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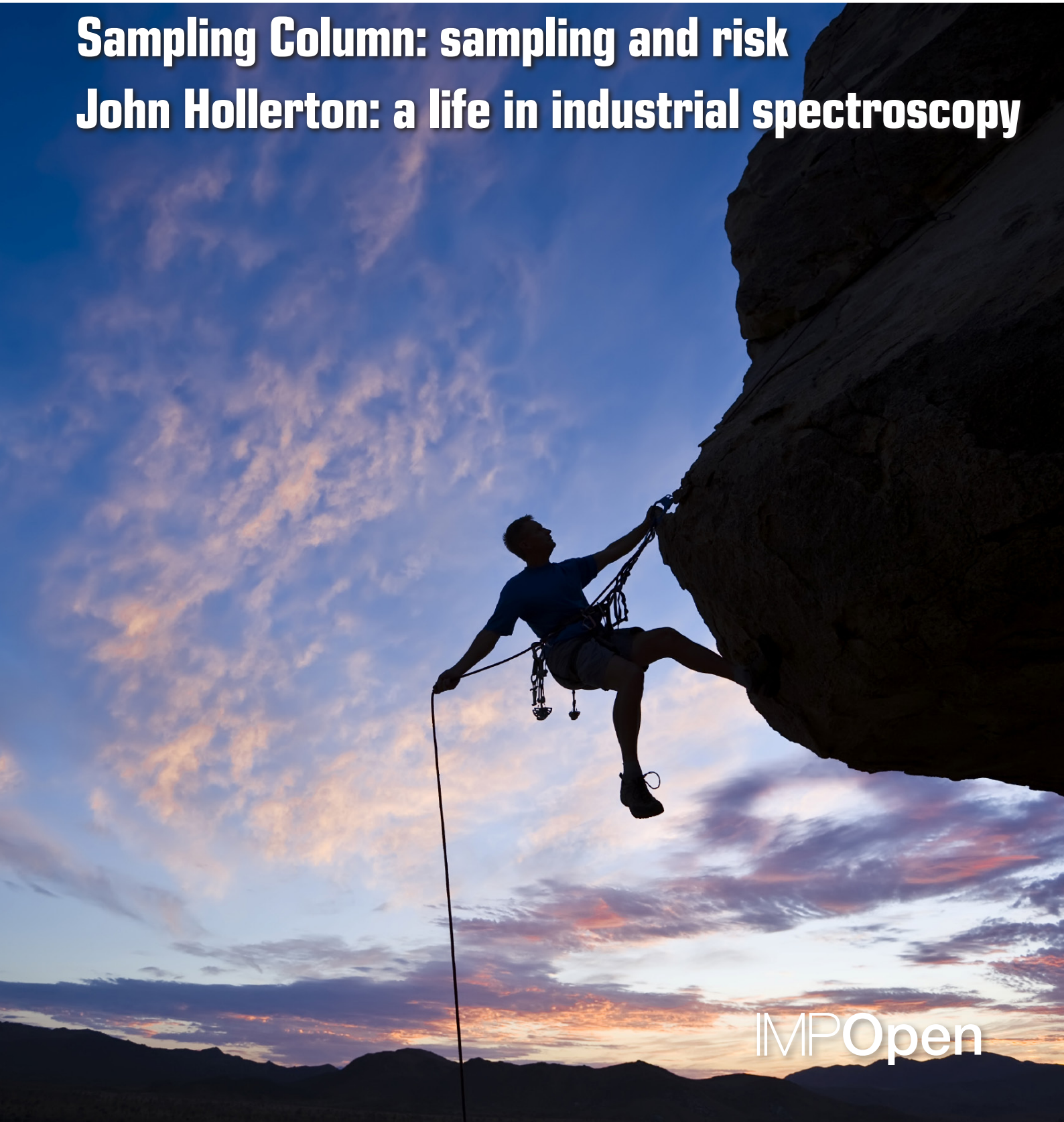
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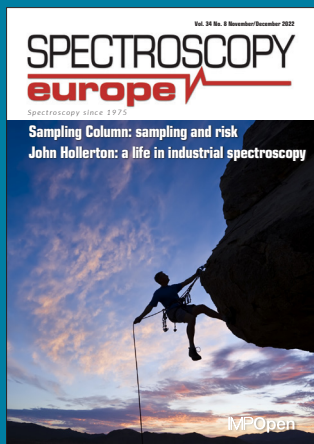
Spectroscopy since 1975

Sampling Column: sampling and risk

John Hollerton: a life in industrial spectroscopy



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Kim Esbensen and Claudia Paoletti hope that a risk assessment scope will allow the sampling community an easier, and perhaps more powerful, way to reach out to business, commerce, trade as well as regulatory and law-enforcement authorities across many societal sectors by also speaking a more business-oriented language beyond traditional "TOS technicalities". See the Sampling Column starting on page 36.

Publisher

Ian Michael
E-mail: ian@impopen.com

Advertising Sales

Ian Michael
IM Publications Open, 6 Charlton Mill,
Charlton, Chichester, West Sussex PO18 0HY,
United Kingdom. Tel: +44-1243-811334,
Fax: +44-1243-811711,
E-mail: ian@impopen.com

Circulation

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Charlton, Chichester, West Sussex PO18 0HY,
United Kingdom. Tel: +44-1243-811334,
Fax: +44-1243-811711,
E-mail: katie@impopen.com

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IMP Open

I know we are all too frequently asked for our feedback and reviews; however, we try to avoid pestering you in this way. The last reader survey was two years ago, and I think this would be a good time to ask you to participate in another: <https://www.spectroscopyeurope.com/2023-survey> Not only are there a lot of new readers who won't have had the opportunity before, but two years after a major change in the way we publish seems significant. As before, no question is "required", but the more you answer the more we will learn!

This is a slightly unbalanced issue, I am afraid. Whilst a number of articles are "in the pipeline", none was ready for this issue. However, we have a wide range of News stories, and I have included many of them since I didn't want to leave any of the interesting stuff out! They

cover many of the diverse technologies that make up "spectroscopy" and the applications we use it for. However, there is even more "good stuff" later in the issue, so please persevere!

In the Tony Davies Column, Tony and Mohan Cashyap interview John Hollerton, who has just retired after a career of over 40 years at GSK (and its many previous names). John has been responsible for many aspects of analytical chemistry at GSK. As Tony says, he is "an innovative ideas man with some interesting stories". There was so much to discuss that the interview will be split over two issues. Part 1 starts on [page 32](#).

Risk is the topic of the Sampling Column. Kim Esbensen and Claudia Paoletti hope that a risk assessment scope will provide the sampling community with an easier, and

perhaps more powerful, way to reach out to business, commerce, trade as well as regulatory and law-enforcement authorities across many societal sectors. It may also speak a more business-oriented language beyond traditional "TOS technicalities". See the Sampling Column starting on [page 36](#).

More applications appear after the columns ([page 41](#)), followed by a Product Focus on Surface Spectroscopy ([page 44](#)), a process NIR Featured Product ([page 46](#)), a wide range of new products ([page 47](#)) and the ever-popular Diary of future events ([page 54](#)).

La Michael

THE FIRST WORD

Use heated ATR when subtracting water signals from IR spectra

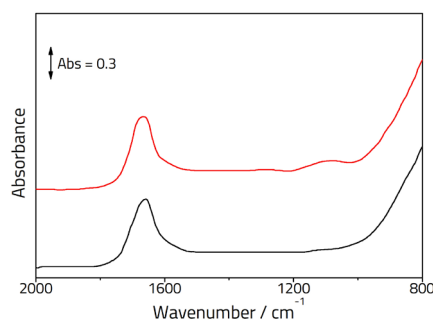
When IR spectra are obtained from aqueous samples, the water content will usually mask signals from any suspended solids or other components of the sample.

If you want to subtract a spectrum of pure water in order to more clearly see the signals from the analytes in solution, it is a good idea to control the temperature of the recorded spectra. The IR spectrum of water is sensitive to small changes in temperature, resulting in erroneous subtraction from samples recorded at a different temperature.

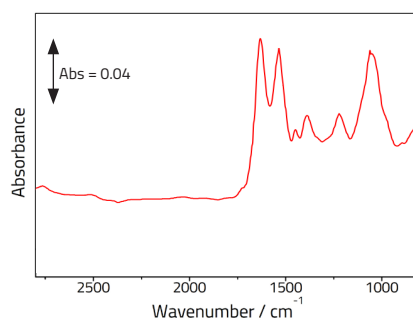
Heated ATR systems offer a simple way to control temperature to within ± 1.0 °C. Specac offer heated options for both the single-bounce Quest ATR (right) and the multi-bounce Gateway ATR (below).



Specac



Top: ATR spectra of an aqueous suspension of yeast cells (red line) and distilled water (black line), showing predominance of spectral features associated with the water molecules.



Bottom: ATR spectra of yeast cells after careful subtraction of the water spectrum above.



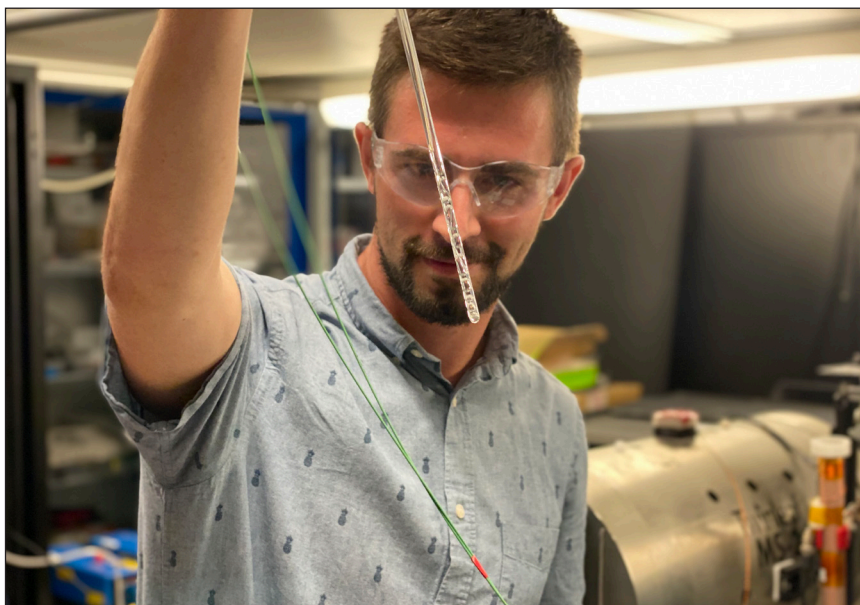
Developments to shrink the size of NMR spectrometers

New method combines zero- to ultralow-field nuclear magnetic resonance with the SABRE-Relay hyperpolarisation technique.

Researchers working at Johannes Gutenberg University Mainz (JGU) and the Helmholtz Institute Mainz (HIM) have now discovered potential new ways to reduce the size of nuclear magnetic resonance (NMR) devices and also any possible associated risk by eliminating the need for strong magnetic fields. This is achieved by combining so-called zero- to ultralow-field NMR with a special hyperpolarisation technique. “This exciting new method is based on an innovative concept. It opens up a whole range of opportunities and overcomes previous disadvantages”, said Dr Danila Barskiy, a Sofja Kovalevskaja Award winner who has been working in the field at JGU and HIM since 2020.

The current generation of NMR devices is—because of the magnets—extremely heavy and expensive. Another complicating factor is the present shortage of liquid helium that is employed as a coolant. “With our new technique we are gradually moving ZULF NMR towards a status of being completely magnet-free, but we still have many challenges to overcome”, stated Barskiy.

To make magnets redundant in this context, Barskiy has come up with the idea of combining zero- to ultralow-field nuclear magnetic resonance (ZULF NMR) with a special technique that makes it possible to hyperpolarise atomic nuclei. ZULF NMR is itself a recently developed form of spectroscopy that provides abundant analytical results without the need for large magnetic fields. Another advantage over high-field NMR is the fact that its signals can also be readily detected in the presence of conductive materials, such as metals. The sensors employed for ZULF NMR, typically optically pumped magnetometers, are



Dr Danila Barskiy conducting an experiment. © Danila Barskiy

highly sensitive, easy to use and are already commercially available. Thus, it is relatively straightforward to assemble a ZULF NMR spectrometer.

However, the generated NMR signal is an issue to be dealt with. The methods that have been used to date to generate the signal are suitable only for the analysis of a limited selection of chemicals or are otherwise associated with exorbitant costs. For this reason, Barskiy has decided to exploit the Signal Amplification by Reversible Exchange (SABRE) hyperpolarisation technique which allows the alignment of nuclear spins at large numbers in solution. There are a number of such techniques that would produce a signal sufficient for detection in ZULF conditions. Central to the SABRE technique is an iridium metal complex that mediates the transfer of the spin order from parahydrogen to a substrate. Barskiy has managed to sidestep the disadvantages resulting from the temporary binding

of the sample to the complex by employing SABRE-Relay, a very recent improvement of the SABRE technique. In this case, SABRE is used to induce polarisation which is then relayed to a secondary substrate. Their work has been published in *Science Advances* (doi.org/ggq5vp).

Dr Barskiy and colleagues have reported on how they were able to detect the signals for methanol and ethanol extracted from a sample of vodka. “This simple example demonstrates how we have been able to extend the application range of ZULF NMR with the help of an inexpensive, rapid and versatile method of hyperpolarisation”, summarised Barskiy. “We hope that we’ve managed to get a little closer to our objective of making feasible the development of compact, portable devices that can be used for the analysis of liquids such as blood and urine and in future, possibly endowing discrimination of particular chemicals such as glucose and amino acids.”

SUCCESS

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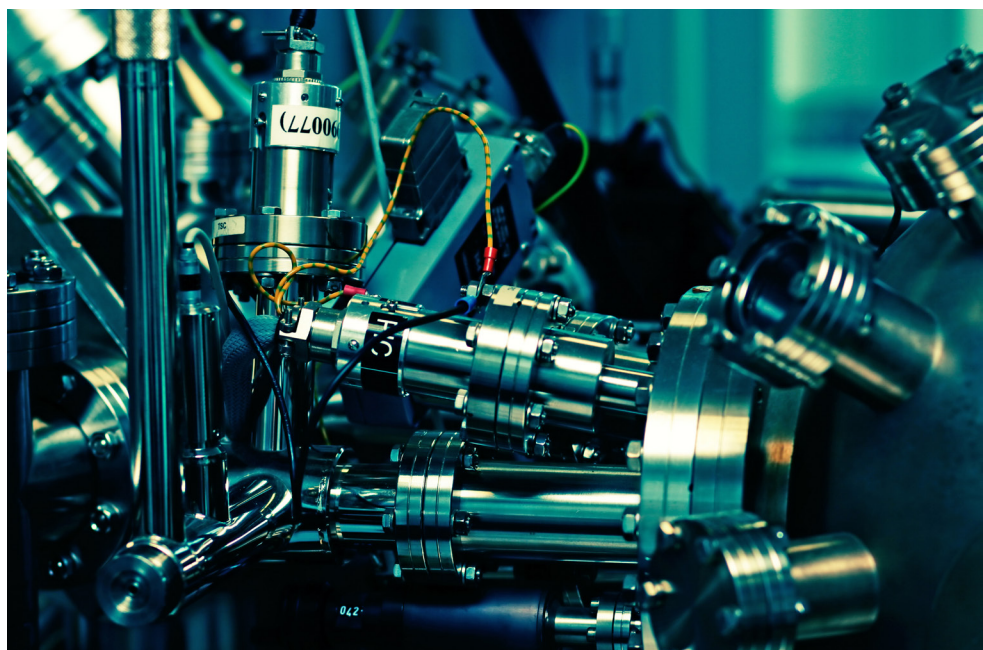
Ultralow-energy SIMS scrapes beyond the surface of nanomaterials

Using ultralow-energy secondary-ion mass spectrometry, researchers are getting a fresh look at MXenes and MAX phases.

Since the initial discovery of what has become a rapidly growing family of two-dimensional layered materials—called MXenes—in 2011, Drexel University researchers have made steady progress in understanding the complex chemical composition and structure, as well as the physical and electrochemical properties, of these exceptionally versatile materials. More than a decade later, advanced instruments and a new approach have allowed the team to peer within the atomic layers to better understand the connection between the materials' form and function.

In a recent paper, published in *Nature Nanotechnology* (doi.org/gqvs5w), researchers from Drexel's College of Engineering and Poland's Warsaw Institute of Technology and Institute of Microelectronics and Photonics reported a new way to look at the atoms that make up MXenes and their precursor materials, MAX phases, using secondary ion mass spectrometry (SIMS). In doing so, the group discovered atoms in locations where they were not expected and imperfections in the two-dimensional materials that could explain some of their unique physical properties. They also demonstrated the existence of an entirely new subfamily of MXenes, called oxycarbides, which are two-dimensional materials where up to 30% of carbon atoms are replaced by oxygen.

This discovery will enable researchers to build new MXenes and other nanomaterials with tunable properties best suited for specific applications from antennas for 5G and 6G wireless communication and shields for electromagnetic interference; to filters for hydrogen production, storage and



separation; to wearable kidneys for dialysis patients.

“Better understanding of the detailed structure and composition of two-dimensional materials will allow us to unlock their full potential”, said Yury Gogotsi, PhD, who led the MXene characterisation research. “We now have a clearer picture of why MXenes behave the way they do and will be able to tailor their structure and therefore behaviours for important new applications.”

While SIMS has been used to study multi-layered materials over the years, the depth resolution has been limited examining the surface of a material (several angstroms). A team led by Pawel Michalowski from Poland's Institute of Microelectronics and Photonics, made a number of improvements to the technique, including adjusting the angle and energy of the beam, how the ejected ions are measured; and cleaning the surface of the samples, which allowed them to

sputter samples layer by layer. This allowed the researchers to view the sample with an atom-level resolution that had not been previously possible.

“The closest technique for analysis of thin layers and surfaces of MXenes is X-ray photoelectron spectroscopy, which we have been using at Drexel starting from the discovery of the first MXene”, said Mark Anayee, a doctoral candidate in Gogotsi's group. “While XPS only gave us a look at the surface of the materials, SIMS lets us analyse the layers beneath the surface. It allows us to ‘remove’ precisely one layer of atoms at a time without disturbing the ones beneath it. This can give us a much clearer picture that would not be possible with any other laboratory technique.”

As the team peeled back the upper layer of atoms, like an archaeologist carefully unearthing a new find, the researchers began to see the subtle features of the chemical scaffolding within the layers of

materials, revealing the unexpected presence and positioning of atoms, and various defects and imperfections.

“We demonstrated the formation of oxygen-containing MXenes, so-called oxycarbides. This represents a new subfamily of MXenes—which is a big discovery!”, said Gogotsi. “Our results suggest that for every carbide MXene, there is an oxycarbide MXene, where oxygen replaces some carbon atoms in the lattice structure.”

Since MAX and MXenes represent a large family of materials, the researchers further explored more complex systems that include multiple metal elements. They made several important observations, including the intermixing of atoms in chromium-titanium carbide MXene—which were previously thought to be separated into

distinct layers. And they confirmed previous findings, such as the complete separation of molybdenum atoms to outer layers and titanium atoms to the inner layer in molybdenum–titanium carbide.

All of these findings are important for developing MXenes with a finely tuned structure and improved properties, according to Gogotsi.

“We can now control not only the total elemental composition of MXenes, but also know in which atomic layers the specific elements like carbon, oxygen or metals are located”, said Gogotsi. “We know that eliminating oxygen helps to increase the environmental stability of titanium carbide MXene and increase its electronic conductivity. Now that we have a better understanding of how much additional oxygen is in the materials, we can adjust the recipe, so to speak, to

produce MXenes that do not have it, and as a result more stable in the environment.”

The team also plans to explore ways to separate layers of chromium and titanium, which will help it develop MXenes with attractive magnetic properties. And now that the SIMS technique has proven to be effective, Gogotsi plans to use it in future research, including his recent \$3 million US Department of Energy-funded effort to explore MXenes for hydrogen storage—an important step toward the development of a new sustainable energy source.

“In many ways, studying MXenes for the last decade has been mapping uncharted territory”, said Gogotsi. “With this new approach, we have better guidance on where to look for new materials and applications.”¹

First images of carbon dioxide emissions in the NIR from commercial aircraft engine

Large-scale, chemical-specific emissions information poised to aid development of greener airplane engines and fuels.

Researchers have used a novel near infrared (NIR) light imaging technique to capture the first cross-sectional images of carbon dioxide in the exhaust plume of a commercial jet engine. This new technology could help accelerate turbine combustion research aimed at developing engines and aviation fuels that are more environmentally friendly.

“This approach, which we call chemical species tomography, provides real-time spatially resolved information for carbon dioxide emissions from a large-scale commercial engine”, said research team leader Michael Lengden from the University of Strathclyde. “This information has not been available before at this industrial scale and is a big improvement over the current industry-standard emissions measurement, which involves taking gas



Researchers developed a technique called chemical species tomography that can capture carbon dioxide exhaust from a commercial airplane engine. To image such a large area, the researchers used a 7-m diameter optical mounting frame (red) located just 3 m from the exit nozzle of the engine. The testing facility is at the Instituto Nacional de Técnica Aeroespacial (INTA) in Madrid. Credit: Gordon Humphries, University of Strathclyde

from the exhaust to a gas analyser system in a different location.”

Chemical species tomography works much like the X-ray-based CT scans used in medicine, except that it uses NIR laser light tuned to the absorption wavelength of a target molecule and requires very fast imaging speeds to capture the dynamic processes of combustion.

Until now it has been impossible to image turbine combustion on test rigs containing a large airplane engine. To solve this problem, four instrumentation research groups in the UK came together to combine their knowledge in gas species measurement in harsh environments, chemical species tomography and optical source development. These teams worked with industrial partners to develop technology that would be practical for industrial research and development.


