figure 1, it was at one time tentatively decided to try to use "resolved families" as DUs, rather than the entire lot, as laid out by Ramsey.[3] The main statistical issue then was whether it was possible to estimate *how many* drums would be needed to characterise (or validate) each family with a desired low "statistical uncertainty". Further comprehensive problem analysis, however, made it clear it was necessary to increase the observation resolution to focus on *individual drums* as the final operative DUs.

Statistical methodology

The basis for the statistical sampling which must be used for this type of nebulous lot is the *non-parametric one-sided tolerance limit*, a test that does not depend on any distribution of measurement results. The statistical theory behind this test is described in many statistical textbooks.[5–7]

Operative statistical approach

Here follows a generic sampling plan that can be applied to hyper-heterogeneous lots in general:

1) Appropriate definition of DUs—in the present scenario, an individual waste drum.

2) **Determine the Data Quality Objectives for the project:** Project management must decide its wish for a **confidence level (X%)** that no more than **Y%** of the drums *may* fail the chemical WAC. The confidence level and Y% shall be determined *a priori*, without any consideration of, or influence from, the statistically required number of samples (see further below). If project management decides to decree 100% confidence that 0% fail WAC criteria (*a common request*), then there is unfortunately nothing that can be done. Then there must be 100% inspection of all DUs and there must be zero sampling and analytical error—this is obviously an impossibility.

3) **Statistical criterion:** Statistical sampling includes the possibility that some failing DUs may be *missed*. This potential is to be balanced by the tremendous reduction in sampling and analytical costs achievable by carrying out statistical sampling of only a *fraction* of the total population of DUs. To determine the sampling effort required, the X confidence and Y percent must be determined *prior* to calculating the required number of drums to be physically sampled. It is the responsibility of project management to decide on its wish *independently* and *a priori* of working out the sampling plan. Most importantly, do not first select the required number of samples to be extracted, for example based on project economics, logistics or some other bracketing factor, and then accept what the confi-

---

[a]In the nuclear waste realm, often waste drums may even have their own internal heterogeneity, i.e. containing 1, 2 or 3 compressed units (called "pucks"), which may then better reflect the optimal resolved DUs of interest, depending on the specific WAC analytes proscribed. For simplicity in this didactic exposé of statistical methodology however, we here stay with DUs being synonymous with drums.

SAMPLING COLUMN

Table 1. Statistically required number of samples to be extracted from a population.[a,b] In this table, "failing" means a maximum amount that *could* fail, not implying that any *will* fail.

Confidence level (X): 90 %			
Y % DUs failing	10 %	5 %	1 %
Number samples	[22]	[45]	[230]
Confidence level (X): 95 %			
Y % DUs failing	10 %	5 %	1 %
Number samples	[29]	[59]	[299]
Confidence level (X): 99 %			
Y % DUs failing	10 %	5 %	1 %
Number samples	[44]	[90]	[459]

[a]The required number of samples can be calculated for *any* combination of confidence level and percent.

[b]If the number of drums required to be sampled approaches the total number (greater that 10 %) in a population (or in a resolved family or another sub-set of the complex lot), the required number of samples can be reduced by application of the so-called *finite population correction*. In this case seek further statistical assistance.

dence level and risk percent based on this number turns out to be. The confidence level and risk percent must *only* be based on considerations of the consequences of an incorrect statistical decision (Table 1).

Statistical clarification: The percent of drums that *may* fail does not imply that any of the unsampled drums *will* fail, just that many *could* possibly fail and that this would be detectable. The number of samples required for *any* combination of confidence and proportion of DUs can be determined from the master equation shown in the Appendix illustration, based on Reference 6.

4) **Action plan:** Select and retrieve required number of drums *at random* from the total population of drums. It is *imperative* that any drum selected in the statistical sampling plan is fully available for sampling and can be extracted without any undue restrictions in practice.

Statistical conclusion: If *none* of the extracted drums fail the chemistry WAC, project management can be "X % confident that no more than Y % of the drums fail the chemical WAC". Since these Data Quality Objectives have been decided *a priori*, this means that the project can dispose of all drums in the population without further verification regarding the operative WAC. It is noted that this statistical test assumes that there is *no* sampling error and *no* analytical error. While this cannot ever be the case, in practice it is imperative that these errors be controlled as much as possible to provide reliable conclusions, see Reference 8. However—and this is the *whopper* of all inferential statistics:

5) If one or more of the DUs *fail* the chemical WAC criteria, the Data Quality Objectives have *not* been met, and additional sampling and analysis of drums must be performed.

In this case there are several options to continue the characterisation project. It is imperative to develop such alternatives in collaboration with all stakeholders and parties involved, frontline scientific and technical personal, project management, overseeing boards a.o.

One possible course of action could be to compare the sampled drums with their radiological profiles to see if there is a *correlation* between the radiological profile and the chemical parameters in the WAC. There could then, perhaps, be established a multivariate data model, aka a chemometric model.[9] If this is the case, it may *perhaps* be possible to classify all the drums in the population into operative sub-populations (*a la* the presently resolved ~40 radiological families) as a basis for repeating steps 1–3 above, specifically now addressing the array of *resolved* sub-populations ("families") *individually*. This approach could be attempted for any relevant WAC (radiological, chemical, physical, other ...). N.B. This model must be validated on *additional* random DUs, since it is easy to constrain a model to fit the available data. The critical issue is to test the model, to validate the model on a *new* set of randomly selected DUs ("test set validation"). The number of samples to verify any model will be that same as initially determined since the data quality objectives do not change. It makes no sense to try out just a moderate number of additional samples. The power of non-parametric statistics lies in the number of DUs with which to cope with hyper-heterogeneous lots; this is a hard problem.

Take home lesson

The objective of this issue's contribution is to present a type of lot heterogeneity for which all types of parametric statistics is not applicable (based on assumed, or proven, normal distribution, nor any other

SAMPLING COLUMN

parametric distribution). While the above approach is illustrated by a lot with rather specific features, it well illustrates the *general characteristic* for which non-parametric statistical inference can deal with complex, partially or wholly, *hidden* structure(s).

Table 1 shows the evergreen question raised when seeking help from statistics: **"how many"** observations or measurements are needed in this generic non-parametric approach, presented for a few typical cases i.e. (90, 95, 99 %) confidence that no more than (10, 5, 1 %) DUs could be failing. The smallest vs the largest necessary number of samples needed to allow this test regimen could be from just a few to thousands, depending on the Data Quality Objectives. The power of generalisation is awesome, since this test scenario is applicable to all kinds of lots (populations) where it is not possible to sample all DUs—that's quite a broad swath of the material world in which sampling is necessary!

A prominent "someone" from the sampling community, not a professional statistician, when presented with this non-parametric approach for the first time, exclaimed: "*But these are magic numbers—they apply to everything, to every lot with such ill-defined characteristics. This is fantastic! Where do these numbers come from?*"

The science fiction author Isaac Asimov (Figure 3) once pronounced: "Any sufficiently developed technology, when assessed on the basis of contemporary knowledge, will be indistinguishable from *magic*".

A perspective from the point of view of confidence vs reliability

John Young (1930–2018), by many considered *the* consummate astronaut, was a.o. the only astronaut to fly both in NASA's Gemini, Apollo and Space Shuttle programmes; he flew in space six times in all. For an absolutely fascinating life's story,
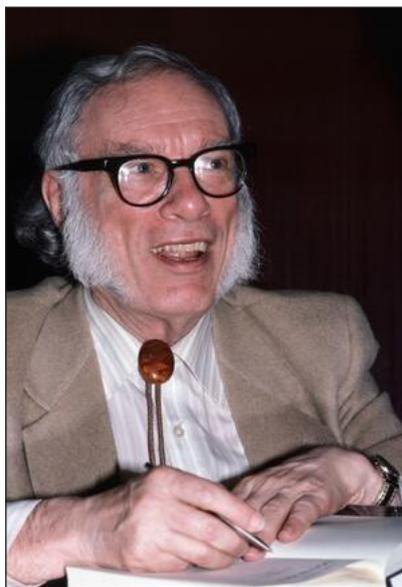

Figure 3. Isaac Asimov: he knew a thing or two about science and technology, and the human condition. Credit: Jim DeLillo/Alamy Stock Photo

see Reference 10; or his entry in Wikipedia.

After a "stellar" career as an active astronaut, in 1987 he took up a newly created post at the Johnson Space Center as Special Assistant for Engineering, Operations and Safety. In this position Young became known, rightly so, as the memo guy, producing

Figure 4. October 1971 portrait photograph of John W. Young. Credit: NASA

literally hundreds of memos on all matters related to crew safety, most definitely not afraid to ruffle more than a few feathers when he felt the need. Safety was foremost in his mind. Young knew better than anyone that space flight is a very risky business, but he also knew the importance of paying attention to detail—and always doing things right.

From this plethora of safety missives, here is a small nugget—a *gem* rather in the present context (Reference 10, pp. 314–315):

"Sometimes the absurdity of bureaucratic logic was tough to take. Consider the case of the solid rocket motor (SRM) igniter. At the flight readiness review for STS-87 (....), we heard a report saying that the solid rocket motor igniter had undergone twelve changes. The changes, along with some other involving the manufacturer, has occasioned the test-firing of six new igniters. Something called "Larson's Binomial Distribution Nomograph on Reliability and Confidence Levels" indicated that firing six igniters with zero failures gave us 89 % reliability with 50 % confidence. To raise that to 95 % reliability with 50 % confidence would take fourteen firings, while raising it to 95 % reliability with 90 % confidence would take forty-three firings. So, stupid me, I asked that we continue firing igniters to upgrade our confidence. Clearly it was far cheaper, I thought, to gain confidence than to experience a failure of the SRM igniter in what was only a flight test."

