Chemistry Update

Newsletter 349, 28 October 2022

Inside this Issue

Calendar of Events

UCAS Visit Days
Dates: 1, 3, 10, 14, 17, 21, 24 & 29 Nov
Time: 12pm—4pm

Seminar: "Molecularly Defined Terpyridine-Based Electrochromic Materials"
Speaker: Dr Olena Zenkina, Ontario Tech
Date: Wednesday 2 November
Time: 1pm—2pm
Location: Online via Zoom

Green Chemistry Seminar
Speaker: Professor Emma Kendrick, University of Birmingham
Date: Thursday 3 November
Time: 1pm—2pm
Location: C/F/106

Seminar: "Collaborative Approach for Catalyst-Controlled Site-Selective and Enantioselective C-H Functionalisation"
Speaker: Professor Huw Davies, Emory University
Date: Tuesday 8 November
Time: 12.30pm—1.20pm
Location: AEW/003, Alcuin East Wing

Seminar: "Discovery Chemistry at Concept Life Sciences – Life in a CRO lab"
Speakers: Dr Matthew Isherwood & Dr Callum Hall
Date: Friday 11 November
Time: 1pm—2pm
Location: C/F/106

Inorganic Early Career Symposium
Speakers: Claire Bakewell, Kings College London; Paul Scattergood, Huddersfield University; Alice Johnson, Sheffield Hallam
Date: Wednesday 16 November
Time: 1pm—3pm
Location: C/B/101

Seminar: "Adventures in catalysis in the pharmaceutical industry"
Speaker: Dr Katherine Wheelhouse, GSK
Date: Friday 18 November
Time: 1pm—2pm
Location: C/F/106

Seminar: "Universal Polymer Crosslinkers"
Speaker: Professor Jeremy Wulff, University of Victoria
Date: Wednesday 23 November
Time: 1pm—2pm
Location: C/B/101

Inaugural Lecture
Speakers: Prof Avtar Matharu & Prof James Lee
Date: Wednesday 23 November
Time: 4pm—5pm
Location: C/A/101
Drinks and nibbles after the event

Seminar: "A career in molecules"
Speaker: Dr Vipul Patel, Grünenthal, Germany
Date: Thursday 24 November
Time: 1pm—2pm
Location: C/F/106

Date of Next Issue:
25 November 2022

York signs ‘Green Chemistry’ commitment

The University of York has signed the Green Chemistry Commitment - a charter to train the next generation of chemists about the key principles of green chemistry.

Green Chemistry aims to remove the adverse impacts of chemistry on the environment by creating greener and more sustainable processes that offer environmentally-sound approaches to chemical products and processes.

The Green Chemistry Commitment is a global initiative to help transform chemistry education by preparing chemistry students with a better understanding of Green Chemistry.

The overarching goal of the Green Chemistry Commitment is to ensure that the next generation of scientists are fully equipped to use methods and chemicals that are benign for human health and the environment – with the potential to have very significant global impact.

Signatories to this initiative, developed by ‘Beyond Benign’, commit to provide Green Chemistry curriculum and specific training to their students. In particular, all students should consider aspects such as the 12 Principles of Green Chemistry, toxicology and the impact chemicals can have on human health and the environment.

In the laboratory, students should be encouraged to explore how sustainable their processes are and develop greener alternatives to chemical processes as a part of the experiments and analysis they carry out.

The Green Chemistry Centre of Excellence (GCCE) at the University of York, led by Professor Helen Sneddon, is a world-leading academic facility for pioneering pure and applied green and sustainable chemical research through a variety of technology platforms.

The GCCE has expertise in developing high quality bespoke teaching on Green and Sustainable Chemistry within its highly successful MSc programme. This experience will be invaluable in ensuring that all students can benefit from the Green Chemistry Commitment.

