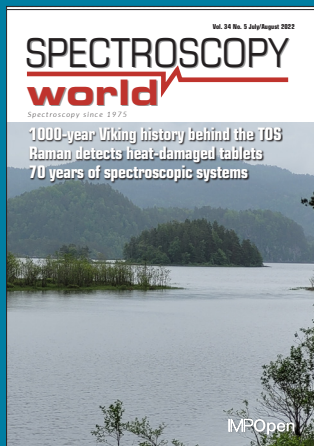


SPECTROSCOPY

world

Spectroscopy since 1975

1000-year Viking history behind the TOS
Raman detects heat-damaged tablets
70 years of spectroscopic systems



Is this the home of the Viking ancestors of the founder of the Theory of Sampling? Find out in the Sampling Column on page 28. Photo credit: Anne J. Cole

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Circulation

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

Spectroscopy World is published by IM
Publications Open LLP, 6 Charlton Mill,
Charlton, Chichester, West Sussex PO18
0HY, United Kingdom.

Vol. 34 No. 5

July/August 2022

ISSN: 2634-2405

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

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I need to start with an apology. This issue is a bit early and the next one will be a bit late. I have to go into hospital and needed to get this published before I do and my stay is going to delay Issue 6, which is likely to be a combined Issue 6/7. I also will not be able to send you my regular fortnightly e-newsletters reliably, although I hope that it may be possible to send some over the summer. However, Issue 6/7 should be a bumper issue we can look forward to!

After the usual selection of interesting, important or unusual News, our article is "Raman spectroscopy analysis for monitoring of chemical composition of aspirin after exposure to plasma flame" by Jasim Jamur. Pharmaceutical products can be damaged by heat or even changed into toxic compounds. This article describes how it may be possible to use Raman

spectroscopy to detect damaged aspirin tablets.

Tony Davies has been reading John Hammond's Quality Matters "Four Generations" series and has started a timeline of significant spectroscopic system developments aligned with Queen Elizabeth's reign as recently celebrated in her Platinum Jubilee. Jumping from Princess Anne the Princess Royal's birth to Heinrich Kaiser certainly makes for a novel approach! Tony hopes that we can turn this into an online resource with your help, and you are encouraged to add your own significant spectroscopic system developments using the form at <https://www.spectroscopyeurope.com/form/td-column-timeline>.

Sampling and Vikings seems to be the next unexpected connection within Kim Esbensen's Sampling Column. Kim has been exploring

an area of Southern Norway from where the founder of the Theory of Sampling, Pierre Gy, believed his ancestors originated. You will have to read the column to find the "smoking axe"! Oh, and there is an interesting report on the 10th World Conference on Sampling and Blending that has just finished.

John Hammond has taken a break from his Four Generations *magnum opus* and reports on the recent meeting of the ISO technical committee on reference materials (ISO TC 334).

The American Society for Mass Spectrometry meeting took place recently and produced a crop of new instrumentation and software, which we report on.

My thanks to all who have contributed to this issue, especially our regular columnists who have adjusted their schedules to meet my revised deadline.

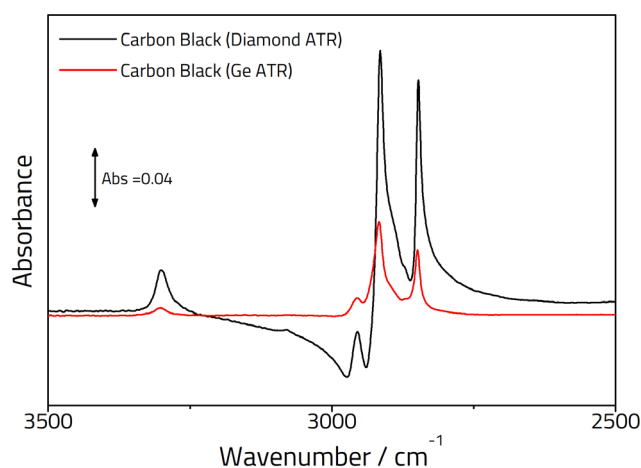
THE FIRST WORD

ATR Spectroscopy of high refractive index samples

ATR spectroscopy relies upon total internal reflection within the ATR crystal at the interface between the crystal and your sample. When the refractive index of the sample approaches that of the crystal light is transmitted into the sample and spectral artefacts are observed in the spectrum.

Carbon Black has a refractive index close to that of diamond and a direct consequence of this is that severe band distortions are observed due to anomalous dispersion, if a diamond ATR is used. This presents as asymmetric peaks, with stronger peaks exhibiting negative dips to higher wavenumbers. These artefacts can be eliminated by simply choosing an ATR crystal with a higher refractive index such as Ge, which then ensures that total internal reflection occurs and a good spectrum is obtained.

Specac



Comparison of spectra of a sample with high refractive index (Carbon Black) recorded on a Diamond and Ge puck. Anomalous dispersion causes severe band distortion when diamond is used (black line), whilst Ge produces the expected spectrum (red line).

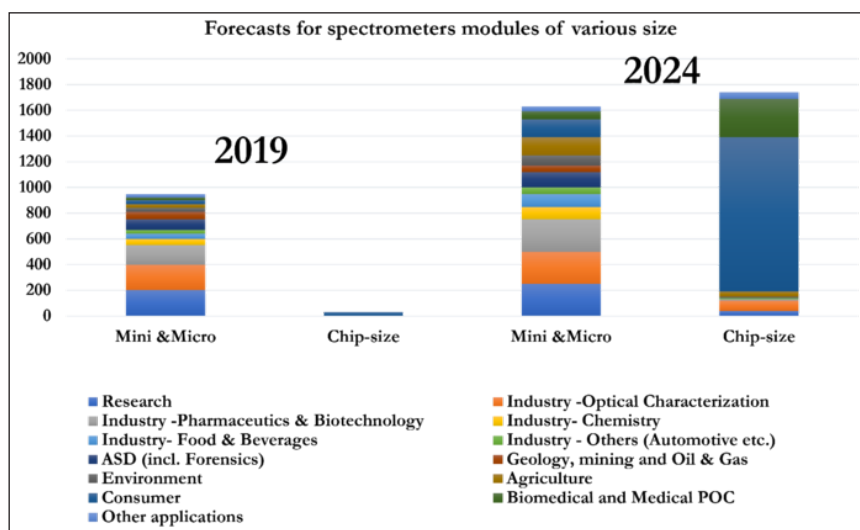
Read our technical
note here

Advances in cost-effective integrated spectrometers

A review of and prediction for the development of chip-based optical spectrometers.

Optical spectrometers are one of the essential types of instruments in numerous fields, including chemical engineering, materials analysis, astronomical science, medical diagnosis and biological sensing. Conventional high-performance spectrometers based on bulky and costly systems can no longer meet the requirements of various emerging application scenarios where the portability, cost, robustness and power-consumption are paramount metrics, such as portable or wearable sensing devices for healthcare, food safety monitoring, smartphone-based spectrometers, drone-based remote sensing and space exploration. During the past decades, substantial progresses have been made by both academia and industry in miniaturising spectrometers while maintaining adequate performance. However, while some work has indeed advanced the state-of-the-art in miniaturised spectrometers, they may suffer from insufficient performance and low technology readiness levels in connection with commercialisation.

In a review paper (doi.org/hzbow), researchers from Nanjing University of Aeronautics and Astronautics, University of Cambridge and University of California at San Diego summarised the recent progresses on miniaturised spectrometers with a special focus on integrated spectrometers based on CMOS-compatible integration platforms that hold great promises for massive fabrication at low cost. The paper starts with a brief market analysis of miniaturised spectrometers, showing their rapid growth, especially the chip-size integrated spectrometers which are predicted to have a disruptive increase in market volume from less than US\$2 million in 2019



Forecast for miniature spectrometers. Credit: Ang Li, Chunhui Yao, Junfei Xia, Huijie Wang, Qixiang Cheng, Richard Penty, Yeshaiahu Fainman and Shilong Pan

to over US\$1.6 billion in 2024. Nevertheless, in general, the footprint reduction of a spectrometer is associated with certain performance degradations regarding its operation bandwidth, resolution, measuring speed, dynamic range or signal-to-noise ratio, making it crucial to customise the spectrometer design for specified applications. Hence, taking the most popular biomedical sensing and industrial chemical detection as examples, the authors summarised a set of key figures of merits in terms of resolution, bandwidth etc., to establish the performance benchmarks for developing the next-generation of integrated spectrometers in various fields.


Afterwards, the paper goes into technological side; the two main categories of integrated spectrometers based on wavelength de-multiplexing (WdM) and wavelength multiplexing (WM) are discussed successively: "As suggested by their names, the WdM spectrometers need to de-multiplex, or in other words, split the incident signals'

spectra, either spatially or temporally, and measure the intensity of individual channel. On-chip WdM spectrometers are typically implemented by dispersive structures. Alternatively, WdM spectrometers can be implemented by using an array of narrowband filters or a single tuneable narrowband filter, whose spectral responses determine the spectral contents arriving at the detector. In contrast, WM spectrometers do not require to split the spectral contents of the spectrum, they typically pro-modulate the entire spectrum and reconstruct it by signal processing using specific algorithms. Dependent on the modulation principle, they can be further divided into Fourier Transform Spectrometers, or Computational Spectrometers." Computational spectrometers, which utilise an array of propagation channels with distinct spectral responses to sample the entire spectrum simultaneously, have recently seen extensive study. However, "even if the computational spectrometers exhibit distinct

advantages in terms of footprint, dynamic range and measurement time, by the nature of using fewer equations to solve many unknown values they are only able to reconstruct sparse spectra, which refer to smooth spectra or spectra with only a few non-zero components. While for dense spectra that contain rapidly changing features such a series of dips and peaks, the number of filters have to be significantly increased in order to

maintain satisfactory performance”, they added.

“To date, silicon photonics is still the most promising platform due to its unique CMOS compatibility. Considering that currently demonstrated integrated spectrometers are still unsatisfactory to the market requirements, we foresee four possible directions for developing the next-generation spectrometers on silicon photonics, involving spectrometers based on active

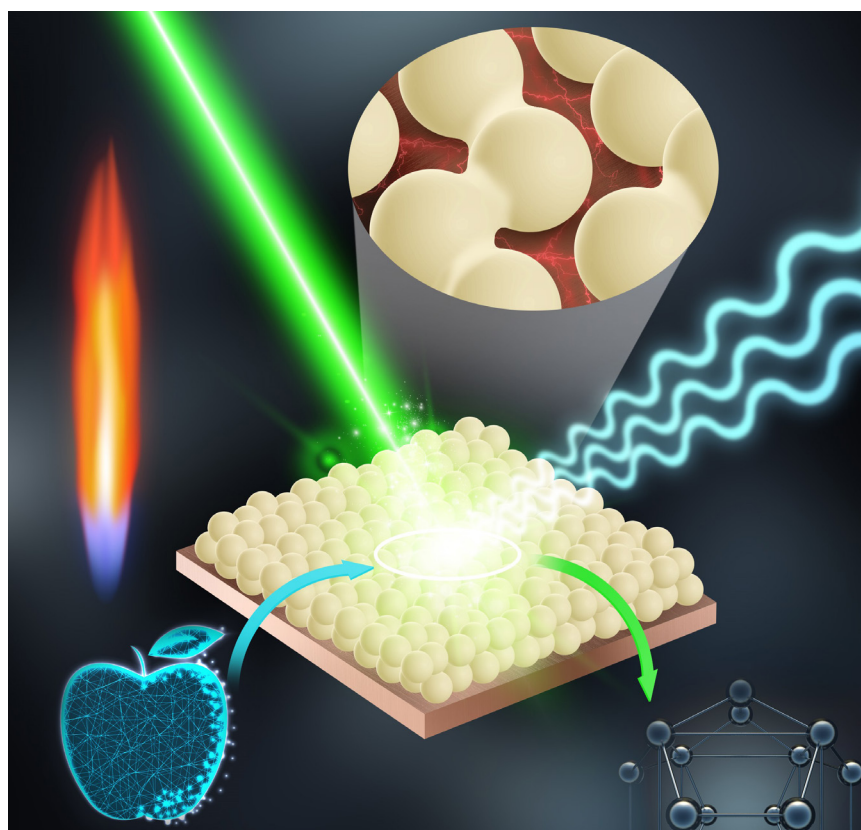
path configuration, spectrometers with programmability, spectrometer systems with parallelism and hybrid integration techniques for spectrometers. We expect to see expanding integration of chip-scale spectrometers into consumer productions within the next few years, providing cost-effective and reliable services to users worldwide”, the authors forecast. 

SERS detects pesticides on fruit in minutes

Flame-sprayed nanoparticles have been used as a SERS substrate to detect low concentrations of parathion-ethyl, a toxic agricultural insecticide that is banned or restricted in most countries.

Researchers at Karolinska Institutet in Sweden have developed a surface-enhanced Raman scattering (SERS)-based sensor for detecting pesticides on fruit in just a few minutes. The technique, described as a proof-of-concept, uses flame-sprayed nanoparticles made from silver to increase the signal of chemicals. While still at an early stage, the researchers hope these nano-sensors could help uncover food pesticides before consumption.

“Reports show that up to half of all fruits sold in the EU contain pesticide residues that in larger quantities have been linked to human health problems”, says Georgios Sotiriou, principal researcher at the Department of Microbiology, Tumor and Cell Biology, Karolinska Institutet, and the study’s corresponding author. “However, current techniques for detecting pesticides on single products before consumption are restricted in practice by the high cost and cumbersome manufacturing of its sensors. To overcome this, we developed inexpensive and reproducible nano-sensors that could be used to monitor traces of fruit pesticides at, for example, the store.”



Flame nanoparticle deposition was used to produce robust nano-sensors that can detect pesticide residues on apple surfaces within minutes. Artwork by Haipeng Li and Georgios A. Sotiriou

The new nano-sensors employ SERS, a powerful sensing technique that can increase the diagnostic signals of biomolecules

on metal surfaces by more than 1 million times. The technology has been used in several research fields, including chemical and

environmental analysis as well as to detect biomarkers for various diseases. However, high production costs and limited batch-to-batch reproducibility have so far hindered widespread application in food safety diagnostics.

In the current study (doi.org/hxvg), the researchers created a SERS nano-sensor by using flame spray—a well-established and cost-effective technique for depositing metallic coating—to deliver small droplets of silver nanoparticles onto a glass surface.

“The flame spray can be used to quickly produce uniform SERS films across large areas, removing one of the key barriers to scalability”, says Haipeng Li, a postdoctoral researcher in Sotiriou’s lab and the study’s first author.


The researchers then fine tuned the distance between the individual

silver nanoparticles to enhance their sensitivity. To test their substance-detecting ability, they applied a thin layer of tracer dye on top of the sensors and used a spectrometer to uncover their molecular fingerprints. The sensors reliably and uniformly detected the molecular signals and their performance remained intact when tested again after 2.5 months, which underscores their shelf life potential and feasibility for large-scale production, according to the researchers.

To test the sensors’ practical application, the researchers calibrated them to detect low concentrations of parathion-ethyl, a toxic agricultural insecticide that is banned or restricted in most countries. A small amount of parathion-ethyl was placed on part of an apple. The residues were later collected with a cotton swab that

was immersed in a solution to dissolve the pesticide molecules. The solution was dropped on the sensor, which confirmed the presence of pesticides.

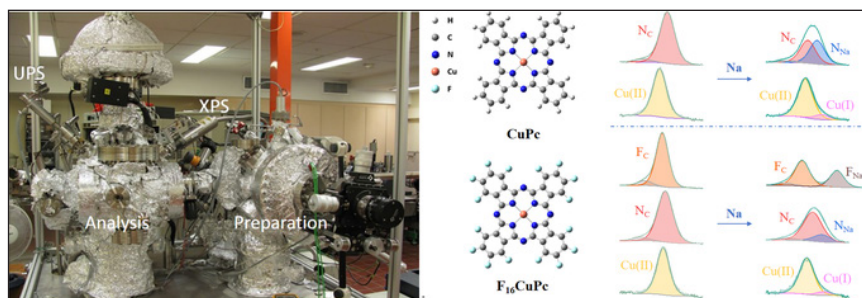
“Our sensors can detect pesticide residues on apple surfaces in a short time of five minutes without destroying the fruit”, Haipeng Li says. “While they need to be validated in larger studies, we offer a proof-of-concept practical application for food safety testing at scale before consumption.”

Next, the researchers want to explore if the nano-sensors can be applied to other areas such as discovering biomarkers for specific diseases at the point-of-care in resource-limited settings. 

Photoelectron spectroscopy helps protect sodium metal anodes

UHV X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy systems have unravelled the Na interaction process at Na/CuPc and Na/F₁₆CuPc interfaces.

Sodium metal batteries (SMBs) have attracted extensive attention because of their high theoretical capacity (1166 mAhg⁻¹), low redox potential (-2.71 V vs SHE), high natural material abundance and low cost. However, the growth of dendrites results in poor battery performance and severe safety problems, inhibiting the commercial application of SMBs. In order to stabilise sodium metal anodes, various methods have been developed to optimise the solid electrolyte interphase (SEI) layer and adjust the electroplating/stripping behaviour of sodium. Among them, developing anode host materials and adding electrolyte additives to build a protective layer are promising and convenient ways. In order to achieve the rational design of advanced anode hosts and



Customer-designed multi-chamber system with ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS) characterisations. Key results of this work. Credit: Yuan Liu, Xu Lian, Zhangdi Xie, Jinlin Yang, Yishui Ding, Wei Chen

electrolyte additives, the understanding of the interaction process between sodium metal and those organic materials is of great significance.

Researchers led by Prof. Wei Chen at National University of Singapore, Singapore, are interested

in the interface protection of sodium metal anodes, which is indispensable for the development of sodium metal batteries. They creatively linked *in situ* interface research methods with the protection of sodium metal anodes. Since the battery system is complicated

with various electrolyte compositions and side reactions, in order to simplify the research system and give direct evidence about the interaction process between sodium metal anodes and the electrolyte additives (or hosts), they used organic molecules as model

systems. Through their customer-designed *in situ* UHV X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) systems, they unravelled the Na interaction process at Na/CuPc and Na/F₁₆CuPc interfaces, especially the effect of fluorination

on sodiophilic sites, which provide insights into the radical design of fluorine-containing electrolyte additives and hosts for the protection of sodium metal anodes. This work was published in *Frontiers of Optoelectronics* (doi.org/gp638c).^{7A}

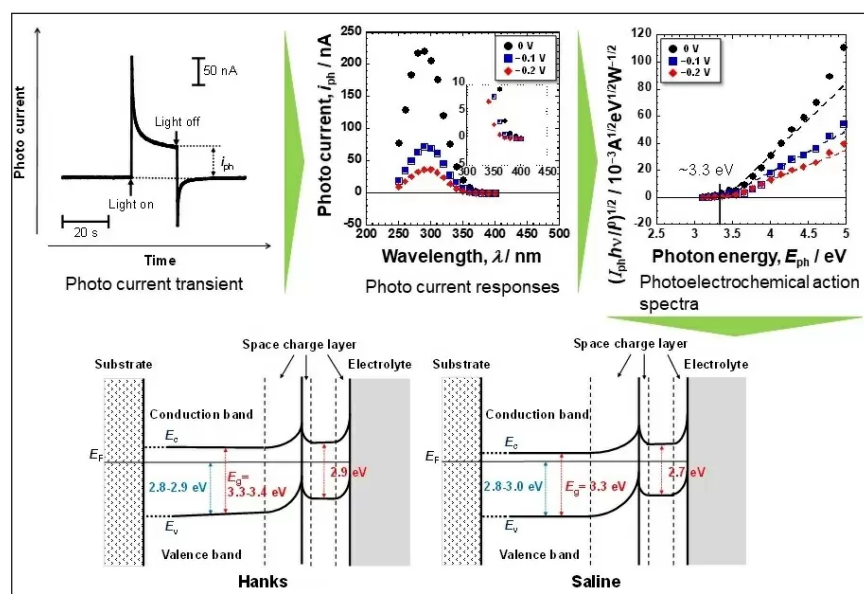
XPS explores biocompatibility of titanium implants

Researchers at Tokyo Medical and Dental University use X-ray photoelectron spectroscopy to discover what gives titanium implants their remarkable biocompatibility: may lead to more affordable medical and dental procedures.