Not related to the present column, but interesting, and funny, is Young's next paragraph:

"So, what was the response to my suggestion? I was told that the plant that manufactured the igniters had been moved. Later, I was told that the manufacturing plant had *not* been moved and, 'therefore', firing six igniters should be enough. 'Therefore?'"

Epilogue: carrying over

So, no magic—just the right kind of inferential statistics to the rescue for this type of "difficult to sample" lot or population.

However, an immediate apropos, which is non-negotiable: all physical sampling of the individual DUs selected and extracted, must be compliant with the stipulations, rules and demands for representative sampling laid down by the TOS. This is an essential approach when the destructive testing is required, no exceptions.

There are many other types of lots with *similar* characteristics as the ones selected for illustration here to be found across a very broad swath of sectors in science, technology, industry, trade and environmental monitoring and control. For example, from the food and feed sector, from which can be found key examples in Reference 11. Or from the mining realm: primary sampling of broken ore accumulations[12,13] as brought to the mill in haphazardly collected truck loads, while sampling for environmental monitoring and control is a field in which the present approach finds extensive applications. It is instructive to acknowledge that the within-DU as well as the between-DU heterogeneity characteristics from such dissimilar application fields, food vs ore are identical, it is just a matter of degree.[2]

Appendix

Where and how to find appropriate "magic numbers"

The Larson *nomogram* (Figure 5) can be used to obtain the required sample numbers presented in this paper. This nomogram was developed in 1966, long before the proliferation of computers, and is based on the binomial distribution. To use the nomogram, draw a line from the desired "confidence" to the "percent" one is willing to allow to fail. The intersection of that line to the line of "*n* Sample size" gives the necessary
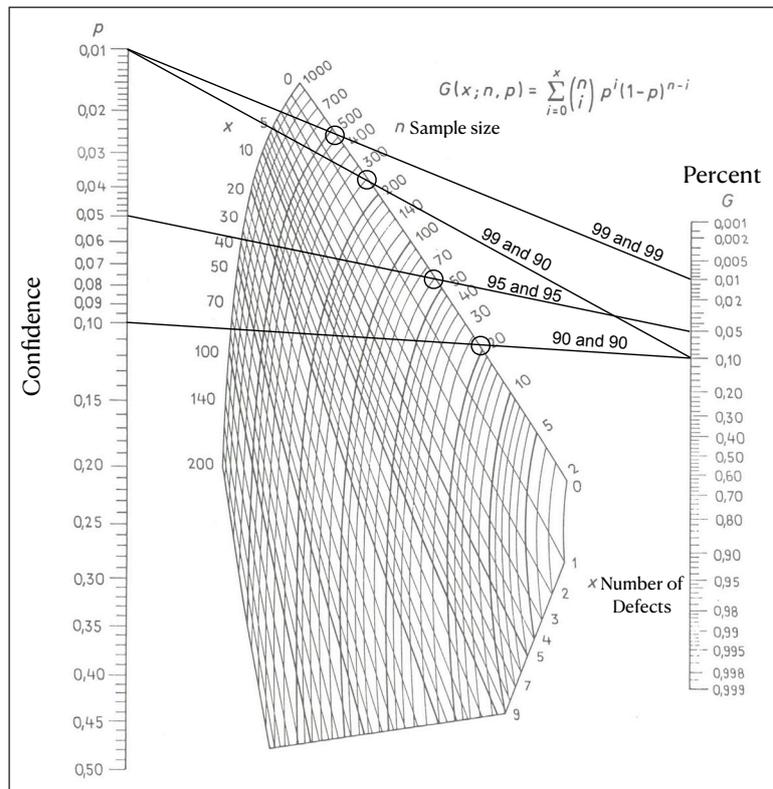
Figure 5. The Larson nomogram. Four circles indicate the required number of samples, found where lines connecting the desired "Confidence" with the desired "Percent" intersect the edge labelled "*n* Sample size". Also note bottom part where this edge is labelled "*x* Number of Defects" (see text). Wikimedia Commons.

number of samples to inspect. With this methodology, an exact determination is impossible, but readings from the nomogram are consistent with calculated values.

Larson developed this nomogram for lot acceptance sampling. Lot acceptance sampling is where and entire lot of individual DUs is accepted or rejected, depending on the acceptable failure rate of individual DUs within the lot. This is very common in statistical quality control. In traditional acceptance sampling any failure rate can be established.

In the scenario presented in this paper, the desired failure rate is *zero*, but that cannot be achieved without 100 % inspection. Therefore, there needs to be balance between the economics of 100 % inspection and the possibility that (a) drum(s) may be mischaracterised.

The Larson nomogram also provides values allowing for *some* defects—notice that many more samples are required in that case. While it is statistically equivalent, this approach (allowing a few defects) is not applicable for the scenario used in this paper since we here show the case in which we are not willing to knowingly allow *any* failing DUs. But this possibility offers an interesting view into even more broad applications, see, for example, References 3, 5, 14–17.

Acknowledgements

SAMPLING COLUMN

References

1. K.H. Esbensen, *Introduction to the Theory and Practice of Sampling*. IM Publications Open (2020). https://doi.org/10.1255/978-1-906715-29-8

2. K.H. Esbensen, "Materials properties: heterogeneity and appropriate sampling modes", *J. AOAC Int.* **98**, 269–274 (2015). https://doi.org/10.5740/jaoacint.14-234

3. C.A. Ramsey, "Considerations for inference to decision units", *J. AOAC Int.* **98(2)**, 288–294 (2015). https://doi.org/10.5740/jaoacint.14-292

4. R. Tuerlinckx and K.H. Esbensen, "Radiological characterisation of nuclear waste—the role of representative sampling", *Spectrosc. Europe* **33(8)**, 33–38 (2022). https://doi.org/10.1255/sew.2021.a56

5. R.E. Walpole, R.H. Myers, S.L. Myers and K. Ye, *Probability and Statistics for Scientists and Engineers*, 9th Edn. Prentice Hall (2011).

6. G.J. Hahn and W.K. Meeker, *Statistical Intervals*. John Wiley & Sons (1991). https://doi.org/10.1002/9780470316771

7. D.R. Helsel, *Nondetects and Data Analysis, Statistics for Censored Environmental Data*. John Wiley & Sons (2005).

8. C. Ramsey, "The effect of sampling error on acceptance sampling for food safety", *Proceedings of the 9th World Conference on Sampling and Blending*, Beijing (2019).

9. K.H. Esbensen and B. Swarbrick, *Multivariate Data Analysis: An Introduction to Multivariate Analysis, Process Analytical Technology and Quality by Design*, 6th Edn. CAMO Publishing (2018). ISBN 978-82-691104-0-1

10. J. Young (with James R. Hansen), *Forever Young: A Life in Adventure in Air and Space*. University Press of Florida (2012). ISBN 978-0-8130-4933-5

11. K.H. Esbensen, C. Paoletti and N. Theix, (Eds), "Special Guest Editor Section (SGE): sampling for food and feed materials", *J. AOAC Int.* **98(2)**, 249–320 (2015).

12. S.C. Dominy, S. Purevgerel and K.H. Esbensen, "Quality and sampling error quantification for gold mineral resource estimation", *Spectrosc. Europe* **32(6)**, 21–27 (2020). https://doi.org/10.1255/sew.2020.a2

13. S.C. Dominy, H.J. Glass, L. O'Connor, C.K. Lam, S. Purevgerel and R.C.A. Minnitt, "Integrating the Theory of Sampling into underground mine grade control strategies", *Minerals* **8(6)**, 232 (2018). https://doi.org/10.3390/min8060232

14. D. Wait, C. Ramsey and J. Maney, "The measurement process", in *Introduction to Environmental Forensics*, 3rd Edn. Academic Press, pp. 65–97 (2015). https://doi.org/10.1016/B978-0-12-404696-2.00004-7

15. C.A. Ramsey and C. Wagner, "Sample quality criteria", *J. AOAC Int.* **98(2)**, 265–268 (2015). https://doi.org/10.5740/jaoacint.14-247

16. C.A. Ramsey and A.D. Hewitt, "A methodology for assessing sample representativeness", *Environ. Forensics* **6(1)**, 71–75 (2005). https://doi.org/10.1080/15275920590913877

17. C.A. Ramsey, "Considerations for sampling contaminants in agricultural soils", *J. AOAC Int.* **98(2)**, 309–315 (2015). https://doi.org/10.5740/jaoacint.14-268

SAMPLING COLUMN
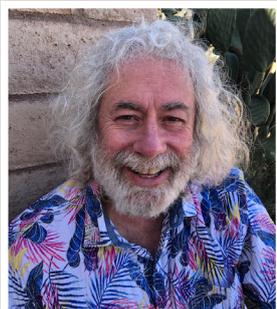
Chuck Ramsey's experience includes seven years with the National Enforcement Investigations Center (NEIC) of USEPA. While with the EPA, Mr Ramsey provided sampling and statistical expertise on all major regulations including Department of Justice, FBI, State Attorney Generals, regional EPA offices, state environmental departments and to industry through professional organisations. Mr Ramsey is involved with the development and review of regulations and guidance documents for sampling and statistics. He is a recognised expert in the areas of statistics and sampling and has served as an expert witness in several enforcement cases. He has given numerous presentations and courses on sampling, statistics and related topics at conferences and workshops. Mr Ramsey has conducted numerous consulting projects in the nuclear energy sector and for the US military, most of which are governed by non-disclosure agreements. Mr Ramsey is currently involved as a consultant in project BESTE (BELGOPROCESS).
chuck@envirostat.org