The chemistry undergraduate degree programme is currently being revised as part of the University of York’s transformative modularisation and semesterisation programme for students starting in 2023, and the GCCE has therefore taken leadership for ensuring that all students will be exposed to the core principles of Green Chemistry and can develop expertise in thinking about, and practising, chemistry in a more sustainable way.

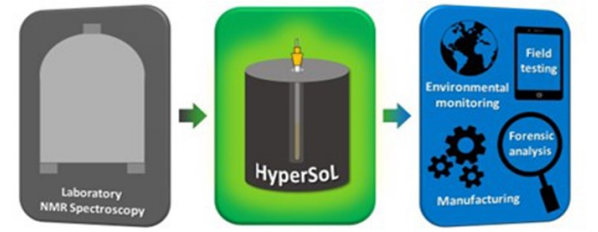
Furthermore, all PhD students in the Department will have new training on the ways in which Green Chemistry can impact on their research, providing a grounding in key principles, and examples of different ways in which they can be used in a research setting.

The Green Chemistry Commitment was signed by Head of Department Professor Caroline Dessent and Dean of the Faculty of Sciences, Professor Andy Dougill.

Reflecting on the commitment, Head of the GCCE, Professor Helen Sneddon said: “In an ideal world, Green Chemistry wouldn't exist as a sub-discipline. We need to move to a way of thinking where sustainability is considered as part of everything we do. Signing this commitment is symbolic of the growing integration of Green Chemistry across all Chemistry teaching and research at York. The next generation of chemists have enormous potential to accelerate the shift to greener chemistry, and it's an honour to be part of that process.”

Major European grant to move NMR spectroscopy beyond the laboratory

An academic in the Department of Chemistry has won a prestigious European Research Council Consolidator (ERC) Grant worth £1.7 million pounds to fund transformative research in NMR spectroscopy.



HyperSoL: Hyperpolarised NMR Solutions beyond the Laboratory

Dr Meghan Halse has received ERC funding for her five-year project: 'Hyperpolarised NMR solutions beyond the laboratory (HyperSol)'. The overall goal is to develop a transformative, portable NMR technology that can be used to solve analytical problems outside of the traditional laboratory environment – from field measurements to use on the factory floor.

Nuclear magnetic resonance (NMR) spectroscopy is a powerful technique that has revolutionised the physical and biological sciences. However, standard NMR spectrometers are large and expensive, meaning they are confined to dedicated technical facilities. The potential for a step-change in NMR exists if the detector could be taken out of the lab and brought to the sample. The challenge is to achieve this without sacrificing the sensitivity and chemical resolving power of laboratory NMR.

The unique innovation of the HyperSoL project will be a new method to amplify the NMR response of both hydrogen and carbon by factors of >1000-fold. This will dramatically enhance both the sensitivity and chemical discrimination of portable NMR devices. The HyperSoL project will develop two approaches based on both commercial and bespoke NMR instrumentation. Harnessing this new portable NMR technology will liberate NMR from the laboratory, transforming the way that it is used in such disparate areas as manufacturing, environmental monitoring, forensics, and field testing.

Reflecting on the award, Dr Halse said: "In science, access to new data drives innovation. Disruptive technologies, such as those being developed here, have the potential to transform research by providing new quantitative information in a simple and cost-effective way."

European Research Council (ERC) Consolidator Grants are highly competitive five-year awards designed to support excellent Principal Investigators at the career stage at which they may still be consolidating their own independent research team or programme. Principal Investigators must demonstrate the ground-breaking nature, ambition and feasibility of their scientific proposal. Currently, as part of the post-Brexit arrangements projects selected for funding by ERC are being financially underwritten by UK Research and Innovation (UKRI).

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.

New Approach to Detecting Reactive Radicals

A new approach, developed in York, allows the detection of short-lived reactive radicals, and has the potential to enhance understanding of chemical reactions, such as those taking place in Earth's atmosphere.