“The teams saw an opportunity to develop world leading instrumentation for the aerospace industry, and to understand emissions and performance improvements from large scale engines”, said Lengden. “With chemical species tomography, we can now start to ‘see’ the

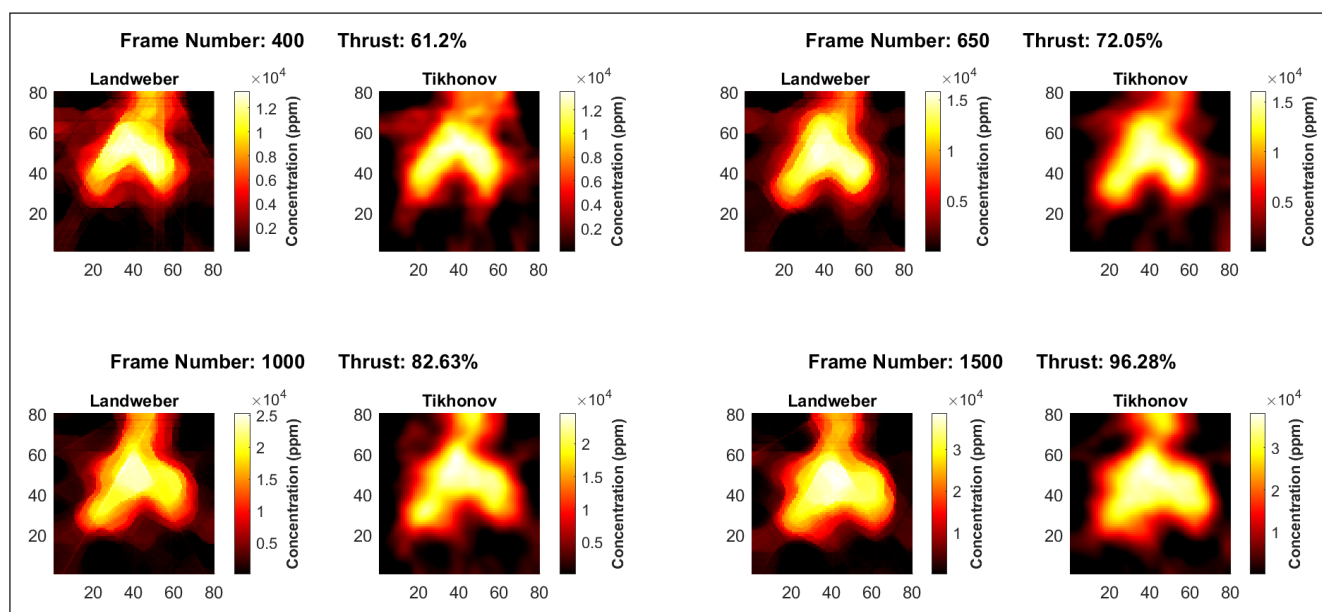
chemical detail of combustion in a real production airplane engine.”

After years of working to fine-tune signal-to-noise ratios, data acquisition methods, imaging techniques and optical sources, the researchers created the first facility capable of acquiring industrial emission measurements at the large scale of a commercial airplane engine. To perform chemical species tomography, 126 beams of NIR laser light are shone through the gas from all around the side at many angles in a way that doesn’t disturb the gas flow. Adequately capturing the exhaust from a commercial airplane engine requires imaging an area up to 1.8 m in diameter. To capture this, the imaging components were mounted on a 7-m diameter frame located just 3 m from the exit nozzle of the engine. The researchers used 126 optical beams to achieve a spatial resolution of about 60 mm in the central region of the engine exhaust.

The researchers used this large-scale setup to perform chemical species tomography of carbon dioxide produced by combustion

in a modern Rolls-Royce Trent gas engine turbine. These engines are typically used on long-haul aircraft and contain a combustor with 18 fuel injectors arranged in a circle. For the tests, researchers recorded data at frame rates of 1.25 Hz and 0.3125 Hz while the engine was operated over the full range of thrust. The resulting images showed that, at all thrust levels, a ring-structure of high carbon dioxide concentration was present in the central region of the engine. There was also a raised region in the middle of the plume, which was likely due to the engine’s shape. The results are published in *Applied Optics* (doi.org/gqwzrr).

The researchers are now working to adapt the new instrument to enable quantitative measurement and imaging of other chemicals produced by turbine combustion in both the aerospace and industrial power generation sectors, and to capture images of temperature. This will enable engineers and scientists developing new turbines and fuels to better understand the combustion process for current and future technologies. 



The researchers used their new chemical species tomography setup to capture the first images of carbon dioxide exhaust from a commercial aircraft engine. At all thrust levels, a ring-structure of high carbon dioxide concentration can be seen in the central region of the engine. Credit: Abhishek Upadhyay, University of Strathclyde

New Auger spectroscopy technique measure properties of a material's surface layer

Physicists at the University of Texas at Arlington have developed a new technique that can measure the properties of the top-most atomic layer of materials without including information from the underlying layers.

Researchers from the Positron Lab in the University of Texas at Arlington (UTA) Department of Physics utilised a process called Auger-mediated positron sticking (AMPS) to develop a novel spectroscopic tool to measure the electronic structure of the surface of materials selectively. The AMPS process, in which positrons (anti-matter of electrons) stick directly to surfaces followed by electron emission, was first observed and described by Saurabh Mukherjee,

a graduate student, along with Alex Weiss, professor and chair of the UTA Department of Physics, and other colleagues in 2010 at UTA.

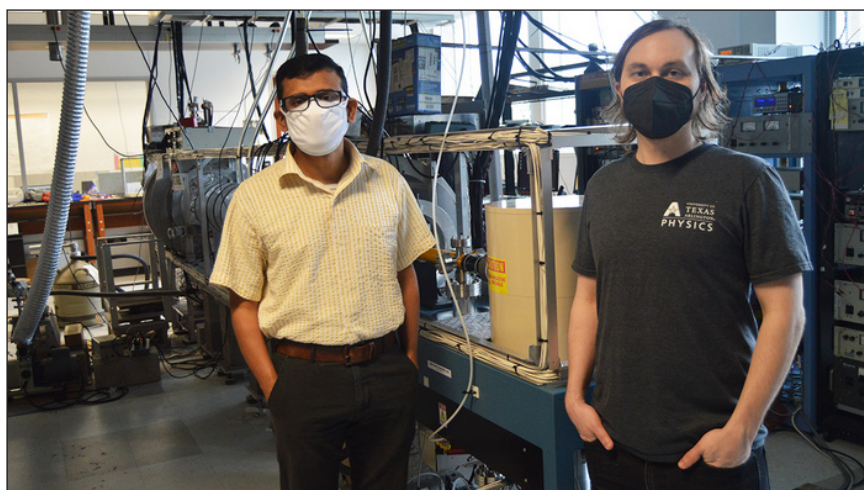
"Alex (Fairchild) and Varghese figured out how to use this phenomenon that we discovered in 2010 to measure the top layer and get information about the electronic structure and the behaviour of the electrons in the top layer", Weiss said. "That will determine a material's many properties, including conductivity, and can have

important implications for building devices."

Alex Fairchild, postdoctoral scholar in the Positron Lab, said the AMPS process is unique because it uses virtual photons to measure the top-most atomic layer. "This is different from typical techniques like photoemission spectroscopy, where a photon penetrates multiple layers into the bulk of a material and, therefore, contains the combined information of the surface and subsurface layers", he said.

"Our AMPS results showed how virtual photons emitted following positron-sticking interact preferably with electrons that extend further into the vacuum than with electrons that were more localised to the atomic site", Varghese Chirayath, assistant professor of research, said. "Our results are thus essential to understand how positrons interact with surface electrons and are extremely important to understand other similarly surface-selective, positron-based techniques."

They have published this work in *Physical Review Letters* (doi.org/gq7wqh).¹



Varghese Chirayath, left, and Alex Fairchild. Credit: UT Arlington

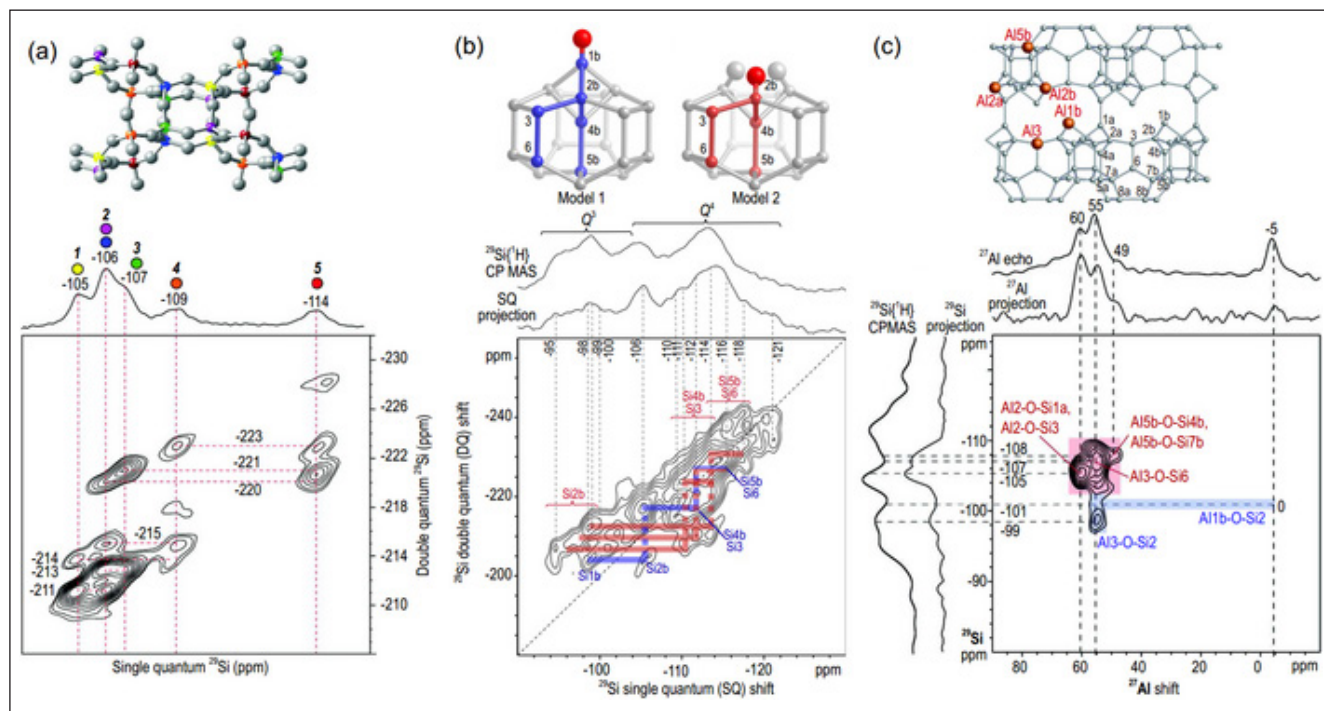
Recent advances in solid-state NMR studies of zeolite catalysts

A new review summarises the recent advances in ssNMR of zeolite catalysts, mainly covering the new applications of ssNMR to investigate zeolite framework structure, catalytically active sites, intermolecular interactions and catalytic reaction mechanisms.

Zeolites are important inorganic crystalline microporous materials with a broad range of applications in catalysis, ion exchange and adsorption/separations. Due to their unique pore structure, high thermal stability and tuneable acid-base property, zeolites are one

kind of the most important heterogeneous catalysts used in the petrochemical and fine chemical industries. The design of efficient zeolites with improved properties depends on the understanding of the structure-activity relationship, which requires fundamental

characterisation of the zeolites. Solid-state NMR (ssNMR) spectroscopy is a well-established tool for the study of zeolites and relevant catalytic reactions because of its advantage in providing atomic-level insights into molecular structure and dynamic behaviour.



(a) 2D refocused INADEQUATE (J -mediated) $^{29}\text{Si}\{^{29}\text{Si}\}$ DQ NMR spectrum of as-synthesised zeolite ITW. (b) DNP-enhanced 2D $^{29}\text{Si}\{^{29}\text{Si}\}$ J -mediated correlation spectrum of calcined Si-SSZ-70. (c) Schematic diagram of the framework structure of Al-SSZ-70 (orange indicates the T sites that are occupied by Al heteroatoms), and 2D $^{27}\text{Al}\{^{29}\text{Si}\}$ J -HMQC NMR spectrum of calcined Al-SSZ-70. Credit: ©Science China Press

In a new review, published in *National Science Review* (doi.org/gqvnkj), scientists at the State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences in Wuhan, China, summarise the recent advances in ssNMR of zeolite catalysts, mainly covering the new applications of ssNMR to investigate zeolite framework structure, catalytically active sites, intermolecular interactions and catalytic reaction mechanisms. The authors also discuss the current limitations and the future prospects of ssNMR for its application in zeolite catalysts.

The authors indicate that, combined with advanced instrumentation and experimental techniques, ssNMR has been demonstrated to be a powerful analytic tool in zeolites characterisation. The direct detection of framework structure and acid sites is enabled by using various 1D and 2D ssNMR methods. The obtained knowledge has made it possible for zeolite scientists to optimise zeolites with improved catalytic performance in many important reactions such as methanol conversion, cracking of hydrocarbons and oligomerisation of alkenes. Meanwhile, 1D and 2D correlation spectroscopy allows ssNMR to probe the internuclear

spatial proximities, which are associated with host-guest and guest-guest interactions in zeolites. The characterisation of various interactions allows scientists to gain better understandings in zeolite synthesis, adsorption/desorption and catalytic reactions. Moreover, the utilisation of ssNMR for the observation and identification of critical active intermediates in zeolite-catalysed reactions has become a key approach for the elucidation of reaction mechanism. The knowledge on the reaction mechanism and the involved intermediates has been applied to the synthesis of new zeolites capable of controlling reaction pathway in a complex reaction such as methanol conversion. \blacktriangledown

Novel focusing quadrupole ion funnel improves detection sensitivity of mass spectrometers

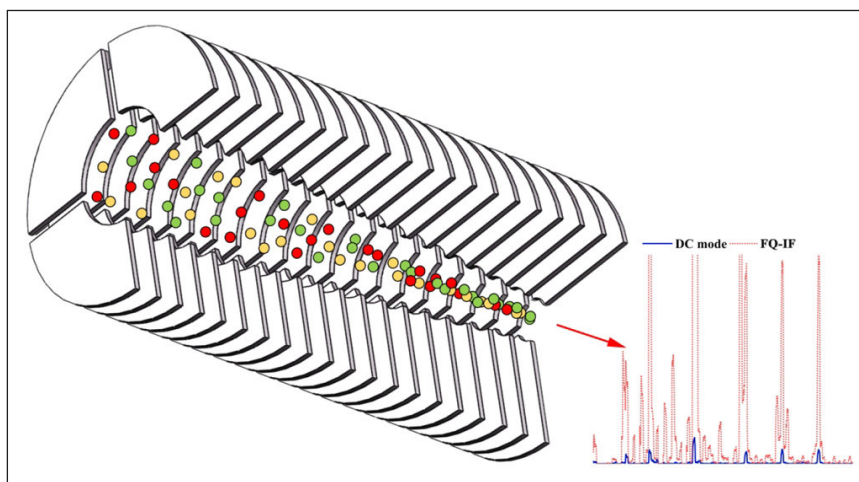
A novel focusing quadrupole ion funnel takes advantage of RF ion focusing technology in proton transfer reaction mass spectrometry and greatly improves its sensitivity.

Researchers from the Hefei Institutes of Physical Science (HFIPS) of the Chinese Academy of Sciences (CAS) have proposed a novel focusing quadrupole ion funnel (FQ-IF) that takes advantage of radio frequency ion focusing technology in proton transfer reaction mass spectrometry (PTR-MS) and greatly improves its sensitivity and endowed it with a better “sense of smell”.

PTR-MS is an important analysis technique for the real-time detection of volatile organic compounds (VOCs). Detection sensitivity is a critical performance in PTR-MS. The successful determination of trace VOCs lies on the sensitivity of the instrument, so sensitivity enhancement is an active area of research.

“The FQ-IF drift tube we developed could improve ion transmission efficiency”, said BAO Xun, “and it offers a suitable collision condition”.

The tube consists of 20 layers of stainless-steel electrodes, each with four quarter rings. The first six layers have a constant bore



The focusing effect of the FQ-IF drift tube. (Image by BAO Xun)

diameter of 22 mm. The later 14 layers taper the inner diameter to 8 mm. The ion transmission efficiency in the drift tube is improved by the radio frequency electric field, which is the key to increase the sensitivity and provides more possibilities for PTR-MS.

The sensitivity of the FQ-IF range now is 13.8–87.9× higher compared to the conventional direct current drift tube, and 1.7–4.8× higher compared to the

ion funnel drift tube. The improvements in the limit of detection for the FQ-IF ranged from 2.7× to 35.7× compared to the conventional direct current drift tube. In addition, the FQ-IF drift tube can be easily coupled to other types of mass spectrometers to increase the detection sensitivity and may offer considerable benefits. They have published this work in *Analytical Chemistry* (doi.org/gqzrmz).¹

Spectrometer on a chip

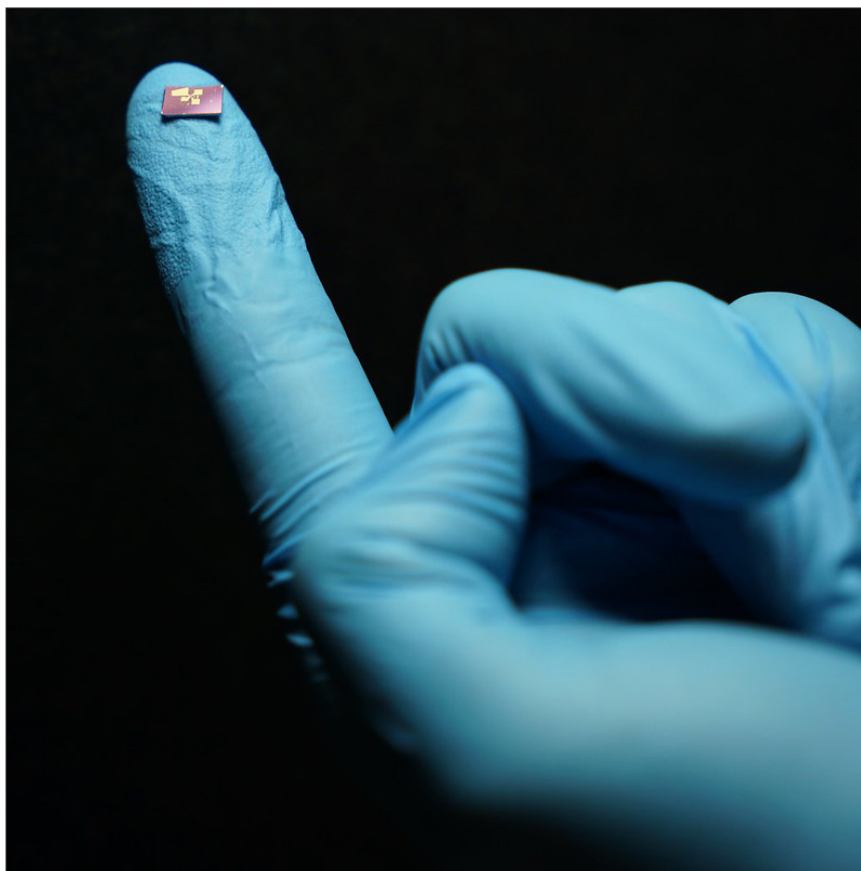
Research involving two-dimensional semiconductors has led to an ultra-tiny spectrometer that fits on a microchip and is operated using artificial intelligence.

Scientists have developed a better tool to measure light, contributing to optical spectrometry in a way that could improve everything from smartphone cameras to environmental monitoring. The study was led by Finland’s Aalto University and resulted in a powerful, ultra-tiny spectrometer that fits on a microchip and is operated using artificial intelligence. The research involved a comparatively new class

of super-thin materials known as two-dimensional semiconductors, and the upshot is a proof of concept for a spectrometer that could be readily incorporated into a variety of technologies—including quality inspection platforms, security sensors, biomedical analysers and space telescopes.

“We’ve demonstrated a way of building spectrometers that are far more miniature than what is

typically used today”, said Ethan Minot, a professor of physics in the Oregon State University College of Science. The new device could fit on the end of a human hair, Minot said. The new research suggests components can be replaced with novel semiconductor materials and AI, allowing spectrometers to be dramatically scaled down in size from the current smallest ones.



Spectrometer on a chip. Credit: Oregon State

“Our spectrometer does not require assembling separate optical and mechanical components or array designs to disperse and filter light”, said Hoon Hahn Yoon, who led

the study with Aalto University colleague Zhipei Sun Yoon. “Moreover, it can achieve a high resolution comparable to benchtop systems but in a much smaller package.”

The device is 100% electrically controllable regarding the wavelengths of light it absorbs, which gives it massive potential for scalability and widespread usability, the researchers say.

“Integrating it directly into portable devices such as smartphones and drones could advance our daily lives”, Yoon said. “Imagine that the next generation of our smartphone cameras could be hyperspectral cameras.” Those hyperspectral cameras could capture and analyse information not just from visible wavelengths but also allow for infrared imaging and analysis.

“It’s exciting that our spectrometer opens up possibilities for all sorts of new everyday gadgets, and instruments to do new science as well”, Minot said.

Minot thinks that as work with two-dimensional semiconductors progresses, “we’ll be rapidly discovering new ways to use their novel optical and electronic properties”. Research into 2D semiconductors has been going on in earnest for only a dozen years, starting with the study of graphene.

“It’s really exciting”, Minot said. “I believe we’ll continue to have interesting breakthroughs by studying two-dimensional semiconductors.”

Details have been published in *Science* (doi.org/gq3qh3).¹⁴

SERS monitors tumour photodynamic therapy

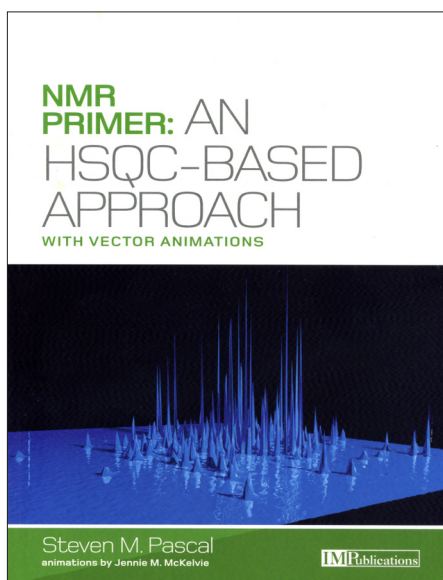
The use of SERS to monitor the photodynamic therapy process of tumours enables understanding of the specific mechanism of the catalytic process of nanozymes.

The equilibrium between reducing species and oxidising species within a tumour’s microenvironment (TME) plays a crucial role in the majority of biological processes, especially the apoptotic cell death process. If the balance of oxidising and reducing molecules is broken by the increase of reactive oxygen species (ROS) concentration, cancer cells will die to achieve the purpose of tumour

treatment. At present, some new chemodynamic therapy and photodynamic therapy (PDT) methods based on nanozyme catalysis are used in the field of tumour therapy, aiming to achieve the effect of *in situ* catalytic production of ROS in tumours. However, most of the studies on the mechanism of this treatment still only focus on the results of the cascade catalytic reaction of the nanozyme, and

cannot monitor the whole treatment process.

