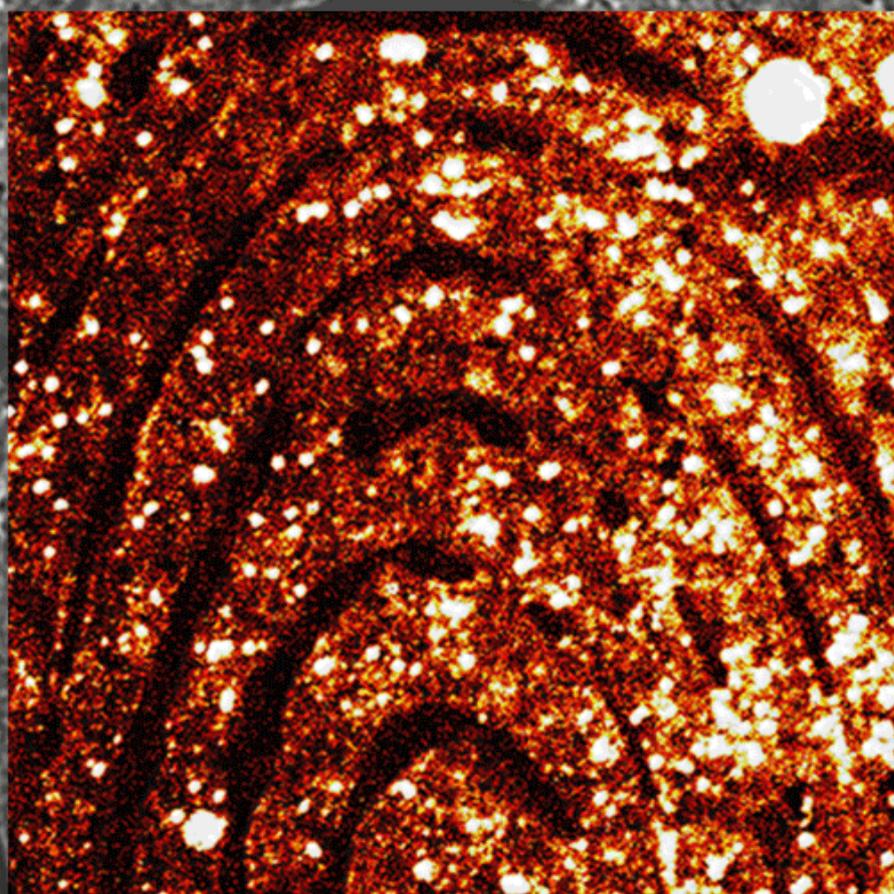


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**New insights in fingerprint chemistry
FAIR data in practice**

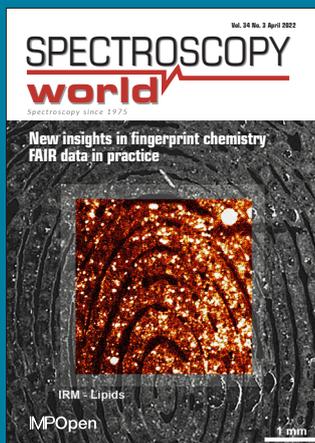


IRM - Lipids

IMPOpen

1 mm





The front cover image is taken from the article, starting on page 22, on spectroscopy and imaging of fingerprints. It shows how X-ray and FT-IR imaging can identify the distribution of different constituents of the fingerprint.

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An interactive issue

At the end of 2021, I indicated that we would be introducing more interactivity into our Digital Editions. This is only available in the flipbook Digital Edition, since PDFs are less good at this sort of thing. Nevertheless, the PDF version contains links to videos.

In the last couple of issues, you may have seen links to videos in both the news and new products sections. This issue sees more of this, with videos from three of our advertisers. Clicking on the video “thumbnail” with the white triangle in a circle will open a popup in which the video plays. You can control the video as normal and even play it in full screen. Give it a go.

Our main article, “Leaving a mark on forensic science: how spectroscopic techniques have revealed new insights in fingerprint chemistry” from Rhiannon Boseley, Daryl Howard, Jitraporn Vongsvivut, Mark Hackett and Simon Lewis, also includes animated figures, which help visualise the location of various chemicals found in fingerprints. Read the article starting on page 22 and get the whole story.

In the Tony Davies Column, “Open publishing FAIR spectra for and by students” by Henry Rzepa and Tony Davies, we have replaced the standard screenshot which would have been used in the past with the live webpage, enabling you to browse around as if you were on the website itself. I think this has

real potential to replace screenshots in many cases. The only problem seems to be intrusive cookie consent popups! Henry and Tony’s contribution really starts to answer the question I asked Tony “how does one actually find FAIR data?”.

There is also a Book Review, something we haven’t included for a long time. I am always interested in receiving these; they don’t need to be as long as this one.

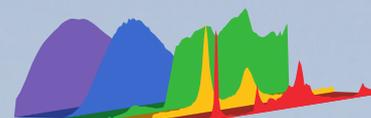
What we haven’t done yet is to include pure audio. Perhaps you have an idea for this? I am always delighted to hear from volunteer authors, so please don’t be shy!



Conference on spectral imaging

July 3–6, Esbjerg, Denmark

Abstract submission deadline: 1 May 2022



IASIM 2022

Keynote speakers

Costanza Cucci (Institute of Applied Physics “Nello Carrara”)

Reflectance Imaging Spectroscopy for artworks, cultural and historical assets

Baowei Fei (The University of Texas at Dallas)

Medical Hyperspectral Imaging

Mauro Dalla Mura (Grenoble Institute of Technology)

Hyperspectral imagery: applications in remote sensing

Marco Veneranda (University of Valladolid)

Raman imaging from terrestrial to planetary applications

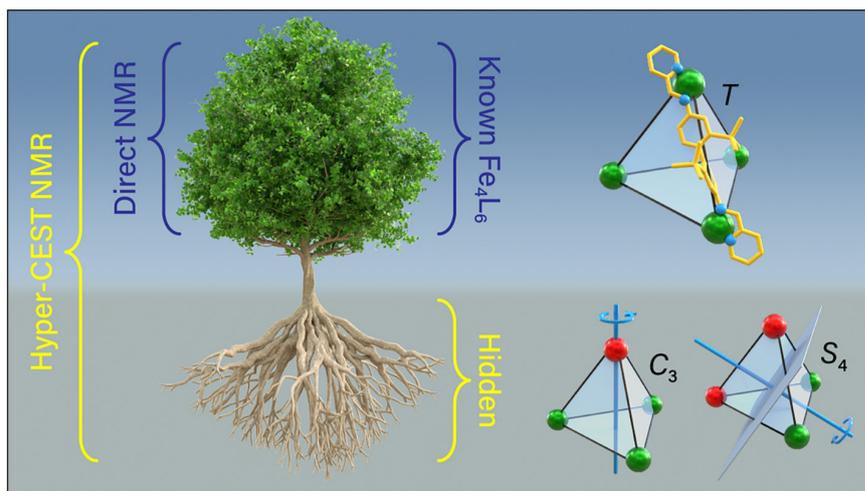
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Hyper-CEST NMR technique reveals missing structure of a novel container molecule

Using the Hyper-CEST NMR technique, researchers have revealed two previously little researched variants of a type of transport container from the class of metal-organic polyhedra (MOPs). This could lead to a novel type of MRI contrast agent.

The concept of a modular construction system proves useful in many applications for assembling complex structures for specific functions from individual, repeated sub-units. In chemistry, the principle can be used to construct a self-assembling network from smaller molecular units that acts as a transport container of a defined size. For example, several metal ions can be linked with organic molecules. These MOPs (metal-organic polyhedra) are used, for instance, to capture greenhouse gases or to pave the way for more effective chemotherapeutic agents by loading them with certain drugs, which they then release in the tumour. Several aspects of the behaviour of these structures have not yet been adequately explored. This is partly because appropriate techniques are not always available to observe the loading and unloading of these MOPs at the molecular level—often, no differences can be measured between the empty and loaded variants for either the container or its contents.

In cooperation with a team from the University of Oulu in Finland, Leif Schröder's research group from the Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP) and the Deutsches Krebsforschungszentrum (DKFZ) has now investigated MOPs that spontaneously assemble in solution from iron ions and an organic compound to form tetrahedra. In the process, the organic struts can be attached differently to the iron "nodes". Essentially, this influences the properties of MOPs, such as their capacity to kill tumour cells. In



Hyper-CEST as ultra-sensitive NMR spectroscopy tool reveals two previously "hidden" structures of metal-organic cages. Visualisation: Barth van Rossum, FMP

the case of the MOP under study, however, it was previously thought that only one of the three theoretically predicted variants existed. The other two variants were considered too unstable, because no analytical methods were able to detect them. Using a new method of magnetic resonance (hyper-CEST NMR), Schröder's team

“MOPs (metal-organic polyhedra) are used, for instance, to capture greenhouse gases or to pave the way for more effective chemotherapeutic agents by loading them with certain drugs, which they then release in the tumour.”

member Jabadurai Jayapaul has now succeeded in demonstrating that these previously unknown variants do exist. The colleagues from Finland were able to confirm the signals of these “hidden”

MOPs using theoretical calculations. Although they only occur in very small proportions, the measurements showed that altering the attachment of struts causes dramatic changes in the loading and unloading of containers. Certain sub-types of containers can be selected to speed up the process. The researchers are now using this knowledge to develop a novel type of contrast agent in MR imaging in which the loading of the container influences the MRI signal. But observations also show that there is greater potential for new insights for further optimising drug carriers. In other words, the first impression gained of these structures may not always be the right one. A substantial part of their nature may remain hidden until we are able to detect them using far more sensitive methods.

This work was published in *Nature Communications* (doi.org/hn7p). 📌

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SERS sensor for faster, more accurate COVID-19 tests

Researchers say the surface enhanced Raman spectroscopy sensor combines accuracy levels approaching those of PCR testing with the speed of rapid antigen tests, and could be used for mass testing.

A COVID-19 sensor developed at Johns Hopkins University could revolutionise virus testing by adding accuracy and speed to a process that frustrated many during the pandemic. The sensor, which requires no sample preparation and minimal operator expertise, offers a strong advantage over existing testing methods, especially for population-wide testing.

“The technique is as simple as putting a drop of saliva on our device and getting a negative or a positive result”, said Ishan Barman, from Johns Hopkins. “The key novelty is that this is a label-free technique, which means no additional chemical modifications like molecular labelling or antibody functionalisation are required. This means the sensor could eventually be used in wearable devices.”

Barman says the new technology addresses the limitations of the two most widely used types of COVID-19 tests: PCR and rapid tests. PCR tests are highly accurate, but require complicated sample preparation, with results taking hours or even days to process in a laboratory. On the other hand, rapid

tests, which look for the existence of antigens, are less successful at detecting early infections and asymptomatic cases and can lead to erroneous results.

The sensor is nearly as sensitive as a PCR test and as convenient as a rapid antigen test. During initial testing, the sensor demonstrated 92% accuracy at detecting SARS-CoV-2 in saliva samples—comparable to that of PCR tests. The sensor was also highly successful at rapidly determining the presence of other viruses, including H1N1 and Zika. The sensor is based on large area nanoimprint lithography, surface enhanced Raman spectroscopy (SERS) and machine learning. It can be used for mass testing in disposable chip formats or on rigid or flexible surfaces.

Key to the method is the large-area, flexible field enhancing metal insulator antenna (FEMIA) array developed by the group. The saliva sample is placed on the material and analysed using SERS. Because the nanostructured FEMIA strengthens the virus’s Raman signal significantly, the system can rapidly detect the presence of a virus, even if only small

traces exist in the sample. Another major innovation of the system is the use of advanced machine learning algorithms to detect very subtle signatures in the spectroscopic data that allow researchers to pinpoint the presence and concentration of the virus (doi.org/hn9x).

“Label-free optical detection, combined with machine learning, allows us to have a single platform that can test for a wide range of viruses with enhanced sensitivity and selectivity, with a very fast turnaround”, said Debadrita Paria from Johns Hopkins.

The sensor material can be placed on any surface, from door-knobs and building entrances to masks and textiles.

“Using state of the art nanoimprint fabrication and transfer printing we have realised highly precise, tuneable and scalable nanomanufacturing of both rigid and flexible COVID sensor substrates, which is important for future implementation not just on chip-based biosensors but also wearables”, said David Gracias from Johns Hopkins. He says the sensor could potentially be integrated with a hand-held testing device for fast screening at crowded places like airports or stadia.

Barman said “we can use this for broad testing against different viruses, for instance, to differentiate between SARS-CoV-2 and H1N1, and even variants. This is a major issue that can’t be readily addressed by current rapid tests.”

The team continues working to further develop and test the technology with patient samples. Johns Hopkins Technology Ventures has applied for patents on the intellectual property associated with it and the team is pursuing license and commercialisation opportunities. 🚀



The new COVID-19 sensor. Credit: Kam Sang Kwok and Aishwarya Pantula / Johns Hopkins University

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

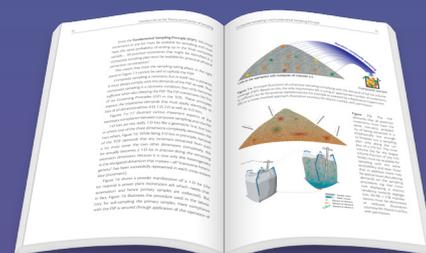
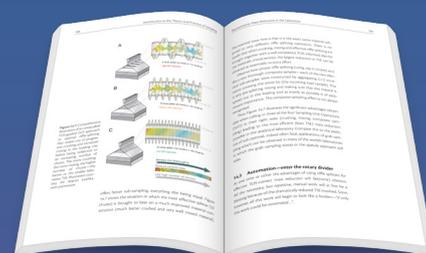
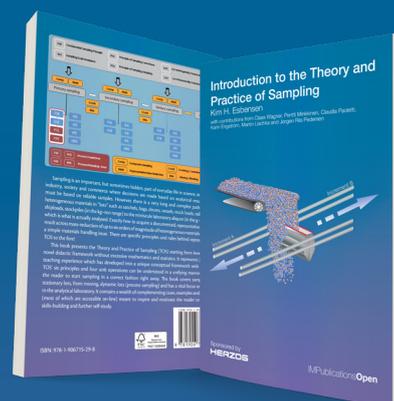
“Sampling is not gambling”. Analytical results forming the basis for decision making in science, technology, industry and society must be relevant, valid and reliable. However, analytical results cannot be detached from the specific conditions under which they originated. Sampling comes to the fore as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



impopen.com/sampling

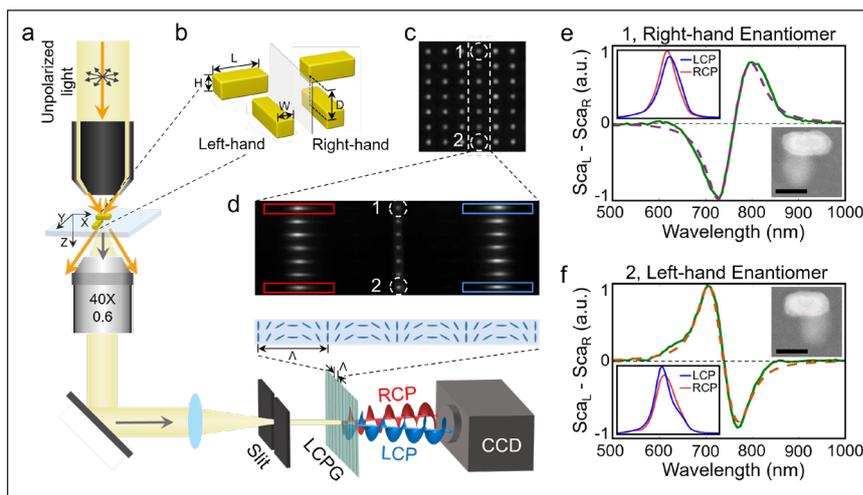
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Snapshot measurement of single nanostructure's circular dichroism

A new CD spectrometer can measure single nanostructures and also be used for weak signal measurements, such as polarised luminescence or Raman scatterings.

