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UNIVERSITY of York

ChemYork

HIGHLIGHTS FROM A LEADING UK CHEMISTRY DEPARTMENT

Digital Chemistry

New Concepts of Dynamic Chemical Bonding

Next Generation Mass Spectrometry

The future of chemistry

PROFESSOR CAROLINE DESSENT, HEAD OF DEPARTMENT, INTRODUCES THE SPRING EDITION OF CHEMYORK.

As I write, the last week of the summer term is upon us, and our undergraduate students are awaiting their final degree results. This is a hectic week for the team of administrative, academic and technical members of staff who share the responsibility for gathering, and compiling all of the exam results. As with many of the things that happen in an academic department, all of this highly professional work goes on "behind the scenes" but this particular activity is one of the most important we undertake each year. In many respects, results week is very much the same as it was decades ago, with long, sunny days, nervous undergraduates and the frenzied checking of marks before they are released. But, the critical thing is that the results must be correct and on time, year after year, and this demands much work to get right. Our team in the exams' office have done an incredible job this year, and I wanted to take this opportunity to especially thank Dr Nigel Lowe, Alison Edmonds, Lisa Mayer and Dr Adrian Whitwood for their exceptional contributions over recent weeks.

> "There is a shared sense of purpose across the Chemistry community that Chemistry must become greener, and this is something that we can look forward to seeing in both research and teaching over the years to come."

Looking over the articles in this month's ChemYork made me reflect on how Chemistry is changing as a discipline. Our Department is leading on the development of a new Master's programme that will teach skills in data science, including programming, artificial intelligence and big data analysis for application across the sciences. Digital Chemistry includes all applications of coding, data analysis, modelling and simulations, and computational methods to chemical problems, and is already revolutionising the way that chemical research is conducted in universities and industry. While we won't be hanging up our lab coats anytime soon, the tools of digital chemistry alongside the increasing automation of synthesis and analysis will certainly change the ways that chemists work. For example, vast data sets of chemical reactions and molecular structures are now being analysed, and then used to predict accelerated routes for synthesising new compounds and materials. Data Science skills are in great demand internationally, and our new Master's course will provide a bridge for our graduating chemists to upskill into this highly sought-after area.

Green and sustainable chemistry is another rapidly growing focus area for chemistry, with the chemical industry increasingly acknowledging the need to incorporate Green principles in the production of chemicals. York Chemistry's Green Chemistry Centre of Excellence (GCCE) has led this field for over 20 years, and continues as an international pioneer in the field, now under the direction of Professor Helen Sneddon. You can read about one of the latest ventures from the GCCE on page 7, involving its partnership with the renewable chemicals company, Circa. There is a shared sense of purpose across the Chemistry community that Chemistry must become greener, and this is

something that we can look forward to seeing in both research and teaching over the years to come.

I hope you enjoy the magazine. I'd like to put in a special mention for the articles on pages 4-6, which showcase some of our recent high-profile research. These include Prof Lucy Carpenter's fascinating discovery of evidence from the marine atmosphere that it has the capacity to "self clean", Dr Paul McGonigal's exceptional new studies on the dynamic nature of bonding in organic molecules, and Profs Dave Smith and Peter O'Brien's incredible work using self-assembled gels to make organometallic compounds safer and easier to use. One thing that is striking about York Chemistry is the genuine delight across the Department when these new discoveries emerge. We celebrate together, are proud of one another, and are happy to embrace the success that grows around us. It's such a privilege to teach and research in an environment where there is so much world-leading science happening every day, and where it goes on in such a mutually supportive way. As much as anything, this is what the future of Chemistry should be.

Front cover image: *Two new additions to the chemistry mass spec lab by Dr Jackie Mosley*

Compiled by *Sophie Packman and David Smith*

Designed by *Cookie Graphic Design*

ChemYork

Department Awards

Easter Conference Prize Success

The 2023 Easter conference season resulted in spectacular success for PhD students and PDRA staff members winning prizes for poster and oral presentations. Across the Department, 16 prize winners were celebrated in the last six weeks at national and international conferences. This success speaks to the strength, quality and diversity of research that is being presented at conferences from the Department.