Scientists from the Tokyo Medical and Dental University (TMDU) used photoelectrochemical measurement and X-ray photoelectron spectroscopy to clarify the source of titanium's biocompatibility when implanted into the body, as with hip replacements and dental implants. They find that its reactivity with the correct ions in the extracellular fluid allows the body to recognise it. This work may lead to new generation medical implants that last longer.

Owing to its excellent strength and resistance to corrosion, titanium is commonly used in medical and dental implants. Over time, doctors have also noticed that patients with titanium implants generate less of an immune response than normally occurs when a foreign material is placed inside the body. This has been explained based on the biocompatibility of titanium. This biocompatibility may generate a problem, such as when screws made from titanium alloys assimilate too much into bone tissue after long-term implantation, which makes them difficult to remove later. Despite numerous studies on biological reactions with implanted materials, the reason for the biocompatibility of titanium remains poorly understood. A more complete explanation of the surface properties that give titanium these features is needed.

Now, a team of researchers led by TMDU has tested thin disks of titanium in a solution containing



Electronic band structures of passive films formed on Ti in Hanks' solution and saline.

ions meant to mimic the extracellular fluid of the body, as well as in saline. They measured how much photoelectrical current was generated when light of various wavelengths was illuminated on the disks. They also performed X-ray photoelectron spectroscopy to characterise the passive films that were naturally present on the surface of the titanium. "Passive films consisted of a very thin TiO₂ layer containing small amounts of Ti₂O₃ and TiO, hydroxyl groups and water. During polarisation in Hanks' solution, calcium and phosphate ions were incorporated or formed calcium phosphate but not

in saline", says Seong-Cheol Kim. Calcium phosphate also formed much more easily, which could help reduce the foreign body response. "The reactivity of titanium with high corrosion resistance, as revealed in this experiment by its electronic band structure, is one of the primary reasons for its excellent biocompatibility among metals", says Takao Hanawa. This research (doi.org/gp69r2) may lead to safer and less expensive implants for hip replacements or dental implants, because titanium is relatively rare and expensive.^{7A}

GC-MS verifies geographical origins of virgin olive oil

GC-MS “fingerprints” of sesquiterpene hydrocarbons have proved to be excellent markers for the geographic origin of olive oil.

Olive oil is one of the most prestigious agri-foods in Spain, which is why adulteration and commercial fraud cases occur when it comes to the origin and varieties of a product with such an economic and business interest. Now, a team from the Faculty of Pharmacy and Food Sciences, Torribera Food and Nutrition Campus and the Institute for Nutrition and Food Safety Research (INSA) of the University of Barcelona presents a new authentication tool to check the geographical origin of virgin olive oil as a control on the quality, tradition and product linked to the territory.

The new methodology, based on gas chromatography-mass spectrometry (GC-MS), has been set as part of the work by the Research Group on Lipid and Bioactive Compounds in the Food Chain (LiBiFOOD) of the UB, aimed at creating analytical tools to verify the authenticity of foods and prevent food fraud. The Institute of Agri-food Research Technology (IRTA) collaborates in these projects too.

In the authentication process of foods, it is important to have analytical strategies that verify the origin of the products and help establishing the official method. The new tool provides a response to this need regarding food safety and traceability and it presents an authentication strategy that can be applied at different geographical scales.

“The new methodology enables us to discriminate between virgin olive oils produced in the European Union and those that are not, apart from classifying them according to the country of origin and verify which oils belong to the Protected Geographical Designations of Origin of the same region or even



adjacent ones”, note researchers Stefania Vichi and Alba Tres, coordinators of the research line in Authentication of Foods and members of the Torribera Food and Nutrition Campus and INSA.

The new geographical authentication strategy is based on the analysis of sesquiterpene hydrocarbons—organic compounds formed by three isoprene units—which



From left to right, Francesc Guardiola, Berta Torres-Cobos, Stefania Vichi, Alba Tres and Beatriz Quintanilla-Casas, from the Faculty of Pharmacy and Food Sciences and INSA of the University of Barcelona. Credit: University of Barcelona

proved to be excellent origin markers for olive oil.

“The cornerstone of an efficient authenticity tool is for it to be based on robust analytical markers. In the case of the geographical authentication of the virgin olive oil, the markers depend largely on the variety of olive tree and the area where it grew, without being significantly influenced by other factors related to the process of extracting or preserving oil”, notes researcher Beatriz Quintanilla-Casas (UB-INSA).

“The sesquiterpene hydrocarbons present in the virgin olive oil meet the requirements from above – she continues – and are robust geographical markers of this commercial product. Also, since they are semi-volatile compounds, they can be easily analysed with a widely used analytical tool—GC-MS—with a previous solid-phase microextraction, a relatively quick and automated procedure which does not require the use of solvents”.

The new protocol uses the sesquiterpene results as a fingerprint to develop geographical discrimination models that enable those oils that show an analytical signal very different from those considered as reference oils to be identified.

“Traditionally, reference methods for the authentication of products are based on the determination of one or a few compounds, so that the legal limits are set to decide whether the product meets certain specifications. Non-directed methods—like fingerprinting—enable using all the available analytical data, instead of focusing on certain compounds like traditional

methods do”, notes researcher Alba Tres.

The innovative nature of the analytical strategy lies in the fact that it proposes geographical markers that have been little studied to date for this purpose. Moreover, the new protocol is based on an analytical technique, which is within the reach of most control laboratory (public and private ones) and it only requires the application of a non-traditional approach.

The process of transforming an analytical method into an official methodology with a legal validity is slow and complicated, especially if the provided innovation is based on an untargeted approach. In the

case of the new technique, created in collaboration of the virgin olive oil producers, the first potential users would be the inspection and control laboratories, certification entities and big marketing companies of the olive oil sector.

The proposal of a geographical authentication strategy presented in the study (doi.org/hzb4) could become a new screening tool applicable to inspections and audits, “in order to contribute to guarantee that the products that reach the market are authentic and therefore reduce the commercial fraud opportunities in the food sector”, concludes the UB team. 📌

Controlling the waveform of ultrashort infrared pulses

An international team of laser physicists of the attoworld team at LMU and the Max Planck Institute of Quantum Optics has achieved unprecedented control over light pulses in the mid-infrared wavelength range.

Ultrashort infrared light pulses are the key to a wide range of technological applications. The oscillating infrared light field can excite molecules in a sample to vibrate at specific frequencies, or drive ultrafast electric currents in semiconductors. Anyone intending to exploit the oscillating waveform of ultrashort light pulses, to drive cutting-edge electro-optical processes for example, faces the same question—how to best control the waveform themselves. The generation of ultrashort pulses with adjustable waveforms has been demonstrated in different wavelength ranges like the UV-visible and the near infrared. Physicists from the attoworld team at the LMU, the Max Planck Institute of Quantum Optics (MPQ) and the Hungarian Center for Molecular Fingerprinting (CMF) have now succeeded in generating ultrashort mid-infrared pulses and precisely controlling their electric-field waveforms. With this infrared waveform manipulator at hand, new possibilities of optical control


for biomedical applications and quantum electronics come into reach.

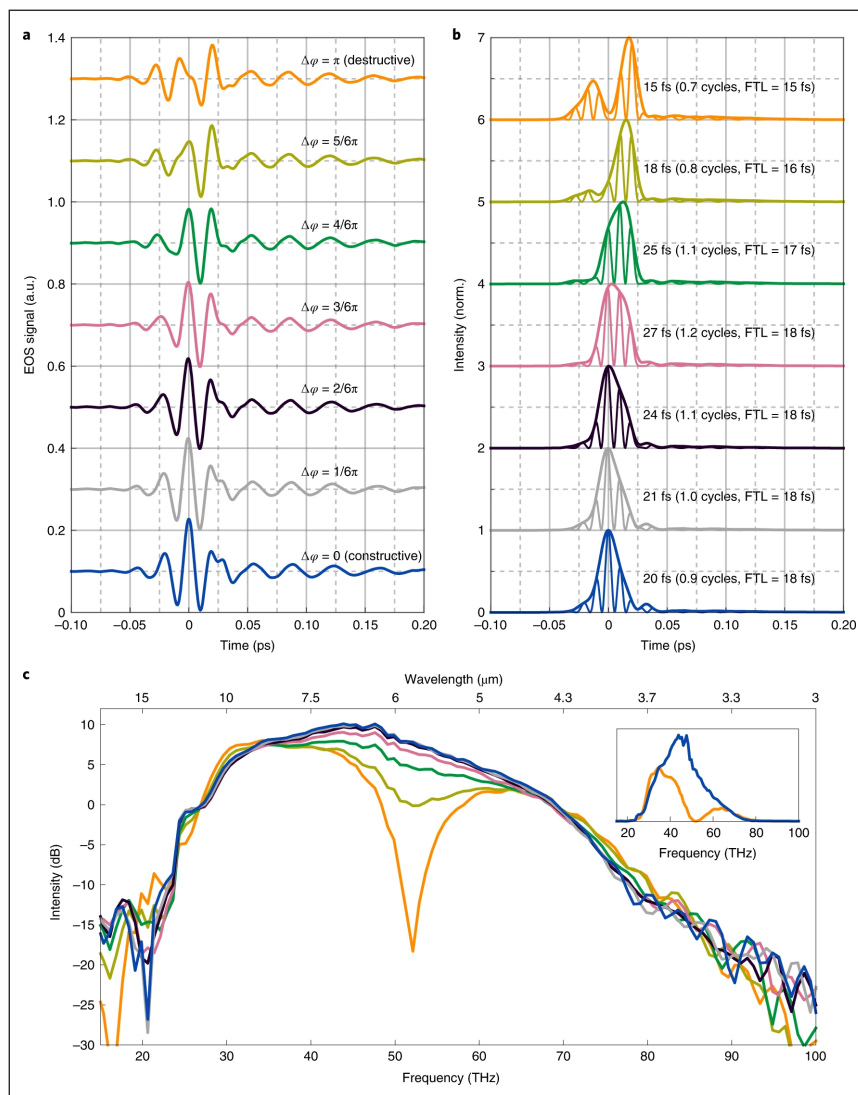
The basis for the new mid-infrared source is a stabilised laser system that generates light pulses with a precisely defined waveform at near infrared wavelengths. The pulses consist of only one oscillation of the light wave and are thus only a few femtoseconds long. When these pulses are sent into a suitable non-linear crystal, the generation of long-wavelength infrared pulses can be induced by taking advantage of complex frequency-mixing processes. In this way, the team succeeded in producing light pulses with an exceptionally large spectral coverage of more than three optical octaves, from 1 μm to 12 μm . The researchers were not only able to understand and simulate the underlying physics of the mixing processes, but also developed a new approach to precisely control the oscillations of the generated mid-infrared light via the tuning of the laser input parameters.

The resulting adjustable waveforms can, for example, selectively trigger certain electronic processes in solids, which could allow to achieve much higher electronic signal processing speeds in future. “On this basis, one could envision the development of light-controlled electronics”, explains Philipp Steinleitner, one of the three lead authors of the study. “If optoelectronic devices were to operate at frequencies of the generated light, you could speed up today’s electronics by at least a factor of 1000.”

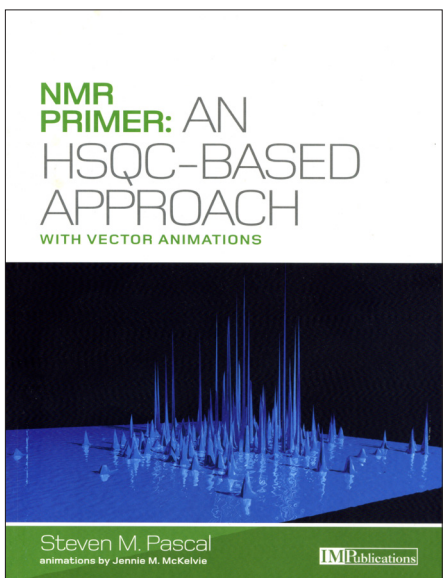
The attoworld physicists are paying particular attention to the use of the new light technology for the spectroscopy of molecules. “With our laser technology, we have significantly expanded the controllable wavelength range in the infrared”, says Nathalie Nagl, also first author of the study (doi.org/gp8x42). “The additional wavelengths give us the opportunity to analyse even more precisely how a mixture of molecules is composed”, she continues.

In the attoworld group, colleagues from the Broadband Infrared Diagnostics (BIRD) team led by Mihaela Zigman and the CMF Research team led by Alexander Weigel are particularly interested in measuring the precise infrared molecular fingerprints of human blood samples. The vision is to identify characteristic signatures that allow the diagnosis of diseases like cancer. A developing tumour, for example, leads to small and highly complex changes in the molecular composition of the blood. The goal is to detect these changes, and to enable the early diagnosis of diseases by measuring the infrared fingerprint of a simple drop of human blood.

“In the future, our laser technology will allow our colleagues to detect previously undetectable changes in specific biomolecules such as proteins or lipids. It thus increases the reliability of future medical diagnostics using infrared laser technology”, says Maciej Kowalczyk, also first author of the study. 



Monolithic-waveform synthesis in the mid-IR range. a, EOS time-domain data for different relative phases $\Delta\varphi$. Constructive interference occurs for a value of 0, whereas the strong modification of the mid-IR waveform for π indicates destructive interference. b, Corresponding intensity envelopes, extracted FWHM pulse durations, number of optical cycles calculated for the spectral centroid and FTL based on the derived spectral intensities. c, Corresponding spectral intensities for different relative phases, as extracted via the Fourier transformation of the time-domain data. Constructive interference occurs for $\Delta\varphi = 0$, whereas the strong spectral dip for $\Delta\varphi = \pi$ indicates destructive interference between the spectrally overlapping components originating from even and odd IPDFG orders. The inset shows the extreme spectra (constructive and destructive) on a linear scale. Reproduced under a CC BY licence from <https://doi.org/10.1038/s41566-022-01001-2>



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

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

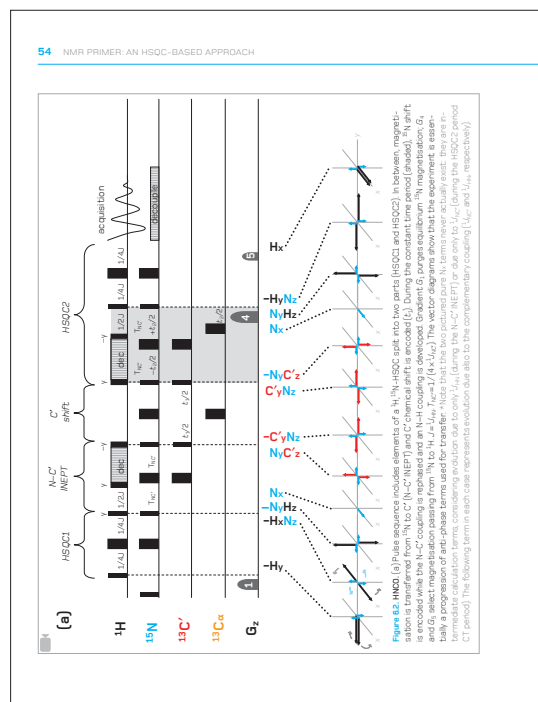
First, a brief introduction to spins, populations, the NMR experiment and relaxation is provided. Evolution due to J-coupling is next described and used to explain magnetisation transfer in the HSQC experiment and several variants. The extraction of structural, sequential and dynamic information is then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

ANIMATIONS

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

BUY THE BOOK

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



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NMR reveals how tau proteins form tangles

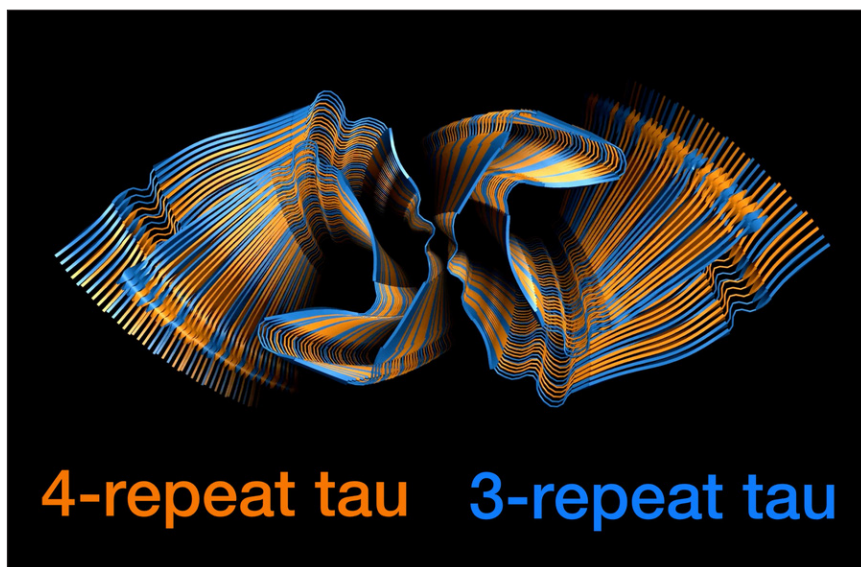
NMR spectroscopy has shown how two types of tau proteins mix together in a nearly random way to generate the tangles seen in the brains of Alzheimer's patients.

One of the hallmarks of Alzheimer's disease is the presence of neurofibrillary tangles in the brain. These tangles, made of tau proteins, impair neurons' ability to function normally and can cause the cells to die. A new study from MIT chemists has revealed how two types of tau proteins, known as 3R and 4R tau, mix together to form these tangles. The researchers found that the tangles can recruit any tau protein in the brain, in a nearly random way. This feature may contribute to the prevalence of Alzheimer's disease, the researchers say.

"Whether the end of an existing filament is a 3R or 4R tau protein, the filament can recruit whichever tau version is in the environment to add onto the growing filament. It is very advantageous for the Alzheimer's disease tau structure to have that property of randomly incorporating either version of the protein", says Mei Hong, an MIT professor of chemistry.

In the healthy brain, tau functions as a stabiliser of microtubules in neurons. Each tau protein is made up of either three or four "repeats," each consisting of 31 amino acid residues. Abnormal versions of either 3R or 4R tau proteins can contribute to a variety of diseases. Chronic traumatic encephalopathy, caused by repetitive head trauma, is linked to abnormal accumulation of both 3R and 4R tau proteins, similar to Alzheimer's disease. However, most other neurodegenerative diseases that involve tau feature abnormal versions of either 3R or 4R proteins, but not both.

In Alzheimer's disease, tau proteins begin to form tangles in response to chemical modifications of the proteins that interfere with their normal function. Each tangle consists of long filaments of 3R and



MIT chemists have used nuclear magnetic resonance (NMR) spectroscopy to reveal how two different forms of the Tau protein mix to form the tangles seen in the brains of Alzheimer's patients. Credit: Aurelio Dregni/Nadia El-Mammeri/Hong Lab at MIT

4R tau proteins, but it wasn't known exactly how the proteins combine at the molecular level to generate these long filaments. One possibility that Hong and her colleagues considered was that the filaments might be made of alternating blocks of many 3R tau proteins or many 4R tau proteins. Or, they hypothesised, individual molecules of 3R and 4R tau might alternate.