Short-lived 'free radicals' play a key role in many chemical processes, including the synthesis of drugs and polymers, in biological systems, and in reaction cycles that occur in the atmosphere. However, detecting these radicals is challenging due to their short lifetimes and low concentrations. Furthermore, in atmospheric field measurements, it can be difficult to detect radicals using existing techniques because of the need for highly complex equipment.

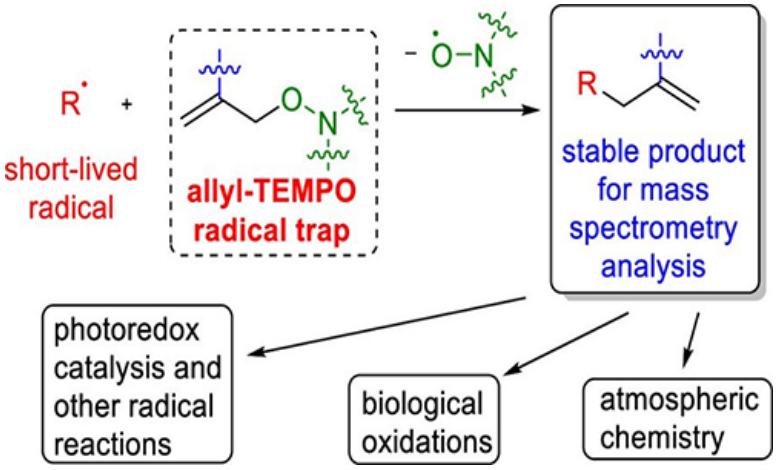


Figure one: Radical trapping by reaction with an allyl-TEMPO trap.

Commonly, in order to detect reactive radicals, they are trapped as more stable, longer-lived species. However, these methods can suffer from poor sensitivity, and in many cases, specific methods have to be employed to detect specific radicals.

In order to solve these problems, and develop a sensitive and general approach to radical-detection, Professor Victor Chechik, working in combination with atmospheric chemists led by Dr Andrew Rickard, has developed a landmark new technique for detecting radicals that could potentially be applied in challenging environmental settings.

These new radical traps enable the easy detection of most short-lived radicals (see Figure one). The approach is based on modifying a known radical trap (TEMPO) to create an innovative new allyl-TEMPO system. The key design feature here is that reaction of a short-lived radical with the trap releases the nitroxide radical and yields a stable, non-radical product. The stability of the non-radical product means that time can be taken to analyse and understand it offline, for instance using laboratory-based mass spectrometry, after the samples have been collected in a field campaign.

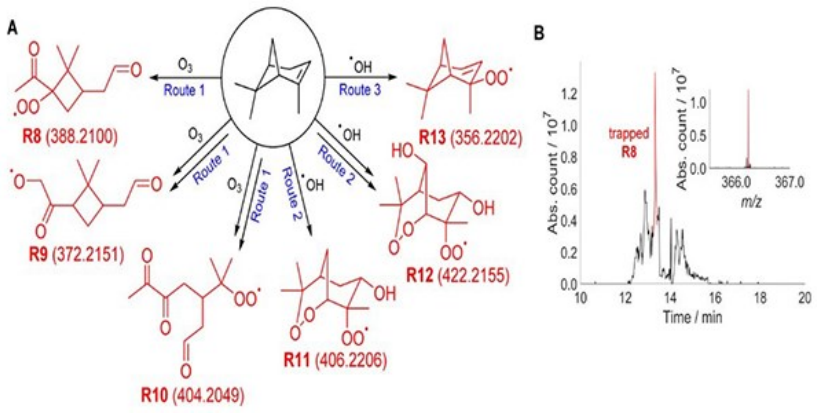


Figure two: The reaction of a terpene with ozone, an important atmospheric process is complex and can go via many routes, the new radical detection approach allowed the researchers to detect a range of intermediate radicals simultaneously.