The 3D conformation of a molecule or nanostructure determines its function. For instance, a left-handed amino acid can be beneficial to health, while its right-handed compartment can be toxic. With today's optical imaging techniques, one can accurately locate a molecule or a nanostructure, but resolving its 3D interior structure requires additional spectroscopic information—CD spectroscopy is the most widely used technique for this purpose. If one can combine CD spectroscopy with an imaging method, real-time tracking and analysis of individual functional nano-units will become possible. This could lead to many important applications in the field of nanoscience and biology.

However, current CD spectrometers rely on the polarisation modulation of excitation light and require sophisticated multi-step measurements, holding the potential of CD spectroscopy from being fully released. To address this issue, a team of scientists, led by Prof. Weihua Zhang and Prof. Yanqing Lu from the College of Engineering and Applied Sciences, Nanjing University, China developed a polarisation-dispersive imaging CD spectrometry technique. The new method operates on the signals instead of the excitation light with the help of a nano-patterned liquid-crystal polarisation grating (LCPG). The LCPG can disperse the left-/right-handed circularly polarised components of optical signals to different directions with equal efficiency (overall diffraction efficiency >95% at optimal wavelength), allowing them to capture the CD spectrum with a single shot. With the new technique, they studied a



a Schematic drawing of the LCPG-based polarisation-dispersive spectrometer. The inset illustrates the director distribution of the liquid crystal in the grating. b Structure of the vertically coupled nanorod pairs used in this work. c Dark-field image of an array of vertically coupled nanorod pairs with different geometrical parameters. The period of the array is $3\mu\text{m}$. d Spectral image of array of nanorod pairs labelled in c. The RCP and LCP components are labelled with red and blue boxes, respectively. e and f are the SCD spectra of sample 1 and 2 in c, respectively. The insets show the correlated SEM image of samples, as well as the left-hand and right-hand circularly polarised components of the scattered light of sample labelled in d. Scalebar: 100nm . Credit: Shuang Zhou, Jie Bian, Peng Chen, Mo Xie, Jie Chao, Wei Hu, Yanqing Lu, and Weihua Zhang

model system, namely the coupled plasmonic nanorod pair using the Born-Kuhn model and theoretically proved that the new method is equivalent to conventional CD spectroscopy when non-polarised excitations are used.

The key component of the new CD spectrometer is the LCPG. Unlike conventional polarisation components, which are commonly difficult to calibrate and sophisticated to use, the LCPG is simple, accurate and robust. "The LCPG is an ideal solution for polarisation-related measurements. First, its accuracy is guaranteed by theory. Mathematically, the space-variant geometric phases for LCP and RCP light generated by the LCPG are

conjugated. As the result, they are always split into the $\pm 1^{\text{th}}$ order of diffractions with absolute equal efficiency. This polarisation dispersion behaviour is non-dispersive, accurate and highly efficient. Second, the LCPG is a mature technique, and high quality LCPGs can routinely be fabricated in research labs. To be honest, we were surprised to see that it worked so well in the single nanostructure CD measurements."

Another important part of single nanostructure CD spectroscopy is how to interpret the data and retrieve sample's interior 3D structural information. In a paper (doi.org/10.1039/c1nr00092g), they studied a special case, coupled plasmonic nanorods,



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*Based on a data comparison, completed by Thermo Fisher Scientific in 2021, of detection limits for OES systems using data published in specifications and applications notes for ARL iSpark and competitors.

and showed that the geometrical parameters are explicitly related to the spectral features. Meanwhile, the scientists pointed out that the spectrum interpretation can be much more complicated:

“A single nanostructure’s CD spectrum is very different from the result of ensembles. In addition to the interior of the nanostructure, the spectrum is also related to its orientation, as well as the

detailed excitation and observation geometries. To fully understand the complexity, more comprehensive theories are needed. We are currently working on it.”

Finally, thanks to the near-unit diffraction efficiency of the LCPG, the polarisation-dispersive CD spectrometer is a perfect tool for weak signal measurements, e.g., the circular polarised luminescence

or Raman scatterings from individual nanostructures. “Besides the plasmonic nanostructures, we also tested the polarisation-dispersive imaging spectrometer with single quantum dot luminescence, and the system works perfectly. We believe that it is even capable of doing single-molecule CD measurements. That is our big goal!”, said Prof. Zhang. 🚀

Single-cell spectroscopy reveals heterogeneity in metal adsorption

A collaborative team of researchers combined a single-cell ICP-MS with XAFS to get a detailed picture of the interaction between precious metals and *Galdieria sulphuraria* cells.

Biosorption is the removal of contaminants from a sample by adsorbing them onto the surface of a biological material. It is expected to provide environmental and economic benefits compared with conventional separation techniques. A team of scientists including a researcher from the University of Tsukuba has analysed the interaction of *Galdieria sulphuraria* algae with precious metals to better understand the biosorption process.

Precious metals—including gold, platinum and palladium—have been detected in the environment at trace levels and the associated health and ecological risks are not well understood. Removing these metals using standard approaches can be challenging because other contaminant elements with generally higher concentrations—iron and copper, for example—provide competition. Biosorption is a potential alternative that could also present financial benefits through recycling of the expensive elements. Understanding and optimising the biosorption of precious metals is, therefore, an important research area.

Massive datasets that consider both the sorption efficiency and capacity of the biomaterials have been accumulated. However, so far, the findings have been averaged over the entire cell population and it has not been possible to assess adsorption at the single-cell level. Now, the Tsukuba team has combined X-ray absorption fine structure (XAFS) spectroscopy—which has been used to analyse the way metals adsorb onto cells—with single-cell inductively coupled plasma mass spectrometry (scICP-MS) to provide the link between the behaviour of the cell population and the nature of the interactions between the metals and the cells at the cell surface.

“Combining XAFS and scICP-MS, and using low metal concentrations, meant that we could get a really close look at the specific interactions taking place at the cell surface”, explains lead author Professor Ayumi Minoda. “We found that the amount of metal adsorbed depended on the metal in question and the acidity of the solution.”

In low acidity conditions gold, platinum and palladium all adsorbed

to the cells. The gold was found to interact with sulfur containing groups at the cell surface, whereas platinum and palladium interacted with both sulfur- and nitrogen-containing groups. Interestingly, at high acidity, only gold and palladium adsorbed onto the cells and only through interaction with sulfur. The distribution pattern of the palladium-adsorbing cells—both the number of cells that adsorbed palladium and the amount of palladium adsorbed—changed drastically. This is the first report to link such interactions to changes in the behaviour of the cell population and clearly demonstrates a differential adsorption mechanism under different environmental conditions.

“The insight achieved is expected to contribute to future engineering of cell surfaces to provide enhanced metal adsorption”, says Professor Minoda. “Optimising the performance of biologically-derived precious metal adsorbents is expected to significantly improve the environmental sustainability of metal recycling and remediation.”

This work was published in *Journal of Hazardous Materials* (doi.org/hpbg). 🚀

Increased repetition of attosecond pulses enables pump-probe spectroscopy

Scientists at the Max Born Institute have managed to generate attosecond pulses at 100kHz repetition rate. This enables new types of experiments in attosecond science.

Attosecond laser pulses in the extreme ultraviolet (XUV) are a unique tool enabling the observation and control of electron dynamics in atoms, molecules and solids. Most attosecond laser sources operate at a pulse repetition rate of 1 kHz, which limits their usefulness in complex experiments. Using a high-power laser system they have developed, scientists at the Max Born Institute (MBI) have managed to generate attosecond pulses at 100 kHz repetition rate. This enables new types of experiments in attosecond science.

Light pulses in the extreme ultraviolet (XUV) region of the electromagnetic spectrum, with durations on the order of 100s of attoseconds, allow scientists to study ultrafast dynamics of electrons in atoms, molecules and solids. Usually, experiments are performed using a sequence of two laser pulses with a controllable time-delay between them. The first pulse excites the system, and the second pulse takes a snapshot of the evolving system, by recording an appropriate observable. Usually, the momentum distributions of ions or electrons or the transient absorption spectrum of the XUV pulse is measured as a function of delay between the two pulses. By repeating the experiment for different timings between the two pulses, a movie of the dynamics under study can be created.

In order to get the most detailed insights into the dynamics of the system under investigation, it is advantageous to measure the available information about the time evolution as completely as possible. In experiments with atomic and molecular targets, it can be advantageous to measure the

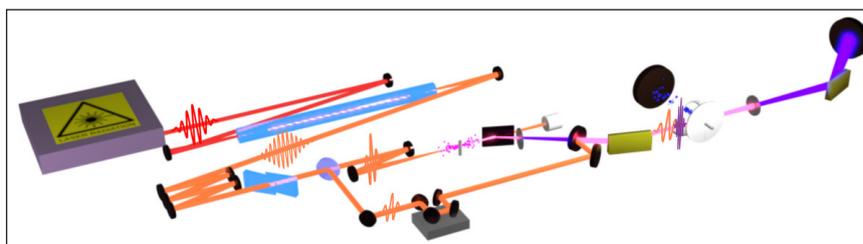


Figure 1. Experimental setup. The home-built OPCPA system provides 7 fs pulses at 100kHz repetition rate. These pulses are shortened to 3.3 fs duration via hollow fibre pulse compression. Attosecond streaking experiments are performed in a purpose-built beamline.

three-dimensional momenta of all charged particles. This can be achieved with a so-called reaction microscope (REMI) apparatus. The scheme works by ensuring single ionisation events for every laser shot and detecting electrons and ions in coincidence. This, however, has the drawback that the detection rate is limited to a fraction (usually 10–20%) of the laser pulse repetition rate. Meaningful pump-probe experiments in a REMI are not possible with 1 kHz class attosecond pulse sources.

MBI has developed a laser system based on optical parametric chirped pulse amplification (OPCPA). In parametric amplification no energy is stored inside the amplification medium, therefore, very little heat is generated. This enables the amplification of laser pulses to much higher average powers than with the current “work-horse” Ti:Sapphire laser, which is most often used in attosecond laboratories around the world. The second advantage of OPCPA technology is the ability to amplify very broad spectra. Our OPCPA laser system directly amplifies few-cycle laser pulses with durations of 7 fs to average powers of 20 W. This is a pulse energy of

200 μ J at 100 kHz repetition rate. They have used this laser system previously to successfully generate attosecond pulse trains.

In many attosecond experiments it is beneficial to have isolated attosecond pulses instead of a train of multiple attosecond pulses. To enable the efficient generation of isolated attosecond pulses, the laser pulses driving the generation process should have pulse durations as close as possible to a single cycle of light. This way the attosecond pulse emission is confined to one point in time leading to isolated attosecond pulses. In order to achieve near-single-cycle laser pulses they have employed the hollow fibre pulse compression technique. The 7 fs pulses are sent through a 1 m long hollow waveguide filled with neon gas for spectral broadening. Using specially designed chirped mirrors the pulses can be compressed to pulse durations as short as 3.3 fs. These pulses consist of only 1.3 optical cycles.

The 1.3 cycle pulses are sent into an attosecond beamline developed at the MBI. The main part of the energy is used to generate isolated attosecond XUV pulses in a gas cell target. After removal of the high

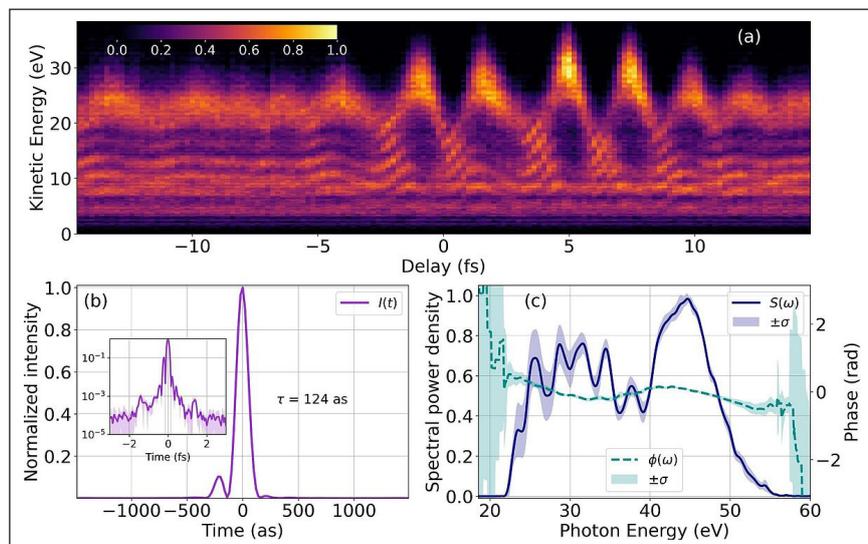


Figure 2. Attosecond streaking results. (a) Measured photoelectron streaking trace. (b) Intensity envelope of retrieved isolated attosecond pulse (inset: the intensity profile on logarithmic scale) (c) Retrieved spectral intensity and spectral phase.

power NIR beam, spectral filtering and focussing, around 10^6 photons per laser shot (corresponding to an unprecedented photon flux of 10^{11} photons per second) are available for experiments.

In order to characterise the generated attosecond XUV pulses,

they performed an attosecond streaking experiment. Essentially the XUV pulse is used to ionise an atomic gas medium (neon in this case), while a strong NIR pulse is used to modulate the XUV generated photoelectron wavepackets. Dependent on the exact timing

of the XUV and NIR pulses, the photoelectrons are accelerated (gain energy) or decelerated (lose energy) leading to a characteristic “streaking trace”. From this data matrix the exact shapes of both the NIR pulse, as well as the XUV pulse can be determined. The attosecond pulse shapes are retrieved using a global optimisation algorithm developed for this project. Careful analysis shows that the main attosecond pulses have a duration of 124 ± 3 as. The main pulse is accompanied by two adjacent satellite pulses. These stem from the attosecond pulse generation half an NIR cycle before and after the main attosecond pulse generation.

The pre- and post-pulse satellites have a relative intensity of only 1×10^{-3} and 6×10^{-4} , respectively.

These high flux isolated attosecond pulses open the door for attosecond pump-probe spectroscopy studies at a repetition rate 1 or 2 orders of magnitude above current implementations.

Read more about this work in the paper in *Optica* (doi.org/hpbk). 🔗

Terahertz circular dichroism for biomolecules

Terahertz circular dichroism may be able to monitor chirality of pharmaceuticals and provide new information on biomolecules’ chirality.

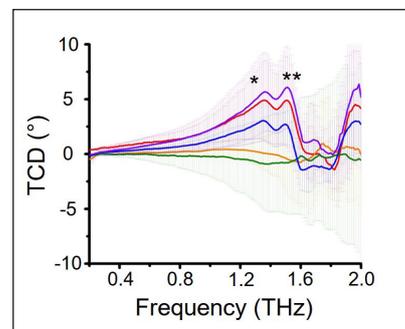
It is not easy to be sure that drugs and supplements with chiral structures are turning in the correct direction. Now, terahertz radiation can probe both the structures of molecular crystals and their twists, research led by the University of Michigan has shown. The researchers hope that the technique could also help diagnose harmful accumulations of twisted molecules in the body, including bladder stones, insulin fibrils and amyloid aggregations such as the plaques that appear in Alzheimer’s disease.