Kim H. Esbensen is an international expert and consultant in sampling (Theory of Sampling, TOS), chemometrics and PAT (Process Analytical Technology). Through a 35-year academic career involving three professorships, he has conducted R&D across a wide range of application fields, primarily in process industries (mining, minerals extraction and processing, bio-fuels, recycling, environmental monitoring, nuclear waste) in environmental science a.o. In 2015 he established an international consultancy (KHE Consulting). Esbensen has been responsible for a university educational programme straddling 30+ years in chemometrics, PAT, TOS, instrumental analysis, Multivariate Image Analysis (MIA), process technology and Philosophy of Science, currently in the form of a continuing education curriculum offered via KHE Consulting. His CV lists ~300 publications and ~400 lectures/presentations. He is a recipient of the Pierre Gy Sampling Gold Medal (2013), and the Russian Chemometrics Society Gold Medal (2012). In 2003 he inaugurated the biannual series of World Conferences on Sampling and Blending (WCSB), now in its 10th edition—https://wcsb10.com. Esbensen is editor of the scientific magazine *TOS Forum* and of the Sampling Column in *Spectroscopy Europe/World*. Esbensen's credentials are documented in full at KHEC's website: https://kheconsult.com. Mr Esbensen is currently involved as a consultant in projects BESTE and NOIR (BELGOPROCESS).
 https://orcid.org/0000-0001-6622-5024
khe.consult@gmail.com

QUALITY MATTERS

Four Generations of Quality: software and data integrity—an essential partnership?

John P. Hammond
Technical Manager, Starna Scientific Limited, 52–54 Fowler Road, Hainault, Essex IG6 3UT, UK

Introduction

As stated in the last article, we will now consider the essential component that controls our modern instrument systems and the associated concept of data integrity that is fundamental to the quality of the data being generated.

Researching this topic, as an article within this Four Generations series, confirmed my statement in the introductory article:

"*As someone who has been involved with the science of analytical measurement and/or spectroscopy for the majority of my adult life, this period of reflection centred not only on the last 12 months, but importantly on the changes since I started in a QA laboratory many years ago.*"

If I related this time frame specifically to the development and evolution of UV/visible instrumentation, once again the chronology of the software and data integrity can be effectively mapped to the timelines, and as in many technical areas impacting on our modern lives, there is the interesting conversion of analogue to digital electronics.

For a more detailed insight into this electronic transition of our scientific instrumentation, no pun intended, see the detailed discussion below.

For both the personal and additional insight into this evolution, I am grateful to, and wish to thank, my colleague at Pye Unicam, Doug Irish, whose History of UV-Vis document[1] provided essential chronology of what had happened before I joined the Unicam organisation in 1988 as a UV Application Specialist. However, whilst the evolution of the Unicam UV/visible instruments over the four generations are used as an example, the change in fundamental electronic hardware (with perhaps one or two exceptions) could be applied to most analytical systems from major vendors found in the laboratory of the day.

This article, therefore, discusses the Four Generations in the previously described time periods and uncovers some of these unique points for discussion.

1st Generation: the years between 1940 and 1975

The Beckman DU spectrophotometer had been developed in 1941 by Arnold Beckman, which introduced an instrumental measurement process capability to the comparison and use of visual colour science, and effectively enabled the quantitative measurement of a chemical species, by use of an associated method calibration process. Approximately 30,000 DU spectrophotometers were manufactured and sold between 1941 and 1976, and, therefore, this, and other key events, provides a convenient break in the chronologic timeline.

From a UK perspective, in the late 1940s the country was

Figure 1. The Beckman DU spectrophotometer. Photo courtesy of the Beckman Institute for Advanced Science and Technology at the University of Illinois Urbana-Champaign

basically bankrupt, with no cash resource to buy American-made instruments. The "Urban Myth" is that the UK government loaned Unicam a Beckman DU instrument for a weekend and in essence asked them to reverse engineer it, essentially copy it; and the Unicam SP 500 was born. The government also loaned an instrument to Hilger Ltd who produced a similar model—the Uvispec.

As previously stated,[2] from a personal perspective, my journey on the Quality path, began in 1975 in a Quality Assurance (QA) laboratory of a fine chemical supplier, which also had a DU spectrophotometer in the laboratory in which I was employed, but more importantly to the discussion of this article, a "modern" UV from one of those other major vendors with the added capability of scanning a wavelength range on the instrument. How this was achieved could now be described as somewhat quaint, in the fact that the wavelength was selected by rotating a thumbwheel which

changed a revolving set of three numbered wheels showing the wavelength in nm, and scanning was produced by engaging a clutch and motor, and watching the wavelength numbers rotate and drive down. As an optional output, this instrument also had the capability to connect a chart recorder for a visual recording of the spectrum. Little did I appreciate at this time that, even in this analogue configuration, the concept of data integrity still existed. Selection of a chart recorder speed that was too fast for the output of the instrument would cause a distortion, i.e. skewing of the peak shape. It wasn't until the microprocessor controlled analogue systems described below arrived that unacceptable scan and/or chart recorder speed combinations were locked out, thereby improving the integrity of the data.

The success of the SP 500 was followed in 1952 by the SP 600, and the SP 700 in 1958. The SP 700 was very much a copy of the Cary 14—then regarded as the "Rolls Royce" of spectro(photo)

metry. Howard Cary was the designer behind the Beckman DU, but left Beckman to set up his own company following a dispute with Beckman over the merits of single- vs double-beam spectro(photo) meters; a debate which subsequently was to be replayed during the development at Unicam of the PU 8700 in the 1980s, but more of this revolutionary instrument later.

Software
So, unsurprisingly in this 1st generation, there is no input into this arena, as all control is truly electronic and analogue.

Data integrity
In selection of incorrect chart speed, we see a fundamental premise of Data Integrity is already in play by posing the question, "… is what is being reported the 'true value'?".

2nd Generation: the years 1975 to 2000
In Pye Unicam's chronology, the SP 1800 and SP 1700 marked the start of using diffraction gratings rather than prisms as the dispersing element, and they were double-beam instruments. The SP 1800 had an analogue readout, and the SP 1700 incorporated a digital display for the first time and could be connected to an external chart recorder.

1976 saw the introduction of the SP 8100, SP 8200 and SP 8250. The mechanics and optics of this family of double-beam scanning instruments were to form the backbone of the main Unicam UV/visible instrument family for many years as they migrated into the PU 8300, 400, 500 and 8800 series. The design was based around an Ebert monochromator and used a high sensitivity end window photomultiplier.

The SP 8200 broke new ground in various ways. It was a microprocessor-controlled instrument, incorporating an Intel 4004 chip, the first

Figure 2. Pye Unicam SP500 UV/visible spectrophotometer. Photo © Ian Michael 2019, reproduced with kind permission of the Pye History Trust, Cambridge, UK.

QUALITY MATTERS

commercially available microprocessor, and very crude by today's standards; but with hindsight the same could be said for the same computer systems that landed the USA Apollo lander on the Moon! The main control panel of the SP 8100—mostly rotary knobs and pushbuttons—was replaced by an array of LEDs and buttons. At the time, there was much debate within Unicam as to who would want to buy one of these new-fangled devices and what benefit did the microprocessor confer? For these reasons, the instrument was made in small quantities by a section of Unicam that specialised in making "one-offs", with a dedicated single software engineer, c.f. the complete reversal of this perception into the modern systems of today. The product became the world's first microprocessor-controlled UV/visible instrument, beating arch-rivals Perkin-Elmer by a couple of weeks in 1978.

The PU 8800 was launched in 1982 and was based on the optics of the SP 8100 series, but with new electronics and a VDU to display results. A Commodore PET computer was purchased in the USA (circa 1979), long before they were available in the UK as Unicam in the UK had access to 110 V and 60 Hz electrical supply. This was used to design the screen displays on the PU 8800 and the similarities in the chunky letters and numbers between the Commodore and the PU 8800 were very evident.

From a personal perspective, the PU 8800 was my "Rolls Royce" UV/visible, and with its superb optical performance, it truly was a system cable of being used as a reference measurement instrument. This was how I was introduced to this concept of certification measurement/value assignment in a Calibration Laboratory; a protocol actively in use and expanded in the Starna CRM laboratory environment of today, albeit that our reference systems, whilst of a

similar optical performance to the PU 8800 are (by necessity) from other leading instrument vendors.

By the early 1980s the basic scanning chassis of the PU 8800 was showing its age and Unicam scanning instruments were not competitive on price in the marketplace. Lessons had been learnt from the PU 8800 with its built in VDU in that the VDU market was fast changing so it was quickly appreciated that any screen had to be an external one.

Major debates were held over the style of user interface and I remember that this was before the appearance of the ubiquitous IBM PC in 1981, which didn't have a PS/2 mouse until 1986. However, even in 1983, Apple was building a reputation for somewhat unique products, and alongside its Apple IIe computer, it released its Lisa business system, where the user interface was a mouse-driven system. This unique and new rodent-based solution resolved to settle

Figure 3. Advertisement for the PU 8700 from *ESN—European Spectroscopy News* 70 (1990).