The researchers set out to explore these possibilities using NMR spectroscopy. They labelled 3R and 4R tau proteins with carbon and nitrogen isotopes and were able to calculate the probabilities that each 3R tau protein is followed by a 4R tau and that each 4R tau is followed by a 3R tau protein in a filament.

To produce their filaments, the researchers began with abnormal tau proteins taken from post-mortem brain samples from Alzheimer's patients. These "seeds"

were added to a solution containing equal concentrations of normal 3R and 4R tau proteins, which were recruited by the seeds to form long filaments. To the researchers' surprise, their NMR analysis showed that the assembly of these 3R and 4R tau proteins in these seeded filaments was nearly random. A 4R tau was about 40% likely to be followed by a 3R tau, while a 3R tau was a little more than 50% likely to be followed by a 4R tau. Overall, 4R proteins made up 60% of the Alzheimer's disease tau filament, even though the pool of available tau proteins was evenly divided between 3R and 4R. Within the human brain, 3R and 4R tau proteins are also found in roughly equal amounts.

This type of assembly, which the researchers call "fluent molecular mixing," may contribute to the prevalence of Alzheimer's disease, compared to diseases that involve


only 4R or 3R tau proteins, Hong says.

“Our interpretation is that this would favour the spread and the growth of the toxic Alzheimer’s disease tau conformation”, she says.

Working with collaborators at the University of Pennsylvania School of Medicine, led by Professor Virginia Lee, the researchers showed that the tau filaments they generated in the lab have a structure very

similar to those seen in human patients with Alzheimer’s disease, but they do not resemble filaments grown exclusively from normal tau proteins. The tau filaments that they generated also replicated the toxic effects of Alzheimer’s tangles, forming aggregates in the dendrites and axons of mouse neurons grown in a lab dish.

The current work (doi.org/gp72fk) focused mainly on the

structure of the rigid inner core of the filaments, but the researchers now hope to further study the structure of the floppier protein segments that extend out from this core. “We would like to figure out just how this protein goes from a healthy and intrinsically disordered state to this toxic, misfolded and beta-sheet rich state in Alzheimer’s disease brains,” Hong says. 

Raman spectroscopy reveals evasive quantum phenomenon

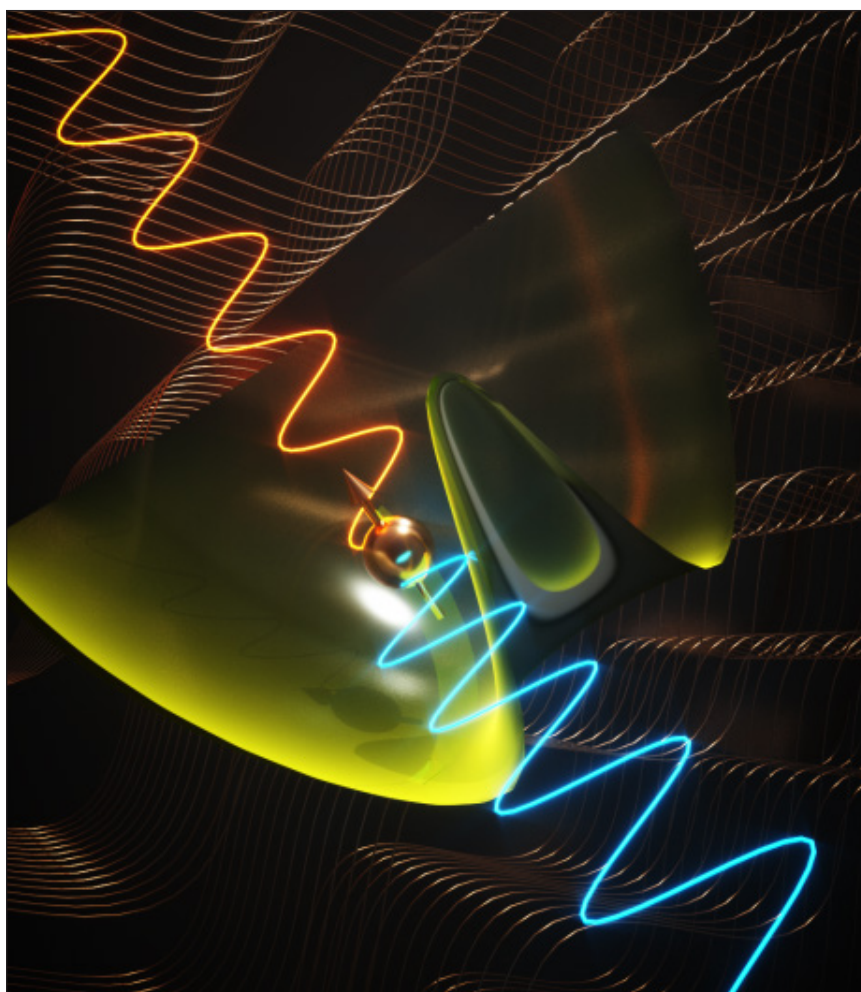
A Quantum Science Center-supported team has captured the first-ever appearance of a previously undetectable quantum excitation known as the axial Higgs mode using Raman spectroscopy.

The axial Higgs mode manifests as a low-energy excitation in rare-earth tellurides, a class of quantum materials notable for exhibiting charge density wave, or CDW, interactions. This behaviour refers to arrangements of interacting electrons in quantum materials that form specific patterns and correlations.

Unlike the regular Higgs mode, which is produced by a Higgs mechanism that provides mass to fundamental particles in the Standard Model of Particle Physics, the axial Higgs mode is visible at room temperature. This characteristic enables more efficient and cost-effective experiments for manipulating quantum materials for various applications—including next-generation memory storage and opto-electronic devices—which would otherwise require extremely cold temperatures.

The team responsible for these results was led by researchers at Boston College and includes scientists from Harvard University, Princeton University, University of Massachusetts Amherst, Yale University, University of Washington and the Chinese Academy of Sciences.

“This result is almost elegant in its simplicity—it’s really rare to find a new particle with a super clean



Researchers recently confirmed the presence of the axial Higgs mode, a particle excitation depicted here as a golden sphere. They used Raman spectroscopy, in which an incoming electric field, shown in blue, was coupled with the particle and subsequently scattered into a different frequency, shown in red. Credit: Ioannis Petrides and Prineha Narang/Harvard University

signature without a lot of fanfare”, said Prineha Narang, an assistant professor at Harvard and a principal investigator through the QSC, a US Department of Energy National Quantum Information Science Research Center headquartered at DOE’s Oak Ridge National Laboratory.

To measure the axial Higgs mode, the researchers used Raman spectroscopy to observe pathway interference, which demonstrates the power of quantum mechanics to control matter. They found this interference of quantum pathways in multiple rare-earth CDW systems, and this phenomenon persisted up to room temperature and was insensitive to the mixing of the axial Higgs mode with nearby phonons, or vibrations in the material.

“Emulating the physics of an axial Higgs mode in a tabletop experiment opens new horizons in our understanding and use of exotic particles”, said Ioannis Petrides, a postdoctoral fellow in Harvard’s NarangLab.


Most notable quantum activity appears only at very low temperatures, which requires dilution refrigerators that rely on a limited supply of liquid helium. Otherwise, the physics of quantum materials tend to be completely invisible or obscured by noise, which can cause certain properties to phase in and out of view so quickly that they cannot be confirmed or properly studied. Although the team did cool their CDW samples, they discovered that the signature, or the wavelength produced by spectroscopy measurements, remained just as clean once the materials warmed up to room temperature.

The researchers anticipate that the axial Higgs mode likely exists elsewhere too, including in superconductors and magnetic materials, which would allow experimentalists to study and optimise quantum systems without relying on extreme conditions or large-scale facilities.

“There is a lot of interest in the axial Higgs mode because it provides a recognisable fingerprint that represents a quantum

system without the need to see all the physics involved”, Narang said. “If you need to study an unknown material to determine whether it’s a spin liquid or a superconductor or something else, the ability to fingerprint the collective mode spectrum allows you to easily characterise it spectroscopically.”

Materials that harbour the axial Higgs mode could even be used as novel quantum sensors capable of categorising other quantum systems, and further studies could potentially lead to a better understanding of pervasive anomalies, such as dark matter, that cannot be explained by the standard model.

This work (doi.org/hzb5) builds on many previous research efforts and marks an important milestone in the hunt for exotic collective modes in quantum materials, including the axial Higgs mode. Narang describes this accomplishment as a significant step forward for multidisciplinary research focused on the intersection between high-energy physics and condensed matter. 

Ultrafast laser spectroscopy probes the charge carrier transfer processes and dynamics within perovskite active layers

New work overviews the crucial charge carrier transfer processes and dynamics within perovskite active layers by means of time-resolved ultrafast laser spectroscopy.

New research provides an overview of how the charge carrier dynamics vary with respect to the crystalline phase of the organic–inorganic perovskite. Despite organic–inorganic lead halide perovskites having attracted enormous scientific attention for energy conversion applications over recent years, the influence of temperature and the type of the employed hole transport layer (HTL) on the charge carrier dynamics and recombination processes in perovskite photovoltaic devices is still largely unexplored. In particular, significant knowledge is missing on how these

crucial parameters for radiative and non-radiative recombinations, as well as for efficient charge extraction vary among different perovskite crystalline phases that are induced by temperature variation.

The research presents micro photoluminescence (μ PL) and ultrafast time-resolved transient absorption spectroscopy (TAS) results in a reference glass/perovskite architecture and two different glass/ITO/HTL/perovskite configurations at temperatures below room temperature. The objective of this work is to probe and shed light on the charge carrier dynamics

of different perovskite crystalline phases, while considering also the effect of the employed hole transport layer (HTL) polymer. Namely, $\text{CH}_3\text{NH}_3\text{PbI}_3$ films were deposited on glass, PEDOT:PSS and PTAA polymers, and the developed glass/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ and glass/ITO/HTL/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ architectures were studied from 85 K up to 215 K in order to explore the charge extraction dynamics of the $\text{CH}_3\text{NH}_3\text{PbI}_3$ orthorhombic and tetragonal crystalline phases. Interestingly enough, the article reports evidence that the charge carrier dynamics at low temperatures, are not only affected

Introduction to the Theory and Practice of Sampling

Kim H. Esbensen

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

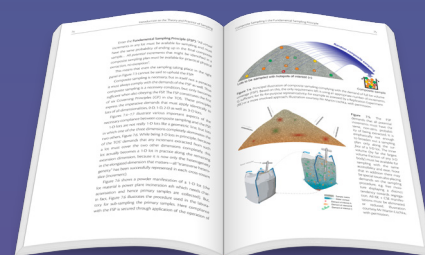
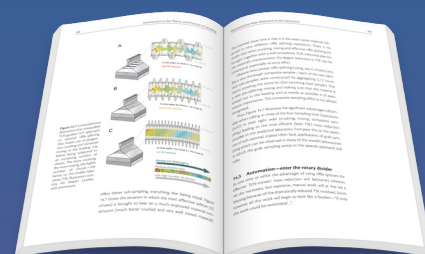
“Sampling is not gambling”. Analytical results forming the basis for decision making in science, technology, industry and society must be relevant, valid and reliable. However, analytical results cannot be detached from the specific conditions under which they originated. Sampling comes to the fore as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

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

“I recommend this book to all newcomers to TOS”

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

“One of the book’s major advantages is the lavish use of carefully designed didactic diagrams”

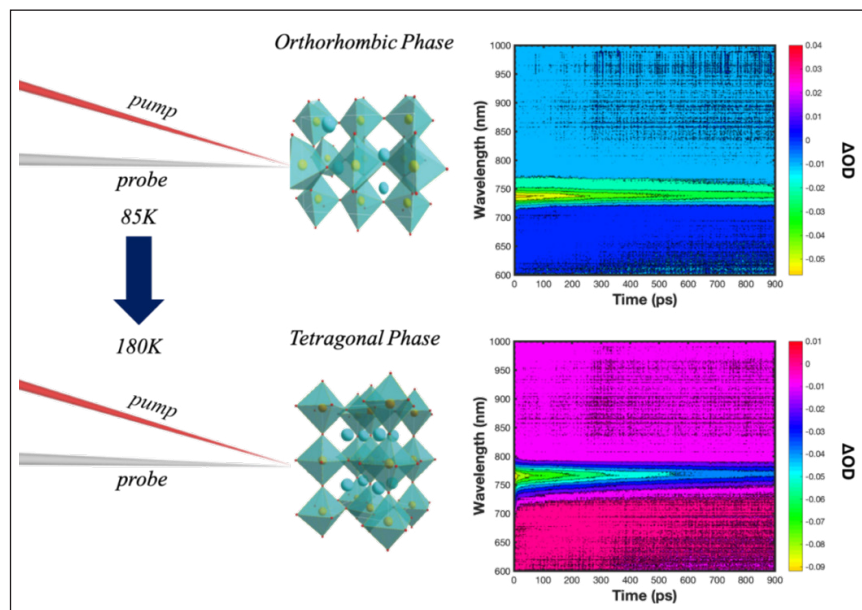


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by the employed hole transport layer, but in addition are strongly correlated to the different perovskite crystal phases.

In particular, μ PL spectroscopy reveals an unusual blueshift of the bandgap with temperature, which is discord of the Varshni behaviour of the typical semiconductor, below 120K for the orthorhombic phase of the perovskite and the dual emission at temperature below of 100K. Moreover, in the three studied temperatures by means of TAS, at 85K (orthorhombic phase), at 120K (coexistence of the orthorhombic and the tetragonal phase) for each peak, and at 180K (tetragonal phase) the glass/ITO/PTAA/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ architecture exhibits faster hole injection from the perovskite layer to the HTL and slower recombination rates (k_2) when compared with the glass/ITO/PEDOT:PSS/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ configuration. It is discussed within the article that this is due to the better crystalline quality of the perovskite film when it is grown on the PTAA polymer. Furthermore, as the temperature increases for each perovskite crystal phase (orthorhombic and tetragonal), the τ_2 time components and k_2 bimolecular recombination rate



decrease, for both configurations. Thus, it was found that the charge carrier dynamics at low temperatures, are not only affected by the employed hole transport layer, as we have already shown for the room temperature measurements but are strongly correlated to the different perovskite crystal phases.

Based on the above, it is believed that the new insights of this article pave the way towards the design of more efficient and stable

PSCs, particularly for low temperature applications, such as the use of PSCs in satellites or in space stations. More importantly, this work (doi.org/gp8t84) demonstrates the validity of TAS as a figure of merit technique on shedding light on the physical origins and mechanisms within and from the perovskite active layers, that are the key component of PSC devices. 

Portable Raman reveals Anne Brontë's hobby

Anne Brontë is renowned as a novelist, but a Raman analysis of her collection of stones has revealed her to be a skilled collector with an active interest in geology who accumulated a collection of attractive specimens before her death aged 29 in 1849.

Anne Brontë is renowned as a novelist and one of three famous sisters, but a detailed scientific analysis of Anne Brontë's collection of stones has revealed her to be a skilled collector with an active interest in geology. The youngest of the Brontë sisters accumulated a collection of attractive specimens before her death aged 29 in 1849.

It was previously thought that she could have collected the items

chiefly for their aesthetic value, however, research by scholars at the University of Aberdeen has revealed that Anne was an informed and skilled participant in the emerging science of geology, which in the mid-19th century was enjoying what would become known as its "golden age". Using portable Raman spectroscopy, researchers analysed Anne's collection which is housed at the Brontë Parsonage

Museum in Haworth in Yorkshire. They found that as well as carnelians and agates which she collected in Scarborough, where she worked as a governess, the collection contained flowstone (a kind of calcium carbonate that formed in a cave like a stalagmite), and a rare kind of red obsidian which originated outside of the UK. It is also likely that Anne would have visited the Rotunda Museum close to

where she stayed in Scarborough, which contained exhibits featuring the area's geology.

Sally Jaspars, a student at the University of Aberdeen's School of Department of English, is studying Anne Brontë as part of her PhD, and contacted Dr Stephen Bowden from the University's School of Geoscience for assistance in analysing the collection. The collaboration also involved Professor Hazel Hutchison of Leeds University and Dr Enrique Lozano Diz at ELODIZ. Their work is published in *Brontë Studies* (doi.org/hzb6).


"This is the first time that Anne's collection has been systematically described and fully identified, and in doing so we add to the body of knowledge on Anne and show her to be scientifically minded and engaging with geology. She was an intelligent and progressive individual who was in tune with the scientific enquiry of the time."

Dr Bowden added: "Our Raman spectroscopy analysis which we



Anne Brontë's collection of stones which is housed at the Brontë Parsonage Museum in Yorkshire © The Bronte Society. The red rocks at the back of the image are Agates and Jasper, and the small grey rock at the far right is Speleotherm, similar to a stalactite or stalagmite. The orange and red pebbles at the centre are Carnelians, while two pieces of red obsidian (post box red with a blocky/slither-like shapes) are visible at the front.

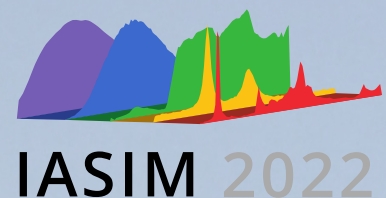
undertook at the Brontë Parsonage Museum shows that Anne Brontë did not just collect pretty stones at random but skilfully accumulated a meaningful collection of semiprecious stones and geological curiosities. Anne's collection comprises

stones that are sufficiently unusual and scarce to show that they were collected deliberately for their geological value, and it's clear that her collection took skill to recognise and collect." 

Conference on spectral imaging

July 3–6, Esbjerg, Denmark

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Hyperspectral imagery: applications in remote sensing

Marco Veneranda (University of Valladolid)
Raman imaging from terrestrial to planetary applications

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Raman spectroscopy analysis for monitoring of chemical composition of aspirin after exposure to plasma flame

Jasim M.S. Jamur

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A Raman spectroscopy method was optimised to examine the chemical changes of aspirin tablets after interaction with helium temperatures. Several aspirin tablets were exposed to plasma-assisted desorption ionisation flame for different times (10, 30, 50, 60, 180 and 300s) and then analysed by Raman spectroscopy using optimal conditions. The changes in chemistry between exposed and fresh (without exposure to plasma) tablets were compared. The vibrational peaks of the aspirin molecule in the Raman spectrum were identified by checking the peak position. The results showed clear spectra with increases in intensity of vibrational peaks until 30s, whereas no spectra were measured for the exposed tablets to plasma flame after 50s. It can, therefore, be assumed that the chemistry structure of aspirin compound might be damaged by exposure to high temperature.