Surface enhanced Raman spectroscopy (SERS) has great potential in monitoring related biochemical reactions in cells. The application of SERS to monitor the photodynamic therapy process of tumours enables further understanding of the specific mechanism of the catalytic process of nanozymes, and obtaining the



NMR PRIMER: AN HSQC-BASED APPROACH (with vector animations) by Steven M. Pascal

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

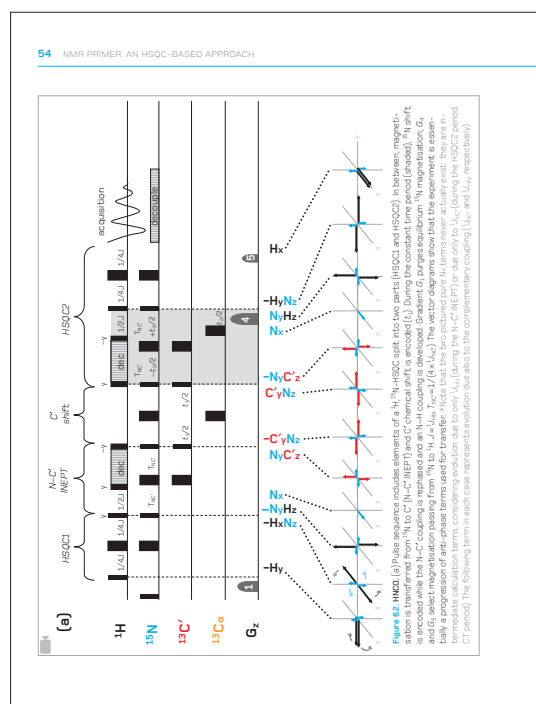
First, a brief introduction to spins, populations, the NMR experiment and relaxation is provided. Evolution due to J-coupling is next described and used to explain magnetisation transfer in the HSQC experiment and several variants. The extraction of structural, sequential and dynamic information is then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

ANIMATIONS

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

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



specific information on the redox state in the TME.

A team of scientists, led by Professor Wei Song, Professor Zhuo Liu and Professor Bing Zhao from Jilin University, China, reported, in *Light Science & Applications* (doi.org/gq2hm2), that cascade nanozymes of Au@CDs could be used for photodynamic therapy of tumour cells. SERS has been used to identify the dynamic change of ROS in TME throughout the whole PDT process, enabling monitoring of the intracellular biochemical reactions with superior sensitivity. This work presents an insightful study about the PDT mechanism based on oxidative stress injury in TME, providing a powerful means for the real-time monitoring of tumour phototherapy.

The researchers designed the Au@CDs cascade nanozyme. In which, CDs are used as a template and capping agent to construct a

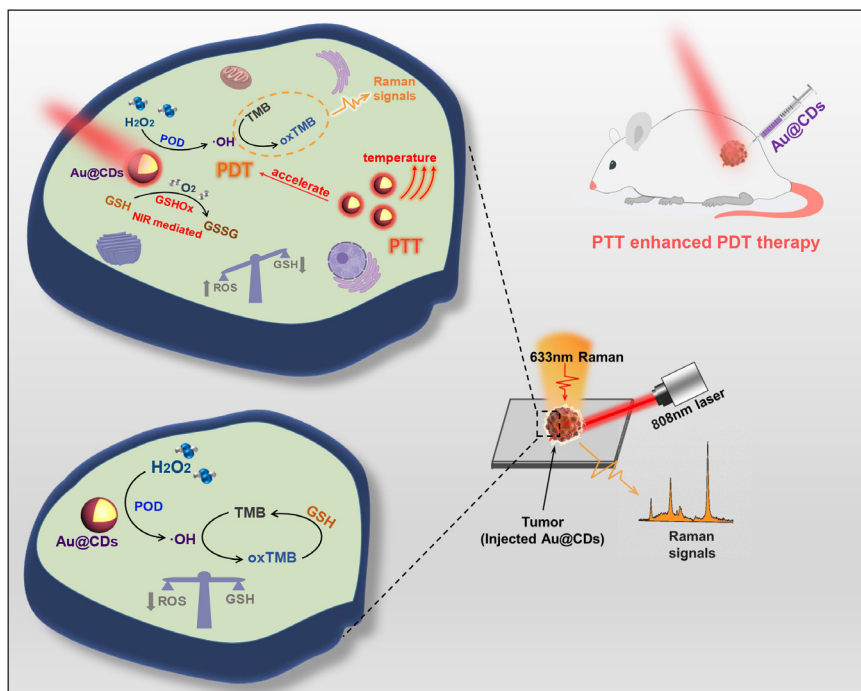


Figure 1. Core-shell structured Au@CDs present a photoinduced-enhanced oxidative stress amplification, which can be efficiently used for tumour catalytic therapy by SERS. Credit: Linjia Li, Jin Yang, Jiahui Wei, Chunhuan Jiang, Zhuo Liu, Bai Yang, Bing Zhao, Wei Song

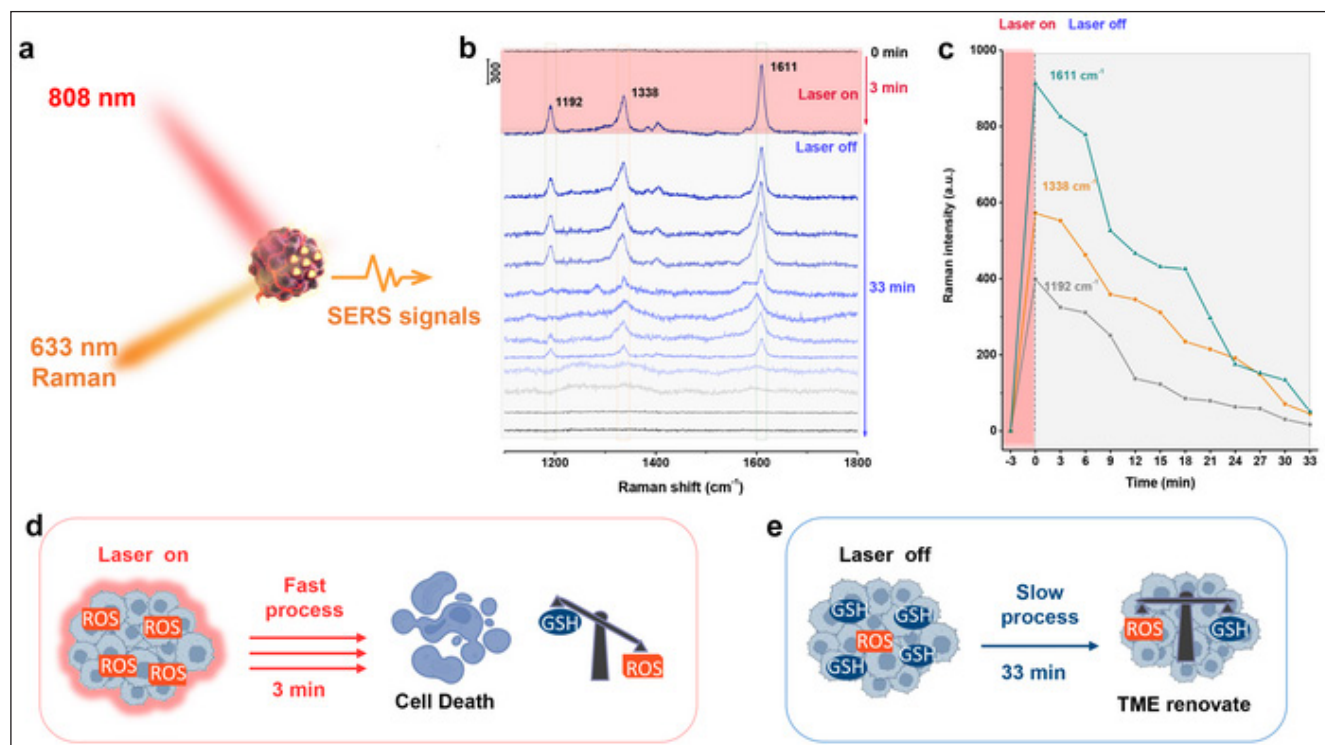


Figure 2. (a–c) Time-dependent SERS spectra during the process of oxidative stress in tumour and (d,e) the breaking and re-repairing processes of redox-homeostasis in TME. Credit: Linjia Li, Jin Yang, Jiahui Wei, Chunhuan Jiang, Zhuo Liu, Bai Yang, Bing Zhao, Wei Song


typical core-shell structure Au@CDs nanoparticles (NPs). Compared with the Au NPs alone, the CDs shell avoids the aggregation of Au nuclei and provides a dense and uniform SERS hotspot. Under the excitation of near infrared (NIR) light at 808 nm, Au@CDs exhibit NIR light-induced enhanced peroxidase-like (POD) and NIR-light-induced glutathione-like oxidase (GSHOX) activity.

Under the irradiation of NIR light, a large number of hot carriers excited by surface plasmon resonance (SPR) can effectively participate in the reaction, and the typical plasma photothermal effect of Au NPs can enhance the POD activity. In addition, Au@CDs mediate glutathione (GSH) to participate in the reaction; which accelerates the generation of ROS and presents the photodynamic treatment effect

of photothermal enhancement. This cascade of nanozyme catalytic processes will rapidly break the redox homeostasis in tumours, generate a large amount of ROS and eventually lead to cancer cell apoptosis (Figure 1).

In order to monitor the photodynamic treatment process, SERS is used to monitor the dynamic change of ROS in the tumour microenvironment during photodynamic therapy by recognising the oxidation products of 3,3',5,5'-tetramethylbenzidine (TMB) substrate molecules. Specifically, the enhanced effect of photothermal property under NIR laser irradiation for PDT processes can catalyse the decomposition of H_2O_2 and the decrease of GSH levels in a very short time, further amplifying the reactive oxygen species damage leading to tumour elimination.

Subsequently, the signals of oxTMB decrease over 33 min upon turning off the NIR laser, which is very slow compared to the increase process mentioned above under laser irradiation (3 min) (Figure 2). This result further suggests that overexpressed reductants (such as GSH) in TME will consume over-expressed ROS again, then until the ROS activity is counteracted and eliminated, the oxidation–reduction equilibrium state will be realised again.

Furthermore, through SERS strategies, a complete oxidative stress process in TMB is obtained, expressing an insightful study about the reaction mechanisms, which provides the most valuable mechanism and data support for the real-time monitoring of tumour phototherapy and normal tissue self-repair. 

Paper spray mass spec can diagnose Parkinson's from skin swabs

A new method to detect Parkinson's disease has been determined by analysing sebum with paper spray mass spectrometry.

The new method has arisen from the observations of Joy Milne, who discovered that she can distinguish Parkinson's disease (PD) in individuals from a distinct body odour before clinical symptoms occur. Joy has hereditary Hyperosmia (a heightened sensitivity to smells) which has been exploited to find that Parkinson's has a distinct odour which is strongest where sebum collects on patient's backs and is less often washed away.

Researchers from The University of Manchester used cotton swabs to sample people and identify the compounds present with mass spectrometry. The method developed involves paper spray ionisation mass spectrometry combined with ion mobility separation and can be performed in as little as 3 min from swab to results.



Professor Perdita Barran at The University of Manchester, who led the research said: "We are tremendously excited by these results which take us closer to making a diagnostic test for Parkinson's Disease that could be used in clinic."

The research, published in *Journal of the American Chemical Society* (doi.org/ggr2x7), used a sample group of 79 people with Parkinson's compared with a healthy control group of 71 people.


Sebum is an oily secretion from sebaceous glands under the skin

which are connected to the endocrine system. The scientists have found that sebum can be used as a diagnostic biofluid, which is rich in hydrophobic endogenous metabolites. Altered sebum production is a well-recognised feature of Parkinson's. The sampling procedure they have developed is simple and non-invasive; sebum is collected in clinics from the upper back of patients and posted in the regular mail to the lab.

Describing the new technique Dr Depanjan Sarkar said: "The sebum is transferred to filter paper from sampling swab, and we then cut this to a triangle, add a drop of solvent, apply a voltage and this transfers compounds from the sebum into the mass spectrometer. When we do this, we find more than 4000 unique compounds of which 500 are different between people with PD compared to the control participants."

The Manchester team now see this as a major step forward towards a clinical method for confirmatory diagnosis of Parkinson's, for which to date there is no diagnostic test based on biomarkers.

Professor Monty Silverdale, Clinical Lead on this study said: "This test has the potential to massively improve the diagnosis and management of people with Parkinson's disease".

The current and future focus is to translate these findings into a test of clinical utility. This exciting new work also opens the door to possibly diagnosing other diseases through non-invasive sebum analysis and the team along with the University of Manchester have launched a spin out company Sebomix Ltd to develop this further. 

Researchers develop NIR non-invasive blood glucose monitoring process

A Raspberry Pi camera is used to capture images that can identify exact value of blood glucose with 90% accuracy.

Maria Valero, and assistant professor of information technology in Kennesaw State's College of Computing and Software Engineering (CCSE) and director of KSU's IoT as a Service Research Group is working to improve the glucose monitoring process for the millions of people around the world affected by diabetes. Valero and her team created a non-invasive process using near infrared (NIR) spectroscopy images that can identify the exact value of blood glucose with 90% accuracy without taking a blood sample. The GlucoCheck process shines NIR light through human tissue, in either the ear or finger, and uses a Raspberry Pi camera to capture images on the other side. Valero's team then uses a model to study the amount of light absorption in those images to determine blood glucose concentration.


"Our pilot study was very successful", she said. "We are excited about how this device will help people with diabetes, which affects about one in every 10 people in the United States."

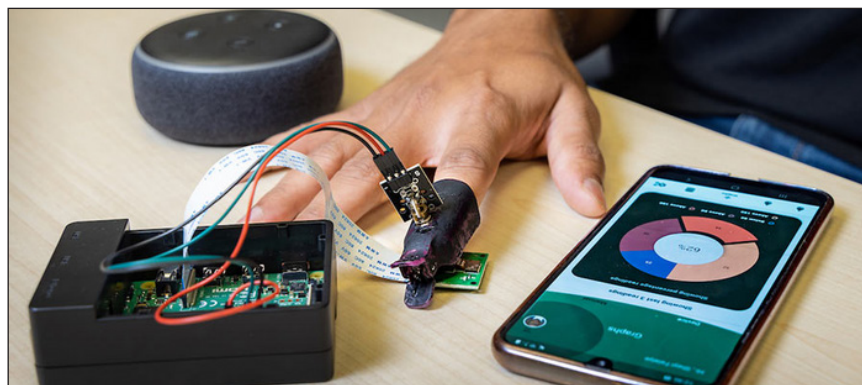
"The way we gather and output the data is novel, and we will

continue to work on ways to improve the glucose estimation model", Valero said. The team has tested the process on nearly 50 people, see *JMIR Formative Research* (doi.org/gqw4qw), so far, but they will continue to assess how the process works on people with a range of skin pigmentations and skin thickness.

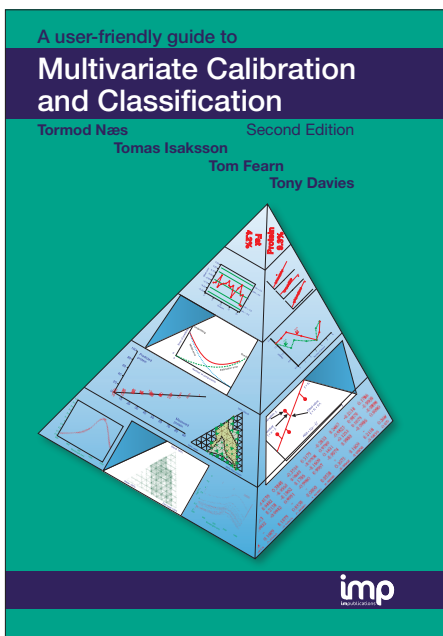
Valero's students have already created a mobile phone application and are working on connecting GlucoCheck to Amazon's virtual assistant, Alexa.

"I am very fortunate to have great students who are extremely motivated and bring a wealth of knowledge to this project", Valero said. "Watching them grow as researchers who want to make a difference in the world using technology is very rewarding."

In addition to her students, Valero has worked closely with Hossain Shahriar, associate professor of information technology, and Katherine Ingram, associate professor of exercise science. Ingram is currently researching gestational diabetes risk, and Shahriar's research focuses on health information technology, data analytics and cybersecurity. 



A new non-invasive blood glucose monitoring process is in development. Credit: Kennesaw State University



A User-Friendly Guide to Multivariate Calibration and Classification

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

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- ▶▶ Basic problems and their solutions
- ▶▶ Univariate calibration and the need for multivariate methods
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"In fact the whole book is particularly well produced by a small publisher who should be a model for larger competitors"

Prof D. Brynn Hibbert (Chemometrics and Intelligent Laboratory Systems)

"I am planning to use this text as a reference for some research projects I am planning to tackle in the near future"

"Clearly, the authors have done a reasonably thorough job on multivariate calibration"

"In conclusion I liked the text. The layout and the figures make it easy to read."

Barry Lavine (Journal of Chemometrics)

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Paul Geladi (NIR news)

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Liquid-interface assisted SERS improves enhancement factor for biomolecules

Label-free trace detection of bio-molecules by liquid-interface assisted surface-enhanced Raman scattering has been realised using a microfluidic chip.

Surface-enhanced Raman scattering (SERS) has attracted attention in biotechnology due to its high sensitivity to localised surface plasmon resonance of nanostructured metals. Trace detection of bio-molecules with large molecular weight remains challenging because treating SERS substrate using coupling or cross-linking agents is required. A new approach applied liquid-interface assisted SERS (LI-SERS) to realise label-free trace detection of bio-molecules. The results suggest it is promising for early-stage diagnosis of virus infection and Alzheimer's Disease.

The SERS technique may be used in the bio-medical field for disease diagnosis at an early stage and also in tumour therapy. Although the enhancement factor of SERS typically ranges from 10^6 to 10^8 due to the use of novel SERS substrates and methods, single-molecule detection by label-free SERS is impracticable because of SERS-blinking, the origin of this phenomenon is due to the escape of analyte molecules from hotspots. Moreover, bio-molecules, including deoxyribonucleic acid (DNA) and proteins, are difficult to detect directly by SERS. Additional treatments with a SERS substrate are needed to bind the bio-molecules.

LI-SERS can achieve a SERS enhancement factor greater than 10^{14} , much higher than the regular SERS method. The microfluidic SERS chip featured an Ag-Cu SERS substrate integrated into an embedded glass microchannel. Hybrid femtosecond (fs) laser processing is used to create the glass micro-channel.

The hybrid fs laser processing enables the creation of more complicated 3-D structures with enhanced functionalities for

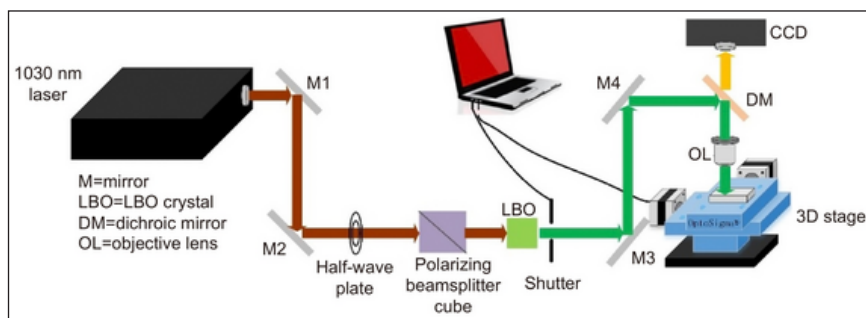


Figure 1. Schematic of laser fabrication system for microfluidic SERS chips. Credit: OEA

biochips, sensors and microelectronic devices. When the interface between the analyte solution and air on the SERS substrate in the microfluidic channel was irradiated by the Raman excitation laser, the LI-SERS intensity was increased by six orders of magnitude compared with regular SERS. The mechanism

of LI-SERS was attributed to the synergetic effect of the Marangoni flow induced by laser irradiation and optical trapping. That laser irradiation would direct the analyte molecules to the hot spots where the collected molecules are trapped by optical force. Consequently, the analyte molecules were immobilised

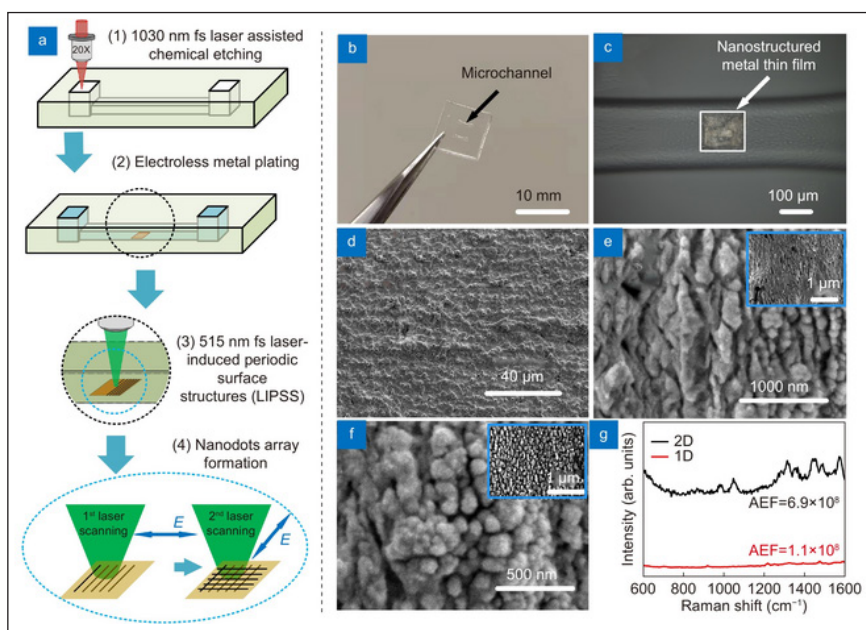


Figure 2. (a) Schematic of the fabrication; (b) photograph of microfluidic SERS chip; (c) optical microscope image showing the SERS substrate. SEM images of (d) original metal film, (e) ripples generated by first laser scanning and (f) nanodots generated by second laser scanning (insert: low magnification of SEM image). (g) Raman spectra of 10^{-9} M Rhodamine 6G (R6G) on 2-D (black) and 1-D (red) nanostructured SERS substrates. Credit: OEA

on the SERS substrate with the achievement of strong Raman scattering.

The researchers demonstrated that the LI-SERS method is applicable for more practical use. It is specifically useful for trace detection of label-free bio-molecules with large molecular masses, including DNA bases, DNA sequences and β -Amyloid ($A\beta$). Owing to the

ultrahigh sensitivity and self-immobilisation of LI-SERS, discrimination of DNA bases and DNA sequences with a detection limit of 1 fM was obtained without requiring additional treatments featuring coupling or cross-linking agents. Moreover, the LI-SERS technique can detect label-free $A\beta$, a biomarker of Alzheimer's Disease, at levels below 1 pM, and with a linear correlation

between the Raman signal and the $A\beta$ concentration in the range 1 nM to 1 pM being achieved. The label-free bio-sensing capability of LI-SERS offers great potential for the early-stage diagnosis of diseases in clinics.

Details of their work are published in *Opto-Electronic Advances* (doi.org/gqstnt).¹

New Raman study reveals how *E. coli* cells evade antibacterial treatment

Raman spectroscopy identifies *E. coli* persisters at single-cell level and reveals their metabolic activity.

The formation of persisters is an important feature of bacteria like *Escherichia coli* (*E. coli*). These noxious cells, being able to go dormant, are highly resistant to antimicrobial treatments and crucially account for various relapsing chronic infections with common symptoms such as severe stomach pain, vomiting and bloody diarrhoea. Formation of persister cells is thought to be one of the most important strategies of bacteria like *E. coli* for survival under drug treatment and harsh conditions. While little is known about how they form and work, primarily due to technical limitations in previous studies.

