# Chemistry Update

Newsletter 345, 24 June 2022

## Inside this Issue



## Calendar of Events

**Active Listening Workshop**
Speaker: Dr Wendy Marie Ingram, Dragonfly Mental Health
Date: Thursday 30 June
Time: 2pm—4pm
Location: Virtual
Register for the event

**Managing Upwards Workshop**
Speaker: Jelena Brasanac, Dragonfly Mental Health
Date: Thursday 7 July
Time: 2pm—4pm
Location: Virtual
Register for the event

**Open Days**
Date: Friday 1 July & Sunday 3 July
Time: 9am—4pm

**Organic Seminar**
Speaker: Dr Stellios Arseniyadis, Queen Mary University of London
Date: Friday 8 July
Time: 1pm—2pm
Location: C/A/101

**Roger Mawby Demonstrator Awards**
Date: Tuesday 5 July
Time: 4pm—5.30pm
Location: C/B/102

**Graduation reception**
Date: Thursday 21 July
Time: 2.30pm—5pm

**Research Seminar: "Rotaxanes and Catenanes as Useful 3D Molecular Scaffolds"**
Speaker: Dr Nick Evans, Lancaster University
Date: Thursday 7 July
Time: 12pm—1pm
Location: C/A/101

Date of Next Issue:
29 July 2022

# York Chemist wins Royal Society of Chemistry Tilden Prize

**Professor David Smith has received the prestigious 2022 Tilden Prize from The Royal Society of Chemistry.**

The Tilden Prizes are awarded annually by the Royal Society of Chemistry to recognise excellence in chemical research, impact and innovation. Recipients of the prizes are established career academics with up to 30 years post-PhD research experience. These research prizes are amongst the most prestigious offered by the Royal Society of Chemistry.

Professor David Smith has been recognised for 'pioneering an understanding of molecular materials based on supramolecular gels'.

Gels are fascinating materials which surround us in everyday life - from hair gel to 'Jelly Babies'. However, while the gels used in everyday life are typically made of polymers, Professor Smith is instead interested in 'supramolecular gels' which reversibly assemble from small molecule building blocks via intermolecular interactions. Such gels are highly tunable and can be programmed by molecular engineering to carry out unique functions.

Over recent years, Professor Smith has developed a new family of hydrogels based on very simple low-cost building blocks, and demonstrated their potential in applications ranging from environmental remediation and catalysis to drug delivery and tissue engineering. His work therefore illustrates that supramolecular chemistry can approach high-tech applications within realistic commercial constraints.

For example, one of Smith's gels has been designed to extract and accumulate precious metals from waste water. The resulting metal-loaded gels can then go on to have applications in their own right, including antibacterial activity (silver), nano-electronics (gold) or catalysis (palladium).

Inspired by his own husband's health problems with cystic fibrosis and organ transplantation, Professor Smith has also created hydrogels capable of supporting cell growth. His research team have created innovative ways of shaping and patterning such gels in order to direct and control cell growth using technologies such as photo-patterning, diffusion and 3D-printing. Such gels have potential future use in growing organs from a patient's own stem cells, which could give rise to organs 'on-demand' and avoid problems with transplant rejection.

Smith and his team have also developed injectable supramolecular microgels which support stem cell growth and have potential applications for tissue repair.

Drug delivery gels explored by the team include a system for nasal delivery that can achieve enhanced uptake into the brain to potentially treat conditions such as Parkinson's Disease.

Smith plays a leading role in Molecular Materials research in the Department of Chemistry – MolMatYork.

This grouping of >30 researchers studies self-assembled, self-organised and nanoscale materials, often based on renewable resources, and applies them in next-generation technologies.

Reflecting on the award, Organic Chemistry Academic Group Leader Professor Ian Fairlamb said: “Dave’s research has been outstanding over many years. He has pioneered new approaches and applications of supramolecular soft matter systems. He leads an inclusive research team, and provides excellent training to his group members, who have gone on to valuable careers in a range of different fields, both in academia and industry.”

Professor Smith added: “I have been privileged to work with some truly remarkable scientists from across the world. This award is a reflection on their talents and the way in which each of them has enriched both the ideas and the culture of my research team.”