QUALITY MATTERS

this debate, and the mouse-driven PU 8700 was born, and launched in 1986. Towards the end of its life in the later years of the 1990s, the requirement to also provide PC-based software, using its own mouse control, provided the obvious, but not easily solved duplicity of process, i.e. a system requiring two mice! However, this requirement for both a "local control" and PC-based interface was to prove both fundamentally attractive, and extremely useful in the next and future generation of instruments.

The PU 8700 was to be a pseudo double-beam instrument (only one beam was accessible in the sample compartment, but to help improve drift figures, a silica plate in the beam reflected 4 % or so of the light onto a photodiode so that in effect a double-beam system was created). Two microprocessors were used—a Z80 to cope with all the low-level instrument control logic, driving stepper motors etc. and a Motorola 68008 to do all the number crunching and graphics display. To get the colours right on the display, advice was sought from the BBC team that developed Teletext and Ceefax. However, the development of the software proved to be Herculean task—experts from Logica were brought in and warned that Unicam had embarked on too big a task as a unique operating system needed to be developed. Work progressed with an army of software engineers (we were constantly reminded of Brookes' *The Mythical Man-Month*,

> Brooks' law is an observation about software project management according to which "adding manpower to a late software project makes it later". It was coined by Fred Brooks in his 1975 book *The Mythical Man-Month*. According to Brooks, under certain conditions, an incremental person when added to a project makes it take more, not less time.

as more and more software engineers and contractors were piled into the project), but eventually the PU 8700 was launched.

Although the performance of the PU 8700 equalled that of double-beam instruments from competitors, its pseudo double-beam design was inevitably a perceived weakness in the marketplace at the time. However, being microprocessor controlled did allow the PU 8700 to use a stepping motor on its monochromator drive, which effectively allowed Stepped Scanning, i.e. stopping the monochromator at each discrete measurement wavelength, thereby eliminating spectral distortion due to the incorrect selection of too fast a scan speed; a design now found in many modern systems and another plus for Data Integrity.

In the late 1990s, the next family of instruments to be developed was the UV Series which reverted to a traditional double-beam design and was based on a stable optical cast base plate. It was available in either a Local Control version, or as a "blind bench" controlled by a PC and Vision software. The quality in the design of these system, like most Unicam products, is seen in the fact that these systems are still in use in many laboratory environments, including at Starna.

As reported in a previous article in this series, the pharmaceutical industry were demanding features to prove the instrument was working correctly when an analysis was carried out and so a major sales thrust of the product was around the sophisticated performance verification facilities built into the hardware and the corresponding software facilities in the Vision control software. In addition, the concept of providing cross-validation of value assignment/measurement by two independent pathways, i.e. dedicated instrument control and PC; both of which had been rigorously validated was invaluable in meeting the above-stated regulatory requirements, and again in many cases is now the *de facto* standard design for modern instrument system. Why this is the case is discussed below.

Software

As with so many of the standards and concepts already discussed in this series of articles, the most dramatic and wide-ranging changes occurred over this last quarter of the twentieth century. We literally went from pure analogue

Figure 4. The UV Series team. Photo courtesy of the Pye History Trust.

electronics, with meter displays and chart recorders, and no software (and/or the associated personnel), to PC and dedicated "local control" systems, where the software required to control these systems was highly developed by a team of skilled engineers, proven to work and more importantly could be shown to have fully tested and compliant with the new and evolving regulations. Sometimes this transition is unkindly referred to as:

"*...string and slide wire to full computer control.***"**

From a UV Series perspective, in parallel with the main instrument development, a significant team continued to refine the Vision PC-based software. Much emphasis was placed on all the aspects of traceability and security required by the pharmaceutical industry as defined in CFR21 - Pt11 by the FDA in America.

Data integrity

Once again, a design consideration of an analogue system relating to the accurate interpretation of the data, thereby ensuring its integrity, is the use of a mirrored scale on a meter display. By use of this simple optical enhancement, the possibility of parallax error caused by viewing a meter display from a non-perpendicular angle is eliminated by ensuring only one needle image is visible when the scale is read. Once the moving meter was replaced by a digital numeric display, it might be perceived that (even using a mirrored scale) a simple number digital number is more accurate than a meter reading? The debate relating to the discussion to this "black box" syndrome started at this point, and continues even more vehemently to this day, as clearly even though digital in presentation, it is just a number, right or wrong?

In the UV Series, having the ability to measure the same reference material within both a Local Control and PC environment, and thereby

cross-validate the data, and ensure its integrity provided invaluable in proving the acceptance of this approach in a regulated environment.

Finally, at the end of the Millennium, and now fading into the mists of time, who can remember the fear that was circulated in the last months by the impending doom of the "Millennium Bug"? Where, because software had only be coded to recognise two digit dates, as the clock struck one second after midnight on 31 December 1999, all internal software clocks would revert to 1 January 1900, with the expected consequences!

Thankfully, the predicted catastrophe didn't materialise, but surely this was a salutary lesson as to how easy the integrity of the data can be compromised.

3rd Generation: the years 2000 to 2020

The Evolution series of instruments was to be the last family of Unicam UV/visible instruments to be developed in Cambridge (around 2002). Certain components of the UV Series were becoming obsolete, and the Evolution was effectively its replacement. Much discussion took place as to what was the primary target market, and it was agreed this should be Life Sciences. The implication of this was for a small beam of light in the sample compartment (to pass through small cells) and a double-beam instrument with a wide beam separation (to allow cell changers to operate). A major innovation was to incorporate a Xenon flash lamp as the light source, so eliminating the need for the traditional Deuterium and Tungsten lamps.

Software

During this period in the consumer marketplace, we see the increasing replacement of desktop PCs

by laptops, and latterly tablets and mobile phones, so we are now all familiar with the user interfaces available on these devices in the form of Apps etc., and we see systems appearing on the marketplace where (in particular) the availability of screens used for tablets etc. are used for this purpose. Also, invariably in a modern laboratory these system(s) are linked together to a central core, via a LIMS system, database etc.

Data integrity

As we have seen in the evolutionary process of the dedicated software systems, on whichever platform for which they are developed, the requirement to ensure the validity of the data, and preserve its integrity has increased almost exponentially. For that reason, given the availability of other commercially based tools, e.g. Excel, this period did see an expansion in the use of these calculation-based tools to provide additional functionality to a system. However, in recent times, a similar discussion/debate revolves around a number producing worksheet, i.e. is it providing the correct answer—"sound familiar", c.f. digital display discussion?

As stated above, linking systems together brings its own headaches with respect to the protection and preservation of the data integrity.

4th Generation: from 2021 forward

So now we have a modern laboratory, with a fully integrated, fully validated LIMS system—what next? As we cannot see into the future, we can only discuss some key concepts currently being considered, and these are listed below as discussion points.

Software

Given the progression and use of software systems into the "Cloud" in many commercial arenas, will this continue for the laboratory of the future?

Data integrity

How to preserve the integrity of the data in these new environments; is Block Chaining a solution to the problem, or (as recently described to me) use of voice-recognition software, to ensure authenticity of the process?

Given that we now have all the components in place to measure, manipulate and produce the quality data required from a system, and perhaps more importantly, prove it, the next article in the series will look at some of the recent uses and applications of these fundamental spectroscopic techniques.

References

1. D. Irish, *UltraViolet and Visible Spectrometry (UV/Vis)*. Pye History Trust. bit.ly/PyeTrust
2. J.P. Hammond, "Four generations of Quality: into the future", *Spectrosc. Europe* **33(2),** 32–35 (2021). https://doi.org/10.1255/sew.2021.a10

John Hammond is an experienced analytical scientist, spectroscopist and technical marketing professional, skilled in the development, production and marketing of analytical systems into highly regulated and controlled industries. A Fellow of the Royal Society of Chemistry (FRSC), executive member of ISO/TC334 and an Expert Advisor to the United States Pharmacopeia, General Chapters, Chemical Analysis committee.
j.p.hammond@starna.com

APPLICATIONS

Separation of butter into phases with the Quest™ heated puck

The Quest ATR with heated puck provides an excellent solution for the analysis of butter and its transition from solid to liquid phase. The use of ATR enables fast and simple analysis of the sample without the need for any preparation, and following analysis it is simple to wipe clean. The software is simple to program and monitor temperature steps. The experimental method outlined here is simple to perform and can be easily reproduced. *Specac*

▶ Download Application Note

Study of polymerisation kinetics of dental materials

The ATR-FTIR method is very useful to characterise the chemistry of dental bonding systems, as a monomeric liquid mixture but also of the separated solids, in this case, inorganic glass fillers. Continuous spectral acquisition during photopolymerisation, without any disconnect from the ATR, allows monitoring of the polymerisation reaction and assessment of the degree of conversion DC (%), with high reproducibility and without the need for normalisation. *Specac*

▶ Download Application Note
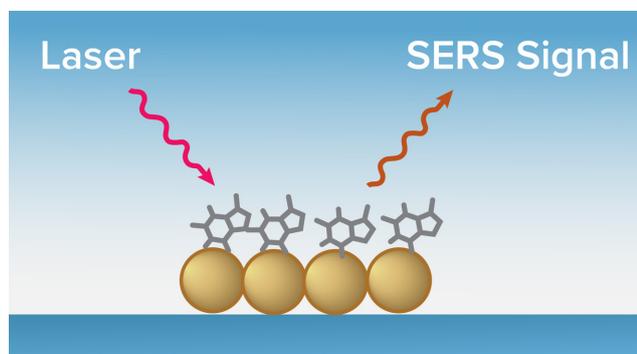
Evaluating a novel approach to SERS