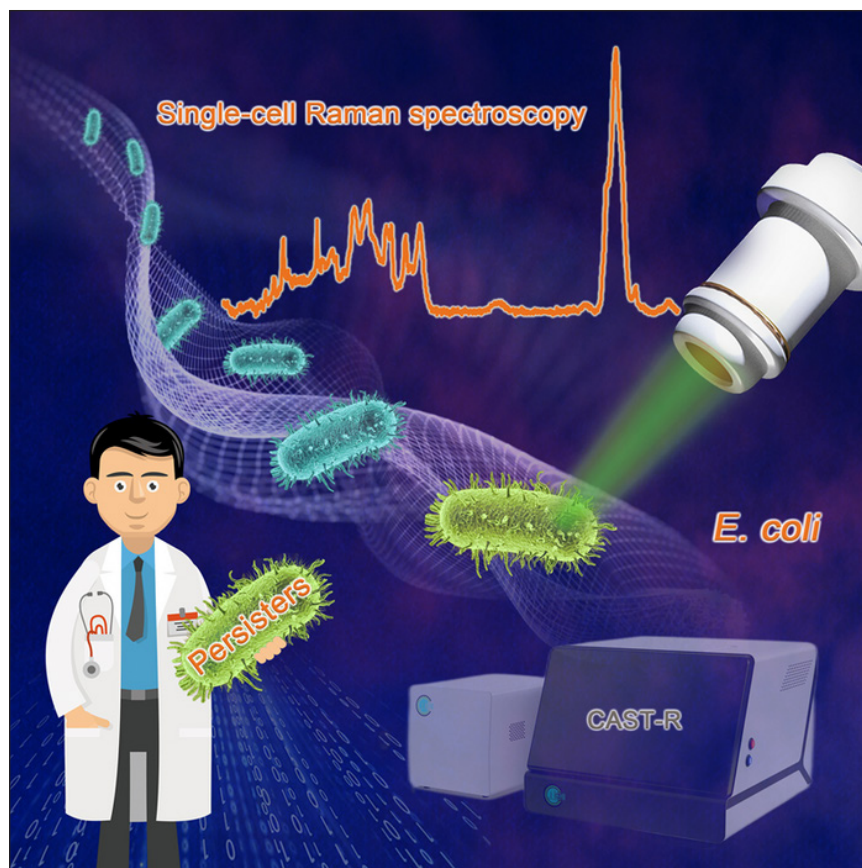
"Currently, majority of the work deals with persisters at the whole population level", said Dr WANG Chuan from The University of Hong Kong. "There are two significant improvements in our study. Firstly, the biochemical synthetic and metabolic activities of *E. coli* persister cells are analysed on the basis of their molecular quantity, instead of merely observing the dividing rate and/or growth state. Secondly, our observations arise from investigations on single cells rather than the 'average' level of the whole population of bacterial persisters."

Such focus on individual cells has been proved to be important for understanding how the persister

cells work. Researchers have used Raman spectroscopy to create a profile of the persister cells that can be used to subsequently identify similar cells.

Traditionally, persister cells have been considered to exist in a

dormant state, as they do not grow while undergoing stress like an antimicrobial treatment. However, researchers find that the metabolic activity of the *E. coli* persister cells is significantly higher than the reference strains of *E. coli*. "This




Raman spectroscopy identifies *E. coli* persisters at the single-cell level. Credit: LIU Yang

important new finding implies that persister cells remain to be active even in their dormant state, and this could be one of the crucial ways they are able to survive a high-dose antimicrobial treatment”, said Prof. JIN Lijian from The University of Hong Kong.

“Based on the advanced Raman spectroscopy technology, our study, published in *Frontiers in Microbiology* (doi.org/gqvm7g), has assessed for the first time the relative levels of biochemical synthesis in *E. coli* persister cells during their formation and resuscitation, indicating that these persister cells may develop intrinsic strategies via downregulating the replication rate while enhancing biosynthesis for survival and subsequent recovery”, said CHEN Rongze, a doctoral student from the Single-Cell Center, Qingdao Institute of Bioenergy and Bioprocess Technology (QIBEBT) of the Chinese Academy of Sciences.

Importantly, this novel study further reveals the metabolic activity of *E. coli* persists under different conditions and an increased level of their metabolic activities as compared to the reference strains of *E. coli*.

Looking ahead, the researchers are hoping that the current findings could lead to additional discoveries in the near future. “Indeed, we have developed a new instrument called CAST-R (Clinical Antimicrobial Susceptibility Test Ramanometry) to identify and characterise the persisters, so that the investigations can be extended to other pathogens and eventually applied in clinics, by disclosing the mechanisms of microbial pathogenicity for developing novel, personalised therapeutic strategies and approaches”, said Prof. XU Jian at the Single-Cell Center who co-led the study. 

Chemically sensitive lidar method

Combines photothermal spectroscopy and lidar, resolving chemical information by detecting sub-nm surface deformations due to photothermal absorption of a pump laser.

Researchers have developed a new laser-based technique that can simultaneously perform lidar and remote chemical measurements. Lidar, which stands for light detection and ranging, uses a laser to measure distances, or ranges. Adding chemical information to lidar measurements could be useful for applications such as remote chemical mapping, detecting trace amounts of chemicals, monitoring industrial processes and quality control.

“By mapping and identifying the composition of the environment, we can augment human interactions and industrial processes of the future with multi-dimensional object information beyond just ranging and detection”, detailed Bibek R. Samanta from Nokia Bell Labs.


The new technique, which combines photothermal spectroscopy and lidar, resolves chemical information by detecting sub-nanometre surface deformations due to photothermal absorption of a pump laser. These photothermal effects are caused by intensity modulations of the pump beam.

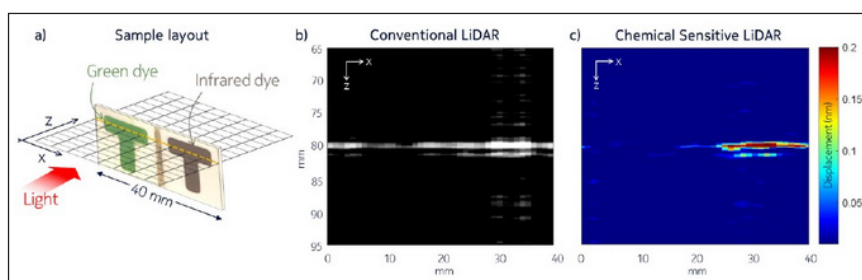
The researchers used a swept-source laser as a probe beam to perform a lidar scan in a frequency-modulated continuous wave configuration. The pump beam was a wavelength-stabilised infrared laser diode laser modulated using

a chopper wheel. Both beams were collimated, combined and focused on the same spot about 8 cm away. For this setup, the researchers estimated an axial resolution of about 150 μm in air and an imaging depth of about 30 cm.

The investigators tested their new approach by using a 3D printed transparent plastic block with 500- μm deep channels containing epoxy resin mixed with either a green acrylic colour or a near infrared (NIR) absorbing dye. They were able to observe surface displacements of 0.2–0.3 nm that resulted from photothermal absorption of the epoxy containing the NIR dye. This agreed with estimated values and was about an order of magnitude greater than the system’s baseline noise.

By scanning the sample laterally, the researchers created a chemically sensitive lidar scan that showed the location of the NIR dye but not the green acrylic resin. Although an infrared laser was used in this demonstration, other wavelengths could be used to identify other materials.

“Using tuneable laser systems and a fast-scanning integrated optical assembly, we plan on implementing spectroscopic identification of common household materials to create a 5D map of the environment”, Samanta further explains. 



Results of displacement obtained from Fourier transform of the phase modulation of 1D scan of the sample. Credit: Nokia Bell Labs

Watching the fate of molecular nitrogen with fs soft X-ray spectroscopy

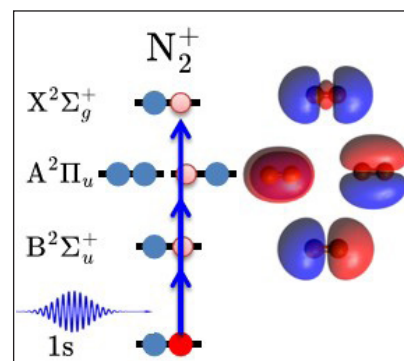
Femtosecond soft X-ray spectroscopy has been used to understand lasing in the forward direction in air upon focusing intense femtosecond light pulses.

The observation of lasing in the forward direction in air upon focusing intense femtosecond light pulses has been a puzzling phenomenon since first observations were reported about two decades ago. Current understanding is that single ionised nitrogen molecules N_2^+ , that are generated by the intense 800 nm laser pulses, are responsible for the lasing at 391 nm or 428 nm. An intense scientific debate has resulted in several models being proposed that all involve three electronic states of N_2^+ , the X, A and B states (see image), with additional roles of vibrational and/or rotational degrees of freedom. Scientists at the Max Born Institute of Nonlinear Optics and Short Pulse Spectroscopy have shed new insight on this using novel ultrashort soft X-ray spectroscopy, with their results published in *Physical Review Letters* ([doi.org/jmmz](https://doi.org/10.1103/PhysRevLett.128.103001)). Standard models for ionisation, population dynamics and lasing do not comply with the obtained results. Instead, the experimental measurements strongly point to a coherent polarisation interplay between the B, X and A states.

The use of ultrashort laser pulses to induce and study ionisation phenomena of small molecules is well established. Typically, the large electric field of a short intense pump pulse causes the ejection of an electron out of a molecule. Often several electronic excited states of the molecular ion may result, where the standard tunnel ionisation mechanism predicts that the degree of excitation will be inversely proportional to the excitation energy (see Figure). For molecular nitrogen this would mean the X ground state will have a higher population than the A and B states. The basic rule for the lasing

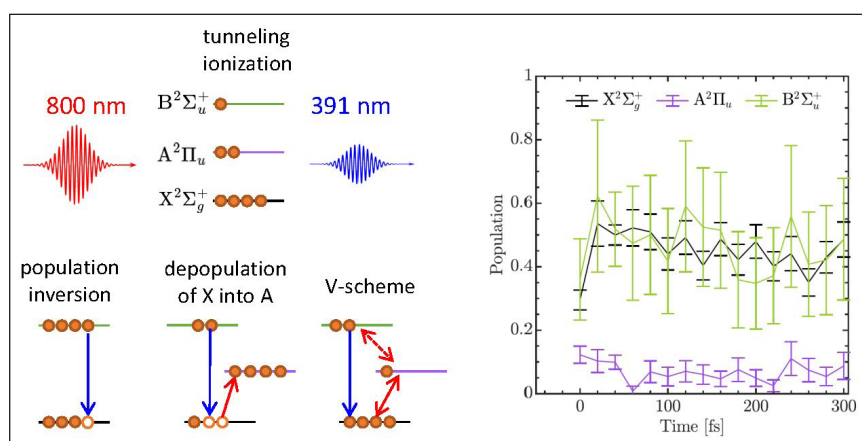
phenomenon, utilised in lasers (light amplification of stimulated emission of radiation), however, is that the population of the excited state should be higher than that of the ground state. For the N_2^+ molecules, this means a higher population in the B state than in the X state would be a necessary condition, contradicting the standard tunnel ionisation model. An experimental verification of the time-dependent population of all three electronic states, that are understood to play a key role in lasing in ionised molecular nitrogen, has until now been lacking. One reason for that is that population changes of the X, A and B states could only be deduced from indirect probing at particular transitions between individual electronic states.

A state-of-the-art table-top laser-based system generating ultrashort



Watching the fate of molecular nitrogen with X-rays, when an electron has been kicked out. Copyright: MBI / E.T.J. Nibbering / C. Kleine


soft X-ray pulses tuned at the nitrogen K-edge has now been used at the Max Born Institute to simultaneously probe the time-dependent population of the X, A and B states (see Figure). Here the transitions of the 1s core to the valence



Level scheme showing the electronic X, A and B states of N_2^+ . Standard tunneling ionisation by the 800 nm pump pulse cannot induce a population inversion between the X and B states, necessary for lasing at the $B \rightarrow X$ transition at 391 nm, shown by blue arrows. Population inversion may occur when the X state gets depopulated by rapid transfer to the A state, as shown with the red arrow. Another possibility is the simultaneous coupling of the 800 nm and 391 nm light fields coupling the three electronic states in a V-level scheme, for which lasing can occur with population inversion. Ultrafast nitrogen K-edge spectroscopy upon strong field ionisation of molecular nitrogen, where the transient population of the X and B states are found to be of similar magnitude while that of the A state remains minor, strongly points to the occurrence of the V-level scheme mechanism. Copyright: MBI / E.T.J. Nibbering / C. Kleine

orbitals of N_2^+ are monitored in real-time. It turns out that directly after the ionisation event the B state has a similar degree of excitation as the X state, while the population of the A state remains remarkably low. With these results the role of the A state as a possible reservoir for a depletion of the X ground state can be excluded. Instead, a coherent interplay of the light fields of the

ionising pump pulse at 800nm and the lasing light field at 391nm wavelengths, coupling the B, X and A states in a so-called V-scheme (see image), is the most plausible underlying mechanism for the observation of lasing in air upon interaction with intense femtosecond laser pulses. Such a interaction scheme enables the so-called lasing without population inversion mechanism.

The potential of the table-top laser-based experimental femto-second soft X-ray spectroscopic method demonstrated by the team at the Max Born Institute will be further capitalised on by exploration of light induced molecular phenomena on time scales of the elementary steps in molecular rearrangements, in the gas phase and in solution phase. 

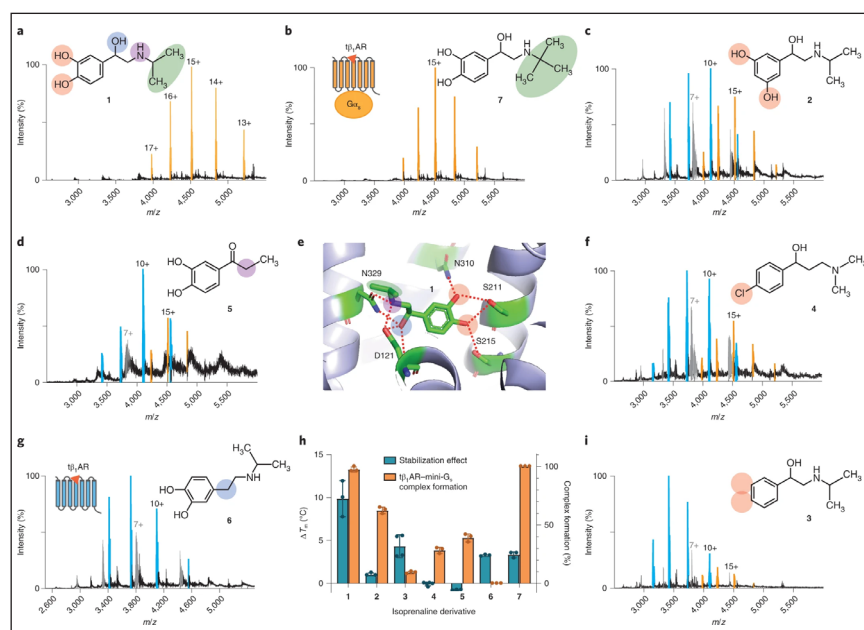
Benefits of native MS in the interrogation of target ecosystems and drug discovery

Native mass spectrometry is shown to be able to interrogate the pharmacology of the beta-1 adrenergic receptor, a G protein-coupled receptor, and has discovered the endogenous zinc ion as a positive allosteric modulator in well-studied receptor.

In a new publication in *Nature Chemistry* (doi.org/jmm7), the authors demonstrate how native MS can be used to investigate the pharmacology of GPCRs using the beta-1 adrenergic receptor (β_1AR) as a model system. Being able to combine the sensitivity and near atomic mass resolution of the mass spectrometer, whilst preserving the receptor-G protein interactions, allowed the authors to monitor, with high sensitivity, the full spectrum of receptor pharmacology *in vitro*. Due to mass differences between different G proteins, the authors were also able to distinguish if a ligand is able to promote biased signalling towards a specific pathway.

The authors also discovered an endogenous zinc molecule associated with the receptor. This cation was shown to be a positive allosteric modulator of β_1AR and demonstrates the potential for native MS to uncover novel insights that may be important for drug discovery. As an example, the regulation of zinc binding or mimicking its mechanism with a small molecule may provide a new avenue for modulating the kinetics or signalling of β_1AR for therapeutic purposes.

These examples highlight two key benefits of utilising native MS



Interrogating the structure–function relationship of isoprenaline derivatives by native MS. a–d,f,g,i, Representative MS spectra of purified β_1AR complexed with mini-Gs in the presence of various isoprenaline derivatives: isoprenaline (a), colterol (b), orci-prenaline (c), 3,4 dihydroxypropiophenone (d), 1-(4-chlorophenyl)-3-(dimethylamino)propan-1-one (f), isopropylidopamine (g) and 1-phenyl-2-(2-propylamino)ethan-1-ol (i). The peaks assigned to the receptor–mini-Gs complex, receptor monomer and mini-Gs are highlighted in orange, blue and grey, respectively, alongside the annotations of their charge states. The structures of the isoprenaline derivatives are illustrated and numbered alongside each spectrum. e, Structure of β_1AR complexed with isoprenaline, showing the critical interactions between the receptor and isoprenaline, denoted by red dashed lines. h, Impact of isoprenaline derivatives on the thermostability and extent of complex formation assessed by MS. Purified β_1AR was pre-incubated with various isoprenaline derivatives before the thermostability assay, and the effect of different isoprenaline derivatives on the degree of stabilisation was determined by the difference in the protein melting point in the presence and absence of isoprenaline. The dots refer to the individual data points and the error bars in h represent the mean \pm s.d. Reproduced from <https://doi.org/10.1038/s41557-022-01041-9> under a CC BY licence.

within drug discovery, namely: reconnecting the two fundamental drivers of pharmacology, binding and function; and interrogation of a native ecosystem with high precision.

Professor Dame Carol Robinson, co-founder of OMass Therapeutics and Chair of the Scientific Advisory Board said: “Our findings

demonstrate that native MS can be used to reconnect the two fundamental drivers of pharmacology, binding and function. From a practical viewpoint, GPCRs had represented a major challenge for native MS. Overcoming these difficulties has allowed us to monitor attenuated G-protein coupling, driven by a wide range of ligands, highlighting

the sensitivity and robustness of our approach. I am also delighted that despite the fact that β_1 AR is a well-studied receptor, we were able to find a previously unknown endogenous zinc molecule associated with the receptor, which could have implications for the design of new allosteric modulators.”¹

LC-MS and EC unlock a new method for testing protein-based drugs

Liquid chromatography-mass spectrometry and an electrochemical flow cell could spark a “paradigm shift” in biopharmaceuticals testing.

New Jersey Institute of Technology (NJIT) researchers have unveiled a new technique using liquid chromatography-mass spectrometry (LC-MS) and an electrochemical (EC) flow cell which they say represents a “paradigm shift” in how pharmaceutical laboratories test and produce new protein-based drugs, such as therapeutic monoclonal antibodies being developed to treat a variety of diseases, from cancers to infectious diseases.

The researchers say their electrochemistry-based approach could allow for safety and quality testing of up-and-coming biotherapeutics to be done at a fraction of the time required by conventional methods, which typically require the lengthy and costly production of certain biomaterials used for sample testing.

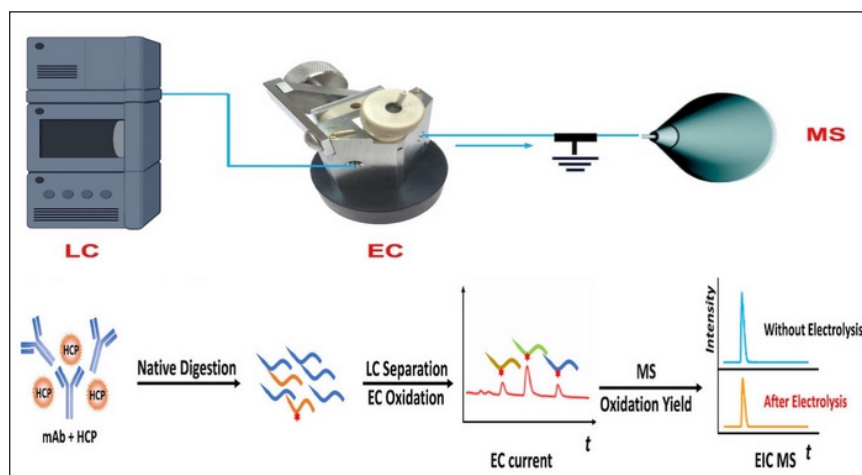
“This method we’ve developed at NJIT has the potential to have a major impact in quantitative proteomics, and it represents a paradigm shift in pharmaceutical industry in terms of monitoring biopharmaceutical product and process impurities for quality control”, said Hao Chen, professor at NJIT’s Department of Chemistry and Environmental Sciences. “With this study, we’ve now demonstrated an approach that can quantify drug product and process impurities much more quickly and

accurately than had been possible. ... We expect it to become very useful to facilitate therapeutic protein and vaccine development for treatment and prevention of different diseases in the future.”

Traditionally such testing, or protein quantitation, involves time-consuming preparation of synthetic isotope-labelled peptides which are used as internal standards to measure total protein concentrations in a sample—helping researchers actively monitor the efficacy and safety of therapeutic protein components throughout the drug development process. To overcome this limitation, Chen’s lab developed

a coulometric mass spectrometry (CMS) approach for absolute quantitation of proteins without the use of standards. The method instead applies liquid chromatography-mass spectrometry and an electrochemical flow cell to rapidly quantify and detect changes in target proteins or peptides based on electrochemical signatures.

“Instead of waiting for weeks to obtain standards or reagents in traditional approaches, one could carry out CMS quantitation experiments right away. Thus, it would facilitate tracking drug impurities discovered during the process and ensure their effective clearance



Workflow of the NJIT team’s CMS method, combining liquid chromatography (LC), electrochemical oxidation (EC) and mass spectrometry (MS)-based quantitative measurement of protein abundance. Credit: NJIT

with process optimisation and control”, said Chen.

“Such an apparatus allows us to separate peptides after protein digestion with liquid chromatography, monitor peptide oxidation in the electrochemical flow cell to produce an electric current and measure the oxidation yield with mass spectrometry”, explained NJIT PhD student Yongling Ai. “The combination of electric current signals along with the oxidation yield provides sufficient information for absolute quantitation of peptides and proteins.”

In their study, published in *Analytical Chemistry* (doi.org/gqwmf7), the team demonstrated its CMS method by achieving absolute quantitation of multiple proteins (β -lactoglobulin B, α -lactalbumin and carbonic anhydrase) in a mixture in one run, without using any standards. Notably, the team also showcased the

method's capabilities for detecting protein deamidation—a common degradation event in therapeutic proteins resulting from physical or chemical stresses throughout the manufacturing process and storage.