In a world of curled molecules, biology often favours right- or

left-handed versions. But quality control for twisted molecules is tough, and monitoring the chiral structures of drugs and supplements kept in storage isn’t usually done.

“The methods most commonly used at pharmaceutical companies are very sensitive to impurities, but measuring chirality is expensive”, said Wonjin Choi, a research fellow in chemical engineering at the University of Michigan.

The new method, published in *Nature Photonics* (doi.org/hpbp) can quickly recognise wrong twists and wrong chemical structures



Terahertz circular dichroism spectra of five different brands of L-carnosine. While three samples show the same pattern of peaks, the measurement suggests possible differences from the remaining two samples. Credit: Wonjin Choi, Kotov Lab

in packaged drugs using terahertz radiation. It was developed by an international team, including researchers at the Federal University of São Carlos, Brazil; Brazilian Biorenewables National Laboratory; University of Notre Dame; and Michigan State University.

“Biomolecules support twisting, long-range vibrations also known as chiral phonons. These vibrations are very sensitive to the structure of molecules and their nanoscale assemblies, creating the fingerprint of a particular chiral structure”, said Nicholas Kotov from Michigan.

The team was able to measure these phonons in the spectra of twisted terahertz light that passed through tested materials. One of these, L-carnosine, is currently used as a nutritional supplement. “If the twist of the molecule is wrong, if

the twist in the way the molecules pack together is not right, or if different materials were mixed in, all of that could be inferred from the spectra”, Kotov said.

John Kruger, professor of veterinary medicine at Michigan State University, provided bladder stones from dogs, and the team discovered their chiral signature. The team hopes that the findings could help enable rapid diagnostics for pets and perhaps later humans. In addition, they studied insulin as it grew into nanofibres that make it inactive. If the terahertz light technology can be adapted for home healthcare, it could verify the quality of insulin.

The team also explored how light can influence structures, rather than just measure them. Calculations carried out by André Farias de Moura, professor of

chemistry at the Federal University of São Carlos and co-corresponding author, show that multiple biomolecules vigorously twist and vibrate when terahertz light generates chiral phonons.

“We foresee new roads ahead—for instance using terahertz waves with tailored polarisation to manipulate large molecular assemblies. It might replace microwaves in many synthesis applications in which the handedness of the molecules matters”, said de Moura.

Based on de Moura’s calculations, Kotov and Choi believe that the twisting vibrations of chiral phonons caused by terahertz light may make disease-causing nanofibres more vulnerable to medical interventions. Future work will explore whether that interaction can be used to break them up. 

Transient measurement of phononic states with covariance-based stochastic spectroscopy

New work demonstrates transient non-linear spectroscopy based on covariance methods and its advantages over mean-value-based approaches. A generalisation of this approach could be a game change in non-linear spectroscopy in the optical region.

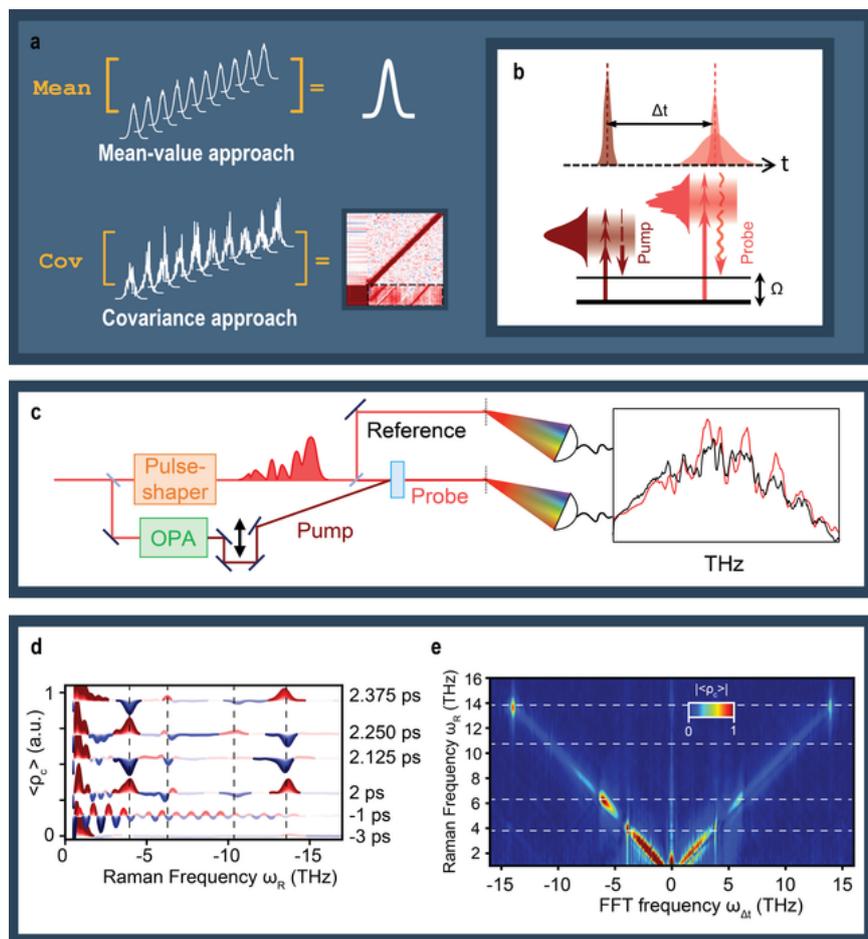
Over the last several decades, ultrafast spectroscopic techniques have played a key and growing role in scientific discoveries in physics, materials science, biology and chemistry, while also proving useful in application-driven projects and device manufacture and characterisation. While the experimental techniques have matured in many ways, they still largely share some key philosophical features: they rely on “well behaved” laser pulses (i.e. as stable as possible); and on integrating or averaging many measurements to reduce the experimental noise to acceptable levels where necessary. These characteristics lead to complicated experimental setups, and expensive lasers which typically are limited to lab-based

environments with large space requirements.

A team of scientists, from Italy, USA and Australia have demonstrated that a fundamentally different approach which benefits from “badly behaved” pulses (i.e. noisy) can retrieve the spectroscopic signal. The team led by Professor Daniele Fausti from the University of Trieste and Elettra Sincrotrone Trieste, Professor Shaul Mukamel from the University of California, Irvine, and Dr Jonathan Tollerud from Swinburne University developed a new ultrafast spectroscopy technique, which instead of making the pulses more stable, utilises noisy pulses and a correlation-based approach for signal detection. Here, the sample is

driven out of equilibrium, and then probed with pulses that are deliberately made “poorly behaved” and display randomised pulse-to-pulse fluctuations in time and frequency. Information from the out-of-equilibrium sample is then encoded into these noisy pulses through non-linear interaction of the light with the material and retrieved by single shot acquisitions.

“The Eureka of my PhD project was realising that every realisation of the experiment is unique and, therefore, measuring the average over many repeated experiments doesn’t tell you the full story”, says Giorgia Sparapassi from Elettra Sincrotrone Trieste. To put it simply, it is common in pump and probe experiments to repeat the measurements thousands



a: A schematic illustrating the paradigmatic difference between mean-value and covariance-based spectroscopy. The covariance-based approach extracts the information embedded in pulse-to-pulse fluctuations, which mean-value ignores. b: In a pump-probe experiment, the pump pulse drives a system out of equilibrium. The noisy probe pulse records the state of the system at a later time through correlations induced by a non-linear interaction with the sample. c: A diagram of the experimental apparatus in which a pulse-shaper introduces fluctuations in the probe pulse, which then interacts with the sample before being recorded by a spectrometer. Comparison with the reference pulse reveals the correlations induced by the sample. d: The vibrational modes are revealed as signals that oscillate between positive (red, correlated) to negative (blue, anti-correlated) as a function of the time delay between pump and probe. e: Among other areas, this covariance-based approach promises to be useful in 2D-Raman spectroscopy, as demonstrated by this pseudo-2D Raman spectrum. Credit: G. Sparapassi, S.M. Cavaletto, J. Tollerud, A. Montanaro, F. Gleran, A. Marciniak, F. Giusti, S. Mukamel and D. Fausti

of times per second so that one can measure even the tiniest changes of the reflectivity or transmissivity in the sample. But it is important to realise that in mean-value-based approaches it is implicitly assumed that all measurements are performed under unchanged conditions, while in truth, each realisation of the experiment is subtly different. “Realising that the subtle difference

between different realisations of the same experiments carry a whole load of information which you miss if you measure the response averaged over many repetitions was the starting point of this research line”, says Professor Fausti who led the project.

In a recent paper (doi.org/hpbq), the authors have brought this concept to time domain spectroscopies and shown that vibrational

modes of quartz can be measured using correlations induced through a Raman interaction of the probe with the out-of-equilibrium material. By scanning the time delay between the noisy probe and a coherent pump pulse (which was used to drive the system out of equilibrium), they show how the degree of correlation over many uniquely randomised pulses can provide new information beyond that provided in mean-value experiments.

In this work, the degree of correlation was quantified using the Pearson Correlation—a basic metric of correlation between two independent quantities—and this relatively simple demonstration has indicated the feasibility of new experimental directions in 2D Raman spectroscopy, an area that has received significant interest but has been impeded by experimental challenges. Dr Tollerud stresses: “There is the incredible opportunity to apply this correlation-based approach to many of the non-linear spectroscopy techniques that have been developed within the mean-value based paradigm”. Professor Mukamel also shares his collaborators’ enthusiasm: “Here we have formalised how to extract time-dependent high-order non-linear signals from intensity correlation functions, rather than mean value, but this is only the first demonstration of an operating principle which could be applied to many other non-equilibrium techniques”.

More broadly, this work demonstrates transient non-linear spectroscopy based on covariance methods and its advantages over mean-value-based approaches. A generalisation of this approach could be a game change in non-linear spectroscopy in the optical region, but also provide a route to retrieve temporal and spectral resolution from stochastic probes, in conditions where noise is unavoidable such as in hard X-ray free-electron lasers based on self-amplified spontaneous emission. 🚀

Synchrotron FT-IR microspectroscopy indicates faster and more effective tooth whitening treatments

Synchrotron FT-IR microspectroscopy has been used to study the side effects of typical tooth whitening treatments, based on oxidation, compared to a new treatment developed through reduction.

Tooth whitening is a common aesthetic treatment around the world. To obtain better results, higher concentrations of oxidising agents and longer application times are needed, but this may increase side effects like hypersensitivity and pulp damage, tooth demineralisation and gingival irritation. Besides, the need to apply these products for hours is not very comfortable for the user. Typical tooth whitening treatments are based on the oxidising power of hydrogen peroxide, which breaks the double bonds of the staining molecules on the teeth's surface making them unable to absorb light. This way the molecule becomes transparent, giving the impression of white teeth.

In recent work (doi.org/hpbt) from the Research Group of Separation Techniques in Chemistry (GTS) from the Universitat Autònoma de Barcelona (UAB) in collaboration with the ALBA Synchrotron, researchers have used bovine incisors as *in vitro* model to study the side effects of whitening treatments. They compared typical whitening treatments (based on oxidation with carbamide peroxide) to a new treatment developed and patented by the authors through reduction via metabisulfite, which also makes the staining molecules colourless. However, metabisulfite offers a faster whitening effect, which permits the use of lower concentrations and shorter application times. Results showed how the whitening effect of the novel treatment is highly improved in terms of application time needed, with the consequent reduction of side effects. This makes it a promising candidate to develop novel whitening treatments.

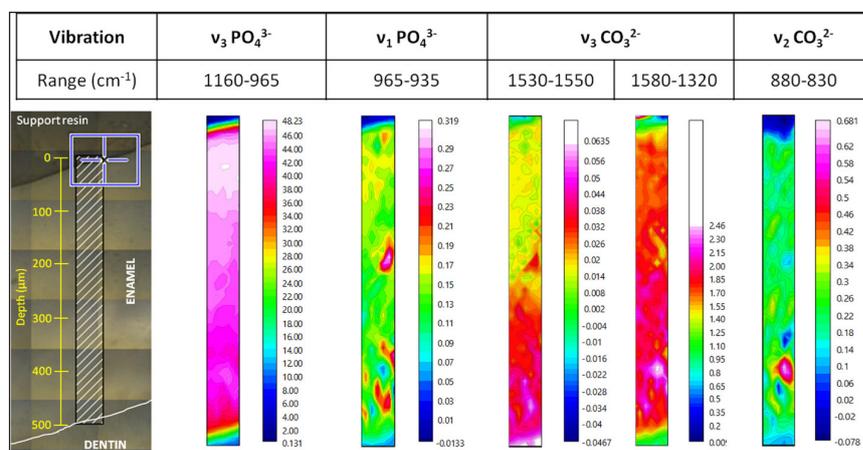


In addition, they found that using oxidising or reducing treatments promotes different mineral changes. This was shown thanks to the chemical imaging performed at the MIRAS beamline of ALBA. It is the first time that synchrotron light has been used to map the bovine incisor's enamel chemically, and to determine the effect of a whitening treatment in terms of chemical mineral modifications, and the extent in depth of these effects.

The team used Fourier transform infrared (FT-IR) microspectroscopy

with synchrotron light, which has enabled the combination of biochemical with spatial information at cellular resolution.

"Synchrotron-based Fourier transform infrared microspectroscopy technique can provide very precise chemical information in small areas, therefore, it is a very suitable technique to study the changes induced by whitening treatments and to characterise the extent of its effects with precision", explains Ibraheem Yousef, the scientist responsible for the MIRAS beamline. 🏆



Chemical distribution of carbonates and phosphates in the middle crown of a bovine incisor control tooth (vertical section).

“Forever” chemicals

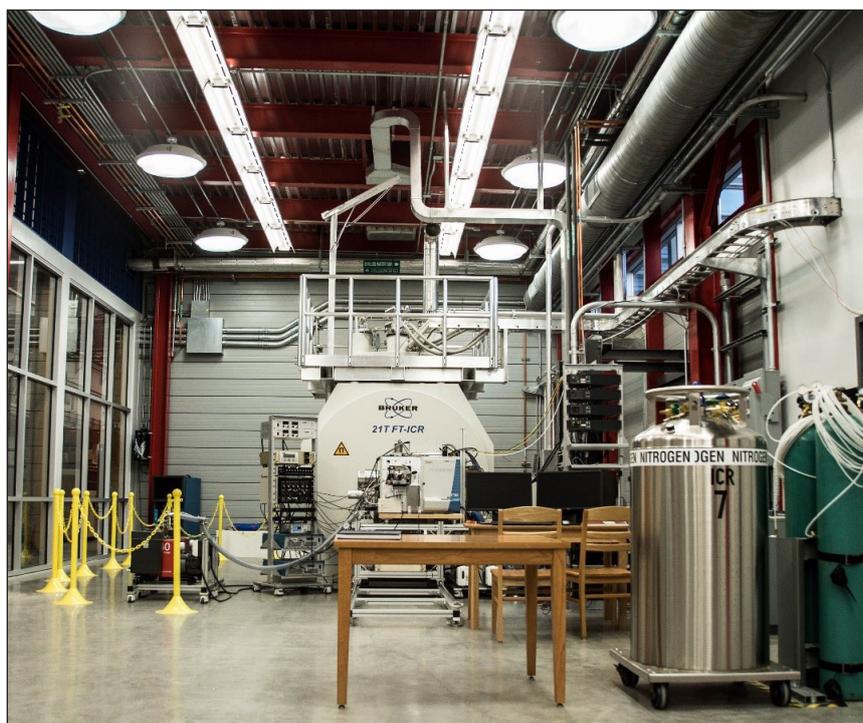
Researchers have developed a more accurate method to discover and document pervasive “forever” chemicals, which have been found in the blood of people and other animals across the globe.