Professor Smith is the latest member of the Department of Chemistry to win a Tilden Prize – previous winners include Professors Duncan Bruce, Lucy Carpenter, Simon Duckett, Robin Perutz and Richard Taylor.

## June is Gypsy, Roma, and Traveller History Month!

This year’s theme of ‘*What Makes a Home*?’ invites everyone to consider how acceptance, community, and cultural connections make a place feel like home. This is a great time to celebrate a spectrum of vibrant and diverse cultures, as well as notable individuals from local communities. We would particularly like to congratulate Violet Cannon, CEO of the York Travellers Trust, whose significant contributions to the local community are being recognised as one of the University’s honorary graduates this year.

GRT History Month also represents an opportunity to learn about the challenges faced by communities across the UK, including barriers to education and health inequalities linked to living conditions.

In a project led by Dr Katherine Manfred, researchers in the Wolfson Atmospheric Chemistry Laboratories are engaging with local community partners on a new RSC-funded outreach project to increase awareness of risks associated with poor air quality. They will be hosting interactive workshops and providing PM2.5 sensors to empower Gypsy, Roma, Traveller, and Showmen communities across Yorkshire to monitor exposure to particulate pollution in areas where they live. For more information about the project, please contact Katherine Manfred (katherine.manfred@york.ac.uk).

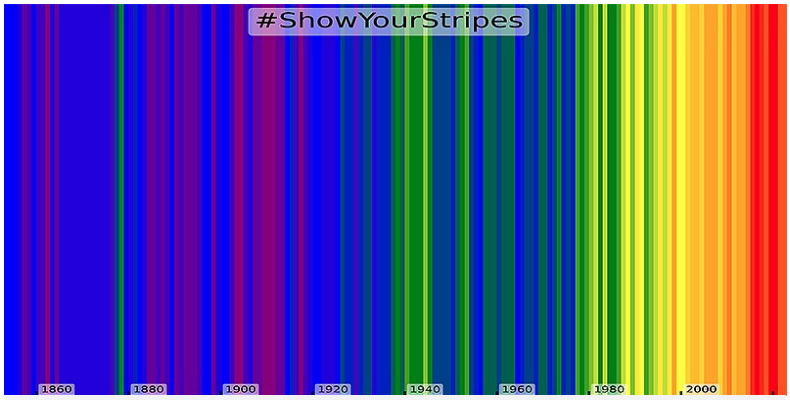
## Chemistry moved up to 7$^{th}$ place in Complete University Guide

*Message from Prof. Caroline Dessent*: The Complete University Guide 2023 has just been published. I'm pleased to let you know that we've moved up one place this year to be ranked at 7$^{th}$ place. The CUG ranking includes both teaching quality and research excellence, so our upward trajectory reflects excellent performance across both our key activities.

View the Chemistry table.

# Show Your Stripes at Pride 2022

**An academic in the Department of Chemistry at the University of York has produced a unique version of the Pride rainbow flag for York Pride celebrations this year and it carries an important additional message.**



Flag in Pride rainbow colours

The rainbow flag for Pride has appeared in many different versions over the years, with variation in colour or pattern carrying different meanings or representing particular identities within the LGBTQ+ community. For Pride 2022, Professor Kevin Cowtan has produced a unique version of the rainbow flag which links in with their own research and illustrates the effects of global warming. It is available in a variety of Pride colours.

The stripes on the flag are the Global Warming Stripes #ShowYourStripes created by Professor Ed Hawkins at the University of Reading, and these vividly show how global average temperatures have risen over the last 170 years, including a dramatic rise over recent decades.

“The historic temperature record is one of the most important measures of how humans are influencing the climate,” said Professor Cowtan. The GloSAT project is extending the record of climate change data back even further, into the pre-industrial period. "Accurate data are essential in assessing the effectiveness of global efforts to limit increases in the Earth’s surface temperature.”

Professor Cowtan’s interest in climate science developed from an interest in science communication. As a Principal Investigator on the GloSAT project, they work with a diverse team of international researchers, including some of the world's top climate scientists.

“Diversity and good science are clearly linked... asking questions which no-one has asked before is central to the practice of science. Diverse teams with people from different backgrounds lead to different perspectives and so better science” said Professor Cowtan.