Professor Chechik says: "We have made radical detection much simpler by detecting a downstream non-radical product. Importantly, we can also easily modify the rate of the radical-trapping reaction, and the ability to detect the product, by subtly tuning the structure of the trap. This makes this approach hugely versatile – it can be applied to a wide range of different reactive radicals, as we demonstrated in the paper."

Dr Rickard adds: “We were delighted to demonstrate that this approach can be used to understand gas-phase atmospheric reactions, such as the ozonolysis of terpenes. As the figure shows, this is a complex reaction system, but it is an important atmospheric process, as terpenes are fast-reacting biogenic compounds emitted by forests. These reactions can potentially form multiple products in small amounts, and the ability to characterise these unambiguously demonstrates the potential of this approach in understanding atmospheric reaction mechanisms. We hope, in the future, to apply the methodology both in the lab and the field to uncover and understand new types of atmospheric reactivity.”

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

New starters

Melanie Boyeson, Primary Science Advisory Teacher in the Humber
Room: TBC; Email: melanie.boyeson@york.ac.uk; Tel: 2523

Dr Katherine Bate, MSc Administrator
Room: C/A/142; Email: kate.bate@york.ac.uk; Tel: 4574

Mattia Barresi, Teaching Lab Apprentice
Room: C/F/101 (office) / C/F/018 (lab); Email: mattia.barresi@york.ac.uk; Tel: 2530

Kelechi Uleanya, PDRA (Dessent group)
Room: C/A/057; Email: kelechi.uleanya@york.ac.uk

Kristof Altus, PDRA in in Organometallic Chemistry and Catalysis
Room: C/E/114; Email: kris.altus@york.ac.uk; Tel: 2538

Kieran Godfree, Teaching Lab Technician
Room: C/F/010; Email: kieran.godfree@york.ac.uk; Tel: 4957

Izzy Hehir, Teaching Lab Facilitator
Room: C/B/103; Email: izzy.hehir@york.ac.uk

Catrin Ellis, Teaching Lab Facilitator
Room: C/B/103; Email: catrin.ellis@york.ac.uk

Adam Richardson, Teaching Lab Facilitator
Room: C/B/103; Email: adam.richardson@york.ac.uk

Joseph Jones, Teaching Lab Facilitator
Room: C/B/103; Email: joe.jones@york.ac.uk

Ethan Ross, Teaching Lab Facilitator
Room: C/B/103; Email: ethan.ross@york.ac.uk

Matthew Cullen, Teaching Lab Facilitator
Room: C/B/103; Email: matthew.cullen@york.ac.uk

Mark Shaw, Deputy Head of Faculty Operations
Room: C/A/136; Email: mark.shaw@york.ac.uk

Uncovering the history of ocean biodiversity from the seafloor

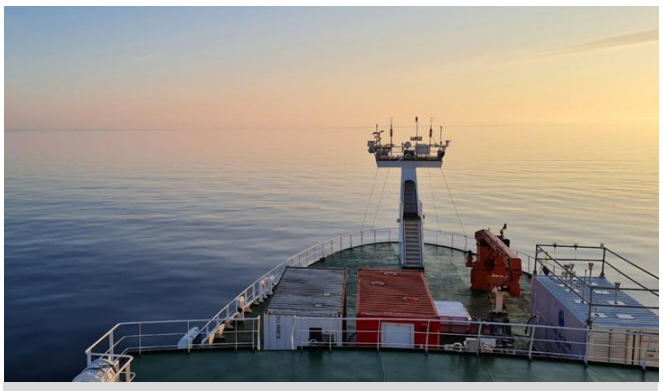
By Ellie Nelson

On 10 April 2022, I departed Southampton on the RRS Discovery for her 150th research cruise. On board were 25 scientists from the SEACHANGE project, including three scientists from the University of York (Ellie Nelson, Department of Chemistry; Dr Harry Robson and Dr Kwaku Afrifa, both Department of Archaeology). This is a six-year project funded by the European Research Council, studying the impact of past major cultural transitions on marine ecosystem functioning and biodiversity. This will help us understand what a "healthy" marine ecosystem looks like, in order to feed into better policy decisions.