US National Science Foundation researchers have developed a more accurate method to discover and document pervasive “forever” chemicals often referred to as PFAS. Studies have documented PFAS in the blood of people and other animals across the globe. Thousands of forever chemicals have been identified, but there could be other potentially hazardous compounds lurking that have not yet been detected. The volume of chemicals and scope of their impact will be brought into clearer focus with the data obtained from this initiative, scientists say.

Per- and polyfluoroalkyl substances (PFAS) are an omnipresent group of thousands of manufactured chemicals, some harmful to people and the environment. The pervasive pollutants can be found in everything from food packaging and cookware to cleaning products, textiles and drinking water. The Colorado State University-based research team is working to classify and catalogue the myriad chemical compounds in the PFAS cohort, data that could be critical to finding solutions to health and environmental damage the chemicals cause.

“We’re not only attempting to resolve the chemical complexity of PFAS, we’re also opening doors for researchers who want to look at treatment, environmental fate and transport, and toxicology”, said Jens Blotvogel, a co-author of the study published in *Environmental Science & Technology* (doi.org/hpdt). “This is giving people the strongest possible magnifying glass to unravel these processes.”

The research team will conduct the survey and chemical analysis using the 21 T Fourier-transform



Researchers are using a 21 T FT-ICR mass spectrometer to identify and analyse “forever” chemicals. Credit: National Maglab

ion cyclotron resonance mass spectrometer at the NSF-funded National High Magnetic Field Lab.

“The first step is understanding what’s there, and then you can figure out the environmental impacts and try to remediate them, but you’ve got to know the chemistry”, said Amy McKenna, an environmental analytical chemist.

“It’s powerful enough to be able to see all of these different PFAS molecules, but it’s also powerful

“We’re not only attempting to resolve the chemical complexity of PFAS, we’re also opening doors for researchers who want to look at treatment, environmental fate and transport, and toxicology”

enough to pick them out of environmental samples that contain many thousands of natural compounds”, said Robert Young.

The team plans to continue investigating why some compounds may go from harmless to harmful when they degrade or are mixed with other compounds. Understanding what the compounds are and how they change will help scientists figure out how to minimise damage from dangerous compounds.

“The long-term goal is to help identify these things so other people know what to look for”, Young said. “As soon as we know what to look for, we can focus on understanding the health and environmental impacts and prioritise treatment or regulatory solutions.”

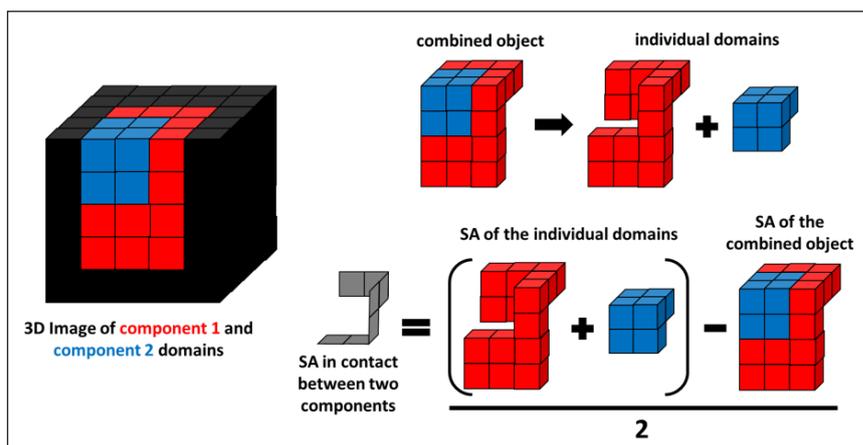
3D chemical images of pharmaceutical tablets

Serial sectioning of pharmaceutical tablets with spectral mapping has enabled full visualisation of the three-dimensional microstructure of a tablet system to be achieved.

Today's pharmaceutical tablets are complex products, and their performance is known to be primarily influenced by the physical and chemical properties of the formulation. The size and spatial arrangement of the active pharmaceutical ingredient (API) within the excipient matrix can influence the bioavailability, dissolution rate and stability of the final drug product.

Vibrational spectroscopic chemical mapping is an established tool within the pharmaceutical industry to examine the size and spatial arrangement of components within tablets. Traditional applications usually involve only examining a single exposed surface area of a sample and thus there are known limitations associated with obtaining domain size statistics from a two-dimensional (2D) chemical image. Recently, the combination of spectroscopic mapping with serial sectioning has enabled full visualisation of the three-dimensional (3D) microstructure of a tablet system to be achieved. A 3D dataset can be reconstructed by stacking individual 2D chemical images collected at regular depth intervals into the sample. To further enhance the added value of 3D spectroscopic mapping methods, this paper, published in *Journal of Spectral Imaging* ([10.1255/jsi.2022.a3](https://doi.org/10.1255/jsi.2022.a3)), outlines the methods required to visualise, process and analyse 3D volumetric data for pharmaceutical applications. This provides a means to quantitatively describe the microstructure of a tablet matrix and is a powerful tool to overcome knowledge gaps in current tablet manufacturing processes, optimising formulation development.

The research team, from the University of Strathclyde and



The 3D domain size distribution of each component in the tablet is important. This figure demonstrates the steps in the process. [10.1255/jsi.2022.a3](https://doi.org/10.1255/jsi.2022.a3)

Pfizer, show how the 3D domain size distribution of each component can be determined and used as a comparative tool to understand how the size and shape of domains change throughout the tablet manufacturing process, from raw materials to tablet compaction. Enhanced knowledge regarding the effect of each processing condition on size and shape of the components may lead to optimised manufacturing processes that produce tablets with desired physical and chemical characteristics. The relative position of a

component within the drug matrix can also be quantified to assess the spatial arrangement of components within the final drug product. Enhanced understanding regarding the 3D microstructure of a new drug product can provide a baseline understanding of the product with the desired attributes. The spatial arrangement of components within OOS samples can now be quantified and with enhanced process understanding, the root cause may be identified to a single manufacturing step. 



Gamma-ray spectrometers can aid archaeological discoveries

Gamma-ray spectrometers, commonly used at nuclear power plants, can be repurposed to help discover ancient buildings or dinosaur bones.

Gamma radiation detectors could be used to help archaeologists scan underground for new finds and could also be applied to discovering dinosaur bones, a new study has shown. A gamma-ray spectrometer—normally used to identify radioactive contamination on nuclear sites—was used for the first time in an archaeological setting at a University of Reading excavation in Roman Silchester, Hampshire, UK. The trials found the devices were able to identify buried buildings or objects by detecting gamma radiation emitted during the natural decay of elements in these materials.

The detectors could, therefore, be a valuable addition to traditional geophysical surveys as they can reveal the composition of objects before they are excavated, and provide clues as to how old objects are, where they came from, or even what a site was used for thousands of years earlier.

Victoria Robinson, a PhD researcher in Archaeology at the University of Reading, who led the trial, said: “Confirming traditional surveys using a different technique is hugely valuable as it takes the guesswork out of archaeology. Until you have fully investigated a site you can never be quite sure what is under the ground, so the more information archaeologists have at their fingertips before they start digging, the better. Radiation detectors aren’t the first thing you’d think of to assist with excavations, but they could be a useful addition to an archaeologist’s toolkit. They are portable and highly versatile, which also offers an advantage over the technology that is currently used.”

A Groundhog Portable Gamma-Ray Spectrometer was tested on



The Groundhog Fusion System trialled at Roman Silchester. Credit: University of Reading

four sites at Silchester in summer 2019. The results are published in the *Journal of Archaeological Prospection* (doi.org/hph3).

The detector was found to be most effective on the site of Silchester’s Roman temple, where it confirmed geophysical surveys locating a buried boundary wall. The position of the wall was indicated by lower radioactivity readings, suggesting the wall was constructed from materials imported from a different geographical area with naturally depleted radioactivity.

Gamma-ray spectrometers pick up naturally-occurring uranium under the ground. As materials and objects are weathered, they release minerals containing uranium, which can then be absorbed by nearby objects, such as bones, over long periods of time. For this reason, dinosaur bones—normally the preserve of palaeontologists and usually only revealed by chance—could potentially be one of the most easily identifiable objects using the detectors.

The detectors penetrate up to a metre into the ground, taking gamma radiation readings at regular intervals to build up an image. They are particularly good at identifying materials that did not originate in the location, as these usually have a very different geochemical composition to the soil and objects surrounding them and, therefore, give contrasting radiation readings. For example, the Welsh blue stone taken to Salisbury to build Stonehenge (<https://bit.ly/shenge>) would be clearly distinguishable within the landscape. Firing clay bricks in a kiln also substantially changes their composition, making them easily detectable using a radiation detector. Places that hosted ancient industrial work such as this often have similarly altered waste material deposited across them, providing a further indication as to what the site was used for.

Currently, there are three main geophysical surveying techniques commonly used on archaeological sites: magnetic, electrical and ground penetrating radar. Each is best applied to different sites. The gamma radiation detectors are more portable than these other technologies, and so can be used for high-resolution surveys while walking around or even mounted to vehicles to cover much larger areas.

The authors concluded that gamma-ray spectrometers could be used alongside other techniques to provide more certainty about what lies underground at archaeological sites. Further trials are planned, using more frequent readings to create a higher-resolution survey image, which could prove to be even clearer than those using other technologies. 🚀

IonSense acquired by Bruker

IonSense, maker of the DART ionisation technology, has been acquired by Bruker. The deal provides financial investments to ramp up development of the DART technology.

IonSense, who produce the ambient DART™ (Direct Analysis in Real Time) ionisation technology, has been acquired by Bruker. The deal provides IonSense with the financial investments to ramp up development of the DART ionisation source technology and increase efforts in developing applications in the applied markets, including food analysis and forensics.

“This merger will help us to accelerate development of DART MS and properly resource robust applications development programmes”, commented the CEO of IonSense,

Jeff Zonderman. “Our vision remains to use DART to empower mass spectrometers to perform better outside their traditional LC and GC workflows. We are committed to continuing sales of our DART sources for coupling with all vendors’ mass spectrometers. In partnership with Bruker, we will leverage their strong presence and reputation in analytical instrumentation, and their investments in IonSense, to introduce our enabling technology to a wider customer audience at a faster pace.”

Commenting on the acquisition, Dr Robert Galvin, VP Applied Markets at Bruker Daltonics, stated: “We are excited about bringing this enabling technology to our customers. We believe that mass spectrometry has a broader potential in a wider range of markets than it has previously been known for. Our financial commitment to DART will ultimately enable more people to have access to the power of mass spectrometry for today’s analytical challenges.” 📈

HORIBA UK joins non-animal technologies partnership

As an industry partner, HORIBA will co-create, support and mentor a four-year research project to explore how spectroscopy can help drive new methods of cell screening and disease diagnosis based on animal-free research.

HORIBA UK announces that it has joined the lifETIME Centre for Doctoral Training (CDT) as an Industry Partner. This partnership aims to provide a new generation of scientists with skills and approaches to reduce and replace the need for animal testing, so transforming drug discovery, toxicology screening and regenerative medicine.

The lifETIME (Engineered Tissues for Discovery, Industry and Medicine) CDT is a partnership between the University of Glasgow, University of Birmingham, Aston University and CÚRAM – Science Foundation Ireland at the National University of Ireland, Galway. Offering fully funded PhD studentships, the CDT focuses on high-value skills training across a range of scientific disciplines to enable research students to develop non-animal technologies (NATs)



HORIBA UK joins the lifETIME Centre for doctoral training in engineered tissues for discovery, industry & medicine

that better mimic physiology and disease.

In partnership with industry, the lifETIME CDT harnesses knowledge-exchange and co-creation in pioneering science to develop bioengineered humanised 3D models, microfluidics, diagnostics and sensing platforms. As an industry partner, HORIBA will co-create, support and mentor a four-year research project to explore how spectroscopy can help drive new methods of cell screening and disease diagnosis based on animal-free research.

In addition to supporting leading research, industry partners such as HORIBA also enable students to experience different industrial roles and strengthen their multi-disciplinary skills to guide their future career choice. Not only in academic/industrial research, but also marketing, regulation, standards or policy. This provides student cohorts with the professional skills

training needed to ultimately enhance industrial and societal impact.

“Our involvement with doctoral training centres keeps us close to cutting-edge UK science, and allows us to give something back through support and nurture of a new generation of scientists”, said Dr Simon FitzGerald, Technical Manager, HORIBA UK. “We are particularly excited to join lifETIME CDT as we can enable and contribute to incredible science that will drive real improvements in disease diagnosis, medicine and clinical science. It covers a broad range of research driven by world-leading scientists, much of which is underpinned by the spectroscopy and measurement technologies that are at the core of HORIBA’s expertise. HORIBA and the lifETIME CDT is a perfect synergy!”

Matthew Dalby, Professor of Cell Engineering at the University of Glasgow, and Director of

the lifETIME CDT, commented, “HORIBA will work with lifETIME to make our models a reality, to reduce and replace the need for animal testing and to offer new skills to our PhD students. The opportunities that this partnership brings are huge—HORIBA’s expertise in spectroscopic and analytical science will be of great benefit for our students and the science they do. The involvement of industry really helps us to deliver enhanced training and opportunities to our students. HORIBA, and our other partner companies, are critical to our success.”

The CDT partnership also facilitates wider networking opportunities between industry partners and the many leading academics involved. This supports the discovery of potential synergies between HORIBA and major research institutions to help identify and develop future technologies for further scientific advancements. 

Calibration partnership for single-chip FT-NIR spectrometers

Si-Ware has announced a partnership with NutriControl Analytical Solutions, a laboratory network based in the Netherlands serving the animal feed, dairy and food sectors.

Si-Ware, manufacturers of the NeoSpectra single-chip FT-NIR spectrometers, has announced a partnership with NutriControl Analytical Solutions, a laboratory network based in the Netherlands serving the animal feed, dairy and food sectors. The partnership will benefit from NutriControl’s calibration experience to provide users of the portable NeoSpectra Scanner with quick, accurate materials sampling capabilities for a broad range of applications.

“We’re excited to partner with NutriControl on this endeavour and pair their NIR calibration expertise with our user-friendly portable technology”, said Ralph Hewitt, vice president of global sales at Si-Ware.



NutriControl develops NIR calibration lines and NIR cloud services

that can be used to analyse feed, grains, dairy products, silages, pet food and many other raw materials. The company’s calibration lines are based on a significant amount of classical wet chemical tests.

“Our customers have long understood the need for accurate materials analysis, and now more than ever, they are searching for portable solutions to conduct real-time sampling and accurate measurements”, said Jörgen van den Ende, managing director at NutriControl. “Through our collaboration with NeoSpectra by Si-Ware, we now have the opportunity to implement our calibration lines on a portable system that will bring value to all global users.” 