Postcards of the Pride Global Warming Stripes will be available from the Chemistry at York team at this year’s York Pride Celebration on the Knavesmire, Saturday 18 June 2022.

# New starters


**Conor MacDonald**, Technician
Room: L0 YSBL labs; Email: conor.macdonald@york.ac.uk; Tel: 8255

**Ruth Winkless**, Research Trainee in Experimental Atmospheric Science
Room: C/G116; Email: rw1462@york.ac.uk; Tel: 1214

# Next Generation ‘SHARPER’ Benchtop NMR Spectroscopy

**An innovative method for enhancing benchtop NMR spectroscopic signals has been reported, opening new possibilities for this simple low-cost technology to be used in settings outside the traditional research lab.**

Benchtop NMR spectrometer

NMR spectroscopy is a hugely powerful analytical technique which allows the structural characterisation of a wide range of molecules and can be used to analyse chemical reactions. However, this method typically requires high-cost instrumentation, with high field magnets, which require cooling with expensive cryogenic fluids. In recent years, low cost, portable benchtop NMR spectrometers have been developed, but these can suffer from relatively low sensitivity and poor signals.

Dr Meghan Halse and PhD student Matheus Rossetto, working with researchers from the University of Edinburgh, have developed and implemented a new experiment which significantly improves the signal internsity on benchtop spectrometers.

This method, the so-called 'SHARPER' experiment, increases the signal-to-noise ratio by a factor of 10 to 30-fold. It achieves this by using a carefully designed magnetic pulse sequence to collapse the target resonance into an extremely narrow singlet. Importantly, the signal is still amenable to quantitative interpretation and therefore this method can still be used in analytical applications like reaction monitoring.

This approach is particularly advantageous when using NMR to anaylse fluroine (19F), which can suffer from poor signal-to-noise ratio Fluorinated organic molecules account for 20% of pharmaceuticals and 60% of agrochemicals produced today. As such, monitoring fluorination reactions and detecting fluorinated compounds are of key importance.

Demonstrating the potential for this methodology to be applied outside the traditional laboratory setting, this method was implemented and optimised during Covid lockdown by remotely connecting to the benchtop NMR spectrometer in the Centre for Hyperpolarisation in Magnetic Resonance (CHyM) in York while working from home. Furthermore the team in York worked remotely with Professor Dušan Uhrín’s team in Edinburgh, using Zoom collaboration to translate the developments in York to a second remotely operated benchtop NMR spectrometer in Edinburgh.

Talking about the research, Dr Halse said: “Benchtop NMR offers the potential to use NMR in wholly new environments as a result of its low cost and portable nature. This ‘SHARPER’ approach significantly improves the spectra that can be obtained and may therefore enable a range of new applications.”

This research has been published in *Chemical Communications*

# Probing and imaging reactions with Nitrogen-SABRE

**Recent research has demonstrated how hyperpolarised NMR methods can be developed to follow reaction processes with much enhanced sensitivity, opening the possibility of creating hyperpolarized pharmaceuticals and following their distribution and reactivity in the human body by MRI.**

Probing chemical processes within the human body is a challenging problem. Positron emission tomography (PET) is a very sensitive technique that uses gamma cameras and long-lived radionuclides, to image changes in metabolic processes, blood flow and agent absorption in the body. Unfortunately, this process can be complex and costly.

Magnetic resonance imaging (MRI) is another, much cheaper, easy-to-implement, powerful diagnostic method, but its inherent low sensitivity means most routine clinical measurements just probe highly abundant water. The ability to detect specific molecules, and interrogate their chemical reactions using MRI would be a game-changing technology.