Prize winners:

- Isabelle Pickles, PDRA - Poster prize winner at the RSC Carbohydrate Group Spring Meeting (Gideon Davies Group)
- Mahima Sharma, PDRA - ECR talk prize at the RSC Carbohydrate Group Spring Meeting (Gideon Davies Group)
- Lorna Tang - PDRA - Poster prize winner at RSC Biotransformations II conference, Burlington House in London and Poster prize winner at 'Novel Enzymes' meeting, Greifswald Germany (Gideon Grogan Group)
- Nick Garland, PhD - Flash presentation prize winner at the National JM iCASE studentship conference in Warwick (Alison Parkin/Duncan MacQuarrie Group)
- Ruhee Dawood - PhD - Johnson Matthey PhD Poster Competition 2023, Dept of Chemistry, University of York (Alyssa Avestro Group)
- Fraser Arnold - PhD - Fossey Memorial Poster Prize, John Fossey Memorial Symposium, University of Birmingham (Alyssa Avestro Group)
- Islam Araar, First poster prize - RSC Organic Division NE Regional Meeting, Northumbria University (Peter O'Brien Group)
- Yuran Wang, First poster prize - RSC Organic Division NE Regional Meeting, Northumbria University (Peter O'Brien Group)
- Kris Altus, PDRA - Poster prize winner RSC Dalton Division Meeting, Warwick (Andrew Weller Group)
- Mat Cross, PhD - Poster prize winner RSC Dalton Division Meeting, Warwick (Andrew Weller Group)
- Helena Lancaster, PhD - Prize honourable mention RSC Dalton Division Meeting, Warwick (Andrew Weller Group)
- Chloe Van Beek, PhD - Poster prize honourable mention RSC Dalton Division Meeting, Warwick (Andrew Weller Group)
- Rosalind Booth, PhD - Faraday Discussion, York (Anne Duhme-Klair Group)
- Lukas Geciauskas, PhD - Poster prize winner RSC Dalton Division Meeting, Warwick (Anne Duhme Klair Group)
- Callum Gater, PhD - Johnson Matthey PhD Poster Competition 2023, Dept of Chemistry, University of York (Simon Duckett Group)
- Promeet Saha, PhD - Johnson Matthey PhD Poster Competition 2023, Dept of Chemistry, University of York (Paul McGonigal Group).

The available prize winners assembled for a photo in the Chemistry Quad.

Centenary Award 2024

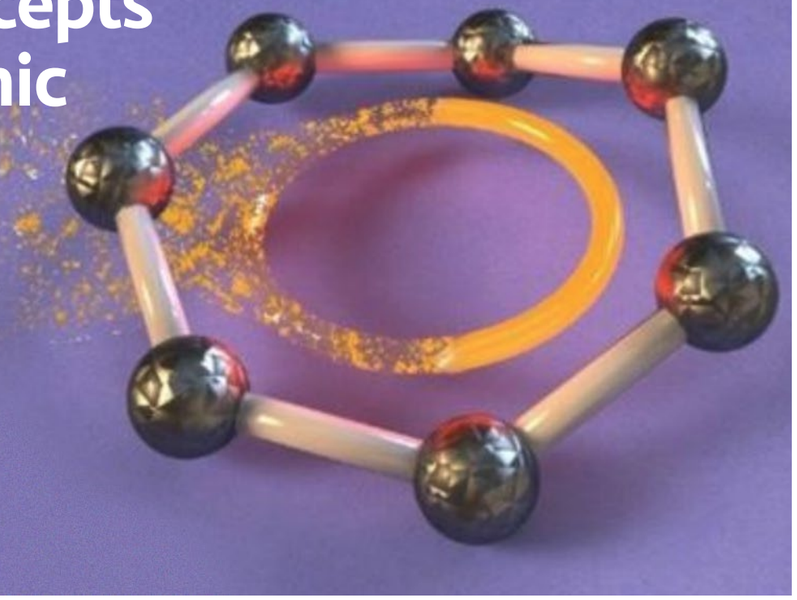
The Biomedical Society has awarded its Centenary Award 2024 to Professor Gideon Davies in recognition of his excellence and achievement in his field of research.

The Centenary Award is awarded annually to a molecular bioscientist based on the impact of their research and a demonstrable commitment to build, support, and nurture talent within the scientific community. Candidates are nominated by their peers and the winners are agreed by a judging panel of respected scientists from across a range of different scientific backgrounds. Winners will receive their prize and deliver an award or medal lecture in 2024. All of the awards and medal lectureships carry prize money and winners will be invited to submit an article to one of the Society's journals.

Professor Davies' research work spans chemistry and biology with a focus on the enzymes that synthesise and degrade carbohydrates and glycans. He is well-known for his work on enzyme mechanism, following the unusual contortions of sugars in enzyme active sites, and building on this to develop inhibitors and more recently activity-based probes. On winning the Centenary Award for 2024, Gideon said "It is especially important to me that this award, beyond research impact, also reflects a commitment to nurture talent within the scientific community. I am so proud of the wonderful, diverse, group of young and early-career scientists I have worked with throughout my career and to see

them thriving in academia, industry, education and child support is the true highlight of my career. I hope the award will inspire other young scientists, from all backgrounds, to dive into the exciting world of the glycosciences."