A new generation of SERS substrates shows promise to combine the convenience of SERS substrates with the reproducibility of SERS performed in solution with a hybrid approach. This note describes the process of using Raman spectroscopy and SERS to detect analytes with concentrations as low as 1 ppm. *Wasatch Photonics*

▶ Download Application Note

Phase and frequency locking of diode lasers

This application note provides an introduction to the principles of laser locking in general and to the more practical aspects of phase and frequency locking of diode lasers. The goal of these application notes is to provide the reader with a conceptual understanding of laser locking but also to help them choose the ideal locking solution for their application. *TOPTICA Photonics AG*

▶ Download Application Note

APPLICATIONS
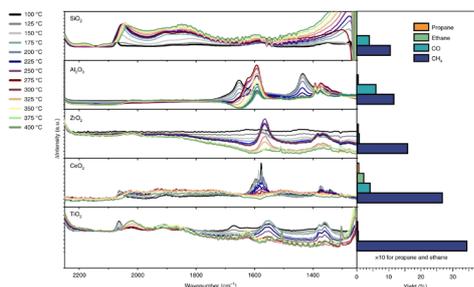
Supported Ni catalysts in action: *operando* infrared spectroscopy

The HTHP cell was used to collect FT-IR spectra of supported Ni catalysts under CO_2 hydrogenation reaction conditions. Differences in spectral features are highlighted for different catalyst and correlated to catalytic performance. The use of *operando* spectroscopy has shown to be a powerful tool to investigate industrially relevant catalysts at work and to find vibrational activity descriptors. The knowledge gained can be used to further guide rational catalysts design, in this case looking for catalysts formulations which favour hydrogen transfer between the active phase and the support. The HTHP cell offers a facile way to study a wide variety of catalysts under different reaction conditions, gas compositions, temperatures and pressures.

Specac

▶ Download Application Note

Watching paint dry, ultra-long duration experiments using the Arrow consumable ATR

This note demonstrates the use of the Arrow silicon ATR system for batch, long-duration experiments on paint samples following the principles of ASTM STP1119, a commonly used transmission method. Arrow makes preparing sample batches for ATR measurement feasible for the first time and is a simple and cost-effective alternative to using multiple KBr windows for this task. We have also shown that spectra recorded on Arrow are amenable to spectral processing using chemometric tools such as PCA.

Specac

▶ Download Application Note
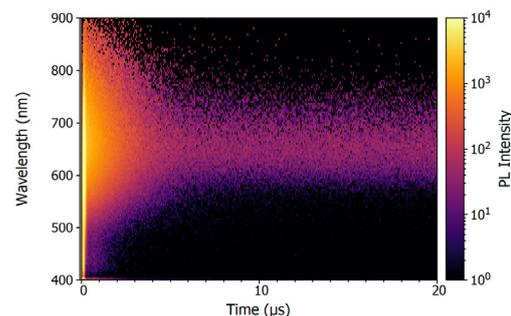
Sb to Mn energy transfer revealed using time-resolved emission spectroscopy

Zero-dimensional (0D) metal halide hybrids are an emerging class of semiconducting materials for optoelectronic applications including light-emitting diodes, lasers and photovoltaics. Heterometallic (comprising more than one type of metal centre) metal halide hybrids, in particular, hold great promise due to the potential for synergistic photo-physical properties depending on the choice of the constituent metal centres. In this application note, time-resolved emission spectroscopy is used to identify the emission pathways in the 0D metal halide hybrid, Tris SbMnCl.

Edinburgh Instruments

▶ Download Application Note
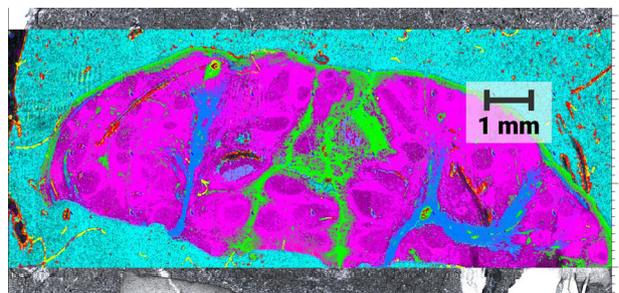
Biological tissue analysis by infrared laser imaging (QCL)

This application note demonstrates the use of IR laser imaging for tissue analysis and the tremendous speed advantages associated with it. FT-IR and IR laser imaging are directly compared and the results presented. The technological innovation that has made this major leap in tissue imaging possible—Bruker's patented spatial coherence reduction technology—is also discussed.

Bruker Optics

▶ Download Application Note

Product Focus on Imaging Spectroscopy

BaySpec
Tel: 1-408-512-5928
Sales@BaySpec.com
www.bayspec.com

OCI™—An Innovative Class of Hyperspectral Imagers

BaySpec's OCI™ hyperspectral imagers address image quality and ease-of-use issues found in legacy imagers with outdated geo-correction or ortho-rectification methods. BaySpec's push-broom imaging can scan at random speeds, fundamentally eliminating artifacts caused by pitch, roll and vibrations.

MORE INFORMATION »

GoldenEye—The Ultimate Snapshot Imager

BaySpec's GoldenEye™ is the only Snapshot hyperspectral imager covering from 400 nm to 1100 nm. Using BaySpec's FT-PI proprietary technology, this novel imager features high sensitivity and is most suitable for low light level applications, such as fluorescence imaging.

MORE INFORMATION »

Bruker Optics GmbH & Co. KG
Tel: +49 (0)7243-504 2000
info.bopt.de@bruker.com
www.bruker.com/optics

FT-IR Microscope LUMOS II

Applications:
- QA/QC
- Microspectroscopic failure analysis
- Microplastic analysis
- Plastic and polymer
- Particle & surface analysis
- Pharmaceuticals

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

MORE INFORMATION »

FT-IR and Laser Imaging Microscope HYPERION II

Applications:
- Materials research
- Tissue Imaging

- Forensics
- Chemicals
- Polymers
- Art & conservation
- Life science

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

MORE INFORMATION »

ClydeHSI
Tel: +44-141-952-9475
info@clydehsi.co.uk
https://www.clydehsi.com

ClydeHSI Hyperspectral Cameras from UV to SWIR (300–2500 nm)

High spectral and spatial resolution, high frame rate push-broom hyperspectral cameras covering the UV-SWIR (300–2500 nm) spectral range, supported by leading data acquisition, visualisation and analysis software. Suitable for a wide range of academic and commercial applications.

MORE INFORMATION »

Gigahertz Optik
Tel: +49 8193 93700 0
info@gigahertz-optik.de
www.gigahertz-optik.de

ISS-15-RGBW

Uniform Light Source in Accordance with EMVA 1288
- Homogeneous light field for applications of camera calibration based on RGBW LEDs
- Precision LED power supply with large dynamic range

- Monitor detector for intensity adjustment
- Software development kit for system integration
- Traceable calibration
  MORE INFORMATION »

ISS-100-LT
Measurement System for the Determination of Veiling Glare

- Interchangeable diameter of baffles for investigation of different FOV in terms of Veiling Glare
- Integrating sphere configured as diffuse illumination source with reference detector
- Additional integrating sphere with black coating for use as a light trap
- Traceable calibration
  MORE INFORMATION »

ISS-50-LU-FE

- Calibration of Fisheye and super-wide angle lenses/cameras
- Three sources with a 3D baffle sub-assembly for the best possible hemispherical light field uniformity
- Filter wheel with correction filters for sample illumination with standard illuminant types A, D50 and D65
- Specimen holder in sphere center with manipulator for precise positioning and contacting of the samples
- Traceable calibration
  MORE INFORMATION »

HORIBA

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

FLIMera—A New Concept in FLIM Imaging

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

Quantum Design UK and Ireland Ltd
Tel: 01372 378822
info@qd-uki.co.uk
www.qd-uki.co.uk

Specim FX10 hyperspectral imaging camera
Specim FX10 camera series is designed for industrial and laboratory use. Specim FX10 cameras work in a line-scan mode in the visible and near-infrared (VNIR) area; Specim FX10 in the 400–1000 nm region, and the colour optimised Specim FX10c camera in the 400–780 nm region.
Specim FX10 cameras are best suited for:

- Vegetation & agriculture
- Phenotyping
- Colour & density in printing
- Display & light source inspection
- Food quality
  MORE INFORMATION »

Specim FX17 hyperspectral imaging camera
Specim FX17 camera is designed for industrial/laboratory use. It works in a line-scan mode, and collects hyperspectral data in the NIR region—900 to 1700 nm.
Applications include:

- Food & feed quality
- Waste sorting
- Recycling
- Moisture measurement
- Threat detection, Security
  MORE INFORMATION »

Specim FX50 hyperspectral imaging camera
Specim FX50 is a high-speed, accurate and efficient camera specifically designed for industrial environments. It works in a line-scan mode and collects hyperspectral data in the MWIR region (2.7–5.3 μm). Applications include:

- Black plastic sorting
- Geology & mining
- Metal industry
  MORE INFORMATION »