Introduction

Further details about the degradation structure of pharmaceutical products are required to improve their stability and determine whether the degradation products and impurities have any toxicity.¹⁻⁴ Temperature is an important component in much of our lives, not least in the climate system, and plays a key role in the chemical change of compounds. Some pharmaceutical compounds are damaged or toxic chemicals produced due to exposure at plasma flame temperatures.⁵ Exposure to these temperatures has been shown to be related to adverse effects in human health

both directly and indirectly. Therefore, these rapid changes are having a serious effect on the environmental and biological impacts of chemical compounds.⁶

Various analytical techniques such as near infrared (NIR), Fourier transform infrared (FT-IR), nuclear magnetic resonance (NMR) and high-performance liquid chromatography (HPLC) have been used to analyse pharmaceutical solid compounds.⁷ Recently, investigators have examined the effects of temperature on the stability of pharmaceutical samples. The thermal stability of aspirin samples after treatment at 40 °C and exposure to a 300 W UV-A lamp for 12 h was studied by Al-Maydama *et al.* and found to be lower to that of the untreated samples using HPLC, photocatalytic, X-ray diffraction (XRD) and scanning electron microscopy (SEM) methods.⁸ In the study by Acharya and co-workers, IR, mass spectrometry and ¹H NMR methods were successfully applied

for analysis of the thermal degradation product obtained from the interaction of aspirin and salicylic acid. This study confirmed that the structure of the new thermal degradation product is different to those of aspirin and salicylic acid.⁹

The chemical composition of artemisinin and *p*-coumaric acid was investigated using HPLC after exposure to high temperature and it showed that the stability of these compounds was affected.¹⁰ However, HPLC is expensive, has long run times and consumes solvents. In the study by Johnsiani *et al.*, several techniques such as NMR, quadrupole time-of-flight mass spectrometry (Q-TOF/MS) and electrospray ionisation collision-induced dissociation tandem mass spectrometry (ESI-CID-MS/MS) were used to study the degradation of sorafenib tosylate after exposure to different stress conditions including temperature.¹¹ Vishnuvardhan and co-workers have shown there was significant degradation of the drug

DOI: [10.1255/sew.2022.a15](https://doi.org/10.1255/sew.2022.a15)

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silodosin under hydrolytic, oxidative and thermal conditions using LC-ESI-MS/MS.¹² HPLC has also been used under these stress conditions to study the behaviour degradation of the drug sofosbuvir.¹³ A positive degradation was also shown for racecadotril during temperature exposure using NMR, GC-MS and LC-MS/MS.¹⁴ Pulsed laser deposition has also been used to study the temperature effect on the chemical structure of copper oxide.¹⁵

Aspirin tablets were used in this investigation as a model sample. In this work, the first part deals with the exposure of several aspirin tablets to plasma flame and the second part identifies the chemical composition of each sample using Raman spectroscopy. The presented work aims to use Raman spectroscopy as a simple and suitable method for analysing the thermal stability of drugs during exposure to temperature.

Experimental Apparatus

Plasma assisted desorption ionisation (PADI) was used as a source of a plasma flame with helium gas. The visible plasma plume emerges from a coaxial helium gas flow with 13.65 MHz RF. The plasma flame was in near-contact (5 mm separation) with the sample under investigation, using a setting of 8W and a carrier gas flow of 224 mL min⁻¹. Helium was used with electric discharge to produce electrons, ions and excited state gas. In addition to those, the energy of helium is higher than other gases such as nitrogen and this is enough to make ions and it can give stable signals.¹⁶

A Raman spectrometer (model Thermo DXR) was used with a spectral range of 3500–50 cm⁻¹. The Raman conditions, such as laser wavelength, laser power, objective, collect exposure time, sample exposure and aperture, were optimised and found to be: 532 nm, 10.0 mW, 10×, 4.0 s, 2 and 50 μm pinhole, respectively.

Chemicals

Aspirin tablets (containing 300 mg aspirin per tablet) were manufactured by Aspar Pharmaceuticals Ltd, UK and helium gas was supplied by British Oxygen Company gases, UK with a purity of 99%.

Preparation of samples

The samples of aspirin tablets were exposed to the PADI plasma for different times after which they were analysed directly by PADI-MS¹⁷ without pretreatment and the spectra were recorded as a function of time.

Procedure

Several samples of aspirin tablets were exposed under atmospheric pressure for different times: 0, 10, 30, 50, 60, 180 and 300 s and then analysed directly by Raman spectroscopy using the optimal conditions previously determined with a total time of 1 min. The temperature in the helium plasma reached 70 °C during the analysis time of 60 s after which it decreased up to 300 s. Therefore, high temperature could be a major factor causing damage to the aspirin molecule.

Results and discussion

The samples of aspirin tablets, after exposure to the plasma flame, were analysed by Raman spectroscopy using the optimal conditions as outlined above. The signal intensity measurements of the exposed samples were compared to that of fresh sample (0 s). The chemical structure of aspirin is shown in Figure 1. In Figure 2, there is a

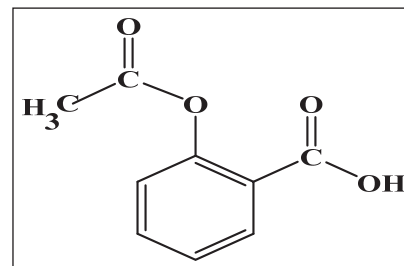


Figure 1. Chemical structure of aspirin.

clear signal intensity of vibrational peaks for 0-s plasma. The carbonyl group (C=O) has a stretching vibration at 1600 cm⁻¹. The vibrations involve C-H and C-CH₃, and were observed at 2950 cm⁻¹ and 1300 cm⁻¹, respectively. Other vibrations, such as C-O-H, O-H and aromatic ring, are shown in Table 1.

In order to investigate the effect of a plasma flame on aspirin chemistry, the intensity and position of vibration peaks were compared between exposed samples and the 0 s one. The analysis results show the six measurements at different

Table 1. Raman identification of vibrations of aspirin.

Peak position (cm ⁻¹)	Vibration
1030	Aromatic rings
1200	C-O-H (OH substitution)
1300	C-CH ₃
1600	(C=O) Stretch
2950	=C-H
3050	O-H

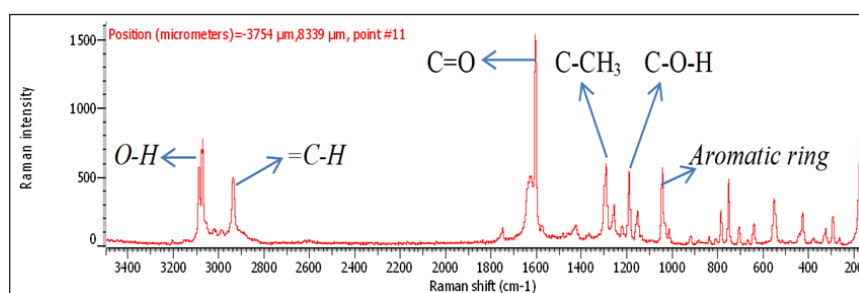


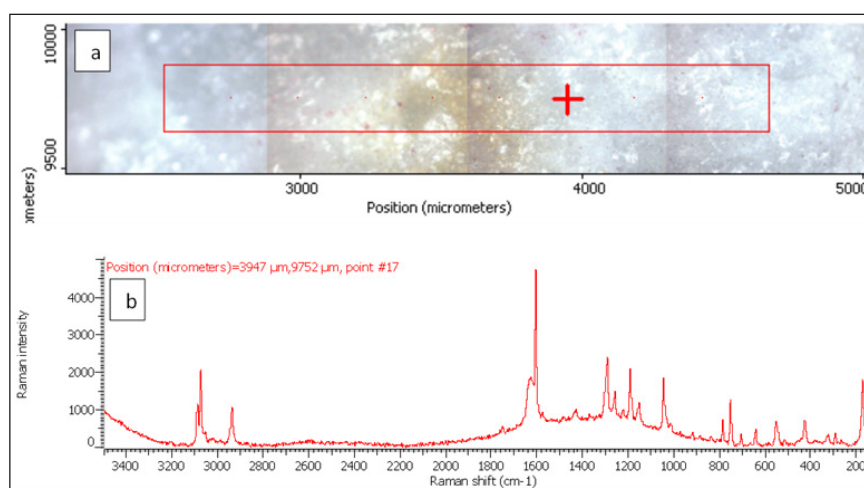
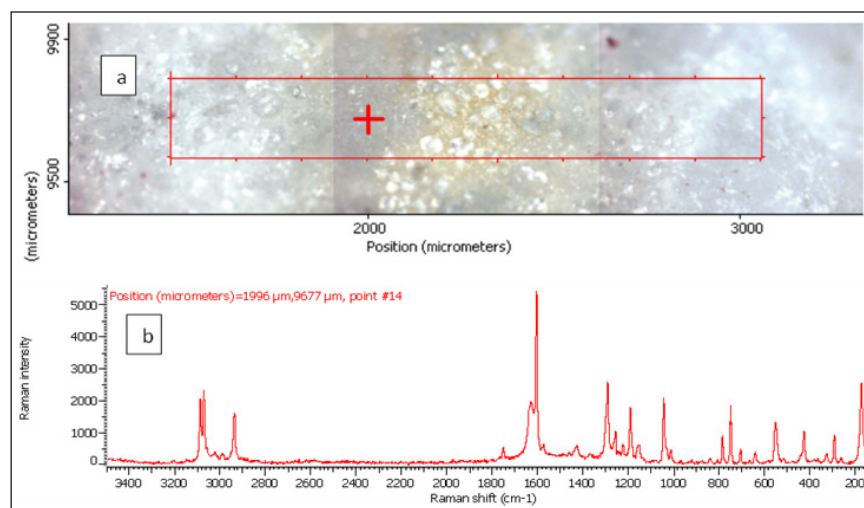
Figure 2. Raman spectrum of 300 mg fresh aspirin tablet (0 s).

Table 2. Peak height of vibrations for fresh and exposed aspirin tablets.

Exposure times (s)	Aromatic rings	C-O-H (OH substitution)	C-CH ₃	(C=O) Stretch	=C-H	O-H
0	550	550	600	1600	550	800
10	1400	1500	1600	4000	1100	2300
30	2000	2500	3000	5500	1700	2600
50	750	500	500	1800	800	1400
60	—	—	—	—	—	—
180	—	—	—	—	—	—
300	—	—	—	—	—	—

exposure times (0, 10, 30, 50, 60, 180 and 300 s). As shown in Table 2, the signal intensity of vibrational peaks increased up to ~30 s, after which it decreased to 50 s. However, no peaks were detected at 1 min, 3 min and 5 min. No important shift in the peak position was found for any vibration. The observed differences in intensities could be attributed to the chemical structure of aspirin tablets not being affected by the plasma flame until 30 s of exposure time, Figures 3 and 4, while it was affected and changed after this time. On the other hand, the change at 50 s was lower compared to those of 60, 180 and 300 s, Figure 5, because after 60 s, the tablets' structure has been changed such that it is no longer detectable by Raman spectroscopy. These results confirm there is no damage to the tablets until after 30 s, after which a little was observed at 50 s, and then the damage increased from 60 s to 300 s.

These results are in agreement with the findings of Al-Maydama *et al.*⁸ which showed that the thermal stability and degradation of aspirin samples after exposure to temperature were changed in comparison to those of the untreated samples. In this previous study, the XRD method showed decreases in peak intensities of treated aspirin samples and this might be attributed to the

**Figure 3.** Raman photo surface (a) and Raman spectrum (b) for aspirin tablet after exposure to plasma flame for 10 s.**Figure 4.** Raman photo surface (a), Raman imaging (b) and Raman spectrum (c) for aspirin tablet after exposure to plasma flame for 30 s.

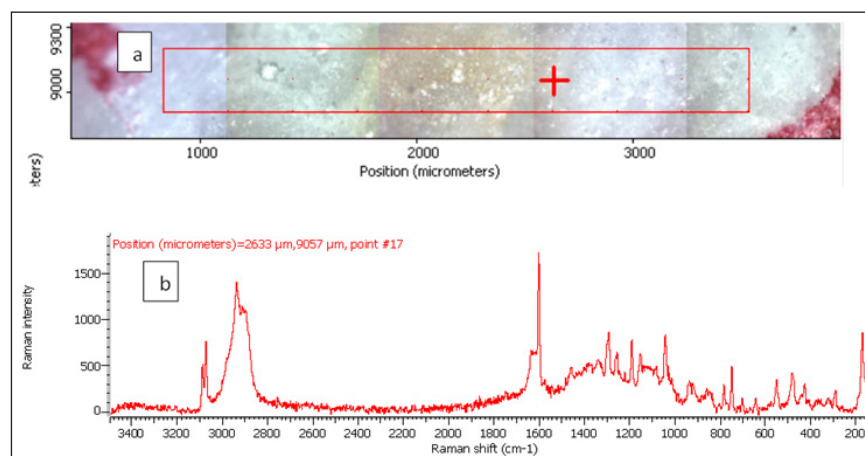


Figure 5. Raman photo surface (a) and Raman spectrum (b) for aspirin tablet after exposure to plasma flame for 50s.

reduction in the crystal structural of the aspirin. In addition, SEM images showed that the surface morphology of the treated samples is changed and the reason for this is that the crystal structure of the treated aspirin particles has a less regular shape than that of the untreated samples. In accordance with the present results, a previous study⁹ has demonstrated that aspirin suffers from degradation during the thermal reaction with salicylic acid.

Conclusions

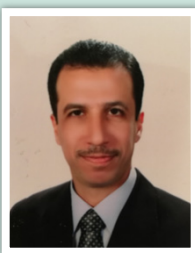
In this investigation, the aim was to show whether the thermal stability of aspirin can be affected by interaction with helium temperatures. The temperature of such conditions was chosen for their impact on aspirin tablets to ensure the quality and safety of pharmaceuticals. This study has shown that the stability of aspirin was changed by exposing to a plasma flame for a long time (≥ 1 min). However, the results have confirmed that the spectra did not show any shift of the vibrational peaks. The results have significant implications for the understanding of how temperature may affect the chemistry of pharmaceutical tablets. Although the current study is based on a small sample, the findings suggest the study should

be repeated using different forms of samples. Further research could also be conducted for the investigation by using other methods of analysis such as infrared (IR) and mass spectrometry.

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Look back and wonder

Antony N. Davies

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

With so much coverage of Queen Elizabeth's remarkable Platinum Jubilee celebrations, not only in the UK but around the world, I was driven to reflect on how our spectroscopic data handling and systems have changed during her long reign. This was rather like wandering around some of the heritage museums, which my family love so much and have visited often in the UK, Germany and the Netherlands. You see so much equipment which was familiar as an everyday tool in our house when growing up and now have to explain to the children exactly what each piece was used for!

I would like to take this opportunity to create a similar timeline. I hope with Ian's permission that we can add to this timeline with contributions from any of you who have particular memories of systems that made a step-change in the way you worked with spectroscopic data.

In the following sections I have made a first attempt to identify "milestones" in the fields of spectroscopic data handling that have been made available to us during the reign of Queen Elizabeth II. I have also added various milestones and incarnations in the life of this journal. A disclaimer—there is no possible way in the space

available that this list cannot fail to miss one of your favourite spectroscopic system developments over the last 70 years (!). So, we would very much like you to tell us about other "milestones" you would like to see put on the timeline using the form at <https://www.spectroscopy-europe.com/form/td-column-timeline>. Please include an image to go with the description. You can see what we have done for some of the entries below; let's see what type of resource we can create together online!

1950s

- 1950: **15 August, Princess Anne the Princess Royal, second child and only daughter of Queen Elizabeth II born.**
- 1951: Heinrich Kaiser gives a seminal lecture on the need for "modern analytical chemistry with physical, primarily spectroscopic methods". Having worked at Carl Zeiss in Jena on spectroscopic instrumentation from 1934 before moving to the state material testing centre of North Rhine-Westphalia in Dortmund, where he took over the management of the spectrochemical laboratory.
- 1952: Kaiser is entrusted with the founding and management of the Institute for Spectrochemistry and Applied Spectroscopy (ISAS). He goes on to help start the Documentation of Molecular Spectroscopy (DMS) efforts collecting reference spectra and associated chemical structure information. Various

collections subsequently published bilingually (English and German side by side) by Butterworths and Verlag Chemie in Weinheim.

- 1953: **June 2 Queen Elizabeth II's Coronation in Westminster Abbey.**

If we go back to the decade immediately after the end of the second world war, spectroscopy as we know it was in its infancy. The need for high quality reference data to support the use and further development of these instrumental analysis techniques is recognised by a few influential scientists such as Heinrich Kaiser and the collection of reference quality data sets begins.

In what was essentially a pre-computing age, extremely clever manual systems were put in place or adapted to suit the needs of the analytical spectroscopist. One such was the DMS Card system shown in Figure 1.

- 1955: First printed version of the Sadtler Spectral Collections.

1960s

- 1960: **19 February Prince Andrew, Duke of York, third child of Queen Elizabeth II born.**
- Mid. 1960s: Chemical structures added to *Chemical Abstracts*.
- 1964: **10 March—Prince Edward, Earl of Wessex, the Queen's youngest son is born.**
- 1965: Work begins on the DENDRAL (from "Dendritic Algorithm") system artificial intelligence at Stanford University by Edward

DOI: [10.1255/sew.2022.a16](https://doi.org/10.1255/sew.2022.a16)

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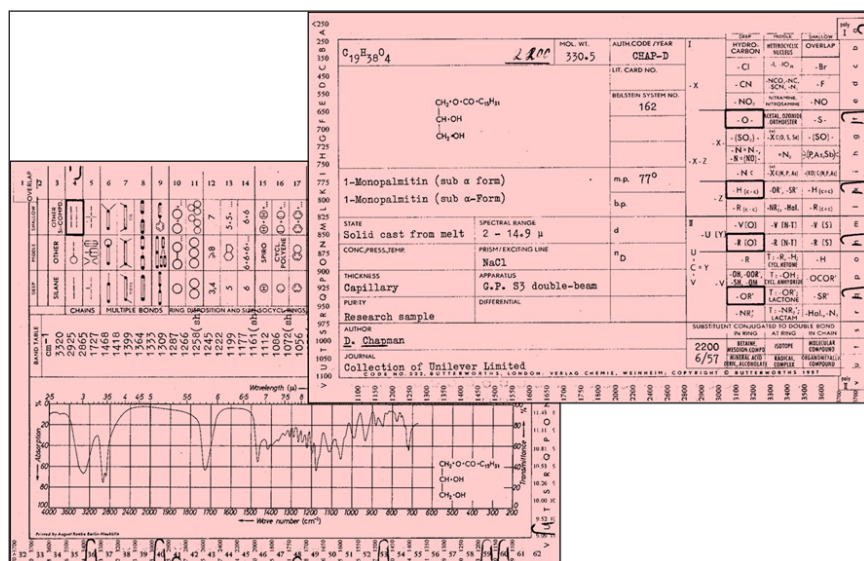


Figure 1. DMS cards, pink indicated organic compounds. Blue cards were for inorganic species.

Feigenbaum, Bruce Buchanan, Joshua Lederberg and Carl Djerassi and their teams. Regarded as the first expert system, it was used to support organic chemists by using mass spectrometric data to suggest molecular structures.¹

- 1969: Bruce Kowalski and co-worker publish works on the use of computers in the analysis of infrared spectra.²
- 1969: First edition of the *Atlas of Mass Spectral Data* (3 Volumes) edited by E. Stenhagen, S. Abrahamsson, University of Goteborg, Sweden and F.W. McLafferty, Cornell University, Ithaca, New York described at the time by a reviewer in the *Journal of Chemical Education* as “a massive compilation (over 6600 compounds)”. 39 sources contributed to this first edition with “the major part of the representing data from Dow and API. The tables are print outs of the computer based storage and retrieval system at the University of Goteborg.”^{3,4}

1970s

- 1972: Protein Data Bank

- 1974: Schrader and Meier publish the first edition of the *Raman/IR Atlas of Organic Compounds*.⁵ Again, here the quality of the analytical sample was paramount in producing top quality data collections. Enormous effort was spent by the technical staff producing this collection in not just buying/obtaining the various chemicals to be measured but

in purifying them. The measurements were carried out just as carefully to avoid saturating the available equipment leading to peak distortions for example. The collection also put emphasis on measuring spectra typical to a compound class—and that is how the spectra are ordered in the Atlas allowing a quick comparison of spectroscopic difference between molecules with similar functional groups. With enormous foresight the data sets were also digitised onto paper tape rolls (Figure 2).