The team successfully quantified several protein degradation products, including a key intermediate of protein degradation, the formation of succinimide, which has never been done before with absolute quantification due to lack of standards, according to the researchers.

“The lack of standards is caused by the challenges in their *de novo* synthesis”, said Chen. “Being able to accurately quantify the deamidation products and intermediates could provide better understanding of therapeutic protein degradation, and potentially create a new way to investigate disease pathologies and aging processes.”

Now, Chen's lab plans to apply their new method for large-scale

quantitation of thousands of proteins in one run. They also plan to improve the sensitivity of their CMS analysis to allow quantifying very low levels of proteins in complex biological samples, which could benefit research efforts ranging from clinical diagnostics and drug discovery to precision medicine for which identification and quantitation of samples at the molecular level is necessary.

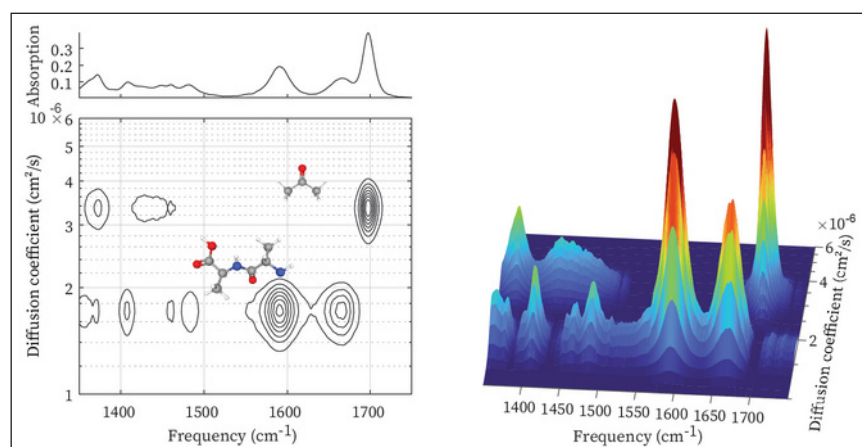
“As proteins perform a vast array of functions within organisms, the importance of absolute protein quantitation is hard to overstate”, said Chen. “CMS should speed up processes for disease diagnosis, drug discovery and development, and it now opens a new door for biologists and biochemists to explore quantities of proteins in the human body that may serve important biological functions or roles as disease biomarkers and drug targets.”

New experimental method IR-DOSY reveals molecular structure and size

Infrared Diffusion-Ordered Spectroscopy separates molecules with different sizes into distinct sets of infrared peaks.

Researchers at the University of Amsterdam have developed a novel approach to infrared spectroscopy that enables simultaneous characterisation of molecular structure and size. Called Infrared Diffusion-Ordered Spectroscopy (IR-DOSY), the method nicely separates molecules with different sizes into distinct sets of infrared (IR) peaks. The researchers foresee analytical applications in fields as diverse as proteins, polymers, pharmaceuticals and biomedicine. They are currently developing a first version of a practical chemical probe implementing the IR-DOSY concept.

Infrared spectroscopy is an important workhorse in the analysis of chemical compounds. It helps to identify molecules based on their functional groups and



IR-DOSY spectra of a mixture of acetone and dialanine, showing which IR peak belongs to which compound. Credit: HIMS

spatial conformation. In general, IR spectroscopy is not sensitive to the size of the molecules. Inspired by an already existing approach in

NMR spectroscopy, the Amsterdam researchers now applied the principle of diffusion ordered spectroscopy to IR. Here, the molecules

present in a sample are separated based on their diffusion behaviour prior to spectral analysis. IR-DOSY relies on the fact that the diffusion of a molecule is determined completely by its size—a concept that was first established by Albert Einstein in his 1905 classic paper on the Brownian motion of microscopic particles.


The IR-DOSY spectrometer creates a spatially inhomogeneous distribution of solute molecules using a simple yet effective flow method that transports both the mixture and pure solvent into a sample chamber. After stopping the flow, the solute molecules start to diffuse into the pure solvent region, at a rate that depends on their diffusion coefficient. The IR absorption is measured at a position in the chamber where there was initially only solvent. As time progresses, the diffusing solute molecules start appearing in the IR beam. In this way, for all types of molecules the individual IR spectra are recorded at different moments in time, depending on their sizes. IR-DOSY thus produces a two-dimensional spectrum with the IR frequency along one axis and the diffusion constant

(or equivalently, the size) along the other axis.

The researchers argue that although the separating power of IR-DOSY is less than that of typical chromatographic methods, it has the advantage that no prior knowledge is required of the chemical structure of the compounds present in the sample. The separating power might even be increased by adding an electrophoresis device to actively separate the species in the sample solution.

Among the anticipated applications are the analysis of protein aggregates and fibrils. Here, IR-DOSY makes it possible to simultaneously investigate monomers, oligomers and fibrils, which typically coexist in a sample. Polymers and plastic nanoparticles constitute another interesting field of research since samples usually contain many different molecules of many sizes. The size-selectivity and structure-sensitivity could also render IR-DOSY useful in the pharmaceutical and biomedical domains. For instance, it has potential to detect trace amounts of small molecules present in pharmaceutical products.

In the biomedical context, it could for instance be used to detect and structurally characterise low-molecular weight species in human blood serum. In all cases, the IR-DOSY analysis provides valuable information about the size or size distribution of the molecules or molecular aggregates in a sample.

The IR-DOSY method was developed in a joint effort of the university's Institute of Physics and the Van 't Hoff Institute for Molecular Sciences, and reported in *Angewandte Chemie* (doi.org/gq44b8). At the latter, Professor Sander Woutersen and Dr Giulia Giubertoni, in collaboration with Dr Saer Samanipour, are now further developing the method into a cost-effective device that can be used by researchers from different disciplines in any laboratory as an analytical or diagnostic tool. For this they were recently awarded a €160,000 "Demonstrator Grant" by the Dutch Research Council NWO. Development of the probe is a joint effort in cooperation with the university's Technology Centre, the technology transfer office IXA and Demonstrator Lab Science Park. 

IR scattering-type scanning near field microscopy reveals Stradivarius violins' secret

IR s-SNOM has shown that the layer between the wood and varnish of two Stradivarius violins contained protein-based compounds, congregating in nano-sized patches.

Stradivarius violins produce elegant music with a level of clarity that is unparalleled by modern instruments, according to some musicians. And it's the finishing touches, mysterious treatments applied hundreds of years ago by Antonio Stradivari, that contribute to their unique look and sound. In a step toward unravelling the secret, researchers report on a nanometre-scale imaging of two of Stradivari's violins, revealing a protein-based layer between the wood and varnish.


Previous studies have reported that some stringed instruments crafted by Stradivari have a hidden coating underneath the shiny varnish. This coating's purpose would have been to fill in and smooth out the wood, influencing the wood's resonance and the sound that's produced. Knowing the components of this film could be key to replicating the historic instruments in modern times. So, Lisa Vaccari, Marco Malagodi and colleagues wanted to find a technique that

would determine the composition of the layer between the wood and varnish of two precious violins—the San Lorenzo 1718 and the Toscano 1690.

Using a technique previously used on historic violins, synchrotron radiation Fourier-transform infrared spectromicroscopy, the team found that both samples had an intermediary layer, but this method couldn't differentiate the layer's composition from the adjacent wood. Then they turned to infrared scattering-type scanning



A nanometre-scale imaging technique has revealed a protein-based layer between the wood and the varnish coating of these two Stradivarius violins. Credit: Adapted from *Analytical Chemistry*, doi: [10.1021/acs.analchem.2c02965](https://doi.org/10.1021/acs.analchem.2c02965)

near field microscopy (IR s-SNOM) to analyse the samples. The IR s-SNOM apparatus includes a microscope that collects images tens of nanometres wide and measures the infrared light scattered from the coating layer and the wood to collect information about their chemical composition. The results of the new method, published in *Analytical Chemistry* (doi.org/gq4m8k), showed that the layer between the wood and varnish of both instruments contained protein-based compounds, congregating in nano-sized patches. Because IR s-SNOM provided a detailed 3D picture of the types of substances on the violin's surface, the researchers say that it could be used in future studies to identify compounds in complex multi-layer cultural heritage samples. 

Mössbauer spectroscopy unlocks properties of pyroxenes

Calcium content determines the peak intensity ratio due to iron ions at Mössbauer spectra in pyroxene.

Pyroxenes are a major group of rock-forming silicate minerals that generally contain calcium, magnesium and iron. Given their abundance, elucidating the physical properties of pyroxenes is deemed vital in the study of rocks and minerals. A research group led by Professor Keiji Shinoda from the Graduate School of Science at Osaka Metropolitan University investigated the status of iron ions in monoclinic pyroxenes, a type of calcium-rich pyroxenes, using Mössbauer spectroscopy on thin sections of single crystals. Their study revealed that in pyroxene crystals consisting of roughly 50% calcium, the tensor that determines the ratios of iron ions at the Mössbauer spectral peaks in the M1 sites—one of two types of cation positions in the pyroxene crystal structure—is independent



Using Mössbauer spectroscopy, Osaka Metropolitan University scientists investigate the iron ion status of pyroxenes, a major group of rock-forming silicate minerals. Their study revealed that in pyroxene crystals consisting of roughly 50% calcium, the tensor that determines the ratios of iron ions at the Mössbauer spectral peaks is independent of the iron content but dependent on the calcium content.

of the iron content but dependent on the calcium content.

The results of this research have clarified one of the physical properties of pyroxenes. These findings, published in *Journal of Mineralogical and Petrological Sciences* (doi.org/gq3pnw), might facilitate detailed future analysis of iron

using Mössbauer spectroscopy on mineral flakes.

“We had expected that the tensor that determines the ratios at the Mössbauer spectral peaks would change if the iron solid solution component changed”, explained Professor Shinoda. “However, we were surprised to find that

the tensor properties actually varied according to the content of calcium, rather than that of iron. This study’s findings provide practical data for researchers who are conducting detailed analysis of iron by Mössbauer spectroscopy on mineral flakes.”

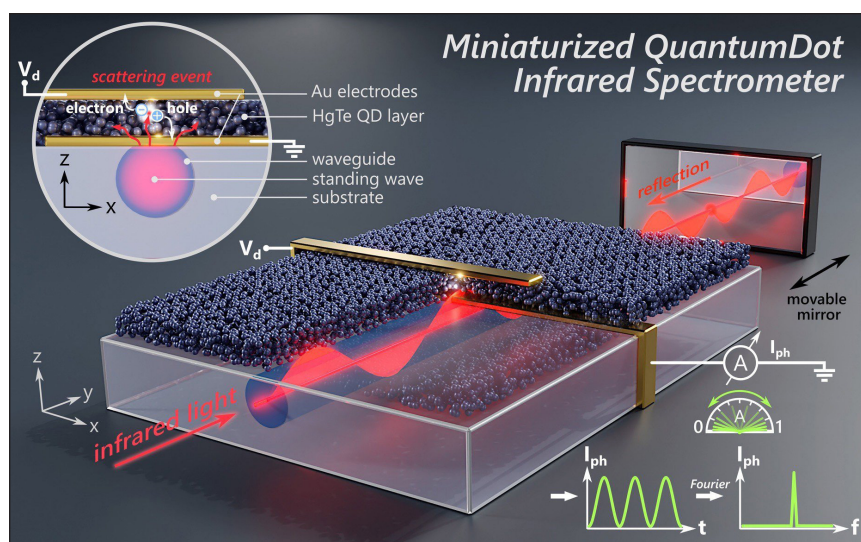
Miniaturised infrared detectors on a chip

A proof-of-concept miniaturised Fourier transform waveguide spectrometer that incorporates a sub-wavelength photodetector as a light sensor has been built.

Miniaturisation of infrared spectrometers will lead to their wider use in consumer electronics, such as smartphones, enabling food control, the detection of hazardous chemicals, air pollution monitoring and wearable electronics. They can be used for the quick and easy detection of certain chemicals without using laboratory equipment. Moreover, they can be useful for the detection of counterfeit medical drugs as well as of greenhouse gases such as methane and CO₂.

A team of scientists at Empa, ETH Zurich, EPFL, the University of Salamanca, Spain, the European Space Agency (ESA) and the University of Basel have built a proof-of-concept miniaturised Fourier transform waveguide spectrometer that incorporates a sub-wavelength photodetector as a light sensor, consisting of colloidal mercury telluride (HgTe) quantum dot and compatible with complementary metal-oxide-semiconductor (CMOS) technology.

The resulting spectrometer exhibits a large spectral bandwidth and moderate spectral resolution of 50 cm⁻¹ at a total active spectrometer volume below 100 μm × 100 μm × 100 μm. This ultra-compact spectrometer design



This is how the IR spectrometer works: the photodetector, fabricated on top of a surface optical waveguide, consists of a bottom gold electrode at the bottom functioning as a scattering centre, a photoactive layer (consisting of colloidal mercury telluride (HgTe) quantum dots) and a top gold electrode. By moving the mirror, the measured photocurrent maps the light intensity of the standing wave, i.e. the IR light. A Fourier transformation of the measured signal gives the optical spectra. Image: Lars Lüder

allows the integration of optical-analytical measurement instruments into consumer electronics and space devices and is detailed in *Nature Photonics* (doi.org/gq4mf6). “The monolithic integration of subwavelength IR photodetectors has a tremendous effect on the scaling of Fourier-transform

waveguide spectrometers”, says Empa researcher Ivan Shorubalko. “But this may also be of great interest for miniaturised Raman spectrometers, biosensors and lab-on-a-chip devices as well as the development of high-resolution snapshot hyperspectral cameras.”

Monitoring cereal bar moisture with HSI: the light source matters

A new study has compared three different illumination systems for moisture prediction using hyperspectral imaging in the visible-near infrared range.

Breakfast, mid-afternoon snack, post-exercise boost? The range and availability of cereal bars has grown enormously in the last years. Whether you like yours moist or on the dry side, consistency is essential. Hyperspectral imaging can be used on the production line to monitor the moisture content; in fact, this should be a fairly simple application with the presence of water bands in the near infrared (NIR). However, there is a drawback. The standard light source is a stabilised-halogen one; these are both expensive and produce significant amounts of heat that can actually dry the cereal bars being analysed!

A new study, published in *Journal of Spectral Imaging* (doi.org/jmm4), has compared three different illumination systems for moisture prediction in the visible-near infrared (vis-NIR) range (from 400 nm to 1000 nm). The hyperspectral images were acquired using three illumination systems including two halogen-based systems (stabilised-halogen and conventional-halogen) and an LED-based



illumination system. The results showed that halogen-based illumination systems combined with a partial least squares model better predicted moisture in bars. Lower accuracies were obtained when the experiment was performed with an LED-based illumination system, which showed double the error of the halogen-based systems. It was concluded that this

is a consequence of the information lost in bands appearing above 850 nm that may be revealing information about the moisture in bars since the second overtone of the water O-H is found at 970 nm. The results demonstrate that conventional halogen-based light systems in the vis-NIR range are a promising method for moisture prediction in cereal bars. ¹

NIR spectroscopy reveals factors relating to hybrid rice eating quality

A high-throughput single-grain quality NIR detection platform has helped evaluate the eating quality of hybrid rice.

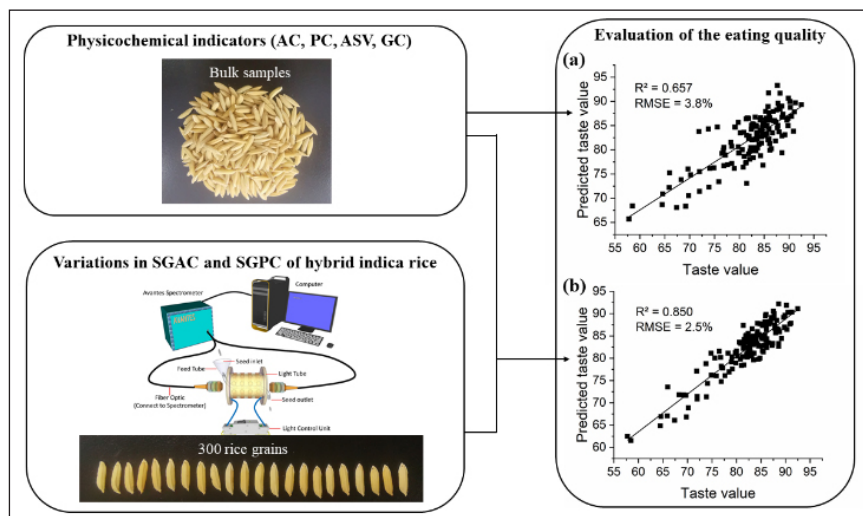
A novel single-grain composition analysis technology has recently been developed to help evaluate the eating quality of hybrid rice, according to a research team led by Prof. WU Yuejin from the Hefei Institutes of Physical Science of the Chinese Academy of Sciences. They found that the eating quality of hybrid rice was not only related to the chemical composition of the rice, but was also influenced by the

variation in single-grain chemical composition.

Rice is one of the major food crops worldwide. Amylose, protein and fat are important quality traits of rice and have important effects on eating quality, storage quality and processing quality. Near infrared (NIR) spectroscopy has the advantages of being non-destructive, rapid and non-polluting in detecting crop quality, but it is hard

to achieve high-throughput accurate detection of single-grain quality traits in isolated populations for genetic breeding.

In their previous study, the researchers designed and manufactured an intelligent single-grain crop quality detection and sorting instrument. Based on this high-throughput single-grain quality NIR detection platform (2–3 grains/second), they developed models



The eating quality model of hybrid indica rice established with physicochemical indicators as independent variables (a), the dispersion indicators of single-grain composition and physicochemical indicators as independent variables (b). (Image by FANG Shuang)

to explore the best conditions for detection and sorting. Accordingly, they determined the amylose and fat content of individual rice grains. They compared the data under two different conditions. Under static measurement conditions. The coefficient of determination (R^2) values were 0.886 and 0.743 for the modelling of amylose and fat

content. And under dynamic measurement conditions, R^2 values were 0.666 and 0.765.

“The process was rapid and non-destructive”, said CHENG Weimin, “and when evaluating the eating quality of hybrid rice, we found the reasons for the varying eating quality of hybrid rice using single-grain quality trait analysis techniques.”

According to the researchers, high-quality hybrid rice has the following characteristics: first, the physicochemical indicators for a large sample size meeting the national standards were the determining requirement, and second, a small variation in the single-grain composition was important.

R^2 of the eating quality model increased from 0.657 to 0.850 when the single-grain composition variations were added to the independent variables (amylose content, protein content, alkali spreading value and gel consistency). In addition, the effect of sterile lines on the eating quality of hybrid rice was greater than that of restorer lines, so selecting high-quality sterile lines was particularly important for the selection of good-tasting combinations.

This is a new method to evaluate the eating quality of hybrid rice and laid the foundation for high yield and quality breeding of hybrid rice. It was reported in *Agriculture* (doi.org/gqzq4b).¹

NIR spectroscopy for non-invasive intracranial pressure monitoring

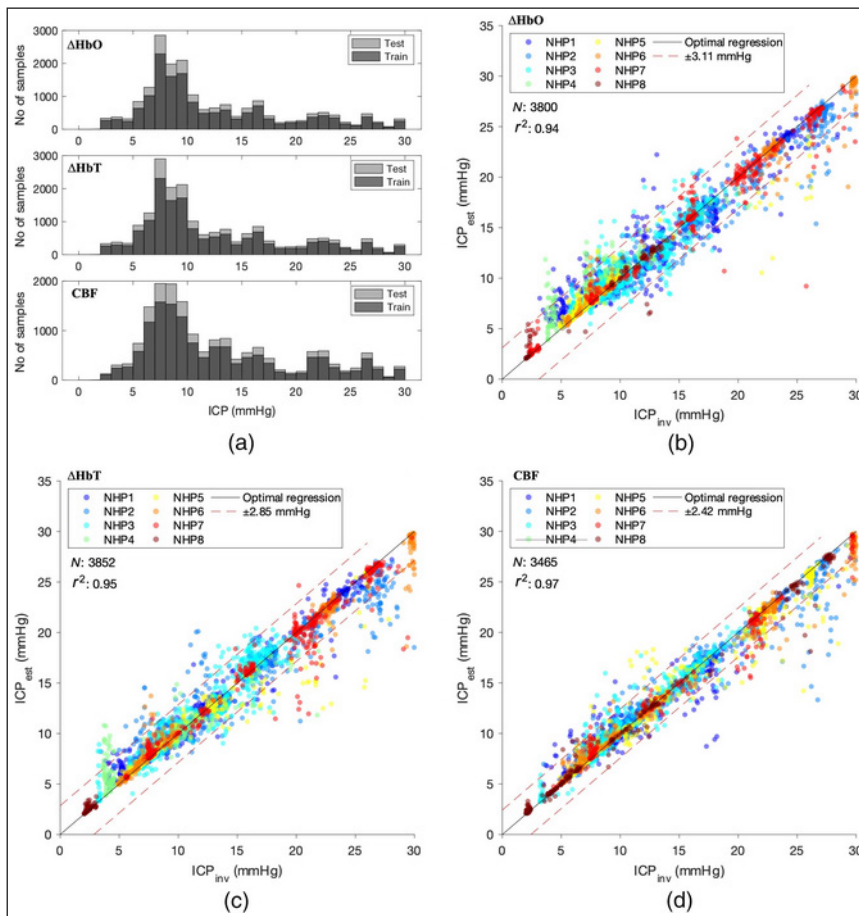
A novel algorithm estimates intracranial pressure based on haemoglobin levels using near infrared spectroscopic cardiac pulse waveforms.

An increase in intracranial pressure (ICP) is a dangerous condition that can be caused by brain bleeds, a brain tumour, cerebral oedema, traumatic brain injury and hydrocephalus. ICP monitoring is thus a key aspect of patient care in patients with these disorders. Additionally, ICP measurements are relevant when estimating cerebral perfusion pressure (CPP), an indicator of cerebral autoregulation (CA). CPP is linked to neuronal function and neurovascular coupling, and CA defines how the brain maintains a constant blood flow. Given

these broad implications and applications in clinical decision-making, precise ICP monitoring is a vital patient management tool. While current tools for ICP monitoring are precise, they can cause haemorrhage or infections and are time-consuming. Although non-invasive alternatives exist, they have limitations such as poor generalisability, low predictive capacity and a lack of reliability. Diffuse correlation spectroscopy (DCS) and near infrared (NIR) spectroscopy are emerging as promising non-invasive solutions. Notably, NIR spectroscopy

has several advantages over other non-invasive methods—low cost, bedside compatibility for long-term and continuous monitoring, along with user independence.