Wasatch Photonics

Wasatch Photonics
Tel: +1 919-544-7785
info@wasatchphotonics.com
https://wasatchphotonics.com
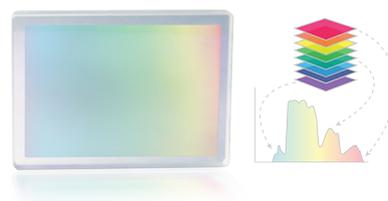
Gratings for Hyperspectral Imaging

- Patented broad bandwidth designs
- Exceptional efficiency for greater sensitivity and faster imaging rates
- Low polarisation sensitivity, uniform efficiency
- Near-zero ghosting & scatter—less stray light
- Low wavefront error for clearer images
- Easy cleaning & handling
- Ideal for NIR imaging to 2500 nm
  MORE INFORMATION »

PRODUCT FOCUS

WITec
focus innovations

WITec GmbH
Tel: +49 (0) 731 140 700
info@WITec.de
www.witec.de

alpha300 R – Confocal Raman Imaging Microscope

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

alpha300 apyron – Fully Automated Raman Imaging Microscope

- Materials research
- Pharmaceutics
- Forensics
- Life science
- Geoscience

- Unprecedented accessibility
- Easily configurable experimental workflow
- Polarisation rotation in excitation and detection available
- Capable of remote operation
  MORE INFORMATION »

alpha300 Ri – Inverted Raman Imaging Microscope

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

RISE Microscopy – Correlative Raman and SEM System

- Materials research
- Pharmaceutics
- Nanotechnology
- Life science
- Geoscience
- Correlative Raman-SEM imaging within a common vacuum chamber
- Automated switching between

Raman and SEM measurements
- Quick correlation of results and image overlay
  MORE INFORMATION »

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 »

Spinsolve Multi X benchtop NMR spectrometer

Magritek's new Spinsolve Multi X benchtop NMR spectrometer can access multiple nuclei in a fully automatic way. All models measure ^1H and ^{19}F, with other X nuclei optionally available: ^7Li, ^{11}B, ^{12}C, ^{15}N, ^{29}Si and ^{31}P (others may be available on request). The spectrometer provides instant switching between nuclei without any loss of sensitivity, and no manual intervention is needed to switch. Both a powerful multi-line solvent suppression method and X-decoupled proton acquisition for all available X nuclei are included. 1D and 2D experiments are calibrated at the factory, so it is possible to switch back and forth without recalibration. The ability to interleave multi-nuclear experiments enables online reaction monitoring. An extensive software library of pre-calibrated protocols is provided for all available nuclei.

   Pulsed field gradient (PFG) experiments are useful to assess the molecular mobility of different molecules dissolved in a mixture. By adding a gradient coil to the Spinsolve Multi X, it can measure the diffusion coefficient of molecules containing any of the nuclei available on the spectrometer.

Magritek
▸ https://link.spectroscopyeurope.com/680-P1-2022

NEW PRODUCTS

IMAGING

Humidity control for imaging

Linkam Scientific Instruments has launched the updated RHGen Relative Humidity (RH) Controller which offers humidity control between 3 % and 95 % RH, at temperatures from ambient to 85 °C, with an upgraded RH sensor and improved connectors, providing environmental control to a variety of Linkam temperature control stages and third-party chambers. The device can be used in conjunction with light microscopy, Raman, FT-IR and X-ray to provide further sample characterisation. The RHGen allows the user to precisely control the humidity around a sample, without the need for an external dry air supply. The device can also be combined with the Inert Gas Regulator, which acts as a regulated pressure interface between the RHGen and an external gas supply to allow inert gases into the chamber, to replicate unique environmental conditions.

Linkam Scientific Instruments

▸ https://link.spectroscopyeurope.com/6060-P1-2022

INFRARED

FT-IR microscope

Thermo Fisher Scientific has introduced the Thermo Scientific Nicolet RaptIR FTIR Microscope, designed to let researchers rapidly locate and identify trace materials, inclusions, impurities and microparticles along with the distribution of these materials within a sample. The microscope includes a large working area and heavy-duty stage, allowing investigation of a wide range of samples up to 4 cm thick and 5 kg in weight. The microscope has clear guidance throughout the entire analytical workflow, and a new wide-area view that enables users to quickly pinpoint areas of interest. Additionally, a diffraction-limited infrared objective lens produces ultra-sharp images.

Thermo Fisher Scientific

▸ https://link.spectroscopyeurope.com/106-P1-2022

FT-IR analysis systems for wine and milk

PerkinElmer has launched a new FT-IR liquid food testing platform including instruments, software and streamlined workflows. As part of the platform, the LQA300 system for wine identifies key quality markers—including alcohol, sugar, acidity, pH and density levels—during every part of the winemaking process, from harvest to bottling. Additional LQA300 system calibrations will be added for other liquid food sample types by the end of

NEW PRODUCTS

2022, including but not limited to beer, alcoholic spirits, edible oils and soft drinks.

The LactoScope 300 system, which expands PerkinElmer's FT-IR dairy portfolio, detects key markers such as fat, protein and lactose levels in milk, cream and whey. Adulterants including urea, ammonium sulfate, maltodextrine, sucrose and water can also be detected in raw and processed milk. Step-by-step pre-developed workflows and intuitive touch screen and software interfaces enable users to simply place liquid samples into the instruments, push a single button and receive results on a 12-inch touch screen in under 45 s, allowing 60 samples to be run each hour.

PerkinElmer

▸ https://link.spectroscopyeurope.com/2200-PF2-W-2022

LASER

Continuously tuneable laser

TOPTICA have introduced the CTL 900 continuously tuneable laser, which is tuneable between 880 nm and 950 nm. This wavelength range is especially useful for resonantly exciting quantum dots, for spectroscopy or addressing, e.g., rare earth ions or the Caesium D1 line. The most important property of this range of lasers is providing wide and continuous tuneability without any mode-hops. They have high power, a narrow linewidth and low drift. Scans can be performed with high resolution. Mode-hops are prevented by a patented opto-mechanical design 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 touchscreen and knobs as well as remotely via PC GUI and command language (Python SDK). A test system mode can characterise components or record spectra.

TOPTICA

▸ https://link.spectroscopyeurope.com/1858-P1-2022

MASS SPECTROMETRY

High-throughput screening mass spectrometry

Bruker has introduced the timsTOF MALDI PharmaPulse® (timsTOF MPP) system, a new high-end solution for unbiased, deep HTS and uHTS based on label-free mass spectrometry. The new timsTOF MPP is now the flagship of Bruker's MALDI PharmaPulse product family which started with the launch of the rapifleX MPP, a MALDI-TOF-based label-free uHTS solution, in 2017. The timsTOF MPP now uses Bruker's Trapped Ion

NEW PRODUCTS

Mobility Spectrometry (TIMS) technology. TIMS enables rapid gas-phase separation of isobars, and even isomers, by exploiting the molecular collisional cross-section. This, in combination with routine 50,000 mass resolution at full speed with QTOF-MS detection enables high levels of assay specificity at HTS speed.

The timsTOF MPP features a dual MALDI/ESI ion source with a 10 kHz smartbeam™ 3D laser to enable uHTS compatible speed and throughput, and is available with the MALDI-2 option for an expanded chemical space. As part of the timsTOF MPP solution, the new MALDI PharmaPulse® 2023 software supports a broad range of HTS applications for drug discovery. Its automation interface allows for timsTOF MPP integration in high throughput environments and works in concert with common scheduling software packages from various vendors. Furthermore, MPP 2023 features seamless transfer of data and results to downstream analysis software, e.g., to Genedata Screener®.

Bruker Daltonics

▶ https://link.spectroscopyeurope.com/2428-P1-2022
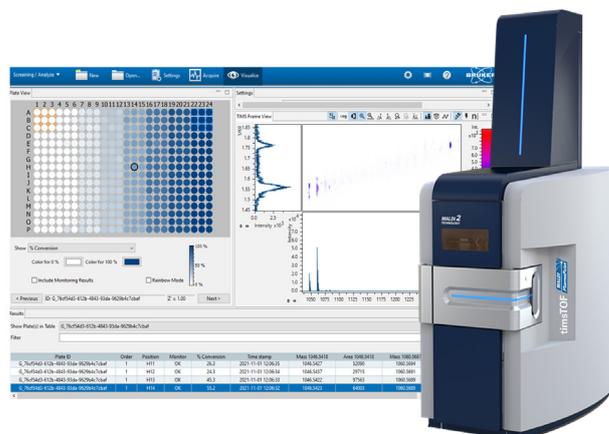
Parallel mass spectrometry

Trace Matters Scientific has introduced two new technologies, SUPER Mass Spec™ and SPion Link™. SUPER Mass Spec™ allows ions produced by a single ion source to be processed in parallel by a network of mass spectrometers. In a SUPER Mass Spec™, each cluster of mass spectrometers (a set of mass spectrometers with identical hardware that work together as a single system) operate in parallel, and therefore, sensitivity, scan speed and dynamic range of each cluster is independently scalable. In addition, a SUPER Mass Spec™ allows for simultaneous analysis of a single sample with different clusters of mass spectrometers, each cluster employing a different type of mass spectrometry technology, such as triple quadrupole, time-of-flight or trapping mass analysers. This provides a multidimensional view of highly complex samples for cross-examination and cross-verification of mass spectrometry data, and promotes deep proteome coverage and quantitative data completeness in bottom-up proteomics workflows.