- 1975: *ESN – European Spectroscopy News* launched by Heyden; a predecessor magazine to *Spectroscopy Europe* and *Spectroscopy World*, starts publication.
- 1976: March 26, Queen Elizabeth sent her first email—probably the first head of state to do so.
- 1976: Milne & Heller publish the introduction to the MSDC/EPA/NIH Mass Spectral Search System, part of the NIH and EPA developed Chemical Information System (CIS). This includes multiple spectroscopic database search strategies.⁶

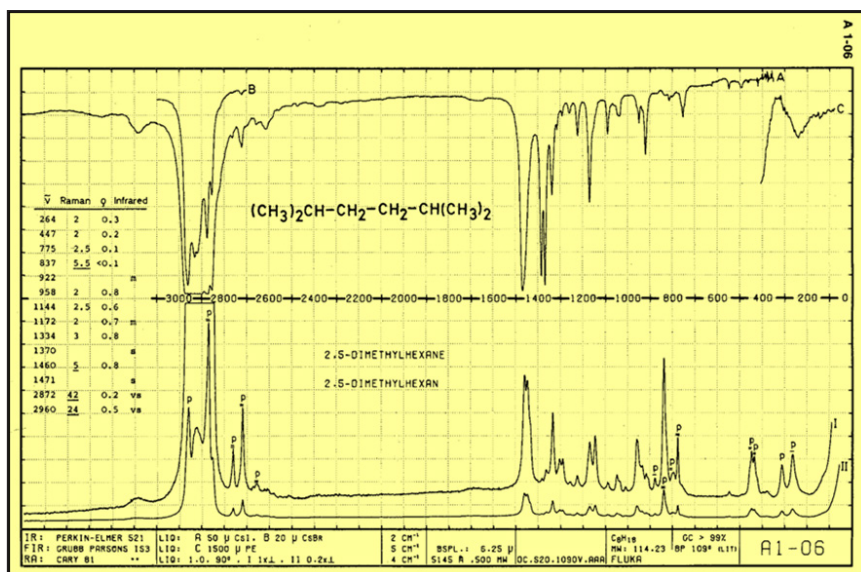


Figure 2. An example page from the Schrader–Meier *Raman/IR Atlas of Organic Compounds*.⁵

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- 1977: **Queen's Silver Jubilee year, Her Majesty first flew in Concorde having followed its development for 11 years.**
- 1978: Wolfgang Bremser publishes the HOSE code—a new substructure code which is a key component in NMR data handling for structure–spectra correlation.⁷

1980s

- 1980: First digital edition of the Sadtler Spectral Collection.
- 1981: **29 July—Charles, Prince of Wales marries Lady Diana Spencer.**
- 1982: The Japanese SDBS Spectral Database System for Organic Compounds is first made available. This is a somewhat unique freely available collection of six different types of spectroscopic analyses and compounds. The database contains an electron impact mass spectra (EI-MS), Fourier transform infrared spectra (FT-IR), both ¹H and ¹³C NMR spectra, laser Raman and electron spin resonance (ESR) spectra. The majority of the spectra were measured at the National Institute of Advanced Industrial Science and Technology (AIST) https://sdb.sdb.aist.go.jp/sdb/cgi-bin/cre_index.cgi
- 1982: Specialist spectroscopy publisher Heyden & Sons Ltd's analytical titles acquired by John Wiley & Sons.
- 1982: **21 June—Queen Elizabeth's grandchild, Prince William, Duke of Cambridge, born to Prince Charles and Princess Diana and, on 9 July, Queen Elizabeth awakes to find a stranger sitting on the edge of her bed, dripping blood from a cut hand.**
- 1988: First JCAMP-DX spectroscopic data transfer standard developed between the academic, industrial and instrument vendor communities with the explicit aim of enabling

the exchange of data between computer systems as a key enabler for the creation of reference spectroscopic databases.

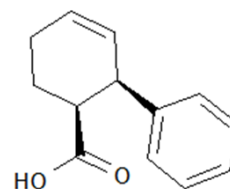
- 1988: Responsibility for the NIST/EPA/NIH Mass Spectral Library passes to the NIST Mass Spectrometry Data Center. A different data quality ethos for collecting mass spectra with each spectrum being critically evaluated has meant that this collection has seemed to lag behind the other large collection of mass spectra.
- 1988: SMILES line notation published.⁸
- 1989: *ESN—European Spectroscopy News* acquired by Aster and becomes *Spectroscopy International* in Europe.
- 1989: *Spectroscopy World* begins publication in the UK.

1990s

- 1992: *Spectroscopy International* acquired by VCH and merges with *Spectroscopy World* to become *Spectroscopy Europe*.
- 1992: SpecInfo online goes live on STN international with 70,000 ¹³C NMR, 17,000 infrared and 6000 NMR spectra of other nuclei (¹⁹F, ¹⁵N, ¹⁷O, ³¹P).⁹
- 1996: August sees the release of the NIST Chemistry Webbook—initially only with data from the NIST Standard Reference Database 19A: NIST Positive Ion Energetics, v. 2.0. For a recent review of all the reference data programmes run in the USA by NBS/NIST see Reference 10.
- 1996: 1–3 September—“Linking and Interpreting Spectra through Molecular Structures” conference includes the Warwick Challenge to the

vendors present to demonstrate the import and export of data of the types that they can handle from the systems of the other vendors present. The conference passes a motion around the need for an analytical reference data archive.

- 1997: August—one year after the NIST Chemistry Webbook went live the first infrared and mass spectra are added to the resource.
- 1998: June—CAS celebrate 18 million substances registered with the chemical structure shown below



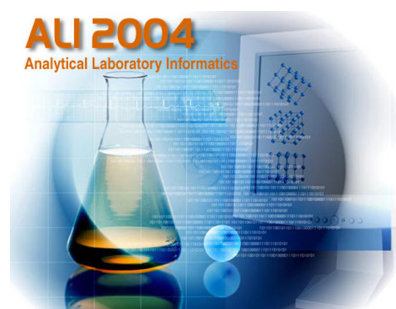
2000s

- 2000: July—CAS reaches 25 million registered entities registered in CAS.
- 2001: October—*Dark Ages II: When the Digital Data Die* by Bryan Bergeron published.
- 2001: the National Metrology Institute of Japan (NMIJ) under National Institute of Advanced Industrial Science and technology (AIST) takes over management and maintenance of the SDBS.
- 2002: **Queen's Golden Jubilee, 50 years.** February—Seminar on Preserving the Record of Science, UNESCO, Paris.
- 2004: June saw the first conference in Analytical Laboratory Informatics, where vendors

Linking and Interpreting Spectra

LSMS

through Molecular Structures



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and scientists will actively work together to define innovative, sophisticated solutions for getting the most from our analytical data.

2000s The New Millennium

- 2013: 22 July—Prince George of Cambridge, born—the Queen's great grandchild and 3rd in line to the throne.
- 2020: January sees the commencement of measures by European Governments to combat COVID-19.

- 2020: 2 April—John Wiley & Sons Inc. announces the acquisition of Bio-Rad Laboratories, Inc.'s Informatics products including the company's spectroscopy software and spectral databases adding, for example, the KnowItAll software suite to Wiley's Science Solutions.

- 2022: 2 June Queen Elizabeth II Platinum Jubilee.

A period that will surely be remembered not only for the Platinum Jubilee but also for the COVID-19 pandemic which impacted so many of us in terrible ways, often exposing deficiencies

in our infrastructure and disaster recovery planning as many were forced to work from home for long periods where the infrastructure we rely on in normal times simply did not stretch. There is a useful resource published by the European Centre for Disease Prevention and Control which documents the timelines that different states adopted various measures to combat the disease.⁹ However, I believe this period will also be remembered for the innovation of our scientists and support staff as well as IT providers (think of the capacity and speed deficiencies of existing video meeting infrastructure at the start of the pandemic and the rise of Zoom calling!) who rose to the challenges and often changed roles and jobs to join the fight against the virus. As I write this many laboratories are still yet to return to pre-COVID tasking especially in the universities attached to medical schools. I salute all those involved in teaching spectroscopy for the multitude of innovative solutions they have found in the last couple of years to still provide a good education to our students in the most difficult of circumstances.

- *Wiley Registry™ of Mass Spectral Data*, is now in its 12th Edition, with 817,290 spectra of 668,435 unique compounds and 785,061 chemical structures.
- NIST/EPA/NIH EI-MS Library, 2020 release, 350,704 spectra of 306,643 compounds and 447,289 retention index values. Keeping up with instrumental developments the NIST Tandem Mass Spectral Library, 2020 release has 1.3 million spectra with 186,000 precursor ions from a variety of both high- and low-resolution fragmentations methods. Much of this data comes from human and plant metabolite studies, drugs and other bio-active compounds.



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In order to be inclusive, the event will be held in hybrid format. Those unable to attend physically are welcome to participate virtually via our online platform.

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Let's build on this resource...

As discussed at the top of the article please send in your own contributions to this list and see what we can generate together!

Stay Safe!

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World Conference on Sampling and Blending WCSB10, June 2022: broadest scientific coverage ever, excited in-person attendees and a 1000-year historical closure

Kim H. Esbensen^a and Elke Thisted^b

^aChairperson WCSB10 Scientific Committee

^bChairperson WCSB10 Organisational Committee

The world community of sampling has reasons to celebrate. The 10th World Conference on Sampling and Blending (WCSB10) took place between 31 May and 2 June 2022 in Kristiansand, Norway. It was the first physical gathering of members of the international sampling community in 2.5 years. A total of 121 in-person attendees from 20 nations together with 19 online attendees who, for one reason or other, could not travel to Norway. In the summer of 2021 when prospects for in-person gatherings of this magnitude were distinctly bleak, the organisational committee nevertheless made a deliberate decision to prepare for success and to go all out for an in-person conference. As it turned out, this paid off beautifully; a total attendance of 140 is right on par with several earlier conferences. From many personal reactions and statements, it was clear that the

international sampling community had been starved of physical interaction. Again and again, delegates declared their excited satisfaction over simply being together again and being able to freely interact vis-à-vis one-another—to the delight of the scientific and organising committees.

A Jubilee conference

WCSB10 was a jubilee conference. It is now 70 years since the first concepts and ideas of what was to become the Theory of Sampling (TOS) were first formulated by Pierre Gy, which has since found application in a growing number of industrial application areas, at first in the “original sectors” of mining, minerals processing and metals (M3), cement a.o. This has in fact been the stable historical status quo until the turn of the millennium when the series of WCSB was initiated. Though the TOS has a clear role to play as an important part of modern society’s drive for sustainable processes and products, there is still a long way to go before this will be fully implemented. In fact, for all the first 20 years of organised activity during 10 World Conferences, there has been a deliberate scientific and technological outreach to

other industry sectors and to society in general as a priority.

This is where WCSB10 was a highly satisfactory success. More than 50% of the contributions addressed application areas *beyond* M3 in technology, industry, society, commerce and trade, e.g. food, feed, agriculture, pharmaceutical production, with special focus on QA/QC/QM, Process Analytical Technologies (PAT), environment, sustainability, circular economy, and also witnessed by the concluding session “Around the world/new developments/going forward”. Likewise, there was substantial coverage of how representative sampling is a necessary element in companies’, corporations’ and organisations’ quality management objectives and environmental goals—and how to optimise the use of natural resources and raw materials (finite and renewable) with considerations of the environmental impact.

WCSB10 specifically targeted the UN world development goals nos 9 and 12, which address sustainable industry, innovation and infrastructure (9) and responsible production and consumption (12). The conference contributed towards fulfilling the aspirations embedded in

DOI: [10.1255/sew.2022.a17](https://doi.org/10.1255/sew.2022.a17)

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these international goals. Thus, WCSB10 lived up to its broader scope, honouring the pronounced sustainable dimension set up by the conference host, the industrial EYDE-Cluster. WCSB10 strengthened a conscious attitude towards sampling quality in the broader sense—and helped foster a proper mindset in many new application fields, technology and industrial sectors.

The conference homepage will be continued as a depository for results, achievements and common as well as individual experiences, not least a plethora of photographs: <https://wcsb10.com/>

Please follow the link on the WCSB10 homepage to see the conference report “Participants from 20 countries at the WCSB conference”.

D3

A special thank you and a strong recommendation goes to the company D3, which was retained to take care of all IT aspects—a task carried out to perfection. The execution of all technical tasks for running the three-day conference went without a glitch. The magnitude of the necessary online facilities could not be predicted before the conference, as many potential participants were unable to make a firm decision GO/NO GO until immediately before the start of the conference due to the different COVID situations across the globe. Thus, WCSB10 had to be ready to accommodate an essentially unknown proportion of online participants and contributors. In close collaboration with the organisational committee, D3 organised a seamless integration of what turned out to be only a small number of pre-recorded or live contributions, while producing full coverage with a perfect streaming facility for all three conference days. All hail to D3 for a thoroughly professional job! <https://www.d-3.no/>

The most important aspect of a modern proceedings is for it to be available OPEN ACCESS for everyone interested, particularly also beyond the immediate target audience. The WCSB10 proceedings can be downloaded free of charge from <https://www.impopen.com/wcsb10>

WCSB7/10 has developed a [complete script](#) for comprehensive, ultra-fast, top-quality proceedings production—available for other conferences should organisers desire.



“Thank you and congratulations to the organising committee of the WCSB10. From feedback I received from colleagues who attended in person, the conference went off very well, despite all the challenges faced.

Due to personal reasons, I was, unfortunately, unable to attend in person, so I can only speak to my experience of the virtual conference, which was brilliantly executed. It is always difficult to get engagement and a good flow during virtual conferences like this, but the WCSB10 team managed to successfully pull it off. With good connection for 99% of the time, well integrated pre-recordings of papers and online contributions, to accommodate those who could not attend. The technically excellent displays of speakers and their presentations really made this a great experience.

This was one of the best online conferences I have ever attended.”
Trevor Bruce

Radisson Blu Caledonian Hotel, Kristiansand

A similar huge appreciation goes to the venue hotel, Radisson Blu Caledonien, for a thoroughly professional collaboration throughout the COVID-uncertain year leading up to the conference start. At ground zero, 29 May–3 June, this was put to the test in full earnest and passed with flying colours—whatever logistical and

practical issues were thrown at the hotel staff and administration were solved promptly and efficiently.

Proceedings

As the immediate exuberance of in-person, or online conferences eventually begins to fade, on the longer historical scale the lasting documentation of any scientific conference is its *proceedings*.

The 2022 WCSB10 Proceedings were edited by Kim H. Esbensen and Anne Jodon Cole.

WCSB10 decided to make use of the then-novel proceedings format and production schedule developed for WCSB7, using the same editor and publisher, allowing contributors the advantages of the shortest possible submission and review deadlines on record. This was a deliberate goal for WCSB10, setting out a modern standard for digital proceedings a.o. cutting down significantly on the duration of the editorial tasks of servicing authors with very different experiences of resubmission, reviewing and revising manuscripts. The final quality of the proceedings provides the scientific touchstone for posterity. Great appreciation goes to the publisher IMP Open, Chichester, UK (<https://www.impopen.com/>)

WCSB10 host organisation and organisational committee

The idea of hosting the World Conference on Sampling and

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Well-deserved recognition to the Organisation Committee (background) with Conference Secretary extraordinaire Kristine Fuller-Gee and Chairperson Elke Thisted (live). Photo credit: WCSB10

Blending in Kristiansand, Norway, arose at the 2017 8th WCSB conference in Perth, Australia. Arranging such an event to spread knowledge on how to sample correctly, discuss current issues in modern industry and get a life-line on how to proceed in a more sustainable direction with less variation in processes, fitted very well with the vision of the industrial EYDE-Cluster, the Norwegian Centre of Expertise (NCE) for Sustainable Process Industry, working for transition towards a sustainable future. Therefore, a proposal for WCSB10 was presented to, and approved by the EYDE-Cluster in 2018. From that day, a compact preparatory committee consisting of Elke Thisted (Glencore 'Nikkelverk'), Marianne Furuholt (EYDE-Cluster) and Kim Esbensen (KHE Consulting) started planning towards WCSB10. The schedule pointed to 2021, but the global COVID situation disrupted the regular biannual WCSB series. However, when the time was again right, a regrouped committee of seven members of, and employees in the EYDE-Cluster as well as partners and professional

friends, went to work again—and the conference was finally ready to be launched in Kristiansand in 2022. A deep gratitude for dedicated hard work and a very agile attitude goes to:

Kristine Fuller-Gee (EYDE-Cluster), Anne Ormshammer (EYDE-Cluster), Ellen Nordgård-Hansen (NORCE), Gro Wickstrøm (GROW), Anne Cole (ReConsider), Kim Esbensen (KHE Consulting) and Elke Thisted (Glencore 'Nikkelverk').

WCSB10 Scientific committee: review corps

Conference proceedings are no better than the peer-reviews involved. Efforts are always directed at securing a corps of reviewers with the optimal scientific competence and experience.

The 2022 WCSB10 corps consisted of Roger Brewer, Stephane Brochot, Trevor Bruce, Quentin Dehaine, Oscar Dominguez, Simon Dominy, Karin Engström, Kim H. Esbensen, Dominique Francois-Bongarcon, Ralph Holmes, Dr Li Huachang, Martin Lischka, Pentti Minkinen, Richard Minnitt, Claudia Paoletti,

Bert Pauels, Francis F. Pitard and Aldwin Vogel.

A very great THANK YOU to all for this essential contribution!

Meeting point: exhibition and poster session

During coffee breaks and a wine tasting event, sponsored by **Elgin wines**, South Africa, conference participants could learn more about sampling equipment, automation and direct analyses of process flows a.o. from conference exhibitors. There were many fruitful discussions at the different stands provided by FLSmidth, Metrohm Process Analytics, Iteca Socadei, Multotec, Scott Automation/Rocklabs and Scantech. It was also possible to chat and discuss at three poster sessions with authors presenting their work spanning a wide coverage of correct sampling and the TOS as well as a call to action regarding the future evolution of the world's only horizontal sampling standard, DS3077.



Testimonials

The weeks immediately after WCSB10 witnessed a flurry of personal impressions and testimonials from happy participants at WCSB10's LinkedIn homepage, which can all be found at <https://www.linkedin.com/company/wcsb10/>

Suffice to quote a fairly "representative" impression from the many personal impressions:

"WCSB10 was a great opportunity to interact with the growing community of scientists and technologists who are applying TOS."

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The conference provided ample opportunity to see the Governing Principles and Sampling Unit Operations applied to industrial processes. The presentations also showed a growing interest in real-time process monitoring through the field of Process Analytical Technology (PAT).

Kristiansand provided a very relaxing atmosphere for the conference. The meeting hall and exhibition spaces were well organised, with good opportunities for relaxing walks together with colleagues, or chats on the balcony of the conference area.

I believe all participants will carry home great memories of this conference, and a renewed and strengthened enthusiasm to keep learning and contributing. WCSB10 leaves an important legacy through our memories, and through the OPEN ACCESS proceedings, which document the current state of our field and of the opportunities to move forward.”

Rodolfo Romanach

Reinvigorated IPGSA Council

The last in-person Council meeting of the International Pierre Gy Sampling Association (IPGSA) took place in August 2019 at WCSB9 in Beijing, after which COVID disruptions ruled for a long time resulting in a pronounced inactivity.