Researchers at Carnegie Mellon University (CMU) have successfully deployed a NIR spectroscopy device to continuously monitor haemoglobin concentration changes. The team built on previous research in which they estimated ICP from cardiac waveform features measured using DCS, and also identified the correlation between relative changes in



The CMU research team evaluated ICP estimator performance on NIR spectroscopy derived average cardiac waveforms (ΔHbO and ΔHbT) against its performance on DCS-based average cardiac waveforms (cerebral blood flow or “CBF”). (a) Histogram of ICP distribution for both train and test sets across all three modalities. More data were available at lower ICP values, especially between 5 mmHg and 10 mmHg. (b)–(d) Correlation plots for ΔHbO , ΔHbT and CBF. Strong coefficient of determination (r^2) for all methods indicates that the model performs well on ICP estimation. Credit: Relander *et al.*, doi: [10.1117/1.NPh.9.4.045001](https://doi.org/10.1117/1.NPh.9.4.045001)

oxyhaemoglobin concentration and ICP. To measure ICP using the NIR spectroscopy data, they developed and trained a random forest (RF) regression algorithm to correlate the morphology of cardiac pulse

waveforms obtained through NIR spectroscopy with intracranial pressure.

To validate their algorithm, they conducted preliminary tests in a preclinical model. They measured

fluctuations in invasive ICP and arterial blood pressure while profiling the changes in haemoglobin concentrations. Following this, they examined the performance of signals derived from the haemoglobin concentration and CBF to accurately verify the precision of their algorithm.

From a proof-of-concept standpoint, the results were very promising. There was a high correlation between the ICP estimated using the RF algorithm and the actual ICP measured using invasive techniques. “We showed, by validating the findings with invasive ICP data, that the trained RF algorithm applied to NIR spectroscopy based cardiac waveforms can be used to estimate ICP with a high degree of precision”, explains Jana Kainerstorfer, Associate Professor of Biomedical Engineering at CMU. Furthermore, the results, published in *Neurophotonics* (doi.org/gq4f54), indicated that the RF algorithm could interpret waveform features extracted from both NIR spectroscopy and DCS, highlighting its useability.

The parameters used in the algorithm can be obtained from NIR spectroscopy measurements, combined with electrocardiograms and mean arterial blood pressure, which are regularly used for clinical evaluation. Thus, if this RF-based platform can produce robust ICP measurements in subsequent human trials, its potential for clinical use would be tremendous. 📈

Clinical LC-MS methods for therapeutic drug monitoring analysis

Shimadzu and Germany's University Medical Center Göttingen are developing new clinical LC-MS methods for a more rapid and flexible therapeutic drug monitoring analysis.

Shimadzu is collaborating with the University Medical Center Göttingen (UMG), one of Germany's leading university medical facilities. The collaboration will focus on the development of new clinical laboratory methods using liquid chromatography-mass spectrometry (LC-MS) for therapeutic drug monitoring (TDM) analysis.

TDM plays a vital role in providing precision medical care. TDM analysis measures the concentration of drugs currently in the blood to determine the required next dosage of a drug, e.g. antibiotics, antiepileptics, antidepressants etc. That means that it is especially important for a clinical laboratory to test a sample and return the result to the doctor as swiftly as possible. This is especially true for emergency patients who require special treatment. Because the standard dosage may not meet their needs in intensive care units, rapid test results are crucial for doctors to properly treat patients and save lives.

The conventional method for conducting TDM tests has been to use an immunoassay. More recently, however, clinical laboratories have been turning to LC-MS systems for this purpose. Among the advantages of LC-MS are greater accuracy and flexibility. Despite this overall superiority, methods using LC-MS have previously been difficult to apply in emergency cases because of the complexity of sample preparation. For instance, the flexibility of




Dr rer. nat. Frank Streit, Head of Clinical Research, University Medical Center Göttingen

the LC-MS system also means that each target group of drugs requires its own column, mobile phase and analysis conditions such as temperature. This means that it can take time to switch methods to start a new sample analysis. And that can make it difficult for a clinical laboratory to quickly return analysis results to the doctors who need them.

However, Shimadzu's CLAM-2030 has shown great potential in simplifying, streamlining and speeding up LC-MS testing. CLAM-2030 is a fully automated sample preparation module for LC-MS. Lab technicians simply place blood collection tubes in position and the module automatically performs

sample pretreatment steps up to LC/MS/MS analysis.

Further developing and testing this potential will form the core of the new collaboration between Shimadzu and UMG. Working together with Professor Andreas Fischer, Dr Frank Streit and other leading experts at UMG, new methods for multiple target groups of drugs will be developed. The team will also use CLAM-2030 to optimise these new methods so that clinical laboratories can switch methods easily and flexibly—and most importantly quickly. This will mean that the more accurate results of LC-MS testing can be used by doctors more rapidly than ever before. 

John Hollerton: a life in industrial analytical spectroscopy, part 1

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

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

^bMASS Informatics, Harpenden, UK

^cHollerton Scientific Software Consultancy, St Albans, UK

Mohan Cashyap mentioned to me recently that an old colleague, John Hollerton, was retiring from a long career at GSK and that we ought to take this opportunity to have a chat with him. Great idea I thought. John is not only a leading industrial analytical scientist, but I know from working with him, Mohan and Ian Michael in the past on the LISMS conference (Linking and Interpreting Spectra through Molecular Structures) that he is also an innovative ideas man with some interesting stories. In fact, our online chat ran well beyond the time we had allocated and was full of insightful observations for industrial colleagues, software and hardware vendors, educators as well as any scientist looking to make career choices at the start or even middle of their careers. We chatted for so long, not only on technological topics but also around people, that we will present the result over two columns to avoid dropping any of the good bits!

Anyway, this will be a slightly different format to the usual

articles (and hopefully a lighter read for dark winter nights!).

Introducing John Hollerton

TD: Thanks for agreeing to speak to *Spectroscopy Europe/World* following your retirement from GSK after so many years. How long did you work within the pharma giant “Glaxo-Wellcome-Smith-Kline-Beckman-Beachams-French” and through how many incarnations?

I joined Glaxo in 1980 which was not long after the Ware R&D site opened, just after Allen & Hanburys became Glaxo. I lived in Ware; I had left university and was looking for a temporary job. I basically had no idea what I wanted to do when I started out, that's for sure.

TD: But over the years you succeeded in becoming one of the top industrial analytical spectroscopists in the UK, but this was not your intention when you started out?

I knew that I liked computers. I knew that I liked analytical chemistry. I also knew that I didn't want to do synthetic chemistry. So really, I knew what I didn't want to do, but I didn't know what I wanted to do. Then having joined Glaxo, I had the opportunity to develop my skills as an analytical chemist and do some computing. I really enjoyed it!

I think I probably changed my job on average every four years. So, had lots of different roles and in my time, I managed all sorts of things from compound registration, physical chemistry, X-ray crystallography, chromatography, mass spectrometry—pretty much the whole gamut of stuff that we that we did over the years.

But fundamentally I was an NMR spectroscopist. That was my primary skill and it was probably the thing that I enjoyed most of all. Once an NMR spectroscopist, probably always an NMR spectroscopist. It keeps your interest. You learn something new every day—and that's remarkable. Even after 40 odd years, I was still learning stuff in NMR which I think is tremendous. I mean, that's the sort of thing that really gets my juices flowing.

But I'm not sure I would class myself as being a top industrial analytical spectroscopist!

TD: OK so how would you define yourself?

I don't know. Just someone who's tried to make a difference in my field. I've probably been vocal, and I quite like presenting so maybe people see me more. A lot of it is about visibility.

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TONY DAVIES COLUMN

TD: There is a phrase which I hate which is “Thought Leader”. But from my interactions with you, limited as they’ve been from both within GSK and from without. You are an ideas person. This is a rare personality trait if I put it that way around. There is a significant number of people who only look to ticking the boxes they are required to tick, and they would be happy doing that. It’s then very difficult to hold a conversation outside of an existing box. You know, it’s often only a limited number of people within some companies that you can hold a conversation with about “Wouldn’t it be great if...”

Yes. I’ve met the same sorts of people. There are lots of people who do their dream job and they do it very, very well, but they don’t tend to look beyond what they do. Maybe one of the things that that’s always driven me is to look at where we ought to be as opposed to where we are today. That’s driven what I’ve done. I’ve always looked at this as “Yeah, but we could do so much better if...”

I do a lot of process thinking. I look at a big process and I try to break it down. What can we change about that big process to make it a better process? It might be more efficient, or it may create more information or more knowledge.

Data is a big driver for me. If we’re doing stuff, why don’t we capture all that we know about what we did? Because even though you might not need it today, it may be really useful tomorrow!

TD: So, coming back to what formed the John Hollerton of today... what were your first instruments?

At university, I had access to a Varian EM360 NMR—that’s 60 MHz, not 360 MHz, because they didn’t exist back then! It was in a really bad state. So, I went to the lecturer who was in charge of

it and asked if I could have a go at trying to make it better? So, I read a book about shiming. Flew right into it and spent hours and hours and hours getting it really badly wrong and worse. And then eventually it gets better, and I actually got it working well. That’s probably my first experience getting onto an analytical system and understanding a little bit about the joy that you have when you finally managed to get a system to work correctly.

TD: So, where did you go to university?

I went to Royal Holloway, which had a brand-new chemistry department then. It was a big, shiny new building. There was a lot of kit there so I was probably fortunate to have access to things that maybe many other undergraduates in those days wouldn’t have had.

When I joined Glaxo, we had EM390s, the 90 MHz version of the EM360 that I had used, so I felt very comfortable with those, and I was very quickly up to speed. I started out mainly doing vibrational spectroscopy

(IR, UV and polarimetry). It was a bit of a production line, pushing out IR spectra because we ran IR on absolutely everything back in those days. The first thing I learned was that UV, as a technique, was often just a stamp collecting exercise. No one did anything with UV data. I successfully lobbied to stop us doing UV unless people had a particular need for it. I think it came to a head when one of the chemists submitted something without a chromophore. I said, just what were you expecting to see? And he said, I was just checking to see there wasn’t a chromophore in it! And it’s like, oh, should I do oxygen NMR to show that there is no oxygen in it?

TD: I think we can see the beginning of a critical thinker prepared to challenge established practice where it doesn’t make sense. Mohan has an interesting question.

MC: If you were to nominate somebody, John, that had the most impact on your career, who would that be and why?

Probably Richard Ernst. And the reason why, because he was the Granddaddy of 2D-NMR and



Figure 1. A Varian EM360 which has been upgraded through the Anasazi Instruments “Refresh Program” (<https://www.aiinmr.com/EM-360-NMR-Refresh-Program>). Image courtesy Anasazi Instruments

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2D-NMR has been the most amazing development for NMR.

In terms of development of my career, I think my first boss, was an amazing person. He just basically allowed people the space to be innovative and do their stuff. I found him and his enthusiasm very, very infectious. I think he probably did more to push my career and also push me. He told me some years later that he would ask me to do something impossible knowing that I would tell him it was impossible, and I would go away and, about three weeks later, come back suggesting that the outcome could be achieved in a different way! So, I think he knew me very well and I think he played me very well. He was a very important influence on my career.

MC: That's a really good answer, actually. If you weren't going to be a spectroscopist and you had your time again, what career would you choose retrospectively and why?

Well, computing is the other area of my career, so I've always had a dual role. So, if I wasn't doing spectroscopy, I would be doing computing, but it would be scientific computing.

In fact, many years ago I was head-hunted by a bank in London to go and work for them. At that point I realised that there was no way on earth I wanted to be in finance. That was not my passion.

I like making things and I like making things that people use. I'm always looking for things, even stuff which is on the edge of what my true employment has been. I've never been constrained, by "you're a spectroscopist—do stuff around spectroscopy".

MC: I know you've been very much a supporter of the use of lab IT systems. Could you expand on the areas with which you have worked

on, and what do you think have become more successful during your career?

Automation of data analysis, particularly complex data analysis, has been one of the things I spend a lot of time on. Automated structure verification (ASV) has been a big area, and I think I've influenced the direction of that for various companies. It's not there yet and I'm famously quoted as saying that ASV will be there in 3 to 5 years. And I've said that every year for the last 20 odd years! One day I'm going to be right, and I think that's probably the big thing. But actually, just removing manual steps from any processes, trying to automate those processes so that people spend that time using their brains, not their fingers. That's something I've done a lot of.

MC: Lab informatics / electronic lab notebooks have been the Holy Grail for many people, but also mean different things to different people. What does it mean to you?

I think terms like electronic lab notebook (ELN), laboratory information management system (LIMS) or scientific data management system (SDMS) are actually very unhelpful terms because there's no definition about what they are. Where they start and where they end. I would rather look at things in terms of an overall process and the bits which make up that process. Part of it will be capturing a thought, an intellectual idea about what you want to do. And I think the ELN captures that. Then you want to execute it and once again the ELN should capture what you've executed. But does it need to be a notebook as such? Probably not. I think it's a very outdated term. It's just there to ease people through that transition from paper to where they need to get, which is electronic capture all the way along the process.

TD: I've had to deal with this issue for so many years. A company would come in with totally fixed ideas about what their software will do, often failing to read the brief. When the company's requirements were explained to them again, they would often respond: "We don't do it like that. We do it like this." Well, no. Vendors need to provide something which supports the way that we are required to work. We will not be changing the way our spectroscopy, our analysts or whatever work to fit around your software. It is astonishing how many companies with really good reputations come in, completely fixated on only one way of working.

Yeah, the software shouldn't design the process. The software should be there to help the process. And everyone's got slightly different processes. You know, you've got the same overall arc, but basically the processes are slightly different. I think ELNs, SDMSs and LIMS, are actually a matter of being able to capture information electronically in a standard form so that it passes right the way through the process from cradle to grave. That's what the Holy Grail is. Are we there? Absolutely not. We're still miles away from that, I think, unfortunately. And there's no reason why we couldn't be there. It's just that there's not been the will or the investment to make it happen.

Anyhow, I think its time for a coffee break before we move into the discussions for part 2!

Thanks for your patience!

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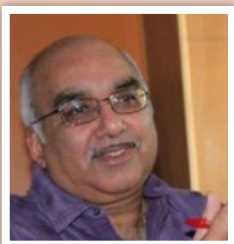
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Tony Davies is a long-standing *Spectroscopy Europe* column editor and recognised thought leader on standardisation and regulatory compliance with a foot in both industrial and academic camps. He spent most of his working life in Germany and the Netherlands,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

<https://orcid.org/0000-0002-3119-4202>

antony.n.davies@gmail.com



Mohan started his professional career as a research chemist in the pharmaceutical industry moving into IT at an early stage and personally overseeing many global transformational projects at corporate level. He is a successful serial investor in technology start-ups including in the med-tech arena where his experience in working in heavily regulated environments brings additional insights above his financial and business acumen. He has actively supported standardisation across industry and vendors scientific systems for decades!

mcashyap@googlemail.com



John Hollerton has worked in pharmaceutical research at GSK for many years as an analytical chemist and informatician. His background is in NMR spectroscopy but has also had a major role in developing informatics solutions to scientific problems. He also has a significant interest in data standards having been a board member of the Allotrope Foundation. He now works as an independent consultant.

<https://orcid.org/0000-0003-1453-9931>

john@hollerton.com

Framing the Theory of Sampling in risk assessment: a compelling perspective for the future

Kim H. Esbensen^a and Claudia Paoletti^b

^aKHEConsulting, Copenhagen, Denmark. E-mail: khe.consult@gmail.com

^bEuropean Food Safety Authority – EFSA, Via Carlo Magno 1/A, 43100 Parma, Italy. E-mail: claudia.paoletti@efsa.europa.eu

Sampling is necessary every time inferences are to be made to take informed, optimal decisions in science, technology, industry, trade and commerce. For reasons extensively addressed over the last two decades, application fields where good sampling practices are a source of economic gain—and bad sampling performance results in significant but unnecessary loss of money, such as the mining/minerals/metals industrial sectors—explicate the role of sampling more than others. In stark contrast to other fields (the realm of food and feed safety assessment is a prime example), sampling is largely perceived as an economic burden and a technical necessity to be fulfilled because of regulatory demands, rather than a vehicle with which to ensure reliable evidence to support management and regulatory decisions. Risk assessment and sampling are both probabilistic disciplines, the first devoted to estimate and minimise economic, safety and other risks, the latter devoted to estimate and mitigate sampling risks (the effects of sampling errors). Here we offer an exposé showing that the Theory of Sampling is an essential discipline and practical tool needed to ensure the best possible estimation of risks in support of both narrow economic objectives (industry, technology, trade, commerce), as well as broader safety decision-making and risk management environmental and biological sciences, and society at large. This contribution offers a novel perspective arguing for proper sampling, one where the economic argument (“what’s in it for me”) for proper sampling is demonstrated in practically all contexts, hereby complementing the compelling 25-author “Economic Arguments for Representative Sampling”.¹

Sampling: a border-crossing discipline

Sampling is a border-crossing discipline relevant every time inferences are to be made for taking informed, optimal decisions in science, technology, industry, trade and commerce. Scientific experiments and technical endeavours are very often dependent upon correct sampling at certain fundamental stages. Trade and international

agreements recommend duplication (or even triplication) of primary samples to allow buyers and sellers performing analyses to compare results for contractual compliance purposes. Market and commercial agreements also rely on sampling for monitoring of quality. Sampling plays a self-evident role in food and feed (F2) safety assessment as representativity of test materials for hazard identification, hazard characterisation and exposure assessment are critical pre-requisites for taking informed decisions regarding public, animal and environmental health. Indeed, potential health risks for humans and animals can only be estimated accurately when exposure scenarios to a given food or feed are realistic, i.e. based on

reliable sampling of food consumption habits. Furthermore, from an analytical perspective, the vast variety of food and feed matrices and commodities, raw or (semi-) processed, pose challenges to develop *appropriate* sampling strategies that best facilitate correct analytical methods. Similar issues exist in other sectors of society, e.g. in pharmaceutical manufacturing. Nonetheless, despite abundant evidence documenting the pervasive relevance of sampling, the Theory of Sampling (TOS) is not (yet) universally accepted.

A confluence of frustration

Over the course of the last 20 years, working alone and together, exploring the application of the

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TOS to very different disciplines and application fields, M3 vs F2, the present authors often felt challenged by meeting two fundamentally contrasting attitudes towards the TOS: **why sampling?** and **who/what benefits from proper sampling?**

In this period, we addressed, analysed and discussed on multiple occasions the likely causes for the divergent attitudes towards the TOS,¹⁻⁵ and arrived at the understanding that different *a priori* motivating factors driving the modes of application of the TOS and practical sampling are the root cause for this. We here choose to focus on the mining/minerals/ metals (M3) and food and feed (F2) sectors as lighthouse examples to illustrate this contrasting mindset. In the M3 sector, incorrect sampling unavoidably translates into hidden or clearly predictable *economic losses*. Consequently, the TOS is here rightly perceived as the main underlying agent *safeguarding business endeavours*.¹ In the equally broad global F2 sector, however, sampling is seen as a tool to verify the accuracy of claims and/or the quality of products, forcing the TOS more to be the operative agent with which to *search for possible problems* or to verify their absence, providing results in a statistical context offering merely degrees of confidence to inform the decision-making process. This is clearly a very different driver for invoking correct TOS when compared to safeguarding information factors for hardcore business interests.

The contra-positioning of the underlying drivers for sampling is a key point dividing the views of samplers, process engineers, managers, regulators: even if from a technical and practical point of view exploration for, and processing of, metalliferous resources is not so different from sampling for, say, aflatoxins in a 60,000-ton shipment of grain kernels—the *motivations* for investing education, intellect,

time and money in correct, representative sampling are *fundamentally different*. In the M3 sector, the better the sampling, the better for business; whereas in the F2 sector the better the sampling, the higher the risk of lot rejection or similar, which always carries a heavy negative economic and/or reputational penalty.

An emerging synoptic TOS framework

The plethora of TOS applications in the last 20 years documents this dichotomy, witnessed by the comprehensive historical record of the Proceedings from ten World Conferences on Sampling and Blending (WCSB) in the period 2003–2022 as well as a trend towards more reflected TOS references in ISO standards a.o. Notably, the technical application of the TOS is virtually identical in all applied fields, including F2 and M3: when sampling heterogeneous materials of any nature, the task for practical sampling is to *counteract* the effects of *the same* sampling errors (SE),

making use of *the same* Sampling Unit Operations (SUO) following *the same* Governing Principles (GP). The purpose of sampling is to conduct the optimal elimination and/or reduction of all eight types of sampling error effects, to deliver a defensible representative analytical aliquot to the laboratory. To be able to do this, all pre-analysis sampling operations must be representative, no exception allowed. In the schematic TOS framework developed by one of the present authors over the past 20 years,⁵ the critical task of eliminating and reducing sampling error effects can also be seen as appropriate *sampling error management*.

In the TOS realm, mitigation (management) of SE is a compound operation driven by the necessary sampling competency, which can range from adequate to non-existing, fighting material heterogeneity, which can range from large to almost non-existing, only using composite sampling. The key principle is clear: all sampling procedures must be representative of

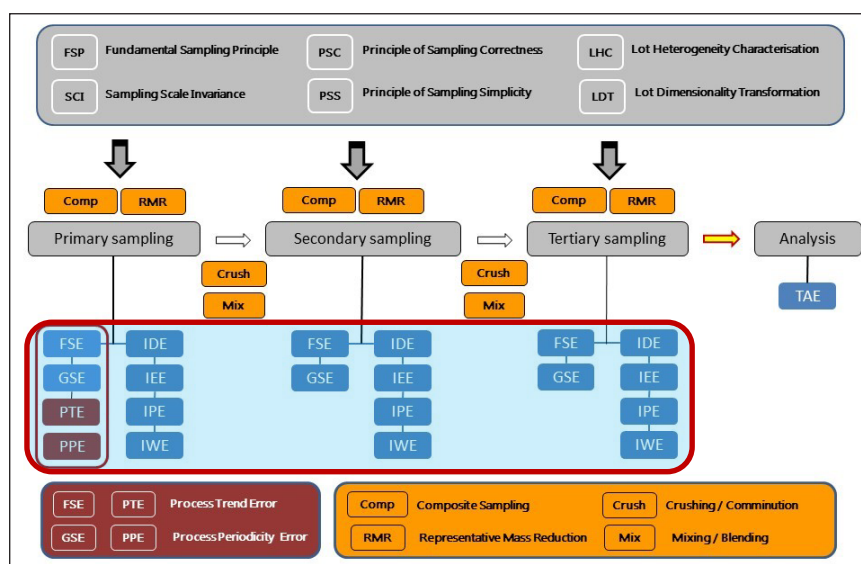


Figure 1. Theory of Sampling (TOS), synoptic overview. Practical sampling is governed by six Governing Principles (GP) [top grey panel], using four Sampling Unit Operations (SUO) [bottom yellow panel] in an informed effort to reduce unwanted sampling error effects, IDE, IEE, IPE, IWE, GSE, FSE ... [blue rectangle]. This constitutes the realm of risk management in the TOS: correct, complete elimination of ISE and reduction of CSE sampling errors (including those occurring in the analytical laboratory). Illustration copyright KHE Consulting, reproduced with permission.

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the original sampling target, the lot. Therefore, the starting point is always the Lot Heterogeneity Characterisation (LHC) which allows the design, implementation and performance of optimal representative sampling with respect to the specific heterogeneity profile of a lot of interest.