Multi-corer returning to the ship after deployment, filled with surface marine sediment.

The purpose of the cruise was to collect marine sediment cores and *Arctica islandica* shells from the North Sea Continental Shelf and the North Iceland Shelf. The cores will be analysed for environmental DNA, radiocarbon dating, and stable isotopes (including $\delta^{18}O$ and Sr/Ca). The shells of *Arctica islandica* will be used for cross-matched floating sclerochronologies (a form of relative dating using the annual bands in long-lived shells, similar to tree-ring dating). These floating sclerochronologies will be "pinned" to a timescale using amino acid dating, performed by Martina Conti and Kirsty Penkman at the NEaar lab here in Chemistry. The inorganic ($\delta^{18}O$, Sr/Ca) and organic (amino acid $\delta^{13}C$ & $\delta^{15}N$) within these shells provide valuable proxies for environment and climate, so out of these dredged shells should come a high resolution and well-dated palaeoenvironmental marine record.

Before we set sail, a mandatory five-day Covid quarantine onboard the Discovery was required to ensure we were safe to sail. To make the most of this additional time, a "floating university" was created where cruise participants shared insights from their research in a series of talks each morning. This was followed by training for each sampling method in the afternoon. On the Friday, we all took one more lateral flow test to make sure the science party and crew were Covid free. Everyone's test came back negative, and we



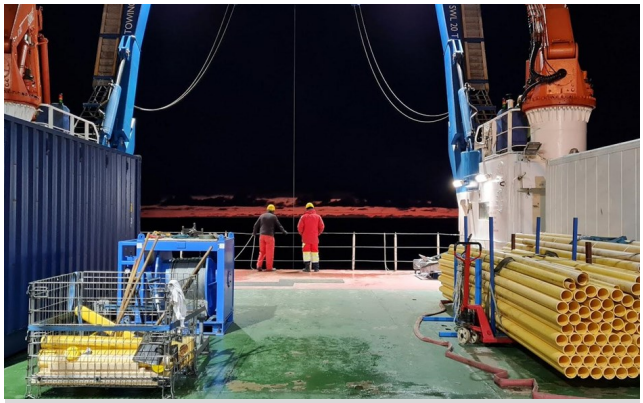
Sunrise over the Skagerrak.

Sorting through samples of *Arctica islandica* following a successful days dredging.

embarked bright and early the next day.

Following departure from Southampton, the RRS Discovery made her way to the Skagerrak (a strait which divides Denmark from Norway and Sweden) where the first sediment cores were collected. We then made our way back to UK waters, gathering sediment cores and *Arctica islandica* from the Fladen Ground, and more cores from Scapa Flow and Shetland. In the first week of May, we arrived in Icelandic waters where we sampled multiple locations on the North Iceland Shelf.

Work was divided into two 12-hour shifts. As a member of the midnight dredging team, I had to wake up at 11.30pm ready to start at midnight. Changing sleep patterns to fit with shift hours was the biggest challenge of the cruise (especially on a noisy ship). However, the positive energy of everyone on board and a constant supply of coffee helped to combat the lack of sleep.



Sunrise on the Fladen Ground.

There were four laboratories onboard the Discovery. The first was a dry lab where the computers that controlled the ship machinery were kept. The second was the wet lab which was used to clean and dry the *Arctica islandica* samples, and to section and package the sections taken from the shallow sediment cores (collected by a mega-corer). This was messy work, requiring waterproofs and frequent cleaning up to remove excess mud. A smaller laboratory, which could be sealed from outside contaminants was used to sample eDNA. In this laboratory, members of the science party were required to wear protective clothing including a body suit, hairnet, mask, sleeves and two pairs of gloves to avoid contamination of the samples. Finally, the longer cores (collected by either a gravity or piston corer) where split in two and described and photographed in another laboratory where they were wrapped up and sealed in specially made boxes for transportation back to the UK.