New Concepts of Dynamic Chemical Bonding



TWO LANDMARK PAPERS, BY A YORK CHEMIST AND THEIR RESEARCH TEAM HAVE OVERTURNED ESTABLISHED DOGMAS IN CHEMICAL BONDING AND DEVELOPED NEW CONCEPTS ABOUT THE DYNAMIC NATURE OF MOLECULES.

The chemical bonding which underpins the structure of molecules lies at the conceptual heart of modern chemistry, being responsible for the structure, stability and function of chemicals such as drugs and organic materials. In two recent papers, both published in Nature Chemistry, York chemist Dr Paul McGonigal has reversed established principles, and demonstrated that carbon-based molecules can be much more dynamic than previously thought.

The first paper explores aromatic molecules, ring-shaped structures which share electrons between their carbon atoms. Aromatic rings prefer to be flat. However, recent research has shown this isn't always the case. Dr McGonigal and his team have now explored how far a ring can be twisted before its aromatic bonding breaks. To do this, they crowded the periphery of a seven-membered 'tropylium' ring and found that low levels of overcrowding made the ring twist, but without breaking its aromatic bonding. Remarkably, the molecule could be twisted by 45° from one end to the other.

By adding progressively larger groups around the edge of the ring, the team then twisted the ring further, eventually causing the aromatic bonding to break. The electrons no longer circle the seven carbon atoms and instead, the ring pinches across its middle to form two smaller rings. Surprisingly, the researchers found there is a balance point, where the ring jumps back and forth between aromatic structure and the two smaller rings. One molecule made in this study spends 90% of its time as the pinched structure and 10% of its time as a larger aromatic ring.

In their second paper, Dr McGonigal and his team set their sights on stereochemistry. When a carbon atom forms four bonds to different groups, the molecule can exist in two mirror image forms. These mirror image forms are vital in medicine because they have different biological activities. Usually, it is impossible to interconvert between these 'enantiomers' because to do so would require a bond to be broken, a process that needs too much energy.

However, the team demonstrated that if the chiral centre was part of a dynamic molecular cage structure, then a simple rearrangement of the cage could lead to inversion of the mirror image form of the molecule. In this way, carbon-based stereochemistry, which is normally considered to be fixed and rigid, became dynamic, fluxional and responsive – a new paradigm in carbon-centred chirality.

Reflecting on the two papers, Dr Paul McGonigal said: "Bonding is such a fundamental part of chemical science – many of the underlying principles having been developed by Linus Pauling and others 100 years ago. To be able to help subvert the view of carbon-based molecules as fixed objects, and to discover new types of dynamic behaviour has been extremely satisfying. We hope, in due course that these intriguing new bonding concepts will be found to apply in other contexts, and potentially used to underpin new applications for more dynamic molecular materials".

The two research papers are published in Nature Chemistry. (Nat. Chem. 2023, 15, 516 and Nat. Chem. 2023, 15, 615.)

Research shows 'self-cleaning' of marine atmosphere

Researchers have shed new light on the 'self-cleaning' capacity of the atmosphere.

This process of self-cleaning is essential to remove gaseous pollutants and regulate greenhouse gases such as methane in the atmosphere. There was already an awareness that the atmosphere had this 'self-cleaning' ability, but in a new study from the Department of Chemistry, experts have now shown a new process that increases the ability of the marine atmosphere to self-cleanse.

Using a combination of aircraft and ground-based observations, scientists were able to confirm the widespread presence of nitrous acid (HONO) in the remote Atlantic troposphere formed by so-called "renoxification", whereby photolysis of aerosol nitrate returns nitrogen oxides (NOx) and HONO to the marine atmosphere. The findings, published in Science Advances 2023, 9, eadd6266, could be highly significant for atmospheric chemistry and largely reconcile widespread uncertainty on the importance of renoxification.

With funding from the Natural Environmental Research Council (NERC), the Wolfson Atmospheric Chemistry Laboratories (WACL) team led extensive observations in and around Cape Verde in August 2019 and February 2020.

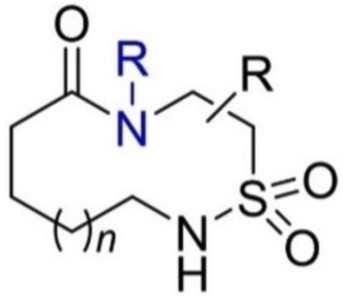
Lead author, Professor Lucy Carpenter said: "Importantly, the observations showed that the efficiency of renoxification increased with relative humidity and decreased with the concentration of nitrate. "This observation reconciled the very large discrepancies in the rates of renoxification found across multiple laboratory and field studies. It was also consistent with renoxification occurring on the surface of aerosols, rather than within their bulk, a new and exciting finding with implications for how this fundamental process is controlled and parameterised in models."