Leaving a mark on forensic science: how spectroscopic techniques have revealed new insights in fingerprint chemistry

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In forensic science, fingerprints are used to connect an individual to a criminal investigation. Their evidential value is reliant on the successful recovery of a fingerprint from a crime scene. Despite a multitude of chemical and physical methods capable of detecting fingerprint residues, there are substantial challenges with fingerprint recovery due to the inherent variability of this biological material. Ongoing research has focused on the development of new or improvement of current fingerprint recovery techniques. Meanwhile, conducting fundamental studies can be valuable to explore the residue itself, to better understand its variation in response to fingerprint treatments.

Spectroscopic methods have played a critical role in the analysis of fingerprints, used to identify the chemical constituents present, examine their degradation over time and compare the chemical variation between donors. Whilst bulk chemical methods have provided an extensive view of the

chemical species present, the heterogeneous nature of fingerprint residues means that a more accurate picture can be obtained when the spatial information is preserved. Chemical imaging methods such as mass spectral imaging and infrared micro-spectroscopy can capture the most comprehensive view of fingerprint chemistry.

Recent scientific advances have made spatially resolved chemical analyses more accessible. Among these powerful methods that can provide an unprecedented view of fingerprint chemistry, only a small number of techniques can analyse natural fingerprint samples without any chemical alteration, treatments or solvent extractions prior to analysis. To capture the most realistic representation of the chemical species naturally present in fingerprint residues, *in situ*, label-free measurements are required. Further, when analysing biological materials, the capability to analyse samples *in situ*, at ambient temperature and pressure, without the need for vacuum conditions, is important for the stability of loosely bound elemental content and the morphology of the sample.

Fourier transform infrared spectroscopy

Fourier transform infrared (FT-IR) spectroscopy has long been used

to characterise unknown samples based on the absorption of IR light by characteristic functional groups of organic molecules. The integration of FT-IR spectroscopy with microscopy (known as FT-IR micro-spectroscopy) further enables classes of biological molecules to be mapped across sample surfaces. Unfortunately, the long wavelengths of IR light (relative to visible light) result in poorer spatial resolution associated with FT-IR micro-spectroscopy than what is generally expected from conventional light microscopy. Nevertheless, the use of high refractive index optical materials in combination with attenuated total reflectance (ATR) modalities, now enable FT-IR micro-spectroscopy to approach micron-scale spatial resolution.¹⁻⁵

FT-IR micro-spectroscopy has been used not only to investigate how the variation in molecular chemistry can be indicative of donor traits, such as age and biological gender, but also to estimate time since fingerprint deposition.^{4,6-8} The identification of components correlating to glandular secretions from the eccrine and sebaceous glands has been characterised and their persistence monitored with variables including temperature and time.⁵ Commonly, fingerprint samples have been analysed with the addition of microscopy (either mapping

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or imaging), to retain spatial information, highlighting the inherent heterogeneous distribution of organic materials across a sample. In particular, coupling a synchrotron light source to a FT-IR imaging instrument provides enhanced spectral quality and improved data collection times. Dorakumbura *et al.* exploited the capabilities of synchrotron FT-IR imaging coupled with the ATR attachment to characterise eccrine and sebaceous material within individual droplets in fingerprint residue.⁹ This method was subsequently applied to monitor the spatio-temporal changes in fingerprint droplets under ambient temperature conditions. Changes in the morphology and chemical composition of the droplet are shown in the immediate hours following deposition (Figure 1), providing a unique perspective of the dynamic nature of this material.¹⁰

X-ray fluorescence microscopy

Research into the inorganic material in latent fingerprints has been limited due to the lack of availability

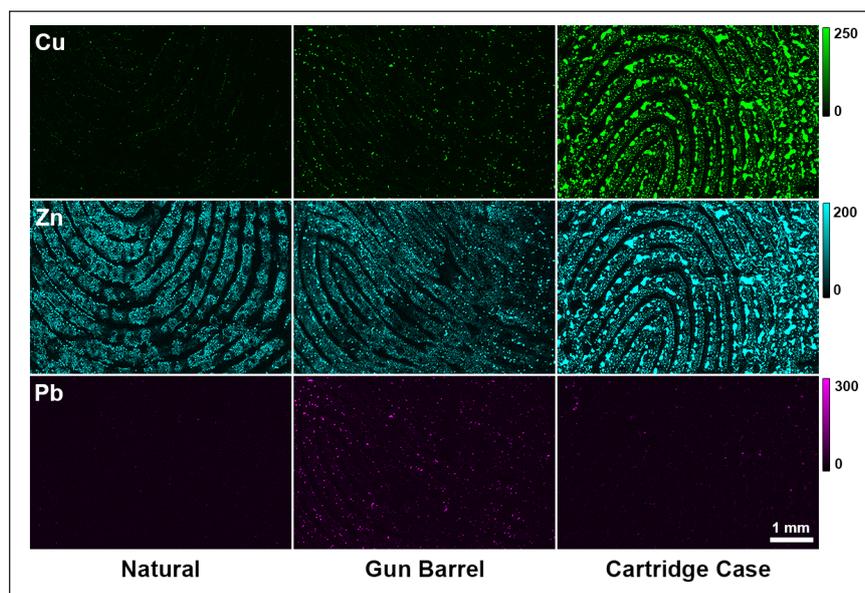


Figure 2. XFM elemental maps from copper, zinc and lead from fingerprints taken following regular activity (left), handling a gun barrel for 30 s (middle) and handling an ammunition cartridge case for 30 s (right). Intensity units are ng cm^{-2} .

in instrumentation with the appropriate sensitivity and spatial resolution required to detect the trace metals present in fingerprint residues. The process of X-ray fluorescence (XRF) inherently lends itself to simultaneous multi-element

mapping, which is of great value across many research applications. Coupling of XRF instrumentation with bright X-ray sources (e.g. synchrotron light sources) now provides the opportunity for rapid acquisition of trace-element maps, at micron spatial resolution.¹¹ Recent work conducted by our group has taken advantage of the brightness of synchrotron-sourced X-rays, using X-ray fluorescence microscopy (XFM) to image the distribution of metals and metal ions in natural fingerprints.¹² Like its organic counterpart, inorganic material is donor dependent, with great variation in the amount and distribution of elemental material present. The elemental material appeared to follow the ridge pattern detail of fingerprint residue, implying it could be an appropriate chemical target for novel fingerprint development methods. Interestingly, donor behaviour, specifically cosmetic use and contact with metal objects can influence the chemistry of inorganic material in fingerprint residues.¹³ This information can be exploited for forensic purposes, with metal

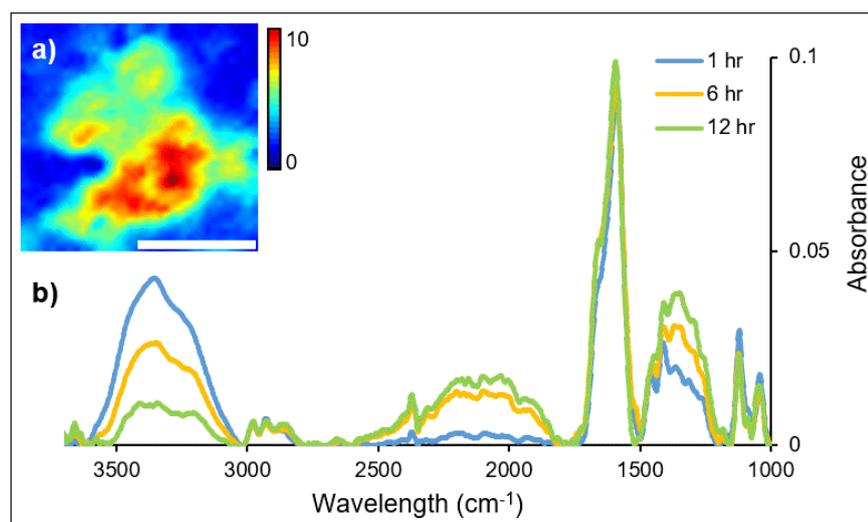


Figure 1. A time-course (12 hour) study of changes in H_2O content during air-drying of a droplet within a natural fingermark, as revealed by synchrotron ATR-FT-IR mapping technique. (a) False colour ATR-FT-IR maps were generated by integrating over the $\nu(\text{O}-\text{H})$ stretching bands of H_2O ($3000\text{--}3500\text{ cm}^{-1}$) as a marker for eccrine material. Scale bar $20\ \mu\text{m}$. (b) Representative synchrotron ATR-FT-IR spectra collected from a droplet within a natural fingermark after 1 hour, 6 hours and 12 hours of air-drying.

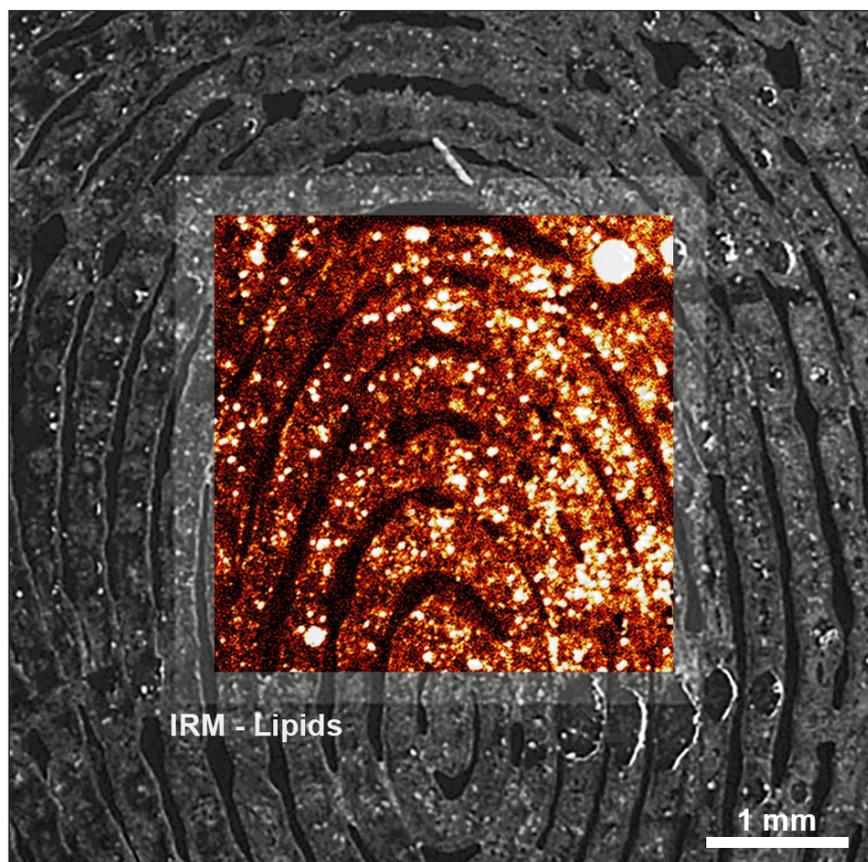


Figure 3. A natural fingerprint deposited on silicon nitride imaged with an optical microscope, XFM elemental mapping showing the zinc distribution, and FT-IR imaging (IRM) showing the distribution of lipid material (false colour image generated by integrating over the C–H stretching band for lipid within the $2800\text{--}3000\text{cm}^{-1}$ spectral range).

profiles characterised to particular criminal activities.

Multi-modal chemical imaging studies

To gain a more holistic view of fingerprint chemistry, a multi-modal workflow combining chemical imaging methods was used to investigate the interactions between organic and inorganic materials.¹² The same fingerprint sample was imaged using infrared micro-spectroscopy (IRM) and XFM, which together allowed the co-location of metals and metal ions within the organic secretions. Figure 3 shows an example of the metal ions, specifically zinc, located within the organic secretions. A broader distribution of exogenous metal ions was more likely to be linked with

external sources such as cosmetic use or secondary metal transfer.¹² This finding is critical to understanding how metal ions can interact with chemical treatments, some of which interact with the organic materials, particularly amino acids present within eccrine sweat.

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Book Review: *NMR Multiplet Interpretation: An Infographic Walk Through*, by Roman A. Valiulin

Reviewed by Abdul Hasib

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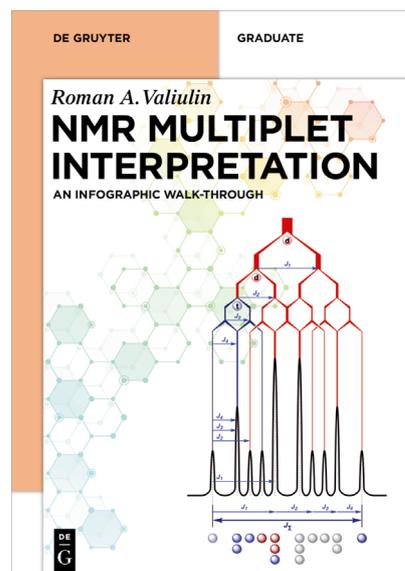
In his article “of studies”, Francis Bacon said “some books are to be tasted, others to be swallowed, and some few to be chewed and digested”¹ and this monograph on proton nuclear magnetic resonance (NMR) spectroscopy, should be “chewed and digested” as Bacon continued to elaborate, “some few to be read wholly, and with diligence and attention”.¹ *NMR Multiplet Interpretation: An Infographic Walk-Through* by Dr Roman A. Valiulin deserves your time perusing it from top to bottom with, as quoted above, “diligence and attention”. This should be the piece that proton NMR spectroscopy readers would, for sure, “try their hand at it”, for “it took over a decade of study, practice, and experience” (preface) to conceptualise followed by the materialisation of this chef-d’oeuvre: the author’s “dream book” (foreword).

It is a “dream book”—a “dream book” of the author having “more visuals than text”, thereby presenting its readers a “study aid” that would function as not only a “portable tutor” but also a useful “analytical kinesthetic” learning

tool (foreword). And it is an infographic book on ¹H NMR, perhaps the first of its kind that, like heteronuclear coupling, has made a juncture between the “realm of science and art” (foreword)—a new initiative by an organic chemist who, as an amateur artist, enjoys dabbling with drawings in his other times. And in parallel, this is a “workbook” for, as the author contends, it “provides a guided work-through of NMR spectra interpretation” on “simple and complex first-order ¹H NMR multiplets” (introduction). Being fundamentally divided into four parts, this booklet discusses the first order multiplets: simple (chapter 2) to complex (chapter 3), followed by the mnemonic rules (chapter 4) and the exercises (with answers) with their increasing difficulty levels (chapter 5).

This book is designed for specifically “developing organic chemists” (introduction), “research chemists” seeking to have a fair dealing with the proton NMR spectra by reliably reporting them for possible publication (preface) as well as the “experienced chemists” who would find more practice regarding proton NMR explanation (introduction), and it is equally targeted for the chemistry undergraduate and graduate students as their chemistry “course companion” (introduction).