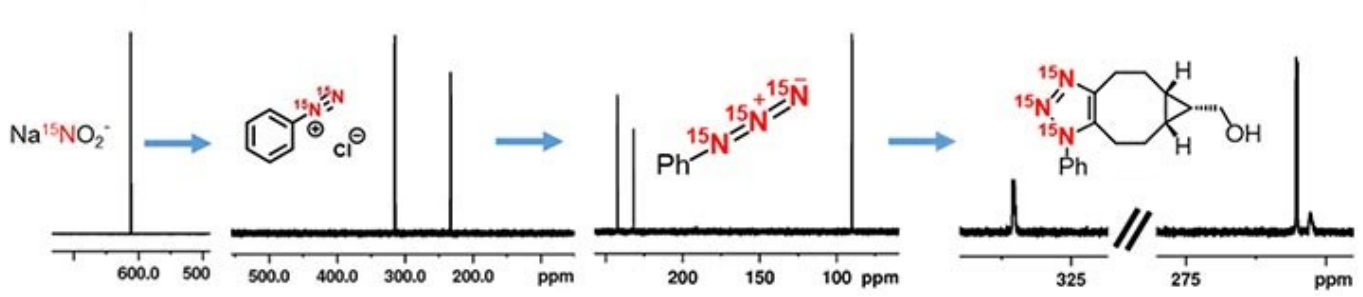



Figure 1. Using $^{15}$N-SABRE to probe a reaction pathway. Signals associated with each key species were detected in the spectrum.

In this new work, Professor Simon Duckett and his research team in the Centre for Hyperpolarisation in Magnetic Resonance describe how the innovative magnetic resonance method, SABRE, developed in their laboratories can be used to improve the detectability of a range of very important 15N-containing species through hyperpolarisation.

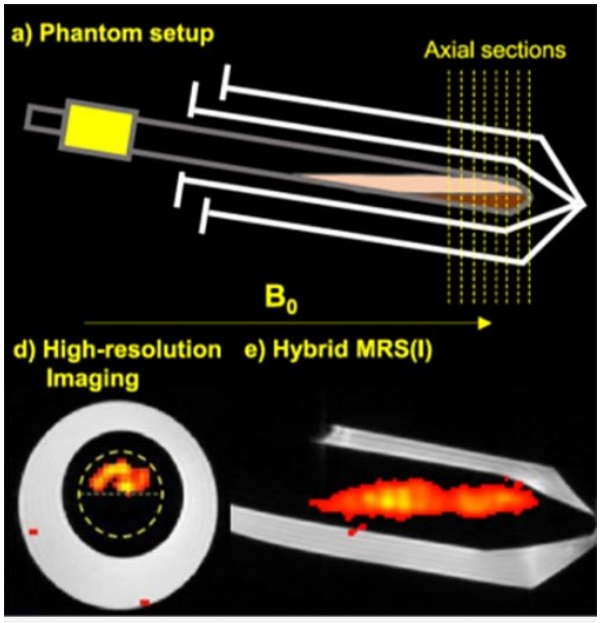



Figure 2. Using High resolution imaging achieved using $^{15}$N-SABRE

This method has been applied to $NO_2^-$ (28% polarization), $ND_3$ (3%), $PhCH_2NH_2$ (5%), $NaN_3$ (3%) and $NO_3^-$ (0.1%). These species are themselves reactive, and can therefore be used to react with other organic molecules and thus incorporate hyperpolarisation. This opens the possibility of developing 'hyperpharmaceuticals' which can be detected within an MRI machine.

The relatively long signal lifetimes allowed the researchers to successfully probe reactivity by NMR over several minutes. For example, in the case of $NO_2^-$ the diazotization of $PhNH_2$ and a subsequent reaction process was monitored. Each step could be followed using the NMR method (see reaction scheme). This indicates that $^{15}$N-SABRE may potentially be used to understand how $^{15}$N-labelled hyperpharmaceuticals

react and interact within a patient.

Professor Duckett and his team then went on to demonstrate that they could detect the signals of these $^{15}N$ species, in a test tube, in a magnetic resonance imaging experiment – the first step in translating the method towards MRI. As can be seen from Figure 2, it was possible to achieve high resolution imaging.

Professor Duckett said: "Taken together, the results of this work indicate that it is possible to use SABRE to achieve high intensity, long-lived magnetic resonance signals which can be used to follow $^{15}N$-labelled reaction process. In the future, we would hope to develop the approach further to follow the distribution and metabolism of hyperpharmaceuticals within a living organism, potentially allowing MRI to achieve transformative steps forward in terms of diagnostic imaging."