Recycling of nitrogen oxides on nitrate aerosol could have important, increasing, and as yet unexplored implications for the trends and distributions of atmospheric oxidants such as tropospheric ozone, an important greenhouse gas.

Expanding Sulfonamide Chemistry

A new synthetic method developed in York that enables the simple synthesis of a wide range of biologically-important cyclic sulfur-containing molecules has been discovered.

These molecules – known as 'sulfonamides' – are common components found in small molecule drugs, used to treat cancer, HIV and various viral and bacterial infectious diseases. Molecules arranged in large rings – also known as 'macrocycles' – are also very important compounds in medicines. However, synthetic methods able to install sulfonamide groups into macrocycles are scarce, thus limiting the ability to use this potentially valuable combination to discover new treatments for disease.



Dr Will Unsworth and his research team have great interest in the development of new and improved synthetic routes to macrocycles and set out to use their expertise to make macrocyclic sulfonamides.

They combined two distinct synthetic strategies, both of which are based on cascade reactions – processes which combine multiple reaction steps into a single operation. Cascade reactions bring several benefits in terms of making synthesis quick and easy, and avoiding the need to handle or isolate potentially toxic intermediates. The team made use of nitro groups or alkenes as masked amines that could be unmasked via reduction or conjugate addition respectively. This allows a diverse range of componds to be simply and efficiently turned into cyclic sulfonamides. These two new reactions allow access to families of previous inaccessible molecules, enabling their biological potential to be properly explored.

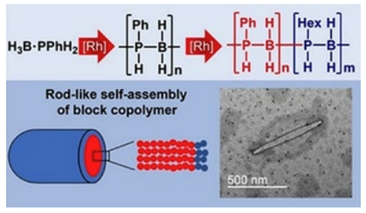
The teamwork on this project exemplifies the collaborative and international ethos in much of the research carried out in the Department of Chemistry. The work to develop one of the two new synthetic methods was led by lead by Chinese PhD student Zhongzhen Yang. The second was led by Ukrainian PhD student Illya Zalessky, who deserves huge credit for driving this research whilst also working to support refugees escaping the war in his homeland. The project was also supported by predictive computational chemistry, conducted by PhD student Ryan Epton and Prof Jason Lynam.

Speaking about the research published in published in Angew. Chem. Int. Ed. 2023, 62, e202217178 Dr Unsworth said: "Although we have worked on ring expansion reactions, we have never explored sulfonamides before. With the discovery of these two new reaction classes, we can now make macrocyclic sulfonamides remarkably easily, which will enable the exploration of their pharmaceutical properties.'

New main-group polymers self-assemble into nanostructured materials

Novel catalytic methods developed in York have provided synthetic access to main-group based block co-polymers for the first time, which self-assemble into nanostructured materials.

Polyphosphinoborane polymers with P–B bonds in their chains based on main-group elements, are chemically-related to technologically ubiquitous carbon-based polymers with C-C bonds (such as polyolefins). As well as being fundamentally interesting as a new class of polymer, polyphosphinoboranes could be used as flame retardants, precursors to high performance ceramics and etch resists in nanolithography.



An important class of polymer are block co-polymers – in which two different types of polymer chain are joined to give a new polymer, which has unique properties. Such polymers often self-assemble in solution to form nano-sized objects which may have many applications in energy research, catalysis, biology and separation science. However, until now, block co-polymers of polyphosphinoboranes could not be made.

Research published as Hot Paper in Angew. Chem. Int. Ed. 2023, 62, e202216106, and led by PhD student James Race, who worked within the Weller Research Group in collaboration with Canadian researcher Ian Manners at the University of Victoria has found a solution to this problem. By developing a new rhodium-based catalyst system for the synthesis of polyphosphinoboranes, and performing detailed mechanistic studies into how the catalyst operates, the team were able to design the synthesis of a polyphosphinoborane block co-polymer, which has more hydrophilic phenyl groups at one end and more hydrophobic hexyl groups at the other. By dissolving these polymers in a solvent mixture of THF/hexane the polymers self-assembled to form nanoscale rods or spheres, where the hydrophobic hexyl groups sit on the outside, and the hydrophilic phenyl groups on the inside.

This work therefore opens up new routes to both the synthesis of main group block co-polymers and their application in assembling nanosized objects.

Reflecting on the next steps, Professor Weller said: "This work shows the possible exciting future applications for main-group polymers and nanomaterials made through atom-efficient catalytic routes.