It should not be a hyperbole, rather a fact of relevance that in spite of being a chemistry graduate nearly a decade ago with a degree required specialisation in organic



chemistry, I have been searching on and off for years to find a book on NMR spectroscopy, more specifically proton magnetic resonance (PMR)² or ¹H NMR etc.³ spectroscopy, or even proton MRS.⁴ It was my hope that it might work as a step-by-step guide in interpreting, in the easiest or a practical way, the PMR spectra obtained from my own graduate work. One might easily be surfeited with the resources on spectroscopy, ranging from books,⁵ spectra analysis software,^{6,7} spectra databases⁸ and handbooks⁵ as well as web pages,⁹⁻¹⁴ blogs, forums etc.¹⁵⁻¹⁷ to the scholarly literature of earlier¹⁸ and contemporary spectroscopists specifically dealing with the interpretative ways of PMR spectra,¹⁹⁻²⁴ yet a reader like me, perhaps alike many other spectroscopy readers, might assume to embrace the situation as depicted by Coleridge:

“day after day, day after day,
 we stuck, nor breath nor motion;
 as idle as a painted ship
 upon a painted ocean”,²⁵

or spend too much time to catch on the spectral matters that could be regarded “sloth” as ascribed in “of studies”.¹ And yes; for many of us could easily get stuck with or be a sluggish learner of NMR spectroscopy, there might have

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BOOK REVIEW

something to which the “causation in the law”²⁶ could be attributed as diagnosed by the present author himself: even if there were “many excellent textbooks” emphasising either the “basic examples or covering complex, rare, and even seemingly obscure ¹H NMR multiplet cases” or the “math and physics that undergird the technique”, those, at their end, would become less “accessible or useful for the organic chemists in their day-to-day research” (preface). Such a paradoxical happening, though unexpected, was inevitable as a result of perhaps adhering to the “general norm of the writers”. Yet, there were some endeavours to challenge this general trend in composing the chemistry books that received a welcome as Azman said in his review of such a book: “this textbook is a refreshing deviation from the norm”²⁷ and the present booklet could be treated in the same fashion. With such a deviation “from the norm” that “many academics would consider ‘mainstream’ or ‘accepted’”²⁷ and invoking the newest approach to learning NMR (the infographic), this book is distinct in itself.

The efficacy of the author’s work could be well understood from the voice of, amongst many authors, Hoye and his co-workers: “the emergence of routine multidimensional NMR spectroscopy has been accompanied by a decline in the learning, teaching, and practice of the important skill of assigning first-order multiplets by inspection”.¹⁹ In this context, this masterwork, as a “visual pedagogical tool” (preface) might be regarded as a “good alternative addition” to the teaching–learning landscape of organic spectroscopy. In addition, the multi-paint facet of the infographics with the author’s selective choice of colour would, for sure, work as fuel to learning a critical subject through visualisation.

Though the merit of this book is unique, originating from the

author’s own journey—a long distance traversed by him as a “student, teaching assistant, graduate and postdoctoral researcher as well as an individual tutor” (introduction and preface) accompanied by his “hobby for art” (foreword)—this workbook lends its “conceptual framework” (preface) from, as its author refers to, the pioneering work of Hoye *et al.*¹⁹ Every work has its own limitations, and this is true for the one under discussion as we are heard from its author: “this book is not intended to be a scientific paper nor a literature review... (preface) and is not intended to be a comprehensive nor exhaustive study of the fundamental theory... (introduction), it omits discussion of NMR theory and should not be used as a comprehensive textbook... readers seeking to become more specialised in the subject-matter may wish to utilise this workbook in conjunction with dedicated coursework on spectroscopy” (preface). Importantly then, one essential tool to searching in a book, i.e. the index, has not been provided. However, this is less important due to the fact that the core discussion has been aesthetically truncated to nearly 50 pages.

At the dénouement of this brief write-up, I should take a position on my own that if I were asked to choose, from a dozen of collections of books discussing ¹H NMR spectra, the only one I would surely have picked up is this infographic book for, with this “guided walk through” work of genius, I have to walk through the “only scholars’ zone” of NMR spectroscopy in spite of being myself one of the common readers of it:

“But I have promises to keep,
And miles to go before I sleep,
And miles to go before I sleep”.²⁸

Now, for the members of the chemistry family: the (organic) chemists, students, amateur collectors or the librarians—it’s your turn to choose yours!

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Open publishing FAIR spectra for and by students

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Ian Michael has challenged us on the topic of Open publishing: with all this focus on Findable data—where is it to be found? To get more data available in a form we can all use requires us all to re-think what we automatically do when we generate new spectra that might be of interest to fellow spectroscopists. Do we leave them to rot on an instrument computer, picking the “best of the best” to land in a peer reviewed publication some time years in the future? Or do we put procedures in place which ensure our work, and the work of our students, will be available to the scientific community for ever? Henry Rzepa has introduced a lovely educational spectroscopic and associated metadata workflow into Imperial College London. This not only ensures the students' spectroscopic data and associated metadata is properly documented, but also made available in a FAIR way for the whole community. It also serves to introduce students to the whole concept of best practice in FAIR data handling and Persistent and Unique Identifiers,

including the registration of the student to receive their own life-long unique publishing ORCID ID.

How did Imperial College arrive at FAIR data publication by university students?

In 2012, the ORCID organisation launched their researcher ID service, and shortly thereafter started to encourage research organisations to promote the concept to their researchers. At Imperial College, a debate was started to define the scope of who should be encouraged to register their ORCID. One sensible, if predictable, plan was to start with the most senior research investigators, who often led large groups and to gradually work down to more junior members. A particular point of view that ended up not being adopted was to start at the other end of the researcher spectrum with undergraduate students, since they after all were the future of research! That latter option continued to resonate, however, and when the design for a new laboratory course for first year undergraduate students in the chemistry department at Imperial College in the first course year was started in 2018, the opportunity to enrol these students in ORCID as part of that course was seized (see Figure 1, Step 1).

This was aided by the design of the course, which was to illustrate laboratory chemical synthesis by asking each student to generate a unique target molecule; more traditional courses involved a small number of previously known targets that all the students made. A careful choice of reaction allowed a large combinatorial design to be implemented in which two reagents (an alcohol and an acid) are combined to form an ester. Although each component is commercially available, the combination of the two would result in a molecule new to science. The next facet of the design was to ask the student to record spectroscopic information for this now unique and newly synthesised molecule, which would include the ¹H NMR spectrum (the ¹³C was deemed too resource demanding for the spectrometer allocated to this course) along with an IR measurement. It was then a short step to encourage the student to formally publish this new data in a manner that the entire community of molecular scientists could potentially benefit from, by making this publication FAIR.¹ This would mean that a simple search for the molecule by anyone based on its registered metadata (see below²) would be possible. Just as importantly, the FAIR attributes would allow a programmed and unsupervised machine to make the same

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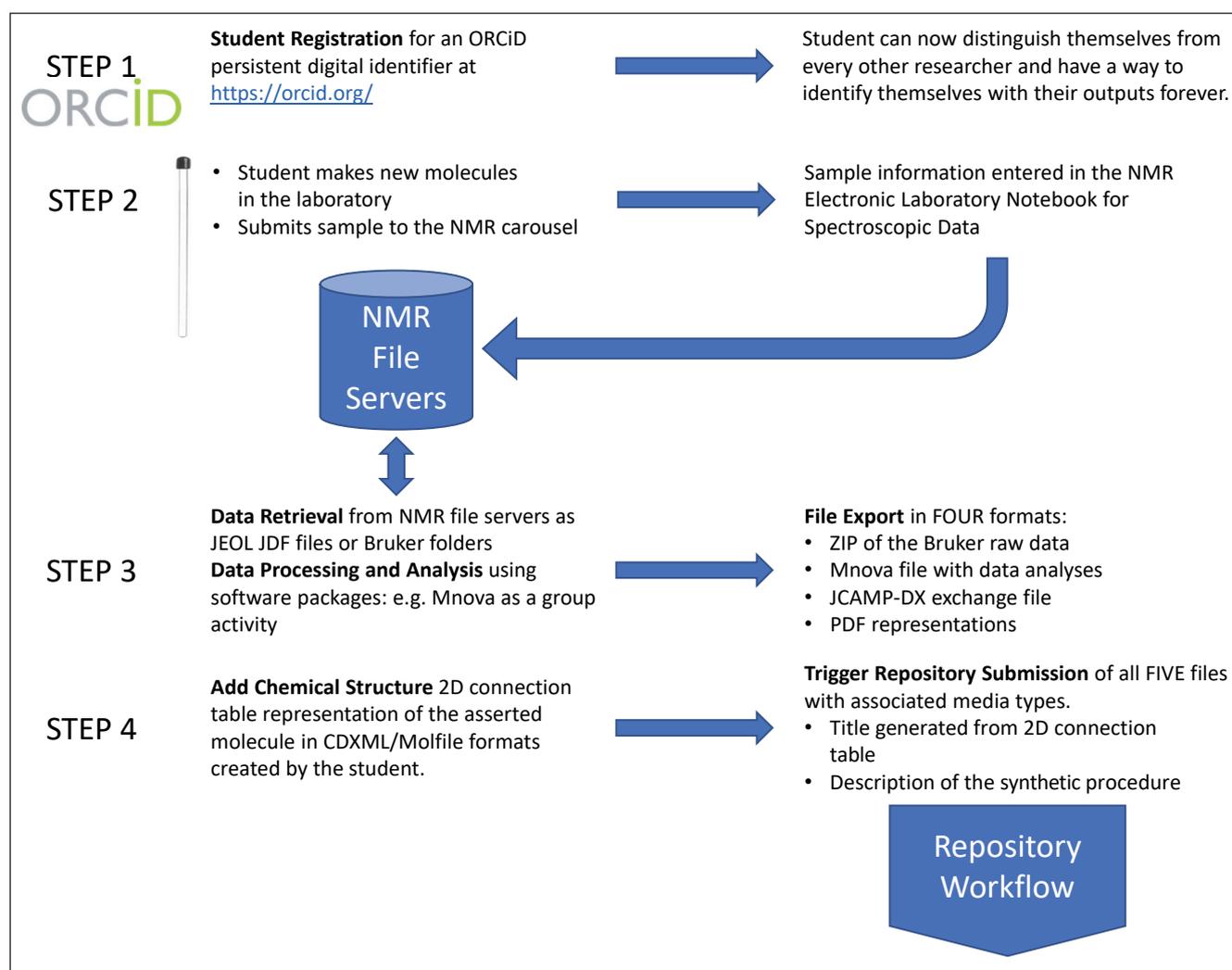


Figure 1. Student introduction to Persistent Identifiers through ORCID ID registration and spectroscopic data generation and analysis of their work.

searches, on any desired scale. The access to this data, its re-use by others and interoperability into new contexts was another benefit of this FAIR specification.

Rather than select a generic, non-subject specific repository such as Zenodo for this task, we already had access to a second generation FAIRsharing registered³ repository that had been custom-designed around rich “FAIR-Enabling” metadata^{4,5} and was already being used as the publication target for an ELN (electronic laboratory notebook) used by students undertaking computational laboratories.^{6,7}

A simple but, at this stage, non-ELN based protocol was developed

for the students to access, analyse and then publish their measured spectroscopic data in this repository.⁸ This experiment is now in its third year and the data acquired can be accessed via the repository collection.⁹

The FAIR publication workflow

The additional workflows associated with this example of FAIR publishing of spectroscopic data is shown in Figure 2. Currently data publication comprises several distinct steps undertaken by the students, a process which could be automated in the future by introducing a spectroscopy-based ELN

analogous to the system used for publishing data acquired in computational chemistry labs in which workflows can automatically generate required metadata.

A metadata model

Since this is about FAIR NMR data, it is useful to look at how the metadata record for an item imparts this aspect. This can take two forms, the media type¹⁰ of the data files uploaded to the repository and the properties of the data as registered in compliance with the DataCite schema. The properties are themselves usefully divided into a core set and a subject-specific set. DataCite core

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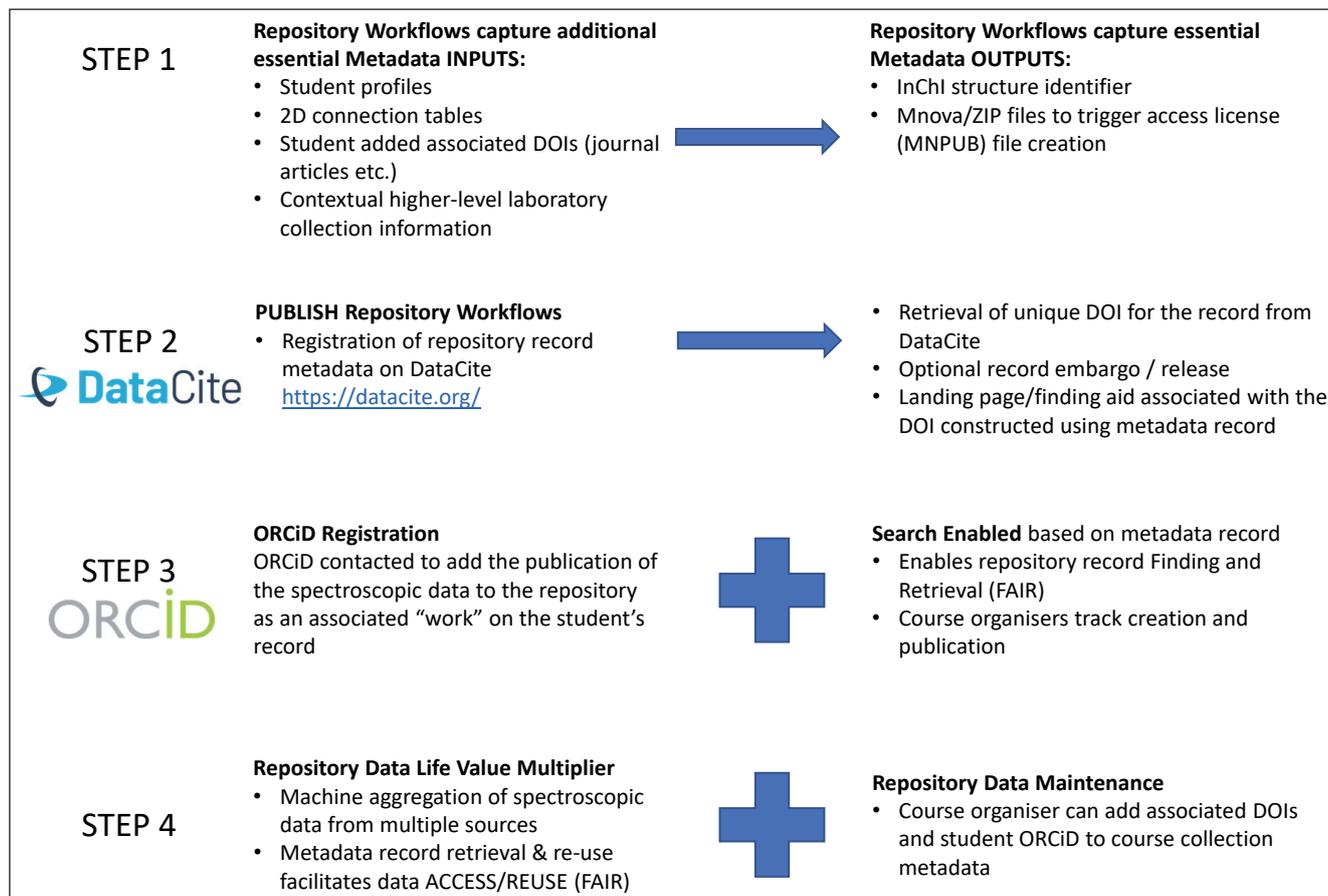


Figure 2. Spectroscopic Data Repository workflows showing interaction with DataCite for DOI generation, ORCID for student data registration and the role in course delivery and monitoring.

properties are fairly well established and include aspects such as the DOI identifier for the data record registration, the ORCID(s) for the creators of the data, title, description, the affiliation identifier in the form of a ROR (Research Organisation Registry), the (re-use) rights identifier scheme, dates and “RelatedIdentifiers”, which can point to further metadata records of other “research objects” if they exist. Other RelatedIdentifiers can point to parent/children relationships involving other collections or datasets, other research objects such as associated journal articles and perhaps in the future instrument and even physical sample identifiers.