This research has been published in *Journal of the American Chemical Society*

## GCCE wins Faraday funding to manufacture advanced electrodes with green solvents

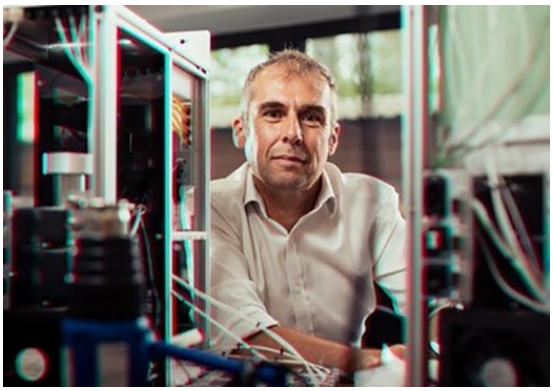

Dr Rob McElroy and Professor James Clark of the Green Chemistry Centre of Excellence (GCCE) have won funding to continue their work on the application of green solvents in battery recycling and manufacturing. This Faraday Institution funded seed project, in collaboration with Professor Emma Kendrick and Dr Dominica Gastol at the University of Birmingham, is a continuation of the UKRI funded R2LiB battery recycling project. In Manufacturing of Advanced Electrodes with Green Solvents (MAEGS), York will be assessing sustainable solvents in binder dissolution and electrode manufacture while Birmingham will be applying such learnings in the production of electrodes which in turn will be used to produce lithium ion batteries. The most successful system(s) will be used in production of pouch cells and their impact on closed loop recycling assessed. This has the potential to reduce the environmental footprint of battery manufacture, improve battery performance over their lifetime and simplify end-of-life recycling.

## The Royal Society's UK Young Academy: an opportunity for Early Career Scientists

*Message from Prof. Caroline Dessent*: The UK Young Academy was launched this month by the Royal Society. This is a major initiative to give Early Career Scientists a better voice and better recognition. It sounds like an excellent opportunity to expand your networks and ensure that early career researchers are heard, so I'd encourage you to apply if you are eligible.

# Lord Lewis Prize recognises academic contributions to air quality and climate policies

**Professor Alastair Lewis has received the prestigious 2022 Lord Lewis Prize from The Royal Society of Chemistry.**



The Lord Lewis Prize is awarded every two years by the Royal Society of Chemistry to recognise distinctive and distinguished chemical or scientific achievements, together with significant contributions to the development of science policy. As such, recipients of the Prize not only perform excellent research, but achieve significant impact in terms of their influence on policy, either at national or international levels.

Professor Alastair Lewis has received the 2022 Lord Lewis Prize for the promotion and application of the chemical sciences to support development of evidence-based policy and regulation in the fields of air pollution and climate change.

Ally Lewis is Professor of Atmospheric Chemistry at the University of York and works in the Wolfson Atmospheric Chemistry Laboratories (WACL). In addition to teaching and research at the University, he is a Science Director at the National Centre for Atmospheric Science (NCAS). Professor Lewis is Chair of the Defra Air Quality Expert Group (AQEG) and the Department for Transport Science Advisory Council where he has a direct input into government decision-making on issues including energy, emissions, air quality and net zero. His personal research focusses on gas phase atmospheric chemistry and chemical metrology, with a particular focus on measurements of air pollutants.

Air pollution is one of the most significant causes of preventable death world-wide and impacts people's health irrespective of whether they live in high, middle- or low-income countries. Developing technologies and policies that improve air quality and deliver on climate objectives is complex since they must be tailored to the geography, transport and energy systems, climate and wider economy of any given location.

Professor Lewis's own area of research includes the development of new technologies to measure pollution, field observations of pollution behaviour and transformation, through to the synthesis of evidence that can support government in managing and reducing national emissions. Indeed, his research is driven by developing science and evidence that supports successful actions and policies, with his team focussed on looking for evidence of interventions that can improve air quality and reduce greenhouse gases simultaneously.

The award recognises that Ally has played a central role in providing scientific advice to Government and Parliament, including the development of the UK clean air strategy, and new post-Brexit air quality standards set out in the Environment Act (2021). Early in the pandemic in 2020 he worked with Defra, the ONS and the Air Quality Expert Group completing a rapid review of the impacts of air quality on mortality rates from COVID-19, identifying inequalities in exposure to pollutants such as $NO_2$ and $PM_{2.5}$.