The second technology, SPion Link™, is a flexible ion guide. Ion transfer is lossless in a wide range of *m/z*, there is no theoretical limit on how long SPion® can be and the ion transfer is extremely fast—close to the speed of sound. SPion Link™ enables fully-automated mass spectrometry workflows to be developed to analyse samples directly from microtiter plates, such as 96-well plates, via custom disposable pipette tips. This provides significant advantages, particularly for clinical applications, where the amount of available sample is typically insignificant. SPion Link™ also minimises reagent use and related costs, eliminates issues with cross-contamination and dead volumes, and allows for a high level

of automation in mass spectrometry workflows essential in reproducibility of mass spectrometry data. It also reduces cost of analysis and minimises exposure of lab personnel to biological samples that may be hazardous.
Trace Matters
▶ https://link.spectroscopyeurope.com/6765-P1-2022

RAMAN

New Raman spectrometer

SphereOptics have announced a new high-performance Raman spectrometer from Wasatch Photonics. The new Raman XL spectrometer series is compatible with ultra-cooled scientific cameras, allowing very long integration times to record even the weakest Raman signals. The systems are available for 532, 633, 785, 830 and 1064 nm excitation. There is a choice between two different numerical apertures: an aperture of f/1.5 maximises the instrument sensitivity. If resolution is more important for the application, an aperture of f/2 can be chosen. There is a further choice between an SMA connector for fibre-optic coupled Raman probes and a cage interface system for free beam coupling. An internal opto-mechanical shutter allows automated dark signal collection. In addition to the standard devices, special OEM versions for integration are available too.
SphereOptics GmbH
▶ https://link.spectroscopyeurope.com/1507-P1-2022

DIARY

Conferences

2022

8 April, London, UK. **Frank Pullen Symposium (FPS22).** https://www.bmss.org.uk/the-pullen-symposium/

11–13 April, Liverpool, UK. **SpringSciX 2022.** springscix@gmail.com, https://springscix.org/

20–22 April, London, UK. **Photoelectron Spectroscopy and the Future of Surface Analysis Faraday Discussion.** https://www.rsc.org/events/detail/45900/photoelectron-spectroscopy-and-the-future-of-surface-analysis-faraday-discussion

8–13 May, Honolulu, Hawaii, United States. **2022 Materials Research Society (MRS) Spring Meeting & Exhibit.** info@mrs.org, https://www.mrs.org/spring2022

10–12 May, Izola, Slovenia. **Sensorfint International Conference.** https://www.sensorfint.eu

10–13 May, Pau, France. **SPECTRATOM 2022.** contact@spectratom.fr, https://spectratom2022.sciencesconf.org

11 May, Sheffield, UK. 8th **BMSS Imaging and MALDI SIG Meeting.** jillian.newton@shu.ac.uk, https://www.eventbrite.com/e/bmss-sig-imaging-symposium-2022-tickets-252980039107

22–26 May, Chiba City, Japan. **Japan Geoscience Union Meeting 2022.** http://www.jpgu.org

30 May–3 June, Gijon, Spain. **Colloquium Spectroscopicum Internationale (CSI) XLII.** csi2021@csi2021spain.com, https://www.csi2021spain.com

31 May–2 June, Kristiansand, Norway. **10th World Conference on Sampling and Blending (WCSB10).** contact@wcsb10.com, https://wcsb10.com

1–4 June, Primošten, Croatia. **Magnetic Moments in Central Europe 2022 (MMCE 2022).** https://mmce2022.hkd.hr

5–9 June, Minneapolis, Minnesota, United States. **70th ASMS Conference.** https://www.asms.org/conferences/annual-conference/future-annual-conferences

12–15 June, Leon, Norway. **10th Nordic Conference on Plasma Spectrochemistry.** yngvar.thomassen@stami.no, http://nordicplasma.com

19–23 June, Dublin, Ireland. **12th International Conference on Clinical Spectroscopy.** http://spec2022.org

19–23 June, Valencia, Spain. **18th International Conference of the Metabolomics Society.** https://www.metabolomics2022.org

20–23 June, Prague, Czech Republic. **29th Symposium on Plasma Physics and Technology.** sppt2020@plasmaconference.cz, https://www.plasmaconference.cz

20–24 June, Champaign, IL, United States. **75th International Symposium on Molecular Spectroscopy.** https://isms.illinois.edu/

24–29 June, Memphis, United States. **31st International Conference on Ion Mobility Spectrometry (ISIMS 2022).** https://www.isims.info/conference-2022

27–29 June, Online, UK. **BNASS 2022.** https://www.rsc.org/events/detail/40623/bnass-2022-the-20th-biennial-national-atomic-spectroscopy-symposium

28 June–1 July, Paris, France. **inArt 2022: 5th International Conference on Innovation in Art Research and Technology.** inart2022@sciencesconf.org, https://inart2022.sciencesconf.org

3–6 July, Esbjerg, Denmark. **International Association of Spectral Imaging Conference (IASIM-2022).** https://2020.iasim.net

3–6 July, Oxford, UK. **British Society for Proteome Research Annual Scientific Meeting.** secretary@bspr.org, http://www.bspr.org

24–28 July, Chicago, United States. **2022 American Association for Clinical Chemistry (AACC) Annual Meeting.** https://www.aacc.org/meetings-and-events/annual-meeting-dates-and-locations

30 July–4 August, Chambersburg, United States. **2022 International Diffuse Reflectance Conference (IDRC).** idrc@cnirs.org, https://cnirs.org/content.aspx?page_id=22&club_id=409746&module_id=500874

8–10 August, Kingston, Canada. **64th ICASS Conference on Analytical Sciences and Spectroscopy.** diane.beauchemin@chem.queensu.ca, http://www.csass.org/ICASS.html

21–25 August, Chicago, United States. **American Chemical Society (ACS) National Fall 2022 Meeting.** natimtgs@asc.org, https://www.acs.org/content/acs/en/meetings/acs-meetings/about/future-meetings.html

26 August–1 September, Scottsdale, United States. **AOAC International Annual 2022 Meeting and Exposition.** meetings@aoac.org, https://www.aoac.org/events/2022-aoac-annual-meeting/

28–31 August, La Jolla, United States. **SMASH 2022—Small Molecule NMR Conference.** https://www.smashnmr.org/

28 August–1 September, Lisbon, Portugal. **8th EuChemS Chemistry Congress.** euchems2022@chemistry.pt, https://euchems2022.eu/

4–8 September, Singapore, Singapore. **SETAC 8th World Congress/12th SETAC Asia-Pacific Biennial Conference.** barbara.koelman@setac.org, https://singapore.setac.org

4–9 September, Brno, Czech Republic. **2022 European Symposium on Analytical Spectrometry (ESAS) & 17th Czech–Slovak Spectroscopic Conference (CSSC).** esas2022@spektroskopie.cz, http://esas-cssc2022.spektroskopie.cz/

13–15 September, Manchester, UK. **42nd BMSS Annual Meeting.** https://www.bmss.org.uk/media-centre/news/bmss42-first-announcement/

13–16 September, Rome, Italy. **12th Hyperspectral Workshop, WHISPERS.** info@ieee-whispers.com, https://www.ieee-whispers.com/

2–7 October, Cincinnati, United States. **Annual Conference of Federation of Analytical Chemistry and Spectroscopy Societies, SciX 2022.** facss@facss.org, http://www.scixconference.org

9–12 October, Denver, United States. **2022 Geological Society of America (GSA) Meeting.** meetings@geosociety.org, http://www.geosociety.org

16–19 October, San Diego, United States. **PANIC 2022.** https://panicnmr.com/conference-schedule-sandiego-2022/

12–16 December, Chicago. **2022 AGU—Advancing Earth and Space Science Fall Meeting.** meetinginfo@agu.org, https://www.agu.org/Events/Meetings/Fall-Meeting-2022

2023

29 January–3 February, Ljubljana, Slovenia. **2023 European Winter Conference on Plasma Spectrochemistry.** http://www.ewcps2021.ki.si

21–23 August, Innsbruck, Austria. **NIR-2023.**

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

Courses
2022

24 March, United States. **CasaXPS Software Training (hands-on)-Online.** j.grant@ieee.org, https://surfaceanalysis.org/Online_Short_Courses.html

2–27 May, Copenhagen, Denmark. **International School of Chemometrics (ISC 2022).** https://www.hypertools.org/isc

25–30 September, Erice, Italy. **International School on Mass Spectrometry (IntSMS).** http://www.spettrometriadimassa.it/intsms2022

15 October, Obergurgl, Austria. **Advanced Study Course on Optical Chemical Sensors (ASCOS).** Christian.W.Huck@uibk.ac.at, http://ascos.org/

Exhibitions
2022

27–28 April, Basel, Switzerland. **Lab Vision.** https://www.spectaris.de/analysen-bio-und-labortechnik/labvision/

21–24 June, Munich, Germany. **analytica 2022.** https://www.analytica.de

22–26 August, Frankfurt, Germany. **ACHEMA.** https://www.achema.de

24–26 November, Istanbul, Turkey. **Turkchem.** http://www.chemshoweurasia.com

DIRECTORY

ATOMIC

Coherent
petra.wallenta@coherent.com
www.coherent.com

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

PerkinElmer, Inc.
www.perkinelmer.com

Thermo Fisher Scientific
info.spectrometry@thermofisher.com
www.thermofisher.com/elemental

Atomic Absorption

PerkinElmer, Inc.
www.perkinelmer.com

Atomic Emission

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

PerkinElmer, Inc.
www.perkinelmer.com

Thermo Fisher Scientific
info.spectrometry@thermofisher.com
www.thermofisher.com/elemental