Currently the DataCite subject-specific metadata are currently less well formalised and standardised;

an ongoing effort to achieve this for chemistry¹¹ is under way under the auspices of IUPAC, the chemistry standards body. In 2016, some subject properties such as the InChI and InChI key chemical identifiers were included in the metadata collection by this repository.^{4,5} These are repository workflow generated from the molecular connection table submitted by the depositor (the CDXML file in the instance above). An example record can be downloaded using the link <https://api.datacite.org/application/vnd.datacite.datacite+xml/10.14469/hpc/10176>, where 10.14469/10176 is the DOI assigned to the data publication. Examples of how this can be exploited are shown below for you to try out.

Examples of FAIR spectroscopic data: how to find them

The metadata registration processes result in a so-called Aggregated Metadata Store (MDS). In this instance stored by DataCite, the selected registration authority. DataCite provide an API (Application Programming Interface) to search the store and they plan to introduce a more human-friendly form. The API calls are relatively human “readable” and a number of them are documented being pertinent for the student data publication project.² They typically operate by specifying the property as defined in the metadata record and its required value (a key-pair) and using Boolean logic can be combined with the media type values to focus the search.

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DataCite Commons titles.title:undergraduate AND synthesis AND laboratory AND (NMR) Q Pages - Support Sign In

Works People Organizations Repositories

5 Works

Synthesis of substituted *N*-phenylmaleimides and use in a Diels-Alder reaction: a green multi-step synthesis for an undergraduate organic chemistry laboratory
Loyd D. Bastin, Manisha Nigam, Sam Martinus, James E. Maloney, Landon L. Benyack & Brendan Gainer
Journal Contribution published 2019 in *figshare Academic Research System*

This paper describes the design and implementation of a minimally hazardous, environmentally friendly, and energy efficient sequential reaction sequence within a sophomore level Organic Chemistry lab course to efficiently synthesize *N*-phenylmaleimide precursors for a Diels-Alder reaction. Substituted *N*-phenylmaleimides are a class of very expensive precursors of considerable interest due to their biological properties and use as intermediates in synthesis. The synthesis described herein produces a substituted *N*-phenylmaleimide in two steps from maleic anhydride and a substituted aniline followed by its Diels-Alder reaction with 2,5-dimethylfuran. The experiment exposes students to the green chemistry principles of atom economy, use of safer chemicals, design for energy efficiency, waste reduction, and inherently safer chemistry for accident prevention and enables students to use ¹H NMR spectroscopy to characterize the products.
DOI registered May 29, 2019 via DataCite.

Text Biological sciences Chemical sciences Health sciences

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Synthesis of substituted *N*-phenylmaleimides and use in a Diels-Alder reaction: a green multi-step synthesis for an undergraduate organic chemistry laboratory
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 DataCite 5

1) This example is based on using keywords present in the title or description of an entry: [https://commons.datacite.org/?query=titles.title:undergraduate+AND+synthesis+AND+laboratory+AND+\(NMR+OR+SPECTRUM\)](https://commons.datacite.org/?query=titles.title:undergraduate+AND+synthesis+AND+laboratory+AND+(NMR+OR+SPECTRUM)) which as we go to press reveals five hits. Three are associated with the course being discussed here and two are from another course. The first three are identified from the metadata as *collections* of items, the collections pointing to “children” as actual *datasets*.

DataCite Commons (relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215 OR relate) Q Pages - Support Sign In

Works People Organizations Repositories

79 Works

1H NMR spectrum of Cumyl ethyl malonate for an undergraduate synthesis laboratory
Henry Rzepa
Results published 2019 in

Ethyl malonyl chloride (234mg, 1.56mmole) was added in one go to a stirred solution of cumyl alcohol (227mg, 1.67mmole) and *N,N*-dimethylaniline (164mg, 1.36mmole) in diethyl ether (2ml). The reaction was exothermic and the mixture went cloudy. After stirring at room temperature over the weekend, the supernatant of the reaction was applied to a column of silica gel and the product eluted with hexane : ethyl acetate (5 : 1) as a sweet-smelling, colourless oil (248mg).
DOI registered October 9, 2019 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/6216>

Ethyl (2-phenylpropan-2-yl) malonate
Henry Rzepa
Results published 2019 in

Ethyl malonyl chloride (234mg, 1.56mmole) was added in one go to a stirred solution of cumyl alcohol (227mg, 1.67mmole) and *N,N*-dimethylaniline (164mg, 1.36mmole) in diethyl ether (2ml). The reaction was exothermic and the mixture went cloudy. After stirring at room temperature over the weekend, the supernatant of the reaction was applied to a column of silica gel and the product eluted with hexane : ethyl acetate (5 : 1) as a sweet-smelling, colourless oil (248mg).
DOI registered December 12, 2019 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/6468>

Publication Year
 2022 13
 2021 19
 2020 45
 2019 2

Work Type
 Dataset 33

License
 CC0-1.0 35

Registration Agency
 DataCite 79

Authors
 Rzepa, Henry 3
 Purcell-Shirley, Oscar 2
 Fu, Haotian 2
 Liu, Murky 2
 Raghavan, Anand 2
 Birchie, Daniel 2

2) These datasets can be found by searching specifically on the three collections identified in the previous search to find the associated children: [https://commons.datacite.org/?query=\(relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/7350+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/8679\)+AND+relatedIdentifiers.relationType:IsPartOf](https://commons.datacite.org/?query=(relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/7350+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/8679)+AND+relatedIdentifiers.relationType:IsPartOf) gives 79 works.

DataCite Commons (media.media_type:chemical/x-mnova* OR media.media_type:cc) Q Pages - Support Sign In

Works People Organizations Repositories

938 Works

hydroxydiphenylborane
Henry Rzepa
Results published 2016 in

Gaussian Calculation
DOI registered July 6, 2016 via DataCite.

1 Citation
Dataset

<https://doi.org/10.14469/hpc/719>

(R)-((1 \rightarrow 4-pyrrolidin-2-yl)methyl)boronic acid hydrochloride
Henry Rzepa
Results published 2016 in

Gaussian Calculation
DOI registered July 7, 2016 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/748>

2,2-diphenyl-1,3,2 λ 4-oxazaborolidine, wB97XD/au-cc-pvdz/SCRF=chloroform
Henry Rzepa
Results published 2016 in

Gaussian Calculation
DOI registered July 7, 2016 via DataCite.

Publication Year
 2022 26
 2021 67
 2020 69
 2019 309
 2018 180
 2017 186
 2016 101

Work Type
 Dataset 69
 Collection 35

License
 CC0-1.0 104

Registration Agency
 DataCite 937
 DataCite 1

Authors
 Rzepa, Henry 186

3) This search adopts a different strategy, which is to search for all datasets with media types associated with NMR data, which in fact returns the globally aggregated set having these metadata properties: [https://commons.datacite.org/?query=\(media.media_type:chemical/x-mnova*+OR+media.media_type:chemical/x-jeol-jdf+OR+media.media_type:chemical/x-jcamp-dx+OR+\(chemical/x-mnpub*+AND+media.media_type:application/zip\)\)](https://commons.datacite.org/?query=(media.media_type:chemical/x-mnova*+OR+media.media_type:chemical/x-jeol-jdf+OR+media.media_type:chemical/x-jcamp-dx+OR+(chemical/x-mnpub*+AND+media.media_type:application/zip)))

DataCite Commons

(((relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215 OR relat...))

Works | People | Organizations | Repositories

68 Works

1H NMR spectrum of Cumyl ethyl malonate for an undergraduate synthesis laboratory

Henry Rzepa
Results published 2019 in

Ethyl malonyl chloride (234mg, 1.56mmole) was added in one go to a stirred solution of cumyl alcohol (227mg, 1.67mmole) and N,N-dimethylaniline (164mg, 1.36mmole) in diethyl ether (2ml). The reaction was exothermic and the mixture went cloudy. After stirring at room temperature over the weekend, the supernatant of the reaction was applied to a column of silica gel and the product eluted with hexane : ethyl acetate (5 : 1) as a sweet-smelling, colourless oil (248mg).

DOI registered October 9, 2019 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/6216>

Ethyl (2-phenylpropan-2-yl) malonate

Henry Rzepa
Results published 2019 in

Ethyl malonyl chloride (234mg, 1.56mmole) was added in one go to a stirred solution of cumyl alcohol (227mg, 1.67mmole) and N,N-dimethylaniline (164mg, 1.36mmole) in diethyl ether (2ml). The reaction was exothermic and the mixture went cloudy. After stirring at room temperature over the weekend, the supernatant of the reaction was applied to a column of silica gel and the product eluted with hexane : ethyl acetate (5 : 1) as a sweet-smelling, colourless oil (248mg).

DOI registered December 12, 2019 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/6468>

5-icosanol 2-methylhept-7-yn-1-yl ester

Publication Year

<input type="checkbox"/> 2022	12
<input type="checkbox"/> 2021	15
<input type="checkbox"/> 2020	39
<input type="checkbox"/> 2019	2

Work Type

<input type="checkbox"/> Dataset	30
----------------------------------	----

License

<input type="checkbox"/> CC0-1.0	30
----------------------------------	----

Registration Agency

<input type="checkbox"/> DataCite	68
-----------------------------------	----

Authors

<input type="checkbox"/> Rzepa, Henry	3
<input type="checkbox"/> Purcell-Shirley, Oscar	2
<input type="checkbox"/> Fu, Haotian	2
<input type="checkbox"/> Raghavan, Anand	2
<input type="checkbox"/> Eapen, Brian	2
<input type="checkbox"/> Davis, Angela	2

DataCite Commons

subjects.subjectScheme:inchikey AND subjects.subject:GTLIMLT

Works | People | Organizations | Repositories

1 Work

4-formyl-2,6-dimethoxyphenyl 2-(4-methoxyphenyl)acetate

Longzheng Cong
Results published 2022 in

Syngalddehyde (0.91 g, 5.0 mmol) was dissolved in acetonitrile (35 mL) with catalyst DMAP (0.06 g, 0.5 mmol) and EDC.HCl (1.25 g, 6.5 mmol). 4-methoxyphenylacetic acid (0.92 g, 5.5 mmol) was then added to the solution and heated to reflux. Upon completion of the reaction, hexane (20 mL) was added to the mixture, and the mixture was then extracted using HCl (20 mL, 1 M), sodium bicarbonate (20 mL, 10 wt%), water (20 mL), saturated sodium chloride (20 mL), and dried with MgSO₄. The solvent was then removed in vacuo and gave the product of white, translucent crystals (0.22 g, 0.67 mmol, 13 % yield).

DOI registered March 1, 2022 via DataCite.

Dataset

<https://doi.org/10.14469/hpc/10176>

Publication Year

<input type="checkbox"/> 2022	1
-------------------------------	---

Work Type

<input type="checkbox"/> Dataset	1
----------------------------------	---

License

<input type="checkbox"/> CC0-1.0	1
----------------------------------	---

Registration Agency

<input type="checkbox"/> DataCite	1
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Authors

<input type="checkbox"/> Cong, Longzheng	1
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<https://orcid.org/0000-0003-2798-5367>

Longzheng Cong

Arvin Cong

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1 Work

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Publication Year

Work Type

License

4) Searches 2 and 3 could be combined into a single search using a Boolean operator (red) to verify that the children previously identified in search 2 actually contain NMR datasets: [https://commons.datacite.org/?query=\(\(relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/7350+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/8679\)\)+AND+relatedIdentifiers.relationType:IsPartOf\)+AND+\(media.media_type:chemical/x-mnova*+OR+media.media_type:chemical/x-jeol-jdf+OR+media.media_type:chemical/x-jcamp-dx+OR+\(chemical/x-mnpub*+AND+media.media_type:application/zip\)\)](https://commons.datacite.org/?query=((relatedIdentifiers.relatedIdentifier:10.14469/hpc/6215+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/7350+OR+relatedIdentifiers.relatedIdentifier:10.14469/hpc/8679))+AND+relatedIdentifiers.relationType:IsPartOf)+AND+(media.media_type:chemical/x-mnova*+OR+media.media_type:chemical/x-jeol-jdf+OR+media.media_type:chemical/x-jcamp-dx+OR+(chemical/x-mnpub*+AND+media.media_type:application/zip)))

5) The next search illustrates hunting for a very specific molecule using its InChI string and of course this search could be combined with other searches if desired using Booleans: <https://commons.datacite.org/?query=subjects.subjectScheme:inchikey+AND+subjects.subject:GTLIMLT+YVRBPEP-UHFF-FAOYSA-N>

6) Clicking on the author's name in Search 5 (Longzheng Cong) leads to a summary page of the author's submissions to the DataCite repository. <https://commons.datacite.org/orcid.org/0000-0003-2798-5367>

The above illustrate a selection of potential searches only. These could be combined as desired with other metadata properties such as author (specified by ORCID), institution (specified by ROR, journal or specific journal article (specified by DOI prefix) and associations with other types of data such as computation, or other types of spectroscopy such as IR spectra or crystal structures etc. The possibilities are vast.

Examples of FAIR spectroscopic data: how to access and re-use them

Following up the result of, say search 5 above, reveals a collection of NMR-related files, in different expressions of the data or different representations of the spectrum. A human can select any of these files for download but is then dependent on specialised software to open the raw data files (in this case the Jeol JDF file or a processed Mnova file). This would normally require possession of a software license allowing access to the program, which might limit access.

To address this specific issue, a further file has been generated by the Imperial repository which provides a free-to-use license to grant access to the data; the MNPUB file. Downloading the MNPUB file(s) specifically grants the user access to the full functionality of the Mnova program to process that dataset. This reinforces one aspect of the A in FAIR; access is not simply about being able to download a dataset but being able to use it in appropriate software to expose the full information the data carries.

FAIR is, however, not just about granting access to people; what about machines? Hidden behind the scenes in the metadata is the following declaration just for them:

```
<relatedIdentifier
relatedIdentifierType="URL"
relationType="HasMetadata">
```

```
https://data.hpc.imperial.ac.uk/resolve/?ore=10176</relatedIdentifier>
```

This specifies how a machine might acquire what might be called a file manifest of further metadata. This manifest contains information on the media types for the files and how to access them, which the machine can exploit.

The future

Clearly the example which Henry has detailed above delivers far more than just a spectroscopic data repository workflow. The students' learnings from such an exercise go way beyond the creation of spectroscopic data. The work shows the importance of the persistent identifiers not only for the data and metadata but also, through the ORCID ID, of their identity as full members of the scientific community.

This work also hammers home the critical and essential importance of carefully created and curated metadata, as much of the functionality illustrated above is achieved with the help of metadata. Importantly, it also depends on community agreement on how that metadata is specified. As noted earlier, an IUPAC working party is expected to produce recommendations on these aspects soon.¹¹ The examples above were produced as proofs-of-concept, but in due course will be harmonised with the emerging recommendations. The next challenge is to encourage all data repositories which contain, for example, NMR spectroscopic data to also adopt these recommendations. When this happens, much richer chemical metadata allowing much more specific searches than the ones above will become enabled.