"Really pleasingly, it was an idea that was initiated by James as a PhD student, and then brought to fruition by his research visit to Ian Manners' labs in Canada. This shows how collaboration and PhD mobility in projects is so important. "

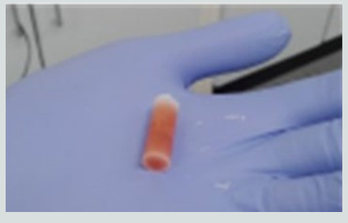
Using Gels to Tame Highly Reactive Chemicals

York chemists have developed an innovative way of using gels to stabilise highly reactive chemicals. This enhances safety and could transform the way organometallic reagents are used in chemical reactions both in research labs and industrial processes.

Recent research published in Nat. Chem. 2023, 15, 319, from a team led by Professors David Smith and Peter O'Brien have reported an innovative encapsulation approach to stabilise sensitive organometallic reagents.

Reactive organometallics based on either lithium or magnesium were mixed with a low-cost hydrocarbon capable of forming a self-assembled gel, which stabilised the organometallic reagent. Reagent lifetime was significantly extended by protection within the gel, which allowed simple handling, delivery and storage, and enabled reproducible reagent portioning. In some cases, the gels could even be held in a glove-protected hand, exposed to air, before dosing into a reaction vessel.

Members of the team, Dr Petr Slavik and Benjamin Trowse, demonstrated that the gels could be used in a wide range of different synthetic organic reactions of high value both in industry and in the academic research community. Some of the reactions proceeded in the absence of all the usual restrictions required for air-sensitive reagents. The purification protocols



were simple and gave the desired products in high yields.

Reflecting on the work Professor Smith said: "We hope to commercialise these gel-stabilised organometallics so that synthetic researchers can perform a wide range of reactions much more safely and easily. There are also potential advantages on an industrial scale, where transport and storage of large amounts of these reagents could be significantly improved."

The team are now extending their approach to organometallics based on different metals, as well as other types of air-sensitive reagents.

Launch of industrial academic partnership

Circa Renewable Chemistry Institute (CRCI)

The Circa Renewable Chemistry Institute (CRCI), a partnership with the GCCE and the renewable chemicals company Circa Group recently held a launch event at Kings Manor. This event included a panel discussion with chemical industry leaders including Croda, Synthomer and the Chemical Industries Association and explored the barriers and critical success factors in the adoption of renewable chemistry.

The new Institute aims to produce and promote bio-based products that are safer and more sustainable for the chemical industry. A significant breakthrough of the partnership so far has been the creation of Cyrene™ - a multipurpose green solvent that often outperforms the toxic petroleum-based materials. Its application extends across pharmaceuticals, paints and coatings, textile recycling, agrochemicals etc. Professor James Clark, Director of the CRCI at the University of York, said: "We have worked with Circa now for nearly a decade, and the strength of the relationship lies in the shared belief that the chemical industry can and will be environmentally responsible and able to transition from fossil-based chemicals to commercially-viable bio-based products.

"We have seen the impact that Cyrene™ has had on the industry, and this is now our inspiration to continue to work on other green products that can be scaled-up to meet the demands of consumers without damaging our environment."

As part of the partnership, Circa and its key customers will have access to all of the latest research from the University. In addition to developing commercial applications for Cyrene™, the team will be looking for the next breakthrough in renewable chemistry.

Nick Smith, Head of Development and Commercialisation for Circa, said: "This partnership provides the skills and expertise of both the Green Chemistry Centre of Excellence and the Biorenewables Development Centre to support application and process development with market leaders who are moving their manufacturing processes to safer and more sustainable products, such as Cyrene™."

Digital Chemistry

2023 SEES A NEW MSC COURSE LAUNCHING IN THE DEPARTMENT. THE MSC DATA SCIENCE WILL BE THE ONLY DEDICATED COURSE IN THE UK FACILITATED BY A CHEMISTRY DEPARTMENT, AND WILL OPERATE AS A COLLABORATIVE VENTURE BETWEEN THE DEPARTMENTS OF CHEMISTRY, BIOLOGY, PHYSICS, ENGINEERING, & TECHNOLOGY (PET), ENVIRONMENT & GEOGRAPHY, AND THE HULL YORK MEDICAL SCHOOL (HYMS).

The aim is to provide accessible and bespoke content designed to appeal to a diverse intake of students who are looking to make a lateral move from a natural/life sciences course towards specialisation in scientific data analysis, analytics, and machine learning.

The new MSc will equip students with the skills needed to ask and answer questions using data across different fields of science, and to navigate new fields and challenges, as the economic and scientific landscape changes. Teaching on the new MSc will comprise of a combination of traditional lectures and 'hands-on' programming, data analysis, analytics, and machine learning workshops and hackathons. The focus is on teaching 'computational thinking' and applied data science skills that can be used to solve real world problems, shifting the focus from theory.