Reflecting on his Lord Lewis award, Ally said: "It is an amazing privilege to given this award, and especially so given the incredible scientists that have received it previously. I'm in a very lucky position

working in WACL - I get the opportunity to explain the fantastic research work done here to decision-makers and then see it translated into practical action."

The Lord Lewis Prize was established in 2008 thanks to a generous donation from Johnson Matthey, and marks the significant contributions of Professor Lord Lewis to both chemistry and the advancement of science policy. There have only been eight winners of the award in total, and Chemistry at York has now been recognised with two of them. The previous Lord Lewis Prize winner from York was Professor Sir John Holman, who received the award for his extensive influence over chemistry education policy.

## SAQN Annual Meeting 2022

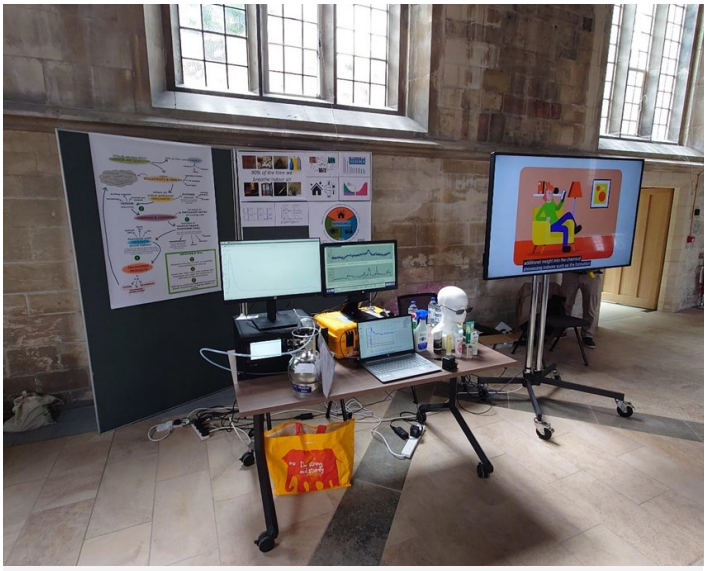
**18 May – 19 May 2022, York**

The SAQN Annual Meeting brings together Science and Technology Facilities Council (STFC) staff, air quality researchers, industry professionals and policy, offering excellent networking opportunities and the chance to learn more about the current and future applications of STFC capabilities to air quality issues. The 2022 meeting took place at the historic Guildhall in the centre of York and was attended by over 80 delegates in person and online.

We were delighted to welcome so many network members to York for our Annual Meeting, our first in person event since the network launch in 2020. With over 60 in person delegates and 20 online delegates, there were plenty of opportunities to talk with contacts old and new. In person delegates enjoyed ‘Netwalking’ around York and the inaugural SAQN Quiz, and everyone discovered more about our funded projects in the ‘Marketplace’, and discussed different ways that STFC capabilities could enhance air quality research.

Content from the meeting is available on the SAQN website.

# Indoor air science and analytical chemistry at the York Festival of Ideas



Readying the science exhibit, with sensor box, greenhouse gas analyser, "Barbara" the disembodied head and some IMPeCCABLE info videos on cooking and cleaning indoors.

Amber and Annie prepping the table of kids' activities – with generous helpings of stickers and pens - inside the beautiful Guildhall.

As part of the York Festival of Ideas, members of Terry Dillon's and Kirsty Penkman's group and Annie Hodgson participated in the Discovery Zone event on Sunday 12 June in the beautiful Guildhall. The event aimed to showcase research being carried out in York with lots of hands-on activities to suit the whole family. The Chemistry stalls were joined by other amazing researchers, including wonderful and interesting exhibits from Psychology and Physics.

**WACL - Indoor air science**

Researchers from WACL brought air monitoring instrumentation and pollution-themed kids activities to the Guildhall for an afternoon of educational fun. Visitors explored emissions from household and personal-care products and a range of food and drinks, whilst $CO_2$, $CH_4$, $H_2O$ and VOC were all monitored in real-time. Younger visitors enjoyed a bit of separation science via paper chromatography and made their own "pollution catchers". Terry Dillon and Annie Hodgson conceived the exhibit, which will be used in forthcoming visits of primary schools to YSOC.