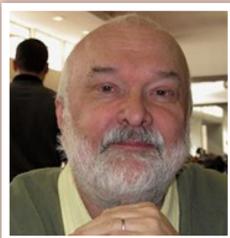
Acknowledgements

We thank Dr Ed Smith for the design and implementation of the synthetic experimental aspects.

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TONY DAVIES COLUMN



Henry Rzepa was trained as an experimental physical organic chemist and then spent three years learning the emerging area of computational chemistry with Michael Dewar in Austin, Texas. Upon joining the staff at Imperial College in 1977, his researches became focussed on computational mechanistic chemistry, NMR and chiroptical spectroscopies and Internet-based Chemical informatics, for which he was awarded the 2012 ACS Skolnik award.

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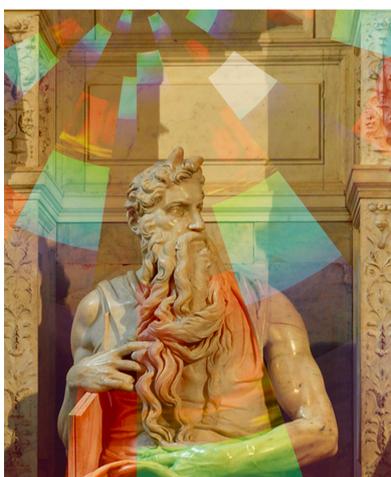


Tony Davies is a long-standing *Spectroscopy Europe* column editor and recognised thought leader on standardisation and regulatory compliance with a foot in both industrial and academic camps. He spent most of his working life in Germany and the Netherlands, most recently as Lead Scientist, Strategic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

<https://orcid.org/0000-0002-3119-4202>
antony.n.davies@gmail.com



Sep 13 - 16 2022
Rome, Italy



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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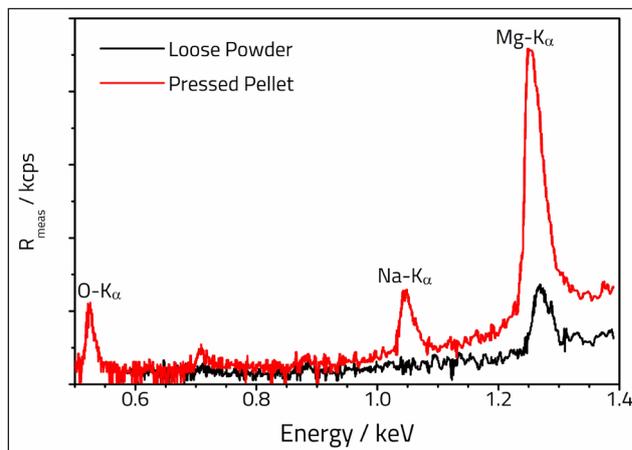


EDXRF analysis of nickel ore as pressed powders in an air environment

Nickel is produced from two very different ores, lateritic and sulfidic. Lateritic ore is found primarily in tropical countries such as Indonesia and mined from various depths beneath the surface, while sulfidic ore is usually found in combination with copper ore and is mined underground. 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. X-ray fluorescence (XRF) spectrometry is a well-established analytical method to determine chemical composition in materials with high accuracy and minimum sample preparation, therefore it is a preferred technique in process and quality control across many industries.

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High throughput, high accuracy sample prep for XRF

Pellet preparation is essential for accurate quantification of sample composition. Compared with XRF measurements on loose powders, the pelletised samples exhibited stronger signal intensities for the lightest elements, which resulted in more accurate quantification of the other elements when using the fundamental parameters method of estimation.

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Thermo Scientific ARL easySpark



The Thermo Scientific ARL easySpark metal analyzer is a benchtop OES instrument with a unique multi-grating/CCD (charge-coupled device)-based optical system. It is designed to meet the challenges and demands of small-to medium-sized plants and laboratories in the metal industry.

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IMAGING

New series of CCD cameras for OEMs

Teledyne Princeton Instruments has released LANSIS, a new spectroscopy detector designed specifically for original equipment manufacturers (OEMs) and system integrators. LANSIS is aimed at instruments using techniques including Raman, optical emission spectroscopy, fluorescence and photoluminescence. The camera can be used for a broad range of clinical and analytical equipment including *in vivo* imaging, life science research, cancer detection, pharmaceuticals, drug discovery, material science, failure analysis for microelectronics etc. Some features specific to LANSIS include permanent vacuum seal technology, a back-illuminated CCD with optional exclusive eXcelon® technology, high average quantum efficiency from UV to NIR and a variety of mounting configurations makes integration of cameras fast and easy, along with a software development toolkit making software integration easy.

The LANSIS family includes a variety of CCD sensor sizes and technologies for spectroscopy and scientific imaging, including back-illuminated, deep-depletion, EMCCD and square-format sensors. Other sensor formats are available to accommodate the requirements of specific system integrators and OEMs.

Teledyne Princeton Instruments

► <https://link.spectroscopyeurope.com/1087-P1-2022>



INFRARED

New IRXross FT-IR spectrophotometer

Shimadzu has introduced the IRXross™ Fourier transform infrared (FT-IR) spectrophotometer. Its P-P values of 55,000 : 1 for one minute of integration enable ultra-high-sensitivity measurements. Users also achieve high-resolution 0.25 cm⁻¹ measurements. In addition, peaks from adjacent gas components are more easily separated using the IRXross compared to its predecessor. High-speed measurement of 20 spectra per second enables faster reaction tracking. It also acquires data with a best-in-class low noise level.

The IRXross FT-IR spectrophotometer includes built-in analytical intelligence, IR Pilot™, for easy start-up and navigation. The standard package includes 23 macro application programs. Even operators unfamiliar with FT-IR spectrophotometry can analyse samples easily by simply selecting the purpose of analysis and attachment they are using. Operators can analyse multiple samples with a single click and do not need to set parameters. Using IR Pilot, users can program the IRXross to specifically support identification testing by making pass/fail judgements for test samples based on verification



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methods specified in pharmacopoeia and official methods. They can also program the system to support contaminant analysis using Shimadzu's proprietary algorithm in combination with a spectral library containing over 550 spectra for substances commonly detected as contaminants.

A wide variety of libraries, including Shimadzu's unique libraries of reagents, polymers and more, is included as standard. Shimadzu also offers LabSolutions™ Software DB IR and LabSolutions CS IR to meet the requirements of Electronic Record and Electronic Signature regulations. In addition, the software includes built-in validation test macros for compliance with requirements from various pharmacopoeia, including USP.

Shimadzu

► <https://link.spectroscopyeurope.com/6348-P1-2022>

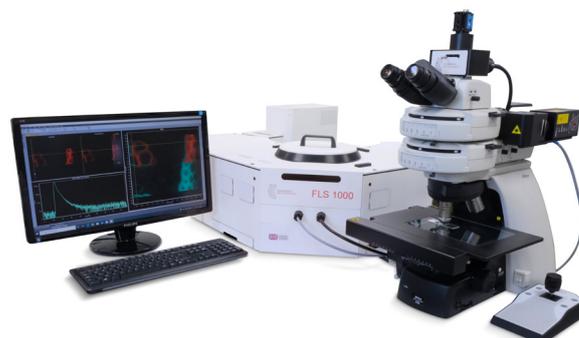
LUMINESCENCE

MicroPL upgrade for photoluminescence spectrometers

Edinburgh Instruments has introduced a new upgrade for its photoluminescence spectrometers. The MicroPL upgrade enables the study of spectral or time-resolved photoluminescence of samples in the microscopic scale by converting an Edinburgh Instruments photoluminescence (PL) spectrometer into a combined spectrometer and microscope system. A wide range of microscope configurations, source coupling and detector options are available enabling both steady state and fluorescence lifetime microscopy, as well as automated maps. It is easy to swap between MicroPL and FLS1000 photoluminescence spectrometer or FS5 spectrofluorometer standard sample holders.

Edinburgh Instruments

► <https://link.spectroscopyeurope.com/670-PFW-1-2022>



MASS SPECTROMETRY

Benchtop tandem quadrupole mass spectrometer

Waters has introduced the new Xevo™ TQ Absolute system, a sensitive and compact benchtop tandem mass spectrometer. It is up to 15× more sensitive for quantifying negatively ionising compounds than its predecessor and is smaller and uses less electricity and gas supply than other high-performance tandem quadrupole mass spectrometers. The Xevo TQ Absolute is designed to help pharmaceutical, food and beverage, and environmental analytical laboratories meet regulations requiring trace-level quantitative mass spectrometry analyses for a broad set of applications. New design features include



guidance on optimal probe positioning for both sensitivity and robustness, and a source shield that helps minimise source contamination by the sample matrix or mobile phase salts.

Waters

▶ <https://link.spectroscopyeurope.com/103-P2-2022>

Intact Mass app for BioAccord

Waters has introduced new software to help biomolecule drug discovery and development. The new Waters™ Intact Mass app allows scientists using the BioAccord™ LC-MS System to confirm the mass of biomolecules and impurities made by synthetic or recombinant processes nearly twice as fast as other commercially available options.

Intact mass analysis is routinely performed during all stages of the development of biological drugs including proteins, peptides, oligonucleotide therapies and conjugates. In early stages of drug discovery, biochemists must analyse hundreds or even thousands of different samples per week. To help speed this process, the Waters Intact Mass app facilitates mass confirmation and purity determination of novel biotherapeutics. The application features intelligent automated deconvolution to process sample results within minutes of their capture, with minimal user input.

Waters

▶ <https://link.spectroscopyeurope.com/103-P1-2022>



Quadrupole system for vacuum process analysis

The new Hiden HPR-30 Series are bolt on vacuum process analysers designed for fast response, high sensitivity analysis of gas and vapour species. Equipped with Hiden's multi-level software package, offering simple control of mass spectrometer parameters and complex manipulation of data and control of external devices. Applications include leak detection, contamination monitoring, process trend analysis and analysis of high mass species and precursors used in ALD and MOCVD. Optional upgrades include the Hiden 3F series triple filter quadrupole system providing enhanced abundance sensitivity, part-per-billion (ppb) detection levels and high contamination resistance, particularly suited to the analysis of aggressive gases in CVD and RIE applications. Standard mass range is 200amu, versions up to 1000amu are offered.

Multiple sampling configurations are available to suit a full range of process pressure and vacuum system geometry requirements. Versions are offered with single or multiple sampling inlets, either unheated or heated to allow sampling of volatile species. Systems can be cart mounted, with height adjustment for maximum compatibility between tools. For pulsed deposition processes,



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time resolved measurements are offered to 50 ns time resolution. The HPR-30 Series are designed to offer a fully featured, flexible and powerful solution for the monitoring of parameters in all aspects of process gas analysis such as leak detection, vacuum quality and precursor monitoring.

Hidden Analytical

► <https://link.spectroscopyeurope.com/672-P1-2022>

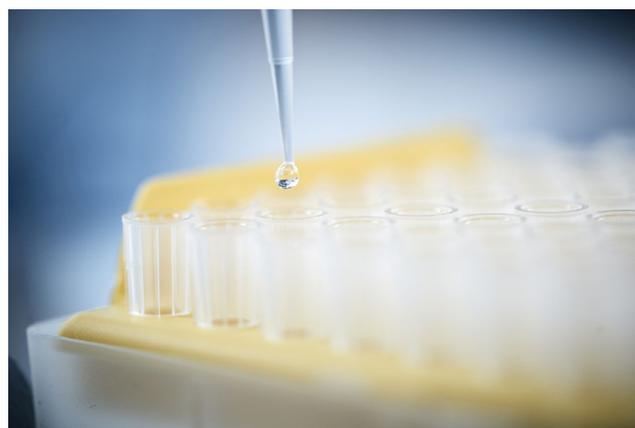
LC-MS sample prep

Evosep has introduced a new and vastly improved generation of Evtips, called Evtip Pure™. The design of Evtip Pure is based on five years of customer feedback added to a thorough review of every single aspect of the Evtip. Evtip Pure improves peptide recovery and increases protein identifications for all sample loads, but especially for low sample loads. This enables deeper proteome coverage, with lower CVs, making them suitable for analysing low sample amounts, e.g. single cell analysis powered by the Evosep Whisper™ Flow Technology.

Evtip Pure not only provides much better chromatographic performance, but also ensures improved results and consistency over time. The improved peak definition and peak width will significantly increase peak capacity and ultimately lead to better performance. The new Evtips will give you more efficient sample binding, significantly improved sensitivity at low loads and visibly sharper and more symmetric peaks at all loads. Retention times are identical ± 1 s using the 60 SPD method.

Evosep

► <https://link.spectroscopyeurope.com/6836-P1-2022>



MAGNETIC RESONANCE

ECZ Luminous NMR spectrometer series

JEOL USA has announced the next generation of their NMR spectrometers: the ECZ Luminous series. This product benefits from spectrometer miniaturisation and improved performance through state-of-the-art digital and high-frequency technologies. The new ECZL series features MFDS (Multi Frequency Drive System) that allows spectroscopists to perform multiple pulse trains on different nuclei on a single RF channel in the same experiment. The STS (Smart Transceiver System), inherited from the previous model, achieves a time resolution of 5 ns for frequency, phase and amplitude modulation, enabling ultra-fast control. The ECZL G series (400 MHz to 1.3 GHz) is the flagship model and supports expansion to more than three channels, with various options for high power amplifiers and high magnetic field gradients. The ECZL R series (400–600 MHz) is a



fixed-configuration high-performance instrument capable of solid-state NMR measurements with less than half the footprint and only one-third the volume of previous models. The ECZL S series (400MHz) has the same architecture and performance as the G and R models, with a configuration that is streamlined for routine solution NMR measurements.

JEOL

▶ <https://link.spectroscopyeurope.com/4220-P1-2022>

RAMAN

Process Raman analyser

Thermo Fisher Scientific has released a new Raman spectroscopic analyser for process monitoring for a variety of applications, including biopharmaceutical manufacturing. The Thermo Scientific Ramina Process Analyzer offers non-destructive and continuous analysis without the need for sample preparation, with rapid system setup and deployment in as little as 15 minutes. The compact system utilises a range of patented probes to maximise the speed and sensitivity of results, enabling fully automated *in situ* measurements to calculate concentrations in a reaction vessel.

The Ramina Process Analyzer offers a rapid and easy-to-use alternative to offline manual or automated wet chemistry testing, and is simpler to install and use compared to traditional Raman process monitoring systems. The Ramina comes with everything the user needs to start collecting data, including a Raman spectrometer and fibre optic probe, as well as a portable monitor, mouse, keyboard and laser safety goggles. It is factory calibrated and its solid-state construction offers long-term stability. Users can also use multiple systems in parallel to test different reaction vessels simultaneously, or combine a number of probes in one vessel.

Thermo Fisher Scientific

▶ <https://link.spectroscopyeurope.com/106-P2-2022>



Conferences

2022

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

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

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

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

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

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

30 May–3 June, Gijón, Spain. **Colloquium Spectroscopicum Internationale (CSI) XLII.** [csi2021@csi2021spain.com](http://csi2021spain.com), <https://www.csi2021spain.com>

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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/>

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>

Courses 2022

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

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

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

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

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

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>

10TH WORLD CONFERENCE ON SAMPLING AND BLENDING



Correct sampling and analysis of raw materials are essential to ensure well-documented product quality and to contribute to a reduced environmental footprint. To this end, the WCSB10 conference covers the latest research and application experience of the Theory of Sampling and Blending.

31 May–2 June 2022, Kristiansand, Norway

<https://wcsb10.com>

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