At the concluding General Assembly session at WCSB10 it was finally possible to take a fresh stock of the duties and obligations. The first point of business on the IPGSA General Assembly agenda was election of a new Council, a task easily accomplished as many members were ready and willing to contribute in the form of several new members and a contingent of Council members willing to carry on. It was decided to augment the number of Council members with two, now totalling 10 (plus four fixed positions: President, Vice-President, Treasurer and Webmaster/Publications) The new IPGSA Council, looking at a time horizon of two to four years ahead was voted in with acclamation.

It is fair to say that WCSB10 marks a generational shift for the IPGSA Council.

At its first meeting in the 2022–2024/2026 period there was an urgent interest and willingness to get to work. The first item will be to bring the IPGSA Foundation in alignment with the new post-COVID realities. After this has been taken care of, the world sampling community will no doubt soon hear what other measures will be taken by the new Council. After a period of 20 years in which focus naturally has been to initiate, grow and secure a firm organisational support, time has come to look ahead with fresh views as all necessary basics are now well in place: the IPGSA association, a bank affiliation (having escaped organisational account slaughter by banks involved in the Panama Paper scandals now cleaning up their reputation), highly successful biannual WCSB conferences, the IPGSA homepage and the publications outlets *TOS Forum* and this



Newly elected IPGSA Council (left-to-right): Elke Thisted, Kim H. Esbensen, Philippe Davin, Karin Engström, Claudia Paoletti, Oscar Dominguez, Rodolfo Romanach, Aldwin Vogel, Martin Lischka, Stephane Brochot, Sheryl Tittlemier, Ralph Holmes. Photo credit: WCSB10

SAMPLING COLUMN



The PGSGM committee (Francis Pitard, Kim H. Esbensen, Pentti Minkkinen, Ralph Holmes, Dominique Francois-Bongarcon), with medal and ready to go—but without the awardee. Photo credit: Rodolfo Romanach.

Sampling Column in *Spectroscopy Europe/World*.

The new IPGSA Council 2022–2026 has the floor going forward...

Pierre Gy Sampling Gold Medal (PGSGM)

A scientific highpoint at all WCSB conferences is the tradition of revealing the recipient of the PGSGM awarded for “Excellence in dissemination and teaching of the Theory of Sampling”.

The PGSGM committee had duly submitted the name of the WCSB10 selectee, the medal had been minted and was present in time for the gala dinner on the penultimate day of the conference, at which the august committee gathered on the stage for the traditional award ceremony. But the 2022 event had a different slant than any before—the recipient was *not present*, neither physically nor online (due to legitimate reasons for absence: he was working at an isolated remote location in the Australian outback).

The Gold medal’s worthy recipient this year is **Dr Simon Dominy**.

To honour Simon, the committee took centre stage at the gala

dinner with an introduction by Kim H. Esbensen, providing the audience the background of the origin and history of the PGSGM, and a salute to Simon by Francis Pitard, giving the reasons for the committee’s selection, i.e. a consistent, impressive dissemination effort over many years.¹

Dr Simon Dominy is a mining geologist-engineer with over 25 years based in operations, consulting and academia. He has experience across mine production, corporate business development and multi-disciplinary studies. Simon has a background in underground operations management and technical/leadership roles, with multi-commodity and continent experience. He has worked across the mine value chain from project studies, through to mine reopening/development, operations and operational improvement. He is a Visiting Associate Professor at the Camborne School of Mines, University of Exeter, UK, and holds technical roles with Novo Resources Corporation, Artemis Resources Ltd and OCX Gold Group. Simon points out that it was his encounter with “Le Bon” Royle c. 1990 that initiated him to the field of sampling. Le Bon Royle was the very first PGSGM recipient (2003).



Simon Dominy, winner of the 2022 Pierre Gy Sampling Gold Medal.

The medal was subsequently delivered by hand to Simon Dominy in Perth, courtesy of two WCSB delegates returning to Australia after the conference. All’s well that ends well ...

WCSB11

The last item on the agenda for the newly elected Council was to decide on the venue of the next conference, WCSB11. There was only one bid, submitted as a perfunctory application commensurate with all the necessary stipulations listed in the IPGSA Foundation. Consequently, the Council unanimously decided that the next venue shall be in Centurion County, Gauteng, South Africa. WCSB11 shall be co-chaired by Dick Minnett (prof. emeritus, WITS) and Terance Nkosi, executive head SHEQ and Technical Assurance, Rand Refinery, Johannesburg (Germiston). IPGSA looks forward to returning to South Africa.

Things to come...

By coincidence, or maybe no coincidence at all? Perhaps the most notable impression of WCSB10 was captured by the snapshot

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The entire WCSB10 organisational and scientific committees, including erstwhile initial member Marianne Furuholmen (left of the only male in this happy group). For good measure keynote speaker Claudia Paoletti joined in the photo fray. Photo credit: WCSB10

below of the full complement of the organisation and scientific committees at a refreshment pause on the 13th floor of the venue hotel. Guess which gender is taking over running the show these days—also in highly technical, specialised scientific disciplines? No worries for the future....

Epilogue: an 1000-year historical closure

Pierre Gy, when engaged about the matter, fondly told about his firm opinion that his family originated from the Normandie region in France, not from the Mediterranean coast (Nice and Cannes) where he lived most of his career. He further clarified that his family name, distinctly non-French, is related to Norwegian Vikings who raided *La Normandie* pretty much exactly 1000 years ago... In fact, Pierre Gy stated with conviction that his family was a direct descendant of one of the *Norman Vikings*! It is a no-brainer to deduct from where and why this region of France got its name.

Fast forward to 1999, when Pierre Gy was an invited speaker at

the Sixth Scandinavian Symposium on Chemometrics (SSC6), Porsgrunn, Norway: <https://bit.ly/GySSC6>

At the symposium Pierre requested a personal favour from the chairman (KHE), asking for directions to a place “near Flekkefjord” he had researched as part of his private preparations for SSC6, to which he wanted to drive himself and his wife after the conference. The chairman went out of his way to accommodate this wish, but could unfortunately not accompany Pierre and Sylvia himself at such short notice. Alas this is one of the things the chairman has since regretted bitterly, because it turned out that the drive was a bit too long and strenuous for the enterprising couple within the time available—much to *their* regret.

Pierre Gy’s intended destination was a small mountain valley “Gyland”, in the Flekkefjord municipality. Gyland is situated in a nearby inland area with a large lake “Kongevoldvannet” surrounded by forests, containing several islands of various sizes. He was of the firm

opinion that he would be able to “close the family history circle” if he could find the location of a former Viking settlement in Gyland—emphasis on *IF* he could find it...

As preparations for WCSB10 were underway, chairpersons KHE and ET debated *if* and *how* perhaps to make a half-day off-conference visit to Gyland—as a surprise for conference participants. *Alas again*, it turned out that this drive was deemed a bit too long and cumbersome, this time because of the already completely full, intense conference programme and schedule, much to *our* regret.

However, the “last man standing” in the aftermath of WCSB10 happened to be KHE, relaxing with a few colleagues and friends after the conference in the hamlet of Tregde (some 40 km west of Kristiansand). After all guests were happily sent off home in many directions, co-editor Anne J. Cole and KHE decided to set time off for a half-day excursion to do a little research in the hamlet of Gyland, which was only slightly more than one hour’s drive away... And luck was present that day: with the help of the proprietor of the local convenience store in town, and a brief telephone conversation with a local history expert, the quest of the roots of Pierre Gy and his family has possibly finally come to light.

Below follows a brief photo documentation from the contemporary hamlet Gyland, with the island “Storøya” in the centre of the dominant lake “Kongevoldvannet”, where archaeological finds have been dated to the “Viking age”.

Looking at the shoreline of Storøya, one would dearly like to believe that this is perhaps closing the gap of the ~1000-year story of the Gy family. This likely *could* be the place of origin of the Viking family that took the name “Gyland” (meaning “from Gyland”). *Perhaps* the raiding parties setting out from the coastal area which is now the Flekkefjord region included

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Lake Kongevoldvannet with the island of Storøya where alleged Viking age archaeological artefacts have been found. View angles of additional photos indicated. © OpenStreetMap contributors, <https://www.openstreetmap.org/copyright>

members from the local neighbourhood—young Vikings eager to prove themselves in raids to foreign lands? Or perhaps equally likely, and much less violent, according to the *Encyclopaedia Britannica* (online version), the Normandy coast was repeatedly raided by



Farm cluster in Gyland anno 2022.
Photo credit: Anne J. Cole

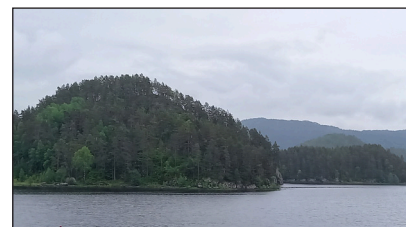
Vikings (“Nordmenn”, “Northmen”) from the 8th century onwards. The French king Charles III the Simple, ceded the territory around Rouen and the mouth of the Seine to Rollo, the chief of the largest Viking group, in the Treaty of St Clair-sur-Epte (911). What followed was a large immigration of Rollo’s countrymen who settled the country and adopted the local culture and language. There is, of course, much more work to do to further document the Gy family history in France in more detail, which is what Pierre Gy had hoped to do. What is known is that as time passed, the name **Gyland** was abbreviated to **Gy**—and the rest, as they say, is history!

Is this the historical background for where, in a sense, “science-backed sampling” originated?

It was a distinct pleasure to try to complete this important family link of the founder of the TOS, alas



Looking across 1000 years of human presence at the island “Storøya”, shown in close-up below. Photo credit: Anne J. Cole



Close-up of “Storøya”, where Viking age artefacts are alleged to have been found. Could this be where “all of science-backed sampling” originated? Photo credit: Anne J. Cole

without his own fulfilment. But this is nevertheless an interesting historical background for the international sampling community.


Reference

1. <http://emps.exeter.ac.uk/csm/staff/sd412/publications>

SAMPLING COLUMN




Kim H. Esbensen is an international expert and consultant in sampling (Theory of Sampling, TOS), chemometrics and PAT (Process Analytical Technology). Through a 35-year academic career involving three professorships, he has conducted R&D across a wide range of application fields, primarily in process industries (mining, minerals extraction and processing, bio-fuels, recycling, environmental monitoring, nuclear waste) in environmental science a.o. In 2015 he established an international consultancy (KHE Consulting). Esbensen has been responsible for a university educational programme straddling 30+ years in chemometrics, PAT, TOS, instrumental analysis, Multivariate Image Analysis (MIA), process technology and Philosophy of Science, currently in the form of a continuing education curriculum offered via KHE Consulting. His CV lists ~300 publications and ~400 lectures/presentations. He is a recipient of the Pierre Gy Sampling Gold Medal (2013), and the Russian Chemometrics Society Gold Medal (2012). In 2003 he inaugurated the biannual series of World Conferences on Sampling and Blending (WCSB), now in its 10th edition—<https://wcsb10.com>. Esbensen is editor of the scientific magazine *TOS Forum* and of the Sampling Column in *Spectroscopy Europe/World*. Esbensen's credentials are documented in full at KHEC's website: <https://kheconsult.com>. Esbensen was head of the Scientific Committee for WCSB10, June 2022 in Kristiansand, Norway.

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Elke Thisted has worked as the Manager of Online Analysis & Development at Glencore Nikkelverk in Kristiansand, Norway, since September 2018. She studied Chemistry at the Technical University in Karlsruhe, Germany, from where she was awarded a MSc (chemistry) in 1998. She received a PhD degree from the Norwegian University of Technology and Science in Trondheim in 2003 in the field of impurities in aluminium electrolysis. From 2004 to 2014 she worked in Elkem, Norway, on method development (measurement, processes and products). Since 2014, she has worked at Glencore Nikkelverk as Lead Process Engineer responsible for process mapping and improvement based on Nikkelverk's business system (LEAN). She has since then worked with variography to broaden applications in the process industry, applying experiences and knowledge gained "in-action" to Glencore Nikkelverk's Online analysis framework. Thisted joined the IPGSA council in 2017. She was Chairperson and head of the organisational committee for WCSB10, June 2022 in Kristiansand, Norway: www.wcsb10.com

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The ISO technical committee on reference materials (ISO TC 334): Annual meeting 2022 and ISO future developments

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Introduction

There has always been and will continue to be collaboration between individual producers of reference materials (RMs), and in many countries around the World, you will find national “mirror” committees reflecting and inputting regional decisions into their appropriate ISO representatives. However, many years ago, RM producers recognised that the growing need by the analytical community for a number and variety of RMs as well as a need for the assurance of the quality of RMs called for collaboration at the international level. This has been achieved through REMCO, the Council Committee on Reference Materials of the International Organization for Standardization (ISO), which celebrated its 40th anniversary in 2016. The evolution of this organisation and its conversion into the formal ISO TC 334 – Reference Material continues in 2022 and beyond, and the key changes are detailed here, in a

report of their latest annual meeting.

The essential role of supporting RM producers and Accreditation Bodies via the ISO 17034 standard¹ route continues as one of the primary mandates of TC 334, but here is the first significant change in this TC.

By definition, an ISO Technical Committee’s main role is to write standards, appropriate to its defined area of expertise. Also, in the language of ISO, a “Guide”, is defined as an informative document which assists an ISO TC in the construction of standards, appropriate to the TC.

However, historically the ISO/REMCO Guides, in some cases, were not designed for this purpose,

but were informative documents for RM producers *per se*. So, the first task that the new TC 334 has to consider is how to meet this requirement and convert these Guides into the appropriate standards, and this conversion essentially forms the basis for the work programme detailed below. To fulfil these conversions, either new or existing appropriate Working Groups were created and/or reinstated, as appropriate. The new committee structure that resulted is shown in Figure 1.

In addition, in a TC structure a Working Group is tasked with a specific project plan, and associated timeframe to investigate (and produce if appropriate) a related standard. Within the old ISO/

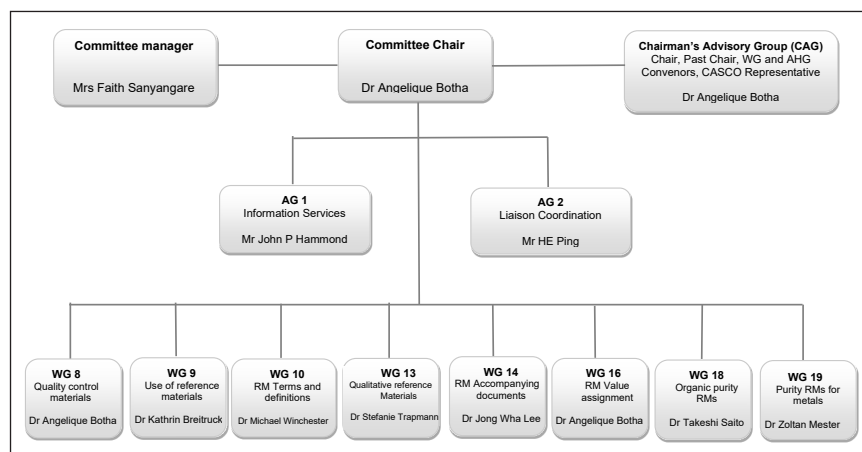


Figure 1. ISO/TC 334 Committee structure (2022).

DOI: [10.1255/sew.2022.a18](https://doi.org/10.1255/sew.2022.a18)

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REMCO structure there were a couple of Working Groups (WG6 – Information Services and WG17 – Liaisons) that, whilst essential to the functioning of the TC, do not meet this requirement. Therefore, a structural rearrangement with respect to these essential requirements was made, converting these two groups to Advisory Group 1 (AG1) and Advisory Group 2 (AG2), respectively.

This article details the 3rd annual meeting of ISO TC 334. Held virtually as a video conference as three sessions on 7 June, 9 June and 14 June, it was well attended with 62, 55 and 52 participants, respectively, on each day.

Work programme

As stated above, the primary task of ISO TC 334 is the conversion of the existing ISO/REMCO series of Guides, into their equivalent ISO 334xx standards as shown in Table 1.

As these new standards still essentially form the support structure to ISO 17034, this relational structure can be redrawn as shown in Figure 2.

As you can see this is not an insignificant amount of work, given the required ISO publication dates in the period December 2023 to August 2024, and therefore, prior to this meeting, it had been discussed and agreed that for ISO

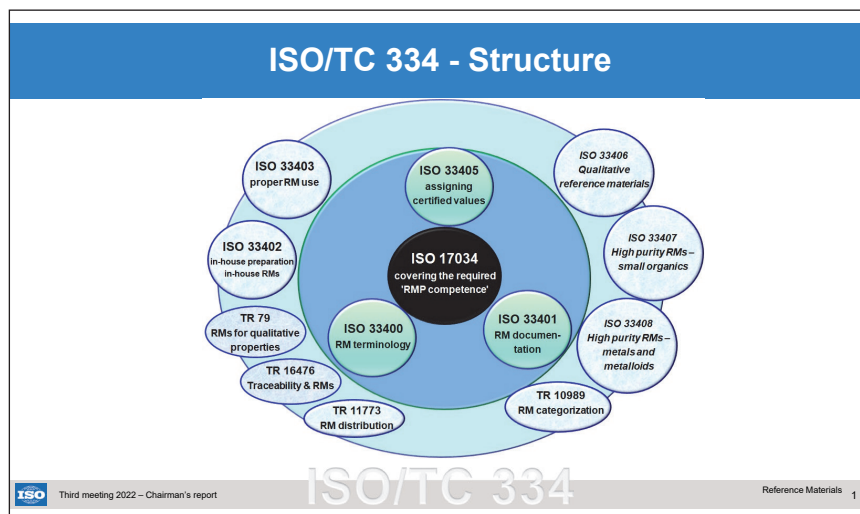


Figure 2. Relationship structure of ISO/TC 334 standards to ISO 17034.

33401/2/3/5 the process would be to simply “fast-track” the transformation of these ISO/REMCO Guides (Guides 31/80/33/35) using a simple international balloting process in TC 334. However, for ISO 33400/6/7/8 (Guides 30/85/86/87), the complete standard development process will be followed, through the appropriate series of draft standards and/or ballots.

For these reasons the meeting essentially split into the following agenda:

- Report of the secretariat

This report, by the SABS, the ISO member for South Africa detailed the current structure of ISO TC334,

which consists of experts in a range of diverse fields from over 40 countries. Anyone interested in getting involved should contact their national ISO member. It also detailed the existing extensive liaisons that ISO TC 334 had inherited from ISO/REMCO, both with similar ISO Technical Committees (TCs) and external international bodies.

- ISO TC 334 Strategic Business Plan

The Strategic Business Plan (SBP) was reviewed and approved. The extension of formal business planning to certain ISO committees is an important measure which forms part of a major review of business. The aim is to align the ISO work programme with expressed business environment needs and trends and to allow these committees to prioritise among different projects, to identify the benefits expected from the availability of International Standards, and to ensure adequate resources for projects throughout their development. It is expected that each committee member participates to the implementation of the Business Planning concept, thereby contributing significantly to the overall effectiveness of international standardisation. The SBP for TC 334 will be made available on the

Table 1. ISO/REMCO Guides / ISO TC 334 Standards.

Working Group	Existing REMCO guide	New TC 334 standard
WG 8: Quality control materials	ISO Guide 80	ISO 33402
WG 9: Use of reference materials	ISO Guide 33	ISO 33403
WG 10: RM Terms and definitions	ISO Guide 30	ISO 33400
WG 13: Qualitative reference materials	ISO Guide 85	ISO 33406
WG 14: RM Accompanying documents	ISO Guide 31	ISO 33401
WG 16: RM Value assignment	ISO Guide 35	ISO 33405
WG 18: Organic purity RMs	ISO Guide 86	ISO 33407
WG 19: Purity RMs for metals	ISO Guide 87	ISO 33408

QUALITY MATTERS

general public area of the ISO TC 334 website.