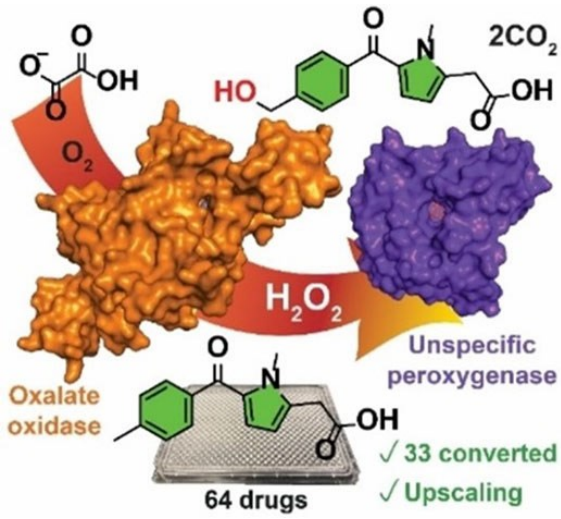
An *Arctica islandica* shell found within a piston core sample.

After four weeks of flat seas and sunny skies, it was in our final week of the cruise that the weather finally turned. A storm forced us to cut the cruise short by a couple of days, but to avoid the harsh weather we sheltered in one of the Westfjords of Iceland, where we joined for the day by a pod of humpbacks.

We arrived at our final destination, Reykjavik, on 11 May with all scientific objectives met and two shipping containers full of samples. I am incredibly grateful for the opportunity to join this cruise. I have gained many new skills including learning new sampling methods and how to work in challenging conditions. I would like to thank everyone involved in the cruise for being such a joy to work with and helping to make this an experience I will never forget! Updates on the progress of the SEACHANGE project can be found at seachange-erc.eu.

Clean oxidation reactions for use in the pharmaceutical industry

Working with a team from AstraZeneca, academics from the Departments of Chemistry and Biology have developed clean and effective enzyme-mediated synthetic methods for use in the pharmaceutical industry.



Oxidation reactions are key processes in synthetic chemistry and of vital importance in the pharmaceutical industry. However, mild and selective transformations often remain elusive. In particular, the oxidation of relatively unreactive C-H bonds often employs transition metal catalysts, an approach which can suffer from poor selectivity and low sustainability.

With this in mind, researchers have turned to using enzymes to try and catalyse such processes. In recent years, certain enzymes have risen to prominence, one such example being unspecific peroxygenase (UPO) enzymes. However, these enzymes require a precisely controlled supply of hydrogen peroxide – enough for the enzyme to work, but not too much to cause its degradation. Practically, this can be difficult to achieve.

In recent research, Professor Gideon Grogan and Dr Jared Cartwright, working together with a team of scientists from AstraZeneca, led by Dr Martin Hayes have developed an innovative solution to this problem. They have used a second enzyme, oxalate oxidase, to provide an *in-situ* source of hydrogen peroxide that can then be utilised by UPO (see Figure).

Oxalate oxidase is a well-known enzyme which produces hydrogen peroxide but has not been used before in combination with a UPO to drive synthetic reactions. In this work, the team demonstrated that this approach works for the oxidation of a diverse range of 33 different drug molecules. They also scaled-up one of the reactions to demonstrate proof of concept.

"Innovations like this provide us with the tools and technologies to make drug synthesis more environmentally friendly. This two enzyme in-one-pot approach ensures optimal hydrogen peroxide levels, enabling rapid access to industrially relevant molecules in a safe and sustainable way." says Dr Hayes.

Professor Grogan explains: "In the human body, pharmaceuticals are very often oxidised by metabolic processes. It is therefore vital for pharmaceutical chemists to test and understand the properties of oxidised drug molecules.