Terry would like to say a big thank you to Amber Yeoman, Cate Mapelli, Yasmin Mueller, Annie Hodgson, Seba Diez and Ashish Kumar who explained the science and entertained the York public on the day, and to Katie Read and Killian Murphy without whom the instruments would never have been ready.

**Analytical chemistry - The chemistry of a bog body**

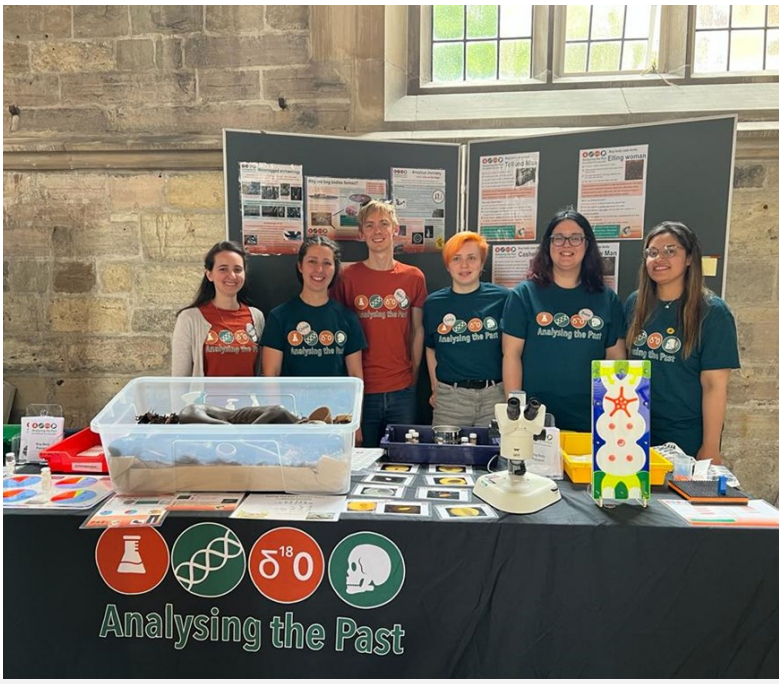
The key role of analytical chemistry was showcased in its application to bog bodies: given their great preservation, we can find out more about their origin, clothing material, last meal, etc.

The "Analysing the past: the chemistry of a bog body" activities included matching elemental composition of textiles with pie charts, running a D and L amino acid randomiser to work out the age of the bog body, looking at 3D-printed pollen grains for working out the season of death and environmental conditions, and using a microscope to identify seeds mimicking the bog body's last meal

to tell us more about geographical location and social status. The visitors enjoyed finding out how chemists and archaeologists work together and we hope they will be inspired to learn more about science and chemistry.

Our centrepiece bog body modelled on Tollund Man and created by artist Dee Dickinson

The stall was set up by Martina Conti and she would like to say a massive thank you to Marc Dickinson, Chloë Baldreki, Sam Presslee, Lucy Wheeler and Fazeelah Munir who helped run a successful event with great enthusiasm. The activities were developed thanks to the Royal Society of Chemistry Outreach Grants won by Kirsty High in 2017 and Martina Conti in 2018, which allowed great puzzles and games to be designed and created by the chemistry workshops team with support from the 3D pollen project for the pollen templates.




Left: Marc, Chloe and Martina explaining our activities to people of all ages.
Right: Team bog body posing with the stall: (left to right) Martina, Chloë, Marc, Lucy, Sam and Fazeelah.

## Online Department suggestion box

The online Equality and Diversity suggestion box has been extended to be a suggestion box for the whole Department. You can submit your thoughts/suggestions/ideas for general Departmental matters as well as matters relating to Equality and Diversity. You can find the Google form at this link.