From particle physics to ecology, and from drug design to climate change, data science skills are in huge demand across the natural sciences and beyond. Graduates equipped with these skills are also able to tap into lucrative opportunities in the private sector in areas such as business intelligence, e-commerce, financial services, and cyber security.

Dr Conor Rankine, Lecturer in Machine Learning & Computational Chemistry, will lead the teaching on the course. The Department will also welcome Dr Alan Lewis, our newest Teaching and Scholarship appointment, who will be joining us from the Max Planck Institute this August to support the venture.

Speaking about the new MSc, Dr Rankine said "Interest [in the course] has been absolutely unprecedented – we've been blown away by the volume of applications. These [machine learning] tools are transforming what we can do and the way we do it across the natural sciences and beyond – and they're here to stay. Computational thinking, which is something of a 21st-century 'survival skill', has evolved to encompass understanding how these tools work and how to work with them – and that's exactly what we want our students to be able to do. I think that the interest we're seeing is a reflection of that – our applicants recognise it."

> "These tools are transforming what we can do and the way we do it across the natural sciences and beyond."

Oak National Academy award to develop science in schools

THE CENTRE FOR INDUSTRY EDUCATION COLLABORATION (CIEC), PART OF THE DEPARTMENT OF CHEMISTRY AND THE UNIVERSITY OF YORK SCIENCE EDUCATION GROUP (UYSEG), HAVE BEEN AWARDED £1.4 MILLION TO DEVELOP ONLINE SCIENCE MATERIALS FOR SCHOOLS. THEY WILL WORK TOGETHER TO DEVELOP LESSON RESOURCES FOR TEACHERS AND PUPILS COVERING THE PRIMARY AND SECONDARY SCIENCE CURRICULUM IN ENGLAND, AGE 5-16.

Working with the Oak National Academy, the curriculum resources will draw on the expertise and work of both groups and will be developed by the CIEC and members of UYSEG's Best Evidence Science Teaching (BEST) project team, working with expert science teachers across the country.

The materials will support an evidence-informed practice, a current key Government initiative in education. The CIEC will produce the primary materials, and UYSEG are developing the secondary school resources.

The CIEC team of six primary science specialists and dedicated science education researchers, who engage in a wide range of primary science initiatives, nationally and internationally, focusing on the development of primary science resources and the delivery of continuing professional development.

Joy Parvin, Director of CIEC said: "As well as developing a full suite of resources for Key Stages 1 and 2, we will be collaborating with our secondary colleagues to smooth the transition from Key Stage 2 to 3, thus building on the knowledge and skills children have gained during their primary years."

Matt Hood, Chief Executive of Oak National Academy, said: "Every part of the education sector – from trusts to publishers to subject associations – are part of this collaboration, forming a coalition of top-tier expertise. It means teachers will have access to some of the smartest curriculum thinking and resource design on tap, something they have told us they want."

CIEC is a collaborative organisation, with current partnerships with many STEM companies across the UK to run Children Challenging Industry, Science Oxford's Thinking Doing Talking Science, Teacher Assessment in Primary Science, National STEM Learning, and the Association for Science Education.

I'm a Scientist – Plastic Zone Outreach Winner

GREEN CHEMISTRY CENTRE OF EXCELLENCE (GCCE) POSTDOCTORAL RESEARCHER, DAN DAY, TOOK PART IN THE 'I'M A SCIENTIST' PLASTIC ZONE OUTREACH EVENT AND WAS VOTED THE WINNER.

The 'I'm a Scientist' programme connects school students with scientists through live online chats and provides them with the opportunity to find out what it's like to pursue a career in science.

As well as answering a range of questions about careers in science, the plastic zone led to lots of questions from students around the environmental issues associated with plastics. This allowed Dan to communicate some of the recent results from the University of York coordinated CHAMPION research project into bio-based polymers. Over the course of the month, he was voted the favourite scientist by the students and was awarded £500 to spend on future outreach activities.

Dan said: "I had such a brilliant time doing the 'I'm a Scientist - Plastic Zone!' I have always enjoyed being involved in outreach activities for young people, and doing it virtually means that you can reach so many more people without geographic restrictions.

It was a pleasure to work with all the moderators and fellow scientists, and I was so impressed by the enthusiasm of the students. I am really grateful to have been voted the favourite scientist by the students. The prize money gives me the opportunity to do more outreach on green plastics, and I am currently having discussions with STEM teachers to help me figure out how I can best provide resources to fit in to the curriculum. I massively recommend all scientists to participate in outreach if they get the opportunity – you can make a big difference to people's lives just by communicating what you do!"

The 'I'm a Scientist' programme is funded by the Royal Society of Chemistry (RSC) and UK Research and Innovation (UKRI). To find out more, or get involved, follow @imascientist on Twitter or visit the website.