The synoptic framework representation of the TOS in Figure 1 has only very recently allowed the sampling community to recognise that proper handling, i.e. management of the gamut of sampling errors is in fact a critical risk management operation,⁶ to be explicated below.

Risk, risk assessment, risk management

The apparently very diverse drivers for applied TOS in the exemplar M3 vs F2 sectors indicated above, can also be seen from a common viewpoint, with a much broader impact, introducing the unifying concepts of *risk*, *risk assessment* and *risk management* in the sampling arena. In the following it is assumed that the reader is familiar with the TOS' basic systemic elements of Governing Principles (GP), Sampling Unit Operations (SUO) and Sampling Error Management rules (SEM), see Figure 1 and basic TOS references as found in References 1 and 5.

Framing the TOS in risk assessment: an outreach perspective for the future

Risk assessment has been defined in many different contexts see, e.g., a Google search.

Positioning the TOS as a risk management task provides a broader perspective, both at the theoretical as well as the practical level, illustrating the far-reaching responsibility vested in the TOS community. This awareness began with the recent publication "Economic arguments for representative sampling", which addresses how to engage

Fundamental risk definitions

Risk: probability that something unknown and/or unwanted happens.

Risk Assessment: the process to identify risks, so they can be minimised, often in order to maximise a critical goal, e.g., economic gains (business scope), consumers protection (societal scope) or quality control (technical quality control/quality assurance/quality management scope).

Risk Management: the process of monitoring and managing risks, optimising success by minimising identified risks as much as possible. Risk management capitalises on data as a reliable asset, for which reason all data must be representative.

Fundamental risk definitions applied to the TOS

TOS Risk: probability of unwanted, unmitigated sampling errors (SE)—both incorrect (ISE) and correct (CSE) sampling errors—resulting in uncontrolled, inflated sampling variability. This is a scenario damaging to every stakeholder.

TOS Risk Assessment: the process to identify the effects of unmitigated sampling errors in terms of ISE + CSE and material heterogeneity—i.e., the total sampling error (TSE)—employing, for example, pairwise sampling, replicated experiments or variographic characterisation, see the TOS literature for technical details.

TOS Risk Management: the process of monitoring and managing sampling error effects, specifically through complete elimination of ISE and the concomitant reduction of CSE, thereby, a.o., eliminating the fatal sampling bias, while complying with the Fundamental Sampling Principle (FSP) at all scales.

better with management, offering more than 25 different points of view.¹ This collective publication expresses well the *status quo* for the International Pierre Gy Sampling Association (IPGSA) and identifies areas where the sampling community needs to expand its activities to promulgate the TOS as a tool necessary for optimal risk management decisions across many disciplines.

Sampling is about providing reliable data and information necessary to take managerial decisions. In some areas such information is sufficient on its own, in others additional considerations must be taken into account.

Discussion

The goal of risk management is not elimination of all risks (which would be an impossibility), but rather getting to know which risks are

worth taking, which must be minimised and which ones have enough of an assured negative pay-out not to take them.

The sampling community should expand its horizon and offer its expertise to all sectors in society where the TOS is a *de facto* essential tool to deliver the appropriate information for critical decision making. Correct sampling is about being accountable for the trust that the business community and society puts into decision-making systems. Society has no other choice: we all consume what is available on the market *trusting* its quality and safety, trusting that the control system has worked as intended.

But "*consumption*" shall be seen here in a context much broader than just human and animal consumption of food and feed, indeed as the responsible *use*

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of resources and commodities. Upon reflection, there are virtually no examples of management decision making in the technical and industrial society that do not rely on sampling-before-analysis considerations along the information flow involved, even if well hidden from immediate reflection. Explicating the risk management scope of what makes sampling representative allows a fresh and powerful look at some of current hindrances for a more successful drive to *go beyond* the TOS' traditional borders. Framed in this perspective, the TOS becomes an essential practical tool needed to ensure the best possible estimation of risks to inform decision making across societal sectors at large, including biological sciences, agro-business, technology, industry, trade, commerce, environment.

Conclusion

Successful risk management considers the full range of risks, examines the relationship among the identified risks and their cascading impact(s). In some areas the number of factors informing management decision is limited, like in the M3 sector where attention is always tightly focused on mitigation of sampling error effects on the business bottom line. In others, like F2, the primary consideration is always human and animal health protection, however, other factors such as economic costs, cost/benefits, technical feasibility and risk perceptions are also considered appropriate. Nonetheless, the TOS is indispensable under either scenario—or beyond.

It is hoped that the risk assessment scope will allow the sampling community an easier, and perhaps more powerful, way to reach out to business, commerce, trade as well as regulating and law-enforcement authorities by starting to speak a more common language beyond

the mere “technicalities” of the TOS.

Disclaimer

Claudia Paoletti is employed by the European Food Safety Authority (EFSA). The positions and opinions presented in this article are those of the authors alone and do not necessarily represent the views or scientific works of EFSA. Kim H. Esbensen is an independent researcher and consultant, having left behind a three-decade university and government employee career in 2015.

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

<https://orcid.org/0000-0001-6622-5024>
khe.consult@gmail.com



Claudia Paoletti did her Master in Biological Science at the University of Rome (Italy) and her PhD in Plant Genetics at the University of Connecticut, USA. She was for three years at Dalhousie University (Canada) studying plant population genetics and biometry. She continued her activity at the Research Institute for Industrial Crops in Bologna (Italy) where she focused on the evaluation of the risks of transgenic crops. In January 2006 she joined the GMO Unit of the European Food Safety Authority (EFSA) first as Team Leader and then as Deputy Head of the Unit. In 2019 she was appointed manager of the programme designed to reorganise the EFSA in preparation for the new European Law on food safety. She has been the Italian expert for the definition of the European Commission sampling plans for GMO detection in conventional seeds. She coordinated the European sampling research project KeLDA and she has been the biometric officer of the EU Community Reference Laboratory for GMOs. She is expert consultant for ISO/IWA committees, OECD, CEN, the European Commission and FAO. She organised international training courses on food/feed safety for the European Commission, UNIDO, PHARE project and universities within and outside Europe. She has over 90 contributions either as book chapters, or as peer-reviewed papers.

claudia.paoletti@efsa.europa.eu

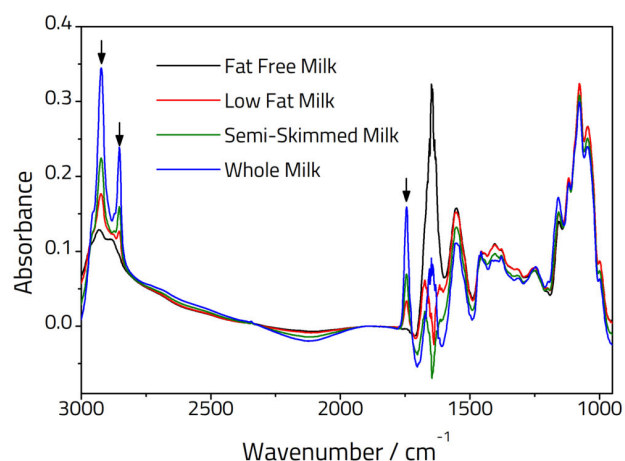


Direct analysis of trace elements in open-ocean seawater

Due to high total dissolved solids (TDS), seawater is considered one of the most difficult matrices to analyse for the presence of heavy metals and other trace elements. Plus, trace elements in open-ocean seawater are even lower than in coastal areas, thus are more challenging to accurately measure using quadrupole ICP-MS. However, PerkinElmer's NexION® 5000 Multi-Quadrupole ICP-MS instrument is a four-quadrupole system which combines two full-length transmission analyser quadrupoles with versatile Universal Cell Technology to achieve interference-free analysis. This work presents a method for the direct analysis of trace elements in seawater samples using the NexION 5000 ICP-MS system, demonstrating superior interference removal capabilities and sensitivity via exceptional detection limits, accuracy and long-term stability.

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Spectra of variable fat content milk types.

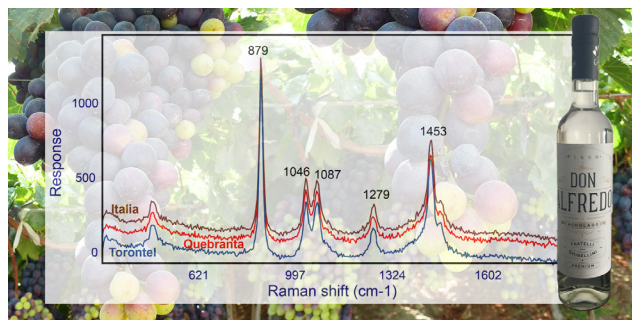
Analysing milk with the Pearl

In 2010, ~10 % of the world's milk was produced by the USA and accounted for 13 % of the food industry turnover in Europe. Monitoring the health of livestock and quality of milk is valuable to the dairy industry. FT-IR spectroscopy is a non-destructive way to determine the

purity of dairy samples. Whilst traditional methods can be time intensive, the Pearl™ accessory is designed for rapid throughput. Sample loading is easy and requires little user-training, saving time and money.

Specac

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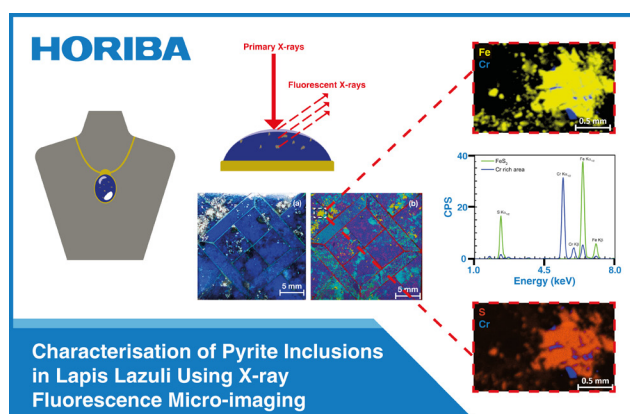


Authentication of Pisco from origin to alcohol content with Raman

Validating authenticity, purity, alcohol content and safety are common problems in the lucrative alcoholic beverage market, particularly when pricing is dependent on origin, variety or alcohol content. Raman spectroscopy is stepping up to close this gap for Pisco, a premium Peruvian liquor, and has excellent potential to do the same for other spirits. This Application Note describes how one group at the Ohio State University is using 1064 nm Raman spectroscopy to distinguish between pure varieties and mixtures, and even identify the specific grape varietal.

Wasatch Photonics

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Characterisation of pyrite inclusions in lapis lazuli using XRF micro-imaging

Lapis lazuli is a blue, semi-precious gemstone of the sodalite group. These rocks are characterised by the presence of clusters of golden-coloured pyrite, whose size can vary making attractive patterns on the

APPLICATIONS

gemstones. μ -XRF imaging can return the elemental distribution in geological samples. It enables the identification of regions of interest and, with the availability of a high-resolution X-ray guide tube, performance of detailed mapping and point analysis. In this application note, pyrite impurities and major elements distribution in a commercial lapis lazuli pendant are studied.

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Determination of impurities in lithium materials

The capability to identify the presence of impurities in lithium (Li) battery materials is critical for manufacturers and suppliers to ensure that the performance of the final battery is not compromised. Li salts used in battery production are generally extracted from brines and, subsequently, have high impurity levels, which can impact battery lifetime, stability and efficiency, therefore, pushing the need for higher purity in these raw materials. For the analysis of Li salts, PerkinElmer's NexION® 5000 Multi-Quadrupole ICP-MS instrument offers outstanding detection limits and interference correction thanks to the combination of its unique multi-quadrupole technology, true quadrupole Universal Cell and other proprietary features.

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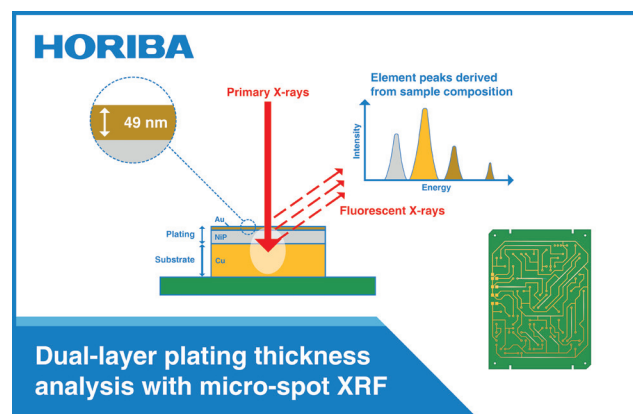
Direct trace-element analysis in cell culture media and raw materials

Raw material preparation and formulation is a known source of elemental content and variation in cell culture media. Other sources of trace metal concentrations

and variability include the leaching of trace metals from bioreactors, preparation vessels and storage containers. Quality control in cell culture media is essential for reducing variability and ensuring improved production yields. In this application note, a wide spectrum of elements in cell culture media samples were analysed with high accuracy and precision using PerkinElmer's NexION® 5000 Multi-Quadrupole ICP-MS instrument, the industry's first four-quadrupole ICP-MS system. The instrument's interference removal capabilities deliver interference-free analysis that in turn leads to extremely low detection limits. Plus, Extended Dynamic Range allows for the analysis of both low- and high-concentration elements within a single analytical run, which, coupled with the High Throughput System, dramatically contribute to the overall accuracy, stability and improved productivity of the system.

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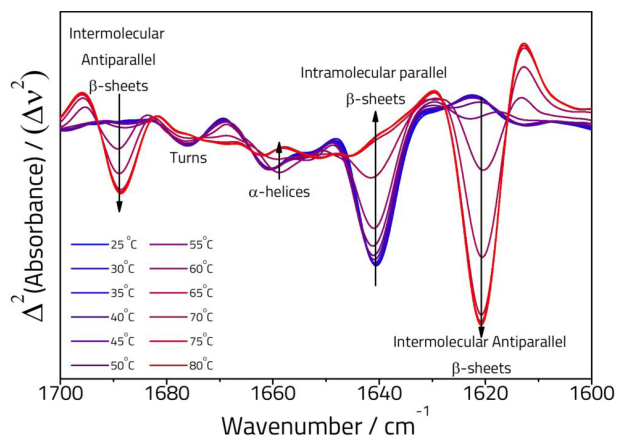


Dual-layer plating thickness analysis with micro-spot XRF

Micro-XRF provides a versatile tool for fast analysis of NiP and Au dual-layer plating thickness on circuit boards without requiring sample preparation. The high spatial resolution capability of the XGT-9000 microscope enables characterisation of coatings on features with dimensions below 1 mm (and as small as 10 μ m). In this note we show that 49 nm Au and 2.5 μ m NiP layers are accurately and reproducibly measured with a 100 μ m micro-spot.

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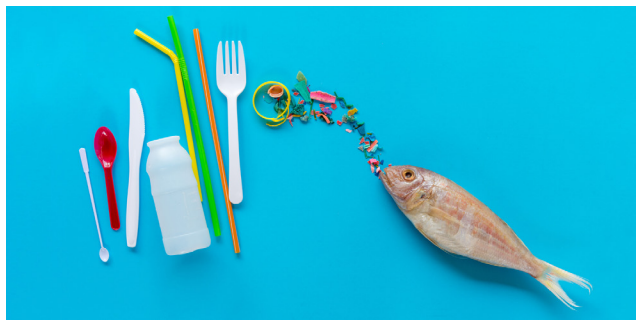


Investigating protein conformational and structural changes using transmission FT-IR spectroscopy

Proteins have been well characterised by FT-IR spectroscopy. The most important regions are the Amide I vibrations at 1700–1600 cm^{-1} , which can be deconvoluted to give information on relative conformational and structural changes in proteins in response to temperature. The measurement is undertaken using a water heating jacket and a transmission cell.

Specac

► [Download Application Note](#)

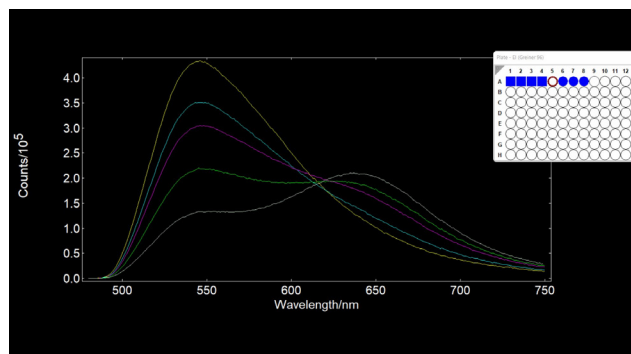


Monitoring microplastics in our oceans

Microplastics in our ocean waters are a growing problem—but how do you collect quick and effective measurements *in situ*, and at the depths needed to properly understand distribution, flow and uptake by ocean life? Filtration-based methods using FT-IR and Raman microscopy are well-proven, but work best for surface measurements where microplastic densities are higher. A collaboration of researchers from Japan and the UK are developing a compact, hybrid system using holography and Raman spectroscopy capable of *in situ* monitoring of particle size, shape and material—offering promise for monitoring at depths where sea life outnumbers the plastics.

Wasatch Photonics

► [Download Application Note](#)



Ratiometric analysis with a fluorescence plate reader

The SC-41 fluorescence Plate Reader enables high-throughput measurements on the FS5 spectrofluorometer via automated measurements of microwell plates. Standard and custom microwell plates can be measured containing up to 384 wells. Both spectral and lifetime measurements can be acquired, a unique feature of the SC-41. This technical note demonstrates the use of the SC-41 Plate Reader for ratio analysis. The emission spectra can be measured from each well where samples contain varying ratios of two fluorophores. The Trend Analysis feature in the Fluoracle software can then be used to plot a calibration curve which allows the determination of the ratio of each fluorophore in unknown samples.

Edinburgh Instruments

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Product Focus on Surface Analysis Instruments

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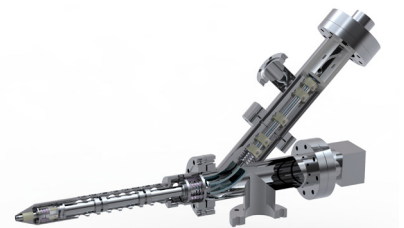
ToF-qSIMS Workstation

The Hidden TOF-qSIMS system is designed for surface analysis and depth profiling applications of a wide range of materials including polymers, pharmaceuticals, superconductors, semiconductors, alloys, optical and functional coatings and dielectrics, with measurement of trace components to sub-ppm levels.

[MORE INFORMATION »](#)

being assisted by the oxygen primary ion beam and provides isotopic sensitivity across the entire periodic table.

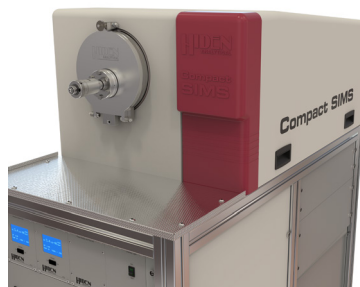
[MORE INFORMATION »](#)



EQS FIB-SIMS

The Hidden EQS SIMS is a high-performance, modular, secondary ion mass spectrometry (SIMS) system. The EQS SIMS analyser is an ideal "add-on" analyser for XPS and focussed ion beam (FIB) electron microscopy systems, where compositional studies can be carried out in the SEM field of view.

[MORE INFORMATION »](#)



Compact SIMS

Designed for fast and easy characterisation of layer structures, surface contamination and impurities with sensitive detection of positive ions

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AXIS Supra+

Our next generation X-ray photoelectron spectrometer, the AXIS Supra+ combines market leading spectroscopic and imaging capabilities with unrivalled automation to ensure high sample throughput and ease of use. X-ray photoelectron spectroscopy provides quantitative, chemical state information from the uppermost 10 nm of the material's surface. Fast, high spatial resolution XPS imaging reveals the lateral distribution of surface chemistry and aids further characterisation with selected area analysis.

MORE INFORMATION »

PIKE Technologies

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<https://www.piketech.com/>

Jackfish Spectroelectrochemical Cell

Jackfish cells are designed for surface-sensitive FT-IR spectroelectrochemistry using the attenuated total reflectance surface-enhanced infrared spectroscopy (ATR-SEIRAS) technique. The Jackfish cells enable fundamental studies of the electrified metal-solution interface.

MORE INFORMATION »

2060 *The* NIR Analyzer

Metrohm Process Analytics has introduced the latest member of the 2060 platform: the 2060 *The* NIR Analyzer. With its high-throughput spectrograph design, this process analyser is suited to inline process monitoring of multiple parameters at the same time.

Maximum flexibility for inline measurements tailored to your needs

The 2060 *The* NIR Analyzer can measure up to five (5) sampling points hundreds of metres away and is available in four different configurations to target multiple applications and industries: 2060 *The* NIR Analyzer, 2060 *The* NIR-R Analyzer, 2060 *The* NIR-Ex Analyzer and 2060 *The* NIR-REx Analyzer (R: Remote; Ex: explosion proof).

Process monitoring taken to a whole new level

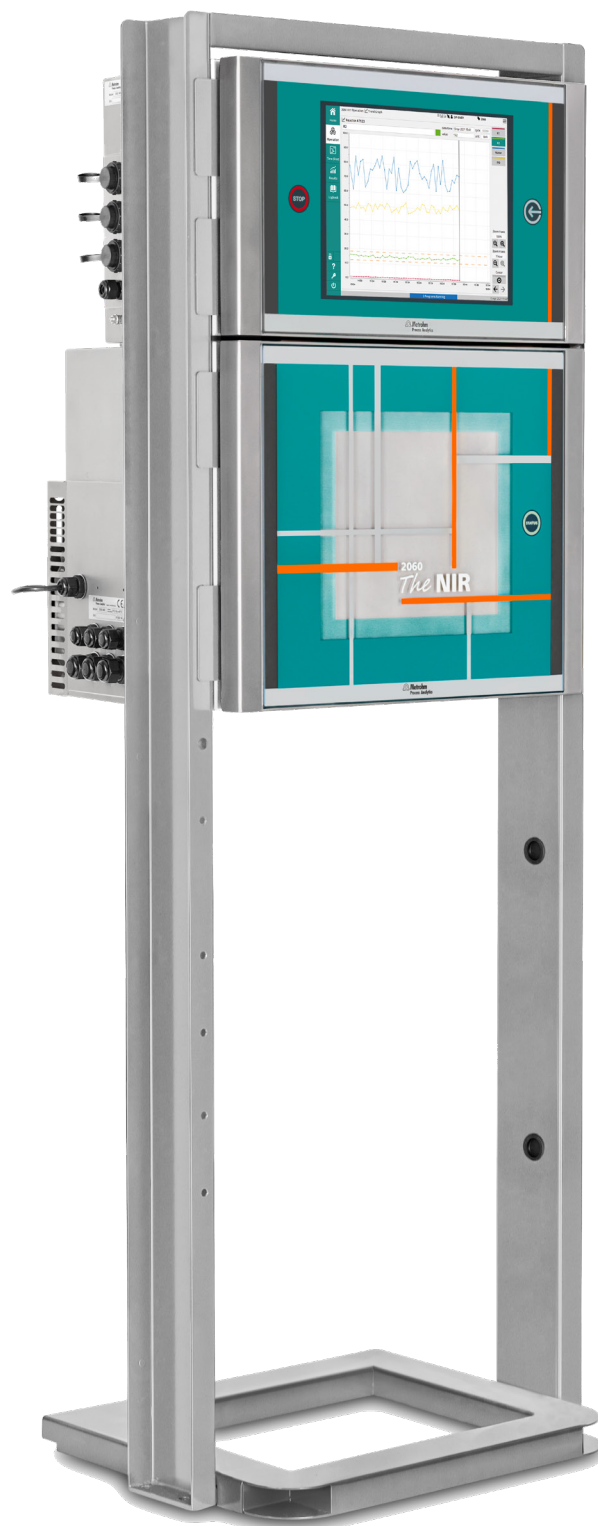
To get the most out of the NIR analysis, smart software are needed: the 2060 *The* NIR Analyzer has the software solutions designed for Process Analytical Technology (PAT). The on-board software products in the 2060 *The* NIR Analyzer—the IMPACT software and the OMNIS software—provide the greatest benefits out of your process analyser. The IMPACT software is the user's interface, with all the possibilities for smart programming, results display and communication protocols to the plant control room. Meanwhile the OMNIS software oversees all data analysis and contains the chemometrics package. As a result of this combination, the 2060 *The* NIR Analyzer is the ideal tool for supporting PAT.