■ Advisory group reports and proposed milestones

□ AG1 : Information services

This group reported on its activities during the previous year, which centred principally on the development, and implementation of ISO TC 334's own website area on the ISO website. This can be found at <https://committee.iso.org/home/tc334>.

□ AG2 : Liaison coordination

As already stated, TC 334 has an extensive liaison network, both with ISO and external international committees, and the reports from these were summarised in this session. In addition, TC 334 member reports were also summarised detailing new RMs, areas of interest etc.

□ Working Group reports and proposed milestones

□ WG8: Quality control materials

□ WG9: Use of RMs

□ WG10: RM Terms and definitions

□ WG13: Qualitative RMs

□ WG14: RM Accompanying documents

□ WG16: RM Value assignment

□ WG18: Organic purity RMs

□ WG19: Purity RMs for metals

These Working Group discussions reviewed the progress of the appropriate standard development, and highlighted progress, areas of concern etc. Work within these groups will continue throughout the upcoming year by the effective use of virtual meeting technology to arrange discussion and/or review meetings.

In conclusion, a very well run and effective meeting held “virtually” over the stated three days, and after a couple of years having to accommodate this process, we are all well versed in turning off cameras, and muting microphones to assist the smooth running of the video conferencing.

Interestingly, one upside appears to be the number of attendees, which was significantly more than any recent face-to-face meeting. However, this has to be balanced by the limited three-hour timeslot around midday to accommodate (as reasonably as possible) time zones from the USA/Canada in the West, to China/Japan in the East, and the informal discussions which invariably result. Therefore, moving forward, the most likely option for

future meetings will be face-to-face with essential hybrid capabilities for those who either cannot, or wish not to, attend in person.

Maybe, similar discussions within ISO have resulted in the following recent statement to all TCs?

“...the President's Committee has decided that decision-making around the modalities for governance and technical meetings be returned to the relevant group and committee leaders, with immediate effect.”

This means that group and committee leaders will have the authority to decide whether a meeting should take place in virtual, hybrid or face-to-face format—without further approval required. To make such decisions, the committee leaders should continue to follow the ISO/IEC Meeting Guidance to ensure a productive and fair experience for all participants.”

References

1. ISO 17034, *General Requirements for the Competence of Reference Material Producers*. International Organization for Standardization (ISO), Geneva, Switzerland (2016).



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

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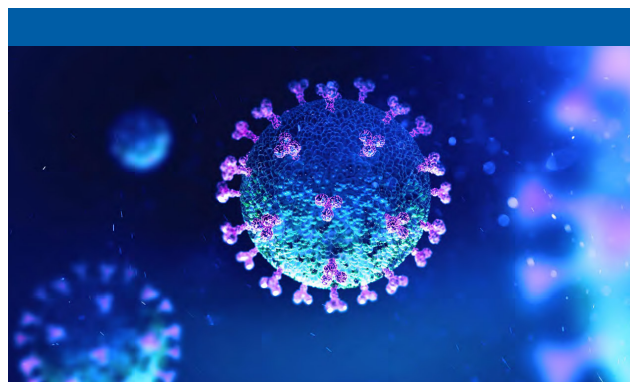
Multi-element analysis of drinking water

The analysis of elemental content is critical to ensuring the quality and safety of drinking water. Regulations such as Directive (EU) 2020/2184 and ISO 17294 provides guidelines for using ICP-MS for water analysis, aiming to protect human health from the adverse effects of its contamination.

ICP-MS technology is ideal for water analysis thanks to its multi-element detection capability combined with low detection limits and high-speed of analysis. However, plasma and matrix-based polyatomic interferences and doubly charged species need to be accounted for by applying mathematical corrections and/or collision/reaction mechanisms. The PerkinElmer NexION® ICP-MS with Universal Cell technology, which can be operated in both Collision and Reaction modes to tackle polyatomic interferences enables laboratories to meet and/or exceed the ISO and EU directives specifications.

PerkinElmer

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THz Raman Spectroscopy

This article introduces THz Raman Spectroscopy as a new analytical tool. Optical interrogation of samples, often involving lasers, is key to several types of automated and high throughput analyses in fields such as drug discovery, flow cytometry for blood assays and DNA sequencing. Most of these life sciences applications entail determining the molecular (chemical) composition of the target, often by using laser induced fluorescence to do spatial mapping. The current world health backdrop where we are running out of non-resistant antibiotics was already creating pressure to conduct drug discovery faster and more intensely than ever.

Coherent

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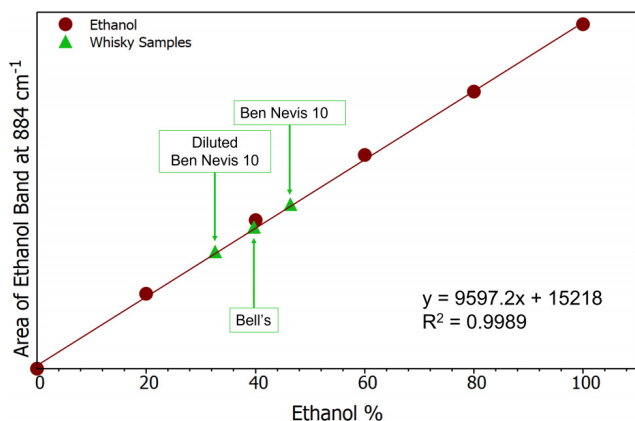
Analysis of nickel ore with the ARL OPTIM'X WDXRF spectrometer

Nickel production has seen increasing demand in recent times as nickel is a key component in lithium-ion batteries, used in electric vehicles. Hence, a fast, accurate and precise method is needed for quantification of these

ores both in the mining and refining processes. The Thermo Scientific™ ARL OPTIM'X™ WDXRF spectrometer is designed for ease of use with minimal operation and maintenance costs. The instrument is fitted with a Goniometer covering elements from fluorine (^{19}F) to uranium (^{238}U). The instrument does not require external or internal water cooling and has 10 times better spectral resolution than a conventional EDXRF instrument as well as superior precision and stability.

Thermo Fisher Scientific

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Whisky analysis by Raman spectroscopy

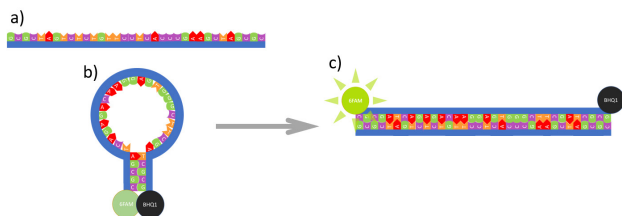
Whisky is made from fermented grain mash, with different grains used to provide the wide variety of whisky flavours available. When bottles of whisky are sold, they will contain a %abv, this relates to how much ethanol is present in the bottle. Commonly, whisky is 40% abv, thus 40% of the bottle should be ethanol. Whisky is an increasingly popular drink, with the Scotch Whisky Association stating 44 bottles of Scotch Whisky are exported every second, with exports worth £4.5 bn in 2021.

Fraudulent sales of drinking alcohol, especially spirits, is a concerning and potentially dangerous way in which vendors try to increase their profits. There are two common ways in which alcohol is sold illegally, first, is the sale of watered down alcohol. This is either done in bulk, where bottles are sold with fraudulent %abvs printed on them, or in bars where spirits are diluted after wholesale purchase. The second issue seen in alcohol fraud is more sinister where methanol, which is toxic to humans, is used in spirits, instead of ethanol.

This application note details how Raman spectroscopy can offer quantitative and qualitative analysis of whisky samples.

Edinburgh Instruments

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Molecular beacon probe fluorescent detection of DNA

Molecular beacon probes are a sequence of nucleotides that can be used to fluorescently detect the presence of a specific sequence of DNA or RNA. The molecular beacon is designed so that a small number of nucleotide bases (between five and seven) at the sequence

terminals are complementary to each other and get paired forming what is called the stem. The formation of the stem creates a loop of the unpaired bases, which is termed the stem loop or hairpin loop. Finally at one end of the nucleotide sequence there is a covalently attached fluorophore and a fluorescence quencher at the other end of the sequence. When the molecular beacon is in this hairpin form, the quencher heavily diminishes the fluorophore fluorescence through Förster Resonance Energy Transfer (FRET) quenching. In this application note, nanomolar concentrations of complementary DNA were quantified using a molecular beacon while controlling the temperature of incubation and measuring the sample emission with a spectrofluorometer.

Edinburgh Instruments

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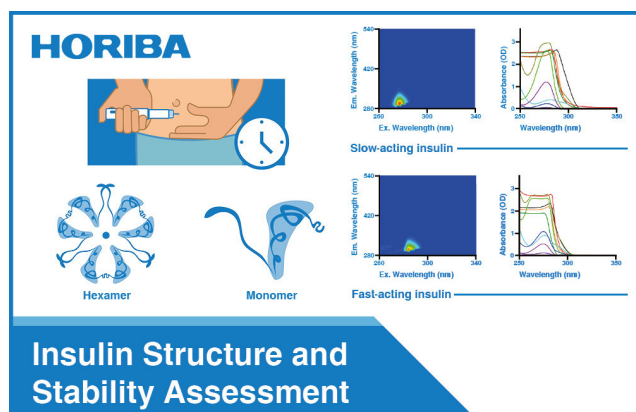


Analysis of traces in aqueous solutions with Thermo Scientific ARL PERFORM'X Advanced WDXRF spectrometer

Analysis of heavy metals and toxic elements as traces in aqueous solutions is becoming increasingly important in view of the environmental concerns. Such analysis demands high sensitivity and accuracy of measurement. The analysis of liquids can be done with ease and minimum sample preparation in XRF. The Thermo Scientific™ ARL™ PERFORM'X series spectrometer used in this analysis is a 2500 watt system.

Thermo Scientific

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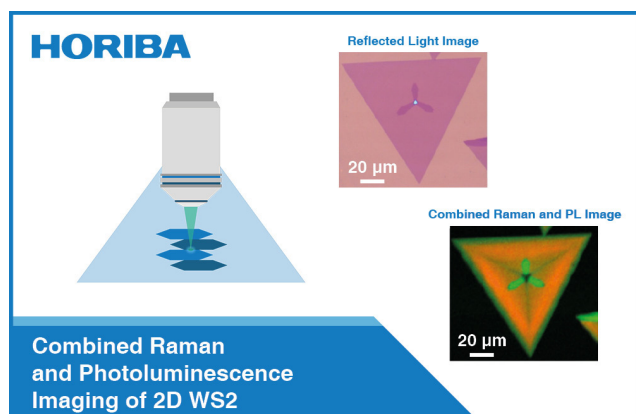
Insulin Structure and Stability Assessment

Insulin structure and stability assessment

Different types of commercial insulin can generally be classified as short-acting or long-acting insulin with the only difference between them being one to three residues in the protein sequence. This difference in sequence, along with controlled pH of storage and delivery, can either trigger or prevent the formation of insulin aggregates in the blood stream, resulting in a slower or faster absorption of the insulin. HORIBA presents in this application note how to characterise protein therapeutic formulations for aggregation behaviour in a matter of seconds with A-TEEM spectroscopy.

HORIBA Scientific

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Combined Raman and Photoluminescence Imaging of 2D WS₂

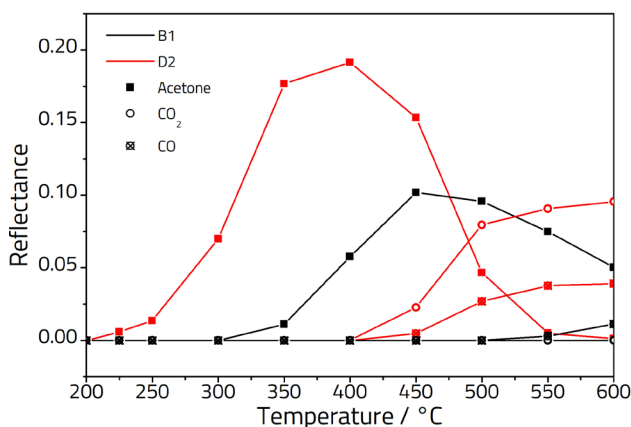
Combined Raman and photoluminescence imaging of 2D WS₂

With their special electronic, optical and optoelectronic properties, tungsten disulfide (WS₂) 2D crystals have recently attracted significant interest as emerging materials for the production of new electronic and optoelectronic devices. Reflected white light microscopy is widely employed to characterise the layers' structure but has limited performance in revealing the spatial variation of composition, optical and electronic properties. In this application note, Raman and photoluminescence

spectral imaging are applied to reveal otherwise invisible spatial variation in chemical/crystal structure.

HORIBA Scientific

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Investigating the dehydrogenation reaction of IPA over catalysts

The thermal reaction of IPA on CeO₂ catalysts has been investigated over a range of temperatures using the Selector™ Environmental Chamber accessory from Specac. The study by Christensen *et al.* clearly demonstrates the critical dependence of reaction parameters on the presence or absence of blocking carbonates on the catalyst surface, which can be controlled by careful treatment of the catalyst.

Specac

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Duetta-2-in-1 fluorescence and absorbance analyser

The Duetta™ combines fluorescence and absorbance spectroscopy in a single compact platform. It offers the fastest fluorescence acquisition of any system with a full-range spectrum (250–1100 nm) taking less than one second. It is an ideal lab partner for reliable, sensitive and fast spectroscopy.

[MORE INFORMATION »](#)



LabRAM Soleil photoluminescence microscope

The LabRAM Soleil offers automated multimodal confocal microscopic imaging. It is the ultimate platform for photoluminescence, electroluminescence and Raman, including QScan laser light-sheet illumination. With HORIBA's AFMs it extends to NanoRaman and NanoPL analysis with sub-20nm resolution.

[MORE INFORMATION »](#)

PRODUCTS AT ASMS 2022

ACD/Labs announces update for its browser-based analytical data processing software

ACD/Labs has announced the first update to its browser-based analytical data processing application, Spectrus JS™. Later in the year, the software will expand its data processing capabilities to new analytical techniques and gain significant enhancements to existing functionalities. With the update, users will be able to process NMR and LC, LC/MS, LC/UV/MS, GC, GC/MS, MS (xG/UV/MS) data in a single software environment, without having to download or install anything on their computer. This release will also introduce ACD/Labs' industry-leading NMR prediction capabilities for spectral simulation, structure assignment and verification.

Spectrus JS is part of the Spectrus® product portfolio, which offers vendor-agnostic data processing/handling solutions for all types of analytical techniques and is paired with established analytical knowledge management and targeted workflow applications. This update extends the distributed data processing capabilities of the platform to xG/UV/MS data and expands its cloud capabilities.

ACD/Labs

▶ <https://link.spectroscopyeurope.com/660-P1-2022>

Agilent MassHunterBioConfirm 12.0

MassHunter BioConfirm 12.0 is software for biopharmaceutical customers. It uses high-resolution mass spectrometry data, this software extracts information to confirm intact protein molecular weights, peptide sequence coverage and location of post-translational modifications (PTMs), and the identification of released glycans. The newest features enable users to rapidly set up workflows for the characterisation of oligonucleotides, meeting the demands of this fast-growing market. MassHunter BioConfirm 12.0 speeds up analysis, supports regulatory compliance and produces answers that users can trust.

Agilent Technologies

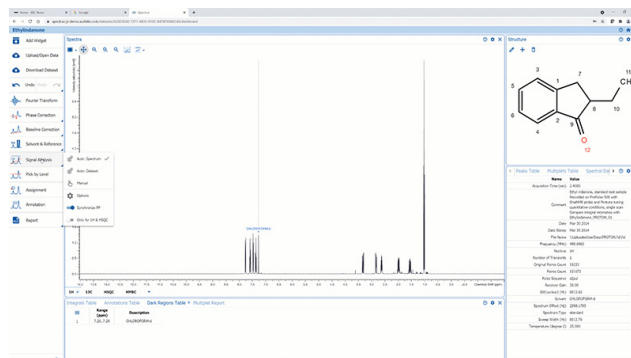
▶ <https://link.spectroscopyeurope.com/105-P4-2022>

Triple quadrupole GC/MS systems

The Agilent 7000E and 7010C triple quadrupole GC/MS systems are the latest iterations of this GC/MS family. The 7000E GC/TQ is a robust and reliable instrument providing optimum operational efficiency for high-throughput labs. The 7010C GC/TQ has been designed to address the most challenging analyses, providing the lowest detection limits to the attogram level.

Agilent Technologies

▶ <https://link.spectroscopyeurope.com/105-P2-2022>



PRODUCTS AT ASMS 2022



Single quadrupole GC/MS instrument

The Agilent 5977C GC/MSD system is the latest of their single quadrupole GC/MS instruments. The introduction of Hydrolnert source in the 5977C allows users to explore hydrogen as a viable alternative to helium as a carrier gas for GC/MS with minimal impact on performance and minimising dependence on helium as a non-renewable resource.

Agilent Technologies

► <https://link.spectroscopyeurope.com/105-P1-2022>

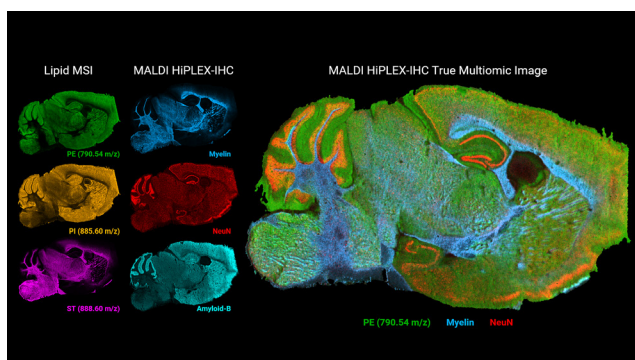


Triple quadrupole LC/MS system

For routine quantitative analysis, the Agilent 6475 triple quadrupole LC/MS system incorporates intelligent reflex, an automated sample reinjection function that intelligently “reflexes” to specific analysis conditions providing immediate validation of results, further improving the speed of analysis and reducing operator involvement. Coupled with 6475, the latest revision of MassHunter Acquisition 12.0 enables data integrity consistent with the regulatory requirements as defined in 21 CFR Part 11 and Annex 11, a key requirement for pharmaceutical and biopharmaceutical manufacturing customers.

Agilent Technologies

► <https://link.spectroscopyeurope.com/105-P3-2022>



Bruker announces developments for highly multiplexed spatial proteomics and multiomic tissue imaging at large field-of-view

Bruker has announced new developments for spatial multiomics of tissue and tumour microenvironments (TME). Following Bruker’s strategic partnership with AmberGen, enhancements have been introduced for MALDI HiPLEX-IHC mass spectrometry imaging. MALDI HiPLEX-IHC represents a breakthrough in multiomics imaging by combining targeted protein expression spatial profiling with unbiased small molecule MALDI imaging to co-localise proteins and small molecules such as glycans, lipids, metabolites or xenobiotics. Using AmberGen’s Miralys™ antibody-based photocleavable peptide mass tags, highly multiplexed IHC staining and photocleavage of peptide markers fit seamlessly into Bruker’s IntelliSlide®-based automated workflows for MALDI imaging.

Novel multiomic imaging enhances spatial high-plex protein imaging with the ability to elucidate metabolic processes in the same tissue section. In addition to mapping tens to over one hundred targeted proteins with high-plex peptide tags, MALDI HiPLEX-IHC can track signalling pathways such as glycosylation, observe lipid spatial profiles for tumour microenvironment

PRODUCTS AT ASMS 2022

segmentation, or simultaneously observe how drugs affect both protein and metabolic states.