Hartshorn Jones Innovation Fund

CHEMISTRY ALUM DR MIKE HARTSHORN AND HIS WIFE DR MICHELLE JONES, HAVE ESTABLISHED A FUND AT YORK TO GIVE EMERGING SCIENTISTS THE CHANCE TO EXPLORE NEW AREAS OF BIOLOGICAL CHEMISTRY RESEARCH.

Whilst at York, funding of this kind gave Mike the opportunity to develop his abilities in molecular graphics, modelling and chemoinformatics. He subsequently developed key software infrastructure in the UK biopharmaceutical industry at the software company, Dotmatics, whose methods have had a global impact on research and discovery in the pharmaceutical sector.

Now, Mike and his family are keen to support the next generation of bright minds in biochemistry.

"I'm delighted to be able to fund additional research and training within the York Structural Biology Laboratory and also other departments at the University.

The opportunities I received from similar funding gave me the best possible start for my career. During a recent visit to the lab, I was impressed to see the progress made by post-graduates in learning truly interdisciplinary skills that had been enabled by the fund."

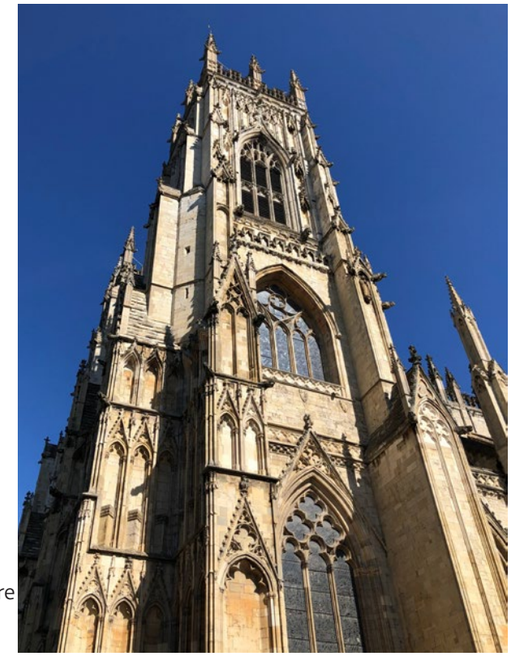
Recent decades have seen accelerating invention and deployment of chemical and biophysical methods to answer significant questions in biology and medicine, however, the constraints of conventional training and funding can limit the opportunities for inventive, early-stage scientists.

Grants made available through the fund enable York researchers to explore new methods and areas of chemical biology.

Thank you to Mike and his family, whose support is having a real impact on students' personal development, the furtherance of scientific research and its wider benefit to society.

Ringing the changes

INSPIRED BY THE EQUALITY, DIVERSITY AND INCLUSION ACTIVITY IN THE DEPARTMENT AND THE SUPPORTIVE AND INCLUSIVE ENVIRONMENT, OUR STUDENT & ACADEMIC SERVICES MANAGER, ALISON EDMONDS, WAS EMPOWERED TO SPEAK OUT AND APPLY SUCH THINKING TO HER INVOLVEMENT OUTSIDE OF THE OFFICE, IN BELLRINGING.



Alison has a long background in bellringing, being involved since a teenager, she met her husband whilst ringing and her children also ring. She recognised that women were not represented equally across the field, there were assumptions that only men were big and strong enough to ring heavy bells, which is untrue.

She identified that there was a lack of opportunities for women to be able to develop and try out the bigger bells in an encouraging and reassuring setting.

In September 2022 Alison organised a Ladies Weekend in York. Over the weekend, three towers were available in Selby Abbey, Leeds Minster and York Minster, with attendees having the opportunity to ring at each location. There were 25 participants, aged 14 upwards, with everyone enjoying a positive and inclusive event.

There is now a network of women, who have a voice and who have proven, without doubt, that they need to be listened to. There are established female groups in ringing centres across the country, Alison has visited Oxford, Cambridge, Birmingham and London, to provide support. She has also presented at conferences, run workshops and given after-dinner speeches about her experiences.

Going forward Alison explains 'I'd like to extend what I've been doing to include young people, who, male and female, don't get opportunities that older men do. The young people are our future, and they won't join us if all they get to do is watch the men do it. The women are under utilised and ready to be involved, so I need to be able to dovetail these two strands effectively to make better use of everyone.'

'I'd also like to organise the National Bellringer's Conference in 2025 along with the Association of Ringing Teachers (ART) of which I am an accredited member. It's a weekend event with about 100 to 150 attendees, and could be entirely hosted in the department. We could use University accommodation at Franklin House, and all the practical sessions could be in York, a 15 minute bus ride away. It would be amazing.'