"This new approach provides easy access to such molecules, giving valuable information to our industrial partner, AstraZeneca. We hope that in the future, oxalate oxidase will go on to find a range of uses in synthetic chemistry as a simple and controlled way of generating the hydrogen peroxide required by other enzymes."

This research has been published in *Angewandte Chemie Int. Ed*.

Pathways to Equity in Research Symposium

Prof Dame Ottoline Leyser offers her views on what equitable research culture looks like. (Paul Shields / UoY)

Prof Anna Vignoles (l) & Lauren Crawford (r) listen as Dr Daniel Smith (centre) responds to a question during panel discussion. (Paul Shields / UoY)

Prof Paul Wakeling (l) speaks with Prof Duncan Bruce & Prof Caroline Dessent during lunch. (Paul Shields / UoY)

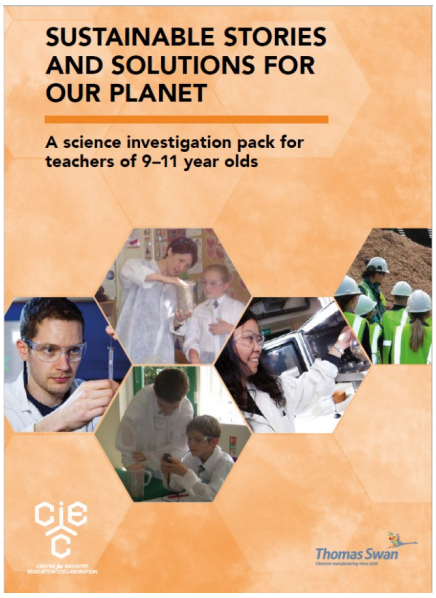
Some of the team who helped organise the event inc. (l-r): Dr Mia Shandell, Dr Katherine Manfred, Dr Connor Prior, Dr Beth Nelson, Dr John Halfacre, Dr Cate Anstöter, Dr Sari Budisulistiorini, Dr Will Drysdale & Megan McLoughlin. (Paul Shields / UoY)

The Department of Chemistry organised and sponsored a symposium in September bringing together national stakeholders and researchers to identify ways to make research funding and culture more equitable. With funding from the department and two external sponsors (GSK and Royal Society of Chemistry), over 120 people registered for the event at the National STEM Learning Centre with an additional 50+ registered virtual attendees. Attendees ranged from undergraduate students to emeritus faculty with expertise across the full breadth of STEM subjects and from a diverse range of backgrounds and lived experiences. Nearly one third were external visitors, extending impacts from the symposium beyond the University of York.

Six talks across the morning and afternoon sessions provided valuable insights from high profile speakers, including: Professor Dame Ottoline Leyser (CEO, UKRI), Professor Anna Vignoles (Director, Leverhulme Trust), and Professor James Wilsdon (REF reform expert). Engagement from such important leaders in steering the UK research landscape ensures that equity and inclusivity considerations remain at the heart of strategy and decision-making. Through a series of focus groups, two live panel discussions, and a networking session, attendees had unique opportunities to discuss ideas with and challenge representatives from funding bodies, publishers, professional institutions, and industry on their future aims.

As Professor Caroline Dessent mentioned in her opening remarks, it was a day that would make a difference as she hoped attendees and speakers would leave with inspiration and ideas for future actions. These actions include, for example, exploring novel mentoring structures such as reverse mentoring with appropriate recognition of additional workload burdens; re-evaluating whether criteria for success allow flexibility for different capabilities and cross-over between academia and industry; and embedding accessibility in promotion and development of technical staff. The value of the event was echoed by speakers and attendees in widely shared social media posts, further increasing visibility of the areas discussed. This event highlighted that the University of York, and the Department of Chemistry in particular, is at the forefront of solution-building to encourage and support diverse talents in scientific research. By focusing on ways to shape a positive environment for different career shapes and impactful research development, it fully embodied York's commitment to serve as a "University for the Public Good" and the University's leadership role within the UK and wider research community in EDI activities.