Bruker

► <https://link.spectroscopyeurope.com/2428-P3-2022>

Bruker has announced its microGRID module for smartbeam 3D MALDI sources for timsTOF fleX systems

Bruker has announced its microGRID module for smartbeam 3D MALDI sources for timsTOF fleX systems. The microGRID improves the MALDI stage to sub-micron precision to correct laser positioning on tissue surfaces down to 5 µm, virtually eliminating any visual artefacts or artefacts in co-registration of MALDI images with optical microscopy. As correction is effective for entire pathology slides, microGRID leverages a large field-of-view for MALDI HiPLEX-IHC protein expression profiling.

Bruker

► <https://link.spectroscopyeurope.com/2428-P4-2022>

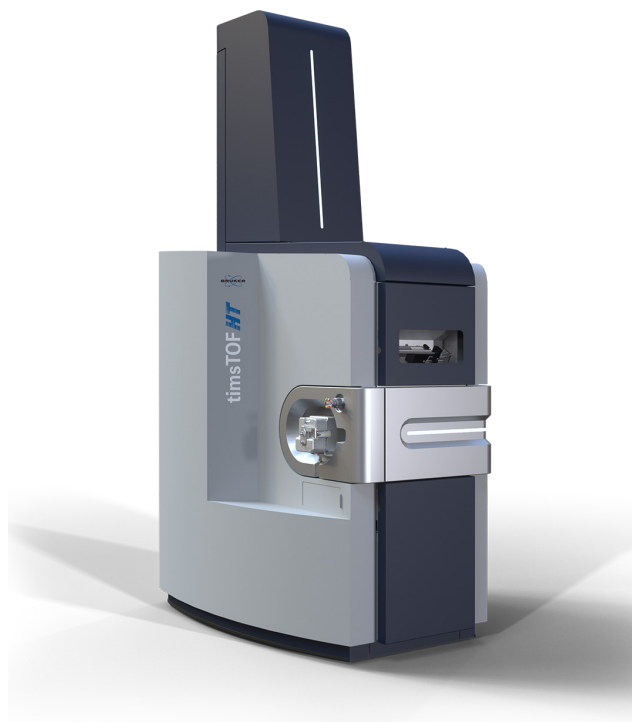


Bruker launches timsTOF HT with greater dynamic range

Bruker has announced the further evolution of their 4D Multiomics timsTOF platform with the launch of the new timsTOF HT system. The timsTOF HT includes a novel 4th-generation TIMS (trapped ion mobility separation) XR cell and 14-bit digitiser for even greater dynamic range, enhanced peptide coverage and more accurate quantitation, particularly in unbiased 4D plasma and tissue proteomics and epiproteomics. These advances are achieved without compromising the ultra-high sensitivity and extreme robustness for high-throughput proteomics, e.g., at 50 samples per day (SPD) or up to 200 SPD, or the high scientific confidence of better than 1% peptide and protein FDRs (false discovery rates), avoiding inherent antigen cross-reactivity in targeted immune-recognition methods. The timsTOF HT instrument can identify over 100k unique tryptic peptides in 60min gradients with accurate quantification of better than 5% CVs for many protein groups in low microgram quantities of a three-proteome mixture, using the diaPASEF technique. The timsTOF HT also is optimised for high-throughput, deep and unbiased plasma proteomics and liquid biopsy biomarker research.

Bruker

► <https://link.spectroscopyeurope.com/2428-P2-2022>



Bruker introduces triple quadrupole mass spectrometer with DART interface

Following their acquisition of IonSense in April 2022, Bruker has introduced the DART-EVOQ[®] triple quadrupole mass spectrometer for high-throughput quantitative

PRODUCTS AT ASMS 2022



analyses. The DART-EVOQ does not require chromatography separations for applied markets analysis in food/beverage, forensics, industrial, security, environmental and pharmaceutical workflows. DART technology removes time-consuming steps to rapidly identify and quantify sample analytes. DART enables novel PoN workflows that are challenging for conventional GC- and LC-mass spectrometers because of the complexity, long analysis times and reduced robustness of front-end chromatography that is required for complex mixture analysis.

Bruker

► <https://link.spectroscopyeurope.com/5073-P3-2022>

SCIEX launches the next generation of data independent acquisition

SCIEX has launched Zeno SWATH DIA, a development of their SWATH technology. Zeno SWATH DIA can enable researchers to discover more potential biomarkers to be used in the development of clinical tests and in the discovery of new therapies. By combining the sensitivity and robustness of the ZenoTOF 7600 system and the high dynamic range of Zeno SWATH DIA, researchers can now routinely quantify up to twice the number of cell and plasma proteins than previously possible with SWATH approaches. The ability to quantify large numbers of lesser abundant proteins that were previously undetectable means that more potential biomarkers can be taken through to verification.

To enable translational research, this performance can be delivered at large scale. Run times can be shortened to as little as 5 min with minimal compromise in proteome coverage. Large population-scale proteomic studies can be achieved in a matter of weeks, without compromising on the depth of information obtained. This means the potential for the development of clinical tests for early detection of disease is vastly increased.

The sensitivity of Zeno SWATH DIA also enables large numbers of proteins to be quantified from sample loadings up to 10-fold lower than previous SWATH approaches. Lower sample loads mean reduced cost per sample in large scale studies, and minimised sample consumption from expensive *in vivo* models during drug development. Additionally, it creates opportunities for large population-scale sample collection methods such as patient-centric microsampling devices.

SCIEX

► <https://link.spectroscopyeurope.com/5073-P1-2022>

SCIEX launches the new SCIEX OS 3.0

SCIEX has launched SCIEX OS software v3.0, which features stMRM, a data rich, scout triggered MRM workflow. stMRM couples improved efficiency with better-quality data across large screening workflows. It

PRODUCTS AT ASMS 2022

utilises the intelligent monitoring of marker compounds to trigger the acquisition of later eluting dependent transitions to identify dependent compounds. stMRM removes analytical dependencies of chromatographic retention times allowing for improved cycle and dwell across compound transitions.

SCIEX OS v3.0 also has the new Central Administration Console. This brings project management, user profiles, permissions and security into a simple and navigable interface. In addition, this launch improves accessibility to SCIEX systems with new language packs. Customers will now be able to operate SCIEX OS software in nine languages, Chinese (simplified), English, French, German, Italian, Japanese, Korean, Portuguese and Spanish.

SCIEX

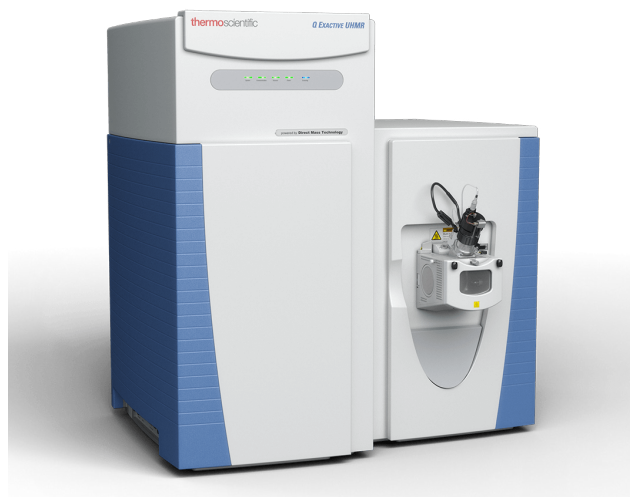
► <https://link.spectroscopyeurope.com/5073-P2-2022>

New MS solution simplifies insights into macromolecular complexes

Thermo Fisher Scientific has introduced the Thermo Scientific Direct Mass Technology mode, which augments Thermo Scientific Q Exactive UHMR Hybrid Quadrupole-Orbitrap mass spectrometers with charge detection capabilities, allowing direct mass determination of hundreds to thousands of individual ions in a single spectrum. As a result, laboratories can measure mass for complex heterogeneous mixtures of multiple charged components, unlocking new and rich insights into proteoforms, biotherapeutics and next-generation drug modalities.

Thermo Fisher Scientific

► <https://link.spectroscopyeurope.com/106-P6-2022>



LC-MS all-in-one toxicology solution

Thermo Fisher Scientific has introduced an all-in-one liquid chromatography-mass spectrometry (LC-MS) toxicology solution to keep pace with the ever-changing landscape of emerging and illicit drugs. The expansion of the Thermo Scientific Tox Explorer Collection onto the Thermo Scientific Orbitrap Exploris Mass Spectrometer platform provides access to ultra-high-resolution mass spectrometry specifically required to identify analytes in complex matrices, increasing laboratory productivity and improving the specificity and selectivity of toxicology analysis. This toxicology solution offers a standardised method with LC retention times that allows users to get up and running fast. It utilises a comprehensive high-resolution accurate mass (HRAM) spectral library that has been expanded to over 1700 compounds, enabling toxicology scientists to screen and quantify a wide and diverse range of compounds, with different hydrophobicities and polarities. The library also includes 212 fentanyl analogues, making it the largest fentanyl HRAM library to date. This solution comes complete



PRODUCTS AT ASMS 2022

with the software, service and support to sustain laboratory productivity.

Thermo Fisher Scientific

► <https://link.spectroscopyeurope.com/106-P7-2022>

Oligonucleotide analysis and biotherapeutic characterisation software

The newest Thermo Scientific BioPharma Finder 5.1 software offers a solution for oligonucleotide analysis and biotherapeutic characterisation workflows, providing increased confidence in results by comprehensively characterising mass spectrometry data using advanced algorithms. Oligonucleotide-based biotherapeutics present unique challenges for characterisation due to their complexity. The new software provides an enhanced suite of built-for-purpose tools to overcome these challenges and meet the needs of this rapidly growing field, quickly and confidently turning complex data into meaningful results. Improvements to the kinetic prediction model for oligonucleotides enable more confident prediction and matching. Improved data review tools and tables offer streamlined review and results reporting of complex oligonucleotide data sets.

Thermo Fisher Scientific

► <https://link.spectroscopyeurope.com/106-P3-2022>

Proteomics research software

The latest Thermo Scientific Proteome Discoverer 3.0 software, in combination with the CHIMERYS intelligent search algorithm by MSAID, use artificial intelligence to more fully interpret data generated by Thermo Scientific Orbitrap mass spectrometers. This innovative approach substantially increases the number of unique peptide

identifications, improves protein coverage and quantitation capabilities, and enables scientists to discover more in their data. The new intelligent search algorithm also facilitates higher throughput analysis and wide-isolation window data-dependent acquisition for synergistic performance enhancements. This deeper mining of data expands the ways in which proteomics scientists can acquire and apply their data.

Thermo Fisher Scientific

► <https://link.spectroscopyeurope.com/106-P4-2022>

Software for untargeted small molecule workflows with new peak detection and quality algorithms

The newest Thermo Scientific Compound Discoverer 3.3 software can be used by small molecule researchers to detect more compounds in less time thanks to a faster and more sensitive peak detection algorithm. Filtering large data sets down to relevant compounds is now easier by using the new peak quality functionality to streamline data processing and review. Improve confidence in compound annotations through MSⁿ spectral tree search capabilities in tandem with the Thermo Scientific mzCloud spectral library to address the most challenging unknown compounds. Compound Discoverer 3.3 software, which has been optimised for processing large datasets and detecting low-abundance compounds, will support scientists in metabolomics, pharmaceutical, environmental, food safety, clinical and forensics applications to acquire the results they need to drive science forward.

Thermo Fisher Scientific

► <https://link.spectroscopyeurope.com/106-P5-2022>



Waters introduce Xevo G3 QToF system

Waters has introduced the new Xevo G3 QToF system, a high-performance, benchtop mass spectrometer for characterising and quantifying thermally-fragile molecules in applications such as biotherapeutics, forensics, metabolite identification, metabolomics and extractables and leachables. The Xevo G3 QToF system is up to 10× more sensitive than its predecessor at transmitting thermally fragile molecules and excels at measuring and characterising denatured or native proteins, peptides and other biotherapeutics. Waters have engineered the Xevo G3 QToF system to reliably give scientists both reproducible and accurate qualitative and quantitative information about molecules in their samples whether in very small or very large amounts.

Waters

► <https://link.spectroscopyeurope.com/103-P3-2022>

PRODUCTS AT ASMS 2022

Coupling UPLC to Waters MRT SELECT SERIES research mass spectrometer

The Waters SELECT SERIES MRT System is now compatible with UPLC-MS with an available electrospray ionisation (ESI) source. Coupling the high resolution MRT System with the ESI source enables scientists to accurately resolve and measure low (<200 ppb) concentrations of sample analytes at UPLC acquisition speeds for metabolomics, metabolite identification or peptide mapping applications. The performance of the SELECT SERIES MRT allows scientists to get the highest quality mass spectrometry data and information faster than any commercial mass spectrometer on the market today, giving scientists a much clearer picture of the structure of their molecules at the isotope level.

Waters

▶ <https://link.spectroscopyeurope.com/103-P5-2022>



New software app for confirming nucleic acid sequence of biotherapeutics

The CONFIRM Sequence app on the waters_connect software platform helps scientists using a Waters LC-MS System to confirm the nucleic acid sequence of therapeutics and identify impurities that could compromise product safety and efficacy. The CONFIRM Sequence app eliminates 50% of the time it takes for post-processing data review, accelerating characterisation and development of nucleic acid therapeutics. The new CONFIRM Sequence app is the first sequencing tool to integrate compliance-ready data acquisition, processing and reporting, making it suitable for deployment in regulated development and Good Manufacturing Practice (GMP) labs.

Waters

▶ <https://link.spectroscopyeurope.com/103-P4-2022>



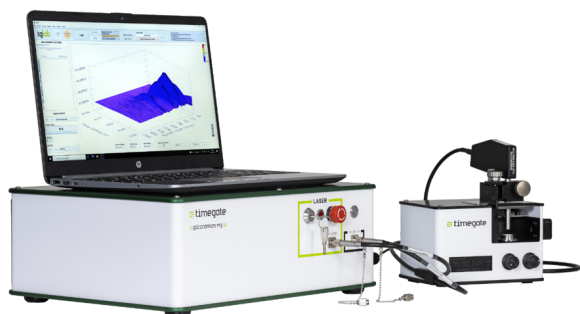
INFRARED

Portable FT-IR spectrometer for emergency response applications

RedWave Technology has introduced the XplorIR, a portable FT-IR spectroscopy gas-identification system developed for emergency response applications. The XplorIR can identify over 5500 gases at low part per million (ppm) concentrations. The XplorIR can identify many dangerous gases, including toxic industrial compounds (TICs), flammables, corrosives, industrial gases and other chemicals at operationally relevant levels.

RedWave Technology

► <https://link.spectroscopyeurope.com/5746-P1-2022>



RAMAN

Process Raman spectrometer

Timegate Instrument Ltd have released their third-generation instrument, the PicoRaman M3, which implements the patented Timegated[®] Raman technology with real fluorescence rejection. The spectrometer offers features including fast and continuous, real-time and online measurements as well as highly specific chemical information and non-destructive analysis. Timegate has reduced the complexity of spectrometer use and developed PicoRaman M3 as a user-friendly, compact and portable design. The instrument allows easy and autoclavable integration with process environment and is free from sample preparation resulting in rapid set-up time. In addition, the PicoRaman M3 enables about 10–40× faster measurements than the previous Timegated[®] Raman instrument generations. Timegate also provides the ProbePro product family, a variety of different probe optics for *in situ*, real-time analysis.

Timegate Instrument

► <https://link.spectroscopyeurope.com/5151-P1-2022>

UV/VIS

Spex NanoSNAP microvolume spectrophotometer

The Spex[®] NanoSNAP[™] is a high-speed microvolume spectrophotometer that is dedicated to life sciences applications, but also provides additional methods for self-defined protocols such as spectrum scanning, multi-wavelength, quantitation and concentration. It assesses the purity of DNA, RNA, proteins and any other type of assay for samples available in small quantities within seconds, using as little as 1 µL of sample with no dilution required. It is versatile, with full wavelength coverage

NEW PRODUCTS

from 190 nm to 1000 nm. It combines high performance along with ease of use thanks to its nano hydrophobic coated sample window, LED viewing light and the cushioning design of the detection arm. Reports are saved on the internal memory and can be easily transferred to USB. Multiple measurement modes are available: Nucleic acids concentration and purity: dsDNA, RNA, ssDNA; Protein A280: BSA, IGG, lysosome and custom proteins; Protein assays: BCA, Bradford, Modified Lowry for protein standard curve protocols; OD 600: Optical density at 600 nm and cells/mL calculation for cell cultures; as well Customised protocols using factor, standard curve and UV-Vis methods.

Spex SamplePrep

▶ <https://link.spectroscopyeurope.com/697-P1-2022>



Conferences

2022

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

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

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

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

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

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

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

21–24 August 2022, Montréal, QC, Canada. **The 61st Annual Conference of Metallurgists.** <https://com.metsoc.org>

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

28–31 August, La Jolla, United States. **SMASH 2022—Small Molecule NMR Conference.** <https://www.smash-nmr.org/>

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

29 August–1 September, Reims, France. **19th European Conference on Spectroscopy of Biological Molecules-ECSBM.** <https://www.univ-reims.fr/ECSBM-2022/>

29 August–2 September, Rome, Italy. **18th Chemometrics in Analytical Chemistry Conference (CAC 2022).** <https://cac2022.sciencesconf.org/>

4–8 September, Singapore, Singapore. **SETAC 8th World Congress/12th SETAC Asia-Pacific Biennial Conference.**

barbara.koelman@setac.org, <https://singapore.setac.org>

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

6–9 September, Prague, Czech Republic. **10th International Symposium on Recent Advances in Food Analysis (RAFA 2022).** rafa2022@vscht.cz, <https://www.rafa2022.eu>

12–14 September 2022, Cairns, Australia. **Australian Near Infrared Spectroscopy Group Conference.** theb.attens@bigpond.au, <https://anisg.com.au>

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

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

14–16 September, Chester, United Kingdom. **Advances in Process Analytics and Control Technologies (APACT 22).** admin@cpact.com, <https://apact.co.uk/>

15–16 September, Paris, France. **9th International Conference on Advanced Applied Raman Spectroscopy (RamanFest2022).** <https://www.raman-festconf.com/2022/index.php>

21–23 September 2022, Málaga, Spain. **IBER2022-XVI Iberian Joint Meeting on Atomic and Molecular Physics.** contact@iber2022.com, <https://iber2022.com/>

25–30 September 2022, Erice, Italy. **International School on Mass Spectrometry (IntSMS).** <http://www.spettrometriadimassa.it/intsms2022>

26–28 September 2022, Ulm, Germany. **18th Confocal Raman Imaging Symposium.** events@witec.de, <https://www.raman-symposium.com/>

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

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

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

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

2023

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

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

21–27 August, Innsbruck, Austria. **NIR-2023.** <https://www.spectroscopyeurope.com/events/nir-2023>

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

Courses

2022

21 August 2022, Montréal, QC, Canada. **Metal Accounting: Key Points to Implement an Efficient System.** <https://com.metsoc.org/short-courses/metal-accounting/>

25–30 September, Erice, Italy. **International School on Mass Spectrometry (IntSMS).** <http://www.spettrometri-adimassa.it/intsms2022>

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

Exhibitions

2022

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

13–16 September 2022, Rome, Italy. **Fourth Spectro Expo.** <https://www.spectroexpo.com>

15–17 September, Hyderabad, India. **analytica Anacon India.** <https://www.analyticaindia.com>

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

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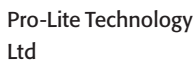
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