CHEMICALS AND RMS

Bureau of Analysed Samples Ltd
enquiries@basrid.co.uk
www.basrid.co.uk

Coherent
petra.wallenta@coherent.com
www.coherent.com

KPM Analytics
sales@kpmanalytics.com
www.kpmanalytics.com

Starna Scientific Limited
sales@starna.com
www.starna.com

Waters Corporation
materials@waters.com
waters.com

DATA HANDLING

ACD/Labs
info@acdlabs.com
www.acdlabs.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

PerkinElmer, Inc.
www.perkinelmer.com

Sepsolve Analytical Ltd
hello@sepsolve.com
www.sepsolve.com

S.T.Japan-Europe GmbH
contact@stjapan.de
www.stjapan.de

Waters Corporation
materials@waters.com
waters.com

GAMMA-RAY

Coherent
petra.wallenta@coherent.com
www.coherent.com

XIA LLC
sales@xia.com
www.xia.com

IMAGING

ABB Measurement & Analytics
ftir@ca.abb.com
abb.com/analytical

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

Coherent
petra.wallenta@coherent.com
www.coherent.com

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

IM Publications Open
info@impopen.com
www.impopen.com

Leonardo UK Ltd
infomarketing@leonardo.com
www.leonardo.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

Quantum Design UK and Ireland Ltd
info@qd-uki.co.uk
www.qd-uki.co.uk

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

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

Waters Corporation
materials@waters.com
waters.com

INFRARED

ABB Measurement & Analytics
ftir@ca.abb.com
abb.com/analytical

AP Technologies Ltd
info@aptechnologies.co.uk
www.aptechnologies.co.uk

BaySpec, Inc.
info@bayspec.com
www.bayspec.com

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

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

IM Publications Open
info@impopen.com
www.impopen.com

KPM Analytics
sales@kpmanalytics.com
www.kpmanalytics.com

Leonardo UK Ltd
infomarketing@leonardo.com
www.leonardo.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

MantiSpectra
info@mantispectra.com
www.mantispectra.com

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Ocean Insight
info@oceaninsight.com
oceaninsight.com

PerkinElmer, Inc.
www.perkinelmer.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

Specac Ltd
sales@specac.co.uk
www.specac.com

Starna Scientific Limited
sales@starna.com
www.starna.com

S.T.Japan-Europe GmbH
contact@stjapan.de
www.stjapan.de

Wasatch Photonics
info@wasatchphotonics.com
www.wasatchphotonics.com

ION MOBILITY

Waters Corporation
materials@waters.com
waters.com

DIRECTORY

LASER

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Ocean Insight
info@oceaninsight.com
oceaninsight.com

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

LUMINESCENCE

AP Technologies Ltd
info@aptechnologies.co.uk
www.aptechnologies.co.uk

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Ocean Insight
info@oceaninsight.com
oceaninsight.com

PerkinElmer, Inc.
www.perkinelmer.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

Quantum Design UK and Ireland Ltd
info@qd-uki.co.uk
www.qd-uki.co.uk

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

Wasatch Photonics
info@wasatchphotonics.com
www.wasatchphotonics.com

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

XIA LLC
sales@xia.com
www.xia.com

MAGNETIC RESONANCE

IM Publications Open
info@impopen.com
www.impopen.com

Magritek GmbH
sales@magritek.com
www.magritek.com

Oxford Instruments
magres@oxinst.com
www.oxinst.com/nmr

MASS SPECTROMETRY

BaySpec, Inc.
info@bayspec.com
www.bayspec.com

Hiden Analytical Ltd
info@hiden.co.uk
www.hidenanalytical.com

IM Publications Open
info@impopen.com
www.impopen.com

PerkinElmer, Inc.
www.perkinelmer.com

Sepsolve Analytical Ltd
hello@sepsolve.com
www.sepsolve.com

Waters Corporation
materials@waters.com
waters.com

MOBILE SPECTROMETERS

AP Technologies Ltd
info@aptechnologies.co.uk
www.aptechnologies.co.uk

BaySpec, Inc.
info@bayspec.com
www.bayspec.com

Bruker Optik GmbH
info.bopt.de@bruker.com
www.bruker.com/optics

B&W Tek LLC
marketing@bwtek.com
bwtek.com

Coherent
petra.wallenta@coherent.com
www.coherent.com

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

Magritek GmbH
sales@magritek.com
www.magritek.com

MantiSpectra
info@mantispectra.com
www.mantispectra.com

Ocean Insight
info@oceaninsight.com
oceaninsight.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

Wasatch Photonics
info@wasatchphotonics.com
www.wasatchphotonics.com

Waters Corporation
materials@waters.com
waters.com

XIA LLC
sales@xia.com
www.xia.com

PHOTONICS & OPTICS

AP Technologies Ltd
info@aptechnologies.co.uk
www.aptechnologies.co.uk

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

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

Leonardo UK Ltd
infomarketing@leonardo.com
www.leonardo.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Quantum Design UK and Ireland Ltd
info@qd-uki.co.uk
www.qd-uki.co.uk

Specac Ltd
sales@specac.co.uk
www.specac.com

Starna Scientific Limited
sales@starna.com
www.starna.com

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

Wasatch Photonics
info@wasatchphotonics.com
www.wasatchphotonics.com

PLASMA SPECTROSCOPY

Coherent
petra.wallenta@coherent.com
www.coherent.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

POLARIMETRY

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Starna Scientific Limited
sales@starna.com
www.starna.com

PROCESS

ABB Measurement & Analytics
ftir@ca.abb.com
abb.com/analytical

DIRECTORY

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

Hiden Analytical Ltd
info@hiden.co.uk
www.hidenanalytical.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

MantiSpectra
info@mantispectra.com
www.mantispectra.com

Magritek GmbH
sales@magritek.com
www.magritek.com

Ocean Insight
info@oceaninsight.com
oceaninsight.com

Starna Scientific Limited
sales@starna.com
www.starna.com

RAMAN

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

B&W Tek LLC
marketing@bwtek.com
bwtek.com

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

IM Publications Open
info@impopen.com
www.impopen.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

Ocean Insight
info@oceaninsight.com
oceaninsight.com

PerkinElmer, Inc.
www.perkinelmer.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

S.T.Japan-Europe GmbH
contact@stjapan.de
www.stjapan.de

Starna Scientific Limited
sales@starna.com
www.starna.com

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

Wasatch Photonics
info@wasatchphotonics.com
www.wasatchphotonics.com

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

RELATED EQUIPMENT

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

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

LTB Lasertechnik Berlin GmbH
info@ltb-berlin.de
www.ltb-berlin.de/en/homepage/

MantiSpectra
info@mantispectra.com
www.mantispectra.com

Magritek GmbH
sales@magritek.com
www.magritek.com

Quantum Design UK and Ireland Ltd
info@qd-uki.co.uk
www.qd-uki.co.uk

Starna Scientific Limited
sales@starna.com
www.starna.com

XIA LLC
sales@xia.com
www.xia.com

DIRECTORY

SAMPLE PREPARATION

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Sepsolve Analytical Ltd
hello@sepsolve.com
www.sepsolve.com

S.T.Japan-Europe GmbH
contact@stjapan.de
www.stjapan.de

Waters Corporation
materials@waters.com
waters.com

SEPARATION SCIENCE

PerkinElmer, Inc.
www.perkinelmer.com

Sepsolve Analytical Ltd
hello@sepsolve.com
www.sepsolve.com

Waters Corporation
materials@waters.com
waters.com

SPECTRORADIOMETRY

ABB Measurement & Analytics
ftir@ca.abb.com
abb.com/analytical

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

SURFACE ANALYSIS

Hiden Analytical Ltd
info@hiden.co.uk
www.hidenanalytical.com

IM Publications Open
info@impopen.com
www.impopen.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Ocean Insight
info@oceaninsight.com
oceaninsight.com

TERAHERTZ

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

TOPTICA Photonics AG
sales@toptica.com
www.toptica.com

UV AND VISIBLE

AP Technologies Ltd
info@aptechnologies.co.uk
www.aptechnologies.co.uk

Coherent
petra.wallenta@coherent.com
www.coherent.com

Edinburgh Instruments Ltd
alison.winn@edinst.com
www.edinst.com

Gigahertz Optik GmbH
info@gigahertz-optik.de
www.gigahertz-optik.de

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

Ocean Insight
info@oceaninsight.com
oceaninsight.com

PerkinElmer, Inc.
www.perkinelmer.com

Pro-Lite Technology Ltd
info@pro-lite.co.uk
www.pro-lite.co.uk

Starna Scientific Limited
sales@starna.com
www.starna.com

X-RAY DIFFRACTION

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Thermo Fisher Scientific
info.spectrometry@thermofisher.com
www.thermofisher.com/elemental

DIRECTORY

X-RAY SPECTROMETRY

HORIBA Scientific
info-sci.fr@horiba.com
www.horiba.com/scientific

IM Publications Open
info@impopen.com
www.impopen.com

Linkam Scientific Instruments
info@linkam.co.uk
www.linkam.co.uk

Quantum Design UK and Ireland Ltd
info@qd-uki.co.uk
www.qd-uki.co.uk

Specac Ltd
sales@specac.co.uk
www.specac.com

Thermo Fisher Scientific
info.spectrometry@thermofisher.com
www.thermofisher.com/elemental

XIA LLC
sales@xia.com
www.xia.com