Centre for Industry Education Collaboration (CIEC) news



The Centre for Industry Education Collaboration (CIEC) has moved offices and is now based opposite the student recruitment team (tel: 01904 322523). As some of you will already know, we support scientists and engineers in industry and academia to communicate their research and processes to primary aged children.

Last month, we launched three new sustainability-focused activities following a year-long collaboration with chemists from Innospec Performance Chemicals. Combining their science with our expertise in communicating science concepts at an appropriate level for primary children, resulted in some very innovative practical problem-solving science activities for teachers to carry out in primary schools. One activity was based on the work that scientists at Innospec have been doing to reformulate personal care products such as shampoo, which are usually sold as liquids, into solid bars. Our resources support teachers and children to compare the relative efficacy of solid and liquid formulations of soap before comparing the transport and packaging costs of solid and liquid preparations.

In recent trials, the resource was well received by teachers and children as it gives a relevant and engaging context in which to tackle the primary science curriculum. The activities also help to raise children's science capital, thus increasing the likelihood of them choosing to study science and pursue STEM careers in the future.

We have followed the same process over many years, to create activities based on chemists' research in the Department, as well as those based in a wide variety of chemical companies.

If you are interested in finding out how CIEC could support your outreach and impact goals, please do drop us an email, so we can arrange a time to meet for a coffee – or catch up at one of the weekly staff meetings.

You can follow us on Linkedin (@centre for industry education collaboration) and Twitter (@ciec_york), and read our blog where we regularly post about our work.

Neurodivergent Network (opportunity)

Do you identify as neurodivergent? Would you be interested in meeting other neurodivergent chemists?

Jon Agirre and Julia Sarju are planning to launch the Neurodivergent Network in November 22.

We hope this network will:

- bring together neurodivergent **students and staff**;
- raise the visibility of neurodivergent scientists;
- act to improve inclusion;
- and facilitate networking and **mentoring**.

Let us know if you are interested in taking part by completing this expression of interest Google form.

KMS Winners Seminar

The Winners of this year's KMS prize each delivered a fantastic talk about their research at a seminar on 12 October. Having been shortlisted from ten nominations, our three winners had been interviewed and selected by an academic panel back in July and each win a prize from the Kathleen Mary Stott Memorial fund.

Winners left to right: Amelia Gilio, Becky Wagner and Pooja Gupta

An audience of over 100 people attended the seminar, followed by a drinks reception to celebrate our winners.

Pooja Gupta (JNB/AJW)

Activating sleeper cells: exploring the bioenergetics of bacterial spore germination

Becky Wagner (DCC/MS)

New methods to determine air pollutant emissions sources in urban areas

Amelia Gilio (GJG)

Engineering Imine Reductases for the Preparation of Pharmaceutical Amines

Congratulations to all nominees as well as our winners, and thank you to the KMS Panel, Jamie Blaza, Meghan Halse, Terry Dillon and Chris Spicer.

Work experience request

We have been approached by a Year 10 student from All Saints RC School in York. They are taking triple science GCSEs. They were enquiring about potential work experience placements in our Chemistry Department to take place between **Monday 27 February and Friday 10 March 2023**.

The student is "very interested in chemistry" and has been achieving grade 9s (that's the highest grade under the new scheme) in science since Year 8. They are considering pursuing chemistry in their future career and would like to gain an insight into the application of chemistry in the lab and real life.

They have a wide range of skills, such as communication, great organisation, and teamwork, which they displayed completing their Bronze Duke of Edinburgh award.They said "as a very enthusiastic student, I would be greatly honoured to be considered for an opportunity for work experience at the University of York."

If anyone is interested in hosting this student for part or all of the time indicated, please get in touch with me. I can provide support in setting up the placement.

Many thanks, Annie Hodgson (Schools Liaison and Outreach Officer) - annie.hodgson@york.ac.uk