# GCCE jointly organises workshop for Going Global Partnership project awarded by British Council

The Green Chemistry Centre of Excellence (GCCE), University of York jointly organised a three-day workshop with the University of Delhi and University of Ladakh on “Green Chemistry Education Today for a Sustainable Tomorrow”. The workshop was held from 27–29 May 2022 at Hotel Maidens, New Delhi under the prestigious Going Global Partnership project awarded by the British Council. The inaugural of the workshop witnessed the presence o f Hon’ble Minister Shri Arjun Ram Meghwal, Minister of Parliamentary Affairs and Culture. He spoke of the need to adopt, practice and implement real green chemistry in day-to-day life.


Professor Anju Srivastava, Hindu College Principal, said “Our efforts were directed towards designing a course on green chemistry education through which talented and potential students can undergo an exchange programme between India and the UK. It was a highly interactive brainstorming session between practitioners and students, wherein students had a working group discussion with the advisors. After engaging discussions between the mentors and students, the various working groups came up with effective suggestions for the course design. With the introduction of the National Education Policy (NEP) 2020, which focuses on internationalisation, this three-day workshop provided a platform for the students to enhance their creativity, critical thinking, and logical decision-making. We saw some thought-provoking research-based interactions by the young members of the Green Chemistry Network Centre. The young students of Hindu College also provided valuable feedback at the workshop”.

Professor Avtar Matharu, Deputy Director of the GCCE, gave a talk covering the internationalisation of higher education, equipping teachers with the latest technology and education methodology, prospects of strengthening our existing education system, and the need to support research, knowledge and innovation to address the local and global challenges of green chemistry.

Other renowned academic experts attending the workshop included Professors R. K. Sharma, GCNC Coordinator, S.K. Mehta, Vice-Chancellor of the University of Ladakh, Balaram Pani, Dean of Colleges of the University of Delhi, and Reena Jain, Vice-Principal of Hindu College. Industrial delegates, Dr Rakeshwar Bandichhor, Vice-President of Dr. Reddy’s Laboratory Ltd., and Dr Manas Sarkar, Dr Mallika Mishra and Mr Sandeep Kumar Jain from Reckitt Benckiser, also interacted with the students. Furthermore, an inspiring lecture by Dr David Constable, Director of ACS GCI, motivated students to think beyond green chemistry and understand the concept of how systems thinking is an integral component. Overall, the conference was deemed a great success.

# CIEC win Chemical Industries Association Reputation Award

Earlier this month, the Centre for Industry Education Collaboration (CIEC) was delighted to receive, along with Johnson Matthey, the Chemical Industries Association (CIA) Reputation Award. The award was given in recognition of their work done through Children Challenging Industry.


A delighted Joy Parvin, pictured here with John Jex, received the award on behalf of CIEC.

CIEC works with industry partners such as Johnson Matthey to help primary aged children to recognise the links between the science that they do in school and the science that happens in industry. Over 4,600 children have visited the Johnson Matthey site as a result of this collaboration. This has led to over 60% of those involved in the project envisaging a career in industry and over 50% stating that they would like to be a scientist or engineer.

If anyone working in the department would like to find out more about CIEC and the work that we do please get in touch at ciec@york.ac.uk.

# Mind your head!

## ACTIVE LISTENING WORKSHOP

with Wendy Marie Ingram, PhD
Co-Founder and CEO of Dragonfly Mental Health

**Thursday, June 30th**
**14:00-16:00 BST**

This Active Listening Workshop provides immediately usable knowledge and skills to improve leader preparedness to recognize, speak with, and refer trainees and team members that may be struggling with mental health issues. In addition, the knowledge and skills gained in this workshop will improve leadership awareness around their own mental health and their preparedness to address it appropriately.

## MANAGING UPWARDS WORKSHOP

with Jelena Brasanac, M.Sc.
Co-Founder and COO of Dragonfly Mental Health

**Thursday, July 7th**
**14:00-16:00 BST**

This Managing Upwards workshop will introduce you to tried and true strategies and techniques that will improve your ability to set expectations, establish and renegotiate healthy boundaries, and anticipate and address issues that arise. Small group practice sessions help you integrate these skills and make them immediately usable in the real world.

As a result of employing these tools your team members, research group, and ultimately your science will benefit. To get the most out of this workshop please fill out the appropriate survey below by following the QR codes provided.

Supervisors PGRs PDRAs

Dragonfly Mental Health

University of York Chemistry