'Finally a personal goal, I'm currently working towards doing a piece of ringing at York Minster that I'm pretty sure no woman has ever done. It will be a peculiar mix of technique, strength and stamina, and I will need some emotional and physical support to get through it. I wish I'd even believed it was possible 20 years ago when I was younger, stronger and more resilient, but it just wasn't ever on the cards.'

> "I'd like to extend what I've been doing to include young people. Women are under utilised and part of the now, so I need to be able to dovetail these two strands effectively."

Next Generation Mass Spectrometry

DR JACKIE MOSELY IS THE LEAD ACADEMIC AT THE CENTRE OF EXCELLENCE IN MASS SPECTROMETRY IN THE DEPARTMENT OF CHEMISTRY. SHE'S PREVIOUSLY BEEN THE CHAIR OF THE BRITISH MASS SPECTROMETRY SOCIETY AND NOW SITS ON THE RSC SEPARATION SCIENCE GROUP AND MANAGES THE FOCUS GROUPS FOR THE INTERNATIONAL MASS SPECTROMETRY FOUNDATION. WE SPOKE TO HER ABOUT ALL THINGS MS.

Where did you originally study? What was your path to York?

I did my PhD at the University of Warwick in Prof. Peter Derrick's mass spectrometry lab, which was home to a mass spectrometer that was the world's largest air freight! I then travelled to the University of Waterloo in Canada, accepting a PDRA post with Prof Terry McMahon, where I started to develop a passion (and patience for) instrumentation.

With a strong background in instrumentation, I was snapped up by Bruker, becoming the Senior Scientist for the UK team. Eventually, academia beckoned once more, and I took up a research fellowship at Durham University, both managing the Chemistry Department's Mass Spectrometry (MS) service, and establishing my own research career. Heading south, I took the post of Reader at Teesside University to establish leading research at the National Horizon Centre. When the opportunity at York came along, I jumped at the chance to work with a great team of people, with amazing students, super facilities, a great location, and with such a strong atmosphere of positivity.

What it is about your area of research that inspires you?

In short, I am nosey. I want to know what everything is, and MS lets me explore this at the molecular level! It is a major analytical measurement technology, as well as one of the most sensitive analytical techniques, and is of strategic importance in all aspects of molecular science, as well as being pivotal across academia, government/institutions and UK industry. To have such a broad reach opens-up doors in the most exciting and unexpected areas of science.

What big research problems are you trying to solve currently and why do they excite you?

We need to squeeze more analytical information out of any experiment, and at the same time samples are becoming more complex. I am currently working with a series of mass spectrometers which have ion mobility separation capability built into them. Ion mobility separation enables me to separate ions based on their size or shape. This is really powerful, and will be a crucial part of understanding the structure of an ion (or molecule) in the future, as we can now measure size (collisional cross section) as well as m/z in one experiment.

What parts of the undergraduate course are you teaching, and how does your expertise help you bring them to life?

I teach MS at a number of stages in the UG course, from second year workshops through to third year and MChem lectures in advanced mass spectrometry. The beauty of MS is that everyone loves to collaborate with you and bring new challenges into your lab. I will always use real data from my research in my lectures to demonstrate underlying principles. Using real life examples from my work puts mass spec into context. For example, when looking at how we can quantify chemicals, I will use data from my research into acrylamide content in food (warning – this has put me off crisps, coffee and pastries, which was pretty much my staple diet!)

What advice do you have for students who are interested in a career in Mass Spectrometry?

Learning practical skills in MS, and developing hands-on experience, will put any good student very much ahead of the class (or recruitment process!). There is currently a huge shortage in this skill sector, and with such a wide range of jobs available, there really is something for everyone. Working for a MS manufacturer will give you access to next generation science. A career in this industry could encompass everything from the pharmaceutical and chemical industries to various agencies where MS is used to monitor water supplies, food safety, public health, and undertake forensic testing. A good skill set in MS, and understanding how to read the data, will let you move throughout this amazing range of opportunities and grow your career.

What does the future for Mass Spectrometry look like? Any upcoming challenges/changes?

This is really interesting, and difficult to answer given the breadth of MS applications. To pull out just a couple of examples in this spectrum: scientists are making great in-roads to mass spectrometry for single cell analyses, providing crucial information about how individual cells respond to disease or treatment, rather than looking at the population level. MS is also a valuable imaging technique. A laser beam can be spatially focused on a surface and map out a molecular image of that surface. This can be used for biological tissues, but also it can screen fingerprints and pull up a 'chemical' fingerprint which not only tells us who someone is but also what they have touched, or imbibed. This is now an accepted technique by the UK Home Office for criminal investigations.