Certified for the harshest environments

In many industries, many production processes are classified as potentially explosive atmospheres, in which higher concentrations of combustible gases, vapours or dusts can occur. This implies that it is vital for the process analysers to be safely operated and to not cause explosions. The 2060 *The* NIR-Ex Analyzer and 2060 *The* NIR-REx Analyzer have been developed for such harsh processes. The pressurised IP66 enclosure directly on the system has the advantage that no further protective shelters are needed. Additionally, all electrical connections are intrinsically safe. This results in an easy implementation to meet IECEx regulations or EU ATEX guidelines.

Metrohm Process Analytics

► <https://link.spectroscopyeurope.com/684-P1-2022>



The 2060 *The* NIR Analyzer by Metrohm Process Analytics

IMAGING

Resonon releases new compact and lightweight NIR hyperspectral imagers



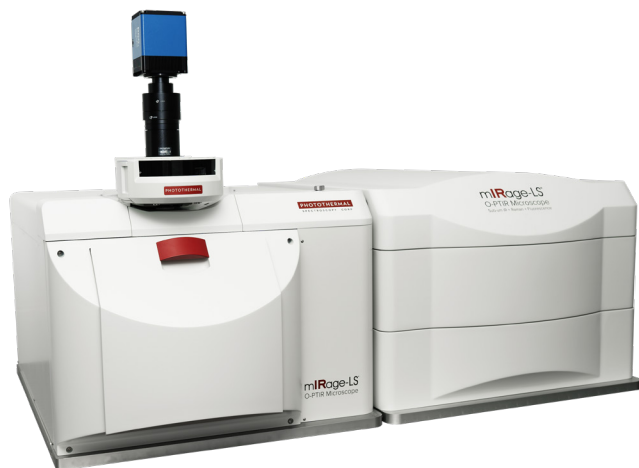
Resonon has released two new NIR range (925–1700 nm) hyperspectral imagers: the Pika IR-L and Pika IR-L+. The new imagers are smaller, nearly three times lighter, and boast improved spectral resolution compared to the current generation of NIR imagers. Their NIR spectral range is particularly suited for delineating land/water boundaries, imaging through low clouds and smoke, classifying a variety of minerals and vegetation covers, as well as contrasting dry and wet soils. Noteworthy applications include survey work, scientific research, precision agriculture and a multitude of commercial applications.

Airborne systems can be acquired as a full kit, including a data acquisition unit, the GPS/IMU unit, georectification software, post-processing and analytical software, a system mount for UAVs or piloted aircraft, radiometric calibration, a calibration target, and a rugged travel case. Resonon also offers RTK systems for very precise geo-location, VNIR downwelling irradiance sensors and training services.

Resonon

► <https://link.spectroscopyeurope.com/6521-P1-2022>

IR and fluorescence microscope



Photothermal Spectroscopy has announced the new miRage-LS sub-500 nm IR multimodal microscope and spectroscopy system uniquely combining, simultaneous Raman and co-located fluorescence microscopy with sub-micron IR in a single platform. Additionally, new developments on their proprietary O-PTIR (Optical Photothermal IR Spectroscopy) technique have improved the IR spatial resolution to <500 nm for life science applications. The new integrated platform combines the benefits of fluorescence microscopy to support fast, easy targeting of molecular features of interest with sub-micron IR spectroscopy to characterise the molecular structure of bio-molecular features, including sub-cellular and tissue applications.

Photothermal Spectroscopy

► <https://link.spectroscopyeurope.com/7036-P1-2022>

Agilent announces chemical imaging system for microplastics analysis

Agilent Technologies have announced the release of its enhanced 8700 LDIR Chemical Imaging System, which has been further optimised for the analysis of microplastics in environmental samples. This newly improved package includes Clarity 1.5 software: a significant upgrade of the speed of analysis, spectral acquisition,

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transformation and library matching, and that provides automated workflows for direct analysis of microplastics on a filter substrate. An innovative, redesigned sample holder allows the on-filter sample to be presented to the instrument more easily and consistently.

The prevalence of microplastics in the environment is a growing concern worldwide, prompting greater scrutiny from governments and increased monitoring of rivers and oceans by environmental agencies. Adequately assessing the prevalence of microplastics in the environment requires researchers to determine the size, shape and chemical identity of plastic particles in a sample. As smaller particles are thought to be the most biologically relevant, this analysis must extend to particles on the micron scale.

Agilent Technologies

► <https://link.spectroscopyeurope.com/105-P5-2022>



Linkam Scientific Instruments announces new NEXUS software

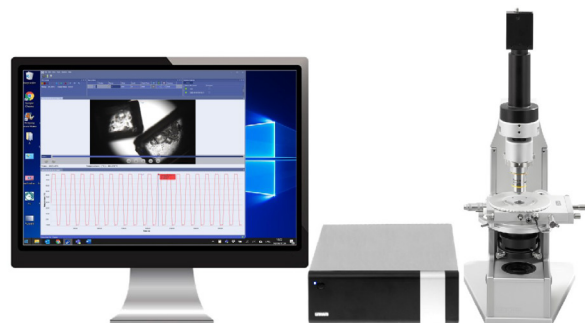
Linkam Scientific Instruments has launched new software, NEXUS, to precisely and record all aspects of heating, cooling, vacuum, humidity and other environmental conditions in a Linkam stage with optional optical measurement capabilities. NEXUS Core is the main NEXUS platform that introduces a range of new specifications to enable a greater degree of experiment control. Users can easily monitor the status of their experiment with the live display feature, quickly creating observations and adjustments that alter the data collection process. The upgraded software ensures precise synchronisation between samples through the live status display in parallel with a real-time temperature chart.

The new optional NEXUS Image Capture Module facilitates automatic image capture at specific points during an experiment. Each image can be stamped with current temperature and other parameters to make offline analysis straightforward. Rewind and review capabilities offer a detailed analysis and can be used during live data recording.

Other optional modules include: Extended Measurements Module, Reporting Module, Thermal Analysis by Surface and the 21CFR11 Module. NEXUS is compatible with Windows, and will initially support the THMS, HFS, LTS, TS, HS, CCR and PE families of the Linkam stages, with expected regular compatibility updates for other stages. Linkam has developed NEXUS to support its T95 and T96 controllers, which are the standard universal controller support for Linkam stages.

Linkam Scientific Instruments

► <https://link.spectroscopyeurope.com/6060-P2-2022>



INFRARED

FT-IR spectrometer for Hazmat responders to identify solid and liquid threats



RedWave Technology today announced the launch of the ProtectIR, their latest emergency response tool for the identification of unknown solid or liquid materials. The ProtectIR can identify more than 22,000 solid and liquid compounds. Emergency response personnel need to chemically identify hazardous materials in order to understand the threat and mitigate the effects when they are intentionally and accidentally released. The ProtectIR identifies most harmful toxic industrial compounds (TICs), chemical warfare agents (CWAs), explosives, narcotics, petroleum products, corrosives and even consumer products.

The ProtectIR uses Fourier transform infrared (FT-IR) spectroscopy. The size of the onboard threat library, coupled with the newest, advanced data analytics and algorithms, enable ProtectIR to identify complex mixtures with a high degree of confidence.

RedWave Technology

► <https://link.spectroscopyeurope.com/5746-P2-2022>

Portable FT-IR spectrometer brings laboratory-grade analysis to the field



Bruker Optics has launched the MOBILE-IR II—a portable, battery-powered Fourier Transform Infrared (FT-IR) spectrometer that delivers the spectral performance of a laboratory benchtop system. The MOBILE-IR II is intended to “mobilise” established use-cases of FT-IR spectroscopy, and also to enable new applications that demand mobility, flexibility and spectral performance. Key application examples include the identification of illegal substances during police or border control operations, the characterisation of recycled goods for sorting, the use in warehouses for mobile incoming goods inspection or in mobile laboratories for the exploration of natural resources.

It has IP65-class protection meaning it is waterproof, dustproof and stable for field applications. A built-in battery powers the device during off-grid operations and safeguards it against power blackouts. The additional IP67 carry-case makes it suitable for outdoor use, e.g., at construction sites or in mining operations.

OPUS® TOUCH software enables intuitive workflow set-up. Wireless operation, cloud service utilisation, database management and multiple other connectivity features enable safe data archiving, while smart user management gives additional security for sensitive data in mobile quality control applications in regulated environments. The MOBILE-IR II also fulfills Good Laboratory Practice (GLP) requirements and offers

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compliance with cGMP/GMP, US, Chinese, European and Japanese Pharmacopeias and 21 CFR Part 11.

Bruker Optics

► <https://link.spectroscopyeurope.com/2200-P1-2022>

MASS SPECTROMETRY

Shimadzu introduces new LCMS-9050 Q-TOF

Shimadzu is introducing the LCMS-9050 Q-TOF, a quadrupole time-of-flight (Q-TOF) mass spectrometer system. A proprietary high precision temperature control system inhibits even tiny mass variations caused by external factors so that the system can be used to measure accurate mass values without worrying about mass calibration. The ultra-stable polarity switching technology enables the simultaneous analysis of positive and negative ions, contributing to new applications development and heightened analysis efficiency. Optional equipment includes the DPiMS™ probe electrospray ionisation unit, SICRIT ion source for LC/GC/direct analysis, MALDI for mass spectrometry imaging and optional fragmentation.

Shimadzu

► <https://link.spectroscopyeurope.com/104-P4-2022>



New SmartVane rotary vane pump for mass spectrometry

Pfeiffer Vacuum has introduced the first rotary vane pump for mass spectrometry with a hermetically sealed pump housing. The SmartVane serves as a backing pump for mass spectrometers. This vacuum pump is designed to ensure that no oil leaks occur, therefore, preventing any contamination. Thanks to the integrated motor, no conventional seal is needed, which means that the SmartVane has longer maintenance intervals. The SmartVane has low noise levels and typical operating pressure <math><10\text{ hPa}</math>. Its compact design makes it easy to incorporate in existing systems. In addition, the pump offers intelligent communication options and can be used as a plug-and-play solution in combination with existing devices.

An additional benefit is the pump's sustainability. The SmartVane has an integrated energy-efficient IPM motor with a stand-by function. Its low power consumption automatically reduces the operating costs and CO_2 footprint.

Pfeiffer Vacuum

► <https://link.spectroscopyeurope.com/1821-P1-2022>



NIR

PET sorting by handheld NIR spectroscopy

trinamiX now supports the flexible differentiation between PET-A and PET-G with its mobile NIR spectroscopy solution. The handheld solution for on-the-spot identification of more than 30 different plastics is supplemented by a new application, which provides information about the type of a PET sample.

Amorphous polyethylene terephthalate (PET-A) is one of the most important thermoplastics. PET-A is a popular material for recyclable packaging of food, cosmetics or hygiene products. PET-G is modified PET that has been combined with glycol. As a result, PET-G features a higher transparency than PET-A, which remains stable even after heating. In addition, molten PET-G has a lower viscosity. These properties favour specific applications in the areas of packaging, 3D printing and visible parts, for example.

The clean separation of PET-G and PET-A is important for several reasons. First, only pure materials can be completely recycled. Due to different melting ranges, recycling a combination of PET-A and PET-G is difficult. In addition, mixtures have a negative effect on the desired properties, such as temperature stability. Ultimately, there is also an economic component: pure PET-G usually achieves higher prices on the market than PET-A.

trinamiX

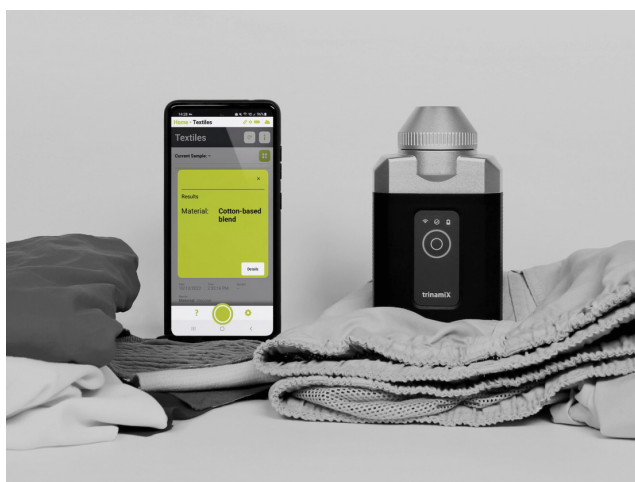
► <https://link.spectroscopyeurope.com/6114-P1-2022>



Handheld NIR spectroscopy textile identification

trinamiX has introduced on-site identification of textiles, enabling more than 15 textile types and compositions to be identified and thus better sorted. Even pieces made of material blends can easily be determined without damaging the material. The solution includes easy-to-use hardware with intelligent data analysis, an intuitive app for fast results and an extensive customer portal where in-depth analyses and reports can be created.

The solution supports a wide range of common textile grades used in clothing, furniture and household goods, for example: acrylic, cotton, nylon 6/6.6, polytrimethylene terephthalate (PTT), polyester, polypropylene (PP), silk, sisal, viscose and wool. Textiles made from more than one material can also be identified. These include blends based on acrylic, cotton, nylon, polyester, silk or wool. For the special requirements of recycling carpets, trinamiX has developed a dedicated application. It supports all common textile and plastic types used in carpets such as nylon 6 and nylon 6.6, polyacrylonitrile (PAN), polyethylene terephthalate (PET), polypropylene (PP), polytrimethylene terephthalate (PTT) and wool.



NEW PRODUCTS

The carpet application is the first one within trinamiX's Mobile NIR Spectroscopy Solution to work offline. This means that the identification of carpet materials can be carried out when there is no connection to the internet. The data is evaluated and stored directly on the device and smartphone, from where it can be uploaded later to the customer portal.

trinamiX

► <https://link.spectroscopyeurope.com/6114-P2-2022>

UV/VIS

New Ocean HR2 spectrometer

Ocean Insight has introduced the Ocean HR2 spectrometer, a high-resolution, configurable spectrometer that provides rapid acquisition speed and excellent thermal stability for applications ranging from plasma monitoring to pharmaceuticals analysis. Ocean HR2 spectrometers are compact and robust, with integration times up to 1 μ s and thermal wavelength drift of 0.06 pixels/ $^{\circ}$ C, helping to ensure reliable spectral performance as temperatures change. Ocean HR2 models cover various wavelengths within the ~190–1150 nm range, with a choice of slit width sizes to help users manage throughput and optical resolution.

The Ocean HR2 spectrometer is compatible with Ocean Insight light sources, accessories and software, allowing users to optimise setups for different applications. Also, each Ocean HR2 spectrometer comes with OceanDirect, a cross-platform Software Developers Kit with an Application Programming Interface. OceanDirect enables users to optimise spectrometer performance, access critical data for analysis and enable High Speed Averaging Mode, a function available with newer-model Ocean Insight spectrometers that dramatically improves spectrometer signal-to-noise ratio performance.

Ocean Insight

► <https://link.spectroscopyeurope.com/689-P1-2022>



X-RAY

Military-approved portable oil analysis now available

AMETEK Spectro Scientific has released a portable oil analysis laboratory that has delivered proven operational benefits for the US Military. Rugged, compact and lightweight, the FieldLab series offers a comprehensive and detailed oil and particulate analysis that enables quick and effective maintenance decisions to be made. FieldLab dramatically shortens analysis turnaround times by providing rapid, accurate results within minutes. This immediately solves challenges where access to remote

NEW PRODUCTS



laboratories is expensive and results can take weeks to be returned, a problem that greatly reduces effectiveness.

FieldLab offers a swift and inexpensive method to gauge potential machine wear by determining the condition of the oil and the presence of metallic wear particles. By measuring oil condition via molecular and viscosity analysis, FieldLab enables customers to extend service life of lubricants used in their applications, optimise labour resources, and minimise disposal costs and environmental impact. Samples can be collected from machines such as gas-powered turbines, generators, diesel engines, gearboxes, pumps and hydraulic systems and immediately tested onsite. The results are available within minutes.

User-friendly with minimal set-up time and no routine calibration required, FieldLab produces easy-to-understand results and diagnostics within minutes in eight different languages. Comprehensive analysis is provided via an X-ray fluorescence system, infrared grating spectrometer and kinematic viscometer. The unique mobile system is battery-operated for instant oil analysis using the touch-panel controller. FieldLab integrates with Spectro Scientific's TruVu 360 expert system and data management software.

AMETEK Spectro Scientific

▶ <https://link.spectroscopyeurope.com/1762-P3-2022>

Conferences

2022

1 December 2022–15 March 2023, Spain. **Fundamentals and Applications of Near Infrared Technology–7th Edn.** ivpl.nirs@gmail.com, <http://www.uco.es/nirsplatform/index.php/overview/29-7th-edition/46-6th-edition>

5–9 December, Kyoto, Japan. **XX CIGR World Congress 2022: Sustainable Agricultural Production - Water, Land, Energy and Food.** cigr2022@convention.co.jp, <http://www.cigr2022.org>

5–8 December, Ljubljana, Slovenia. **22nd European Meeting on Environmental Chemistry (EMEC22).** <https://www.emec22.com/>

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>

13–17 December, Indore, India. **IX International Conference on Perspectives in Vibrational Spectroscopy (ICOPVS-2022).** icopvs2022@gmail.com, <https://icopvs2022.in/>

19 December, London, United Kingdom. **Infrared and Raman Discussion Group Christmas Meeting 2022.** Chris.Stapleton@bruker.com, <https://irdg.us11.list-manage.com/track/click?u=3d2a3239204739e7c75f43831&id=3ffc74f1ac&e=fe93f5497d>

2023

6–11 January, Thiruvananthapuram, Kerala, India. **National Workshop on Fluorescence and Raman Spectroscopy.** <https://fluorescenceindia.org/workshop/fcsxiii/>

11–14 January, Trivandrum, Kerala, India. **Celebrating 50 years of Fluorescence Correlation Spectroscopy.** <https://fluorescenceindia.org/workshop/fcs50>

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

1 February, Macclesfield, United Kingdom. **BMSS Ambient Ionisation Special Interest Group.** admin@bmss.org.uk, <https://www.bmss.org.uk/bmss-ambient-ionisation-sig-meeting-2023/>

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

19–22 March, Philadelphia, PA, United States. **Pittcon 2023.** <https://www.pittcon.org>

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

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

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

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

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

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

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

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

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

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

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

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

2024

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

Courses

2022

5–6 December, United Kingdom. **BMSS Introduction to MS Course (Virtual-Zoom).** admin@bmss.org.uk, <https://www.bmss.org.uk/education/introduction-to-ms-course/>

2023

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

Exhibitions

2023

19–22 March, Philadelphia, PA, United States. **Pittcon 2023.** <https://www.pittcon.org>

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

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

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

2024

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

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info@ahf.de
www.ahf.de



Coherent
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www.coherent.com



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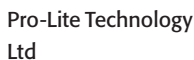
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Medway Optics Ltd
medwayoptics@aol.com
www.medwayoptics.com

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



tec5USA Inc
sales@tec5usa.com
www.tec5usa.com



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

MantiSpectra
info@mantispectra.com
www.mantispectra.com



MEDWAY OPTICS LTD

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



Ocean Insight
info@oceaninsight.com
oceaninsight.com



PerkinElmer, Inc.
www.perkinelmer.com

DIRECTORY

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S.T.JAPAN
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Wasatch Photonics

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

tec5USA Inc
sales@tec5usa.com
www.tec5usa.com

Wasatch Photonics
info@wasatchphotonics.com
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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

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

tec5USA Inc
sales@tec5usa.com
www.tec5usa.com

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

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info@ahf.de
www.ahf.de

APTechnologies 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

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

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

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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

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BaySpec, Inc.

info@bayspec.com
www.bayspec.com



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



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info@impopen.com
www.impopen.com



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www.perkinelmer.com



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hello@sepsolve.com
www.sepsolve.com



Waters Corporation
materials@waters.com
waters.com

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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

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



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

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AHF analysentechnik AG
info@ahf.de
www.ahf.de



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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

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

DIRECTORY



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



Bruker Optics GmbH & Co. KG

info.bopt.de@bruker.com

www.bruker.com/optics



Hidden Analytical Ltd

info@hidden.co.uk

www.hiddenanalytical.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

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



tec5USA Inc

sales@tec5usa.com

www.tec5usa.com

RAMAN



AHF analysentechnik AG

info@ahf.de

www.ahf.de



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



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Ocean Insight

info@oceaninsight.com

oceaninsight.com



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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



tec5USA Inc
sales@tec5usa.com
www.tec5usa.com



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



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info@wasatchphotonics.com
www.wasatchphotonics.com



WITec GmbH
info@witec.de
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info.bopt.de@bruker.com
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info-sci.fr@horiba.com
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www.linkam.co.uk

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info@ltb-berlin.de
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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



tec5USA Inc
sales@tec5usa.com
www.tec5usa.com



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

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AHF analysentechnik AG
info@ahf.de
www.ahf.de



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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



tec5USA Inc
sales@tec5usa.com
www.tec5usa.com



Waters Corporation
materials@waters.com
waters.com

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www.perkinelmer.com



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



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sales@tec5usa.com
www.tec5usa.com



Waters Corporation
materials@waters.com
waters.com

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



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

SURFACE ANALYSIS



Hidden Analytical Ltd
info@hidden.co.uk
www.hiddenanalytical.com



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info@impopen.com
www.impopen.com



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



Ocean Insight
info@oceaninsight.com
oceaninsight.com



tec5USA Inc
sales@tec5usa.com
www.tec5usa.com

DIRECTORY

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



tec5USA Inc

sales@tec5usa.com
www.tec5usa.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

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HORIBA Scientific

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



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info@linkam.co.uk
www.linkam.co.uk



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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