issue 14 | spring 2024

UNIVERSITY of York

ChemYork

HIGHLIGHTS FROM A LEADING UK CHEMISTRY DEPARTMENT

How clean is your home?

New Fellow joins YSBL

Kharkiv-York Partnership

Semester Time

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

As I write, we have just returned from our Easter break. After two quiet weeks, it's very good to see the Department full of students again. I very much hope that you all enjoyed the Easter holiday and found some opportunity to get out and about and appreciate Spring. This has been something of a challenge in York given the amount of rainfall we've experienced recently. King's Staith and the famous King's Arms seem to have been flooded more often than they've been dry since Christmas. Indeed, so much standing water has collected in our Chemistry quadrangle that it's become popular with some of the local ducks; a novelty that we hope is temporary.

This academic year has been the first year of Semesters at the University of York. Thus, the end of the Easter break now marks the beginning of the second half of the second semester, rather than the beginning of the Summer term. The University decided to move from terms to semesters several years ago and, while a huge amount of planning went into delivering the new structures, it is only by living through a semesterised academic year that you can get a proper feeling for how the highs and lows of the year have changed.

> "It is not the strongest of the species that survive, nor the most intelligent, but the one most responsive to change.
>
> **Charles Darwin**

In Chemistry, we decided to use Semesterisation as an opportunity to refresh and renew our entire undergraduate course. This has been an enormous undertaking that has involved staff across the department and we are grateful to all those who made it happen, including those who have written new material and all those who led the changes across course structure, lab delivery and admin support. Truly a multidimensional jigsaw puzzle was solved. Through the restructuring, we've thought carefully about the order in which we teach core topics, removed duplicated material where it occurred, and introduced a range of new material to ensure that the course reflects contemporary chemistry. Although this has been a huge amount of work, we're confident the new course will ensure that our undergraduates are better prepared for their next destination at the end of their studies, whether that is for a PhD, work in industry, or in a non-Chemistry focused career. While we still have half a semester to go, the feedback from students and staff about the restructured course has been overwhelmingly positive. Rebalancing work across the full academic year has removed some of the pinch points for students and staff, and there is a definite 'air of spring' and renewal across the department, as well as pride in being part of a team delivering a new and improved chemistry course.

This year has brought other significant changes to the Chemistry Department. At the end of September, three long-serving members of our academic staff retired; Dr Brian Grievson, our Year-in-Industry lead, and Professors Brendan Keely (Analytical Chemistry), and Mike North (Green Chemistry). Between them, they gave over 65 years of service to the Department and they will be very genuinely missed by staff and students alike.

We were very deeply saddened to lose Professor Paul Clarke, who died in November 2023, almost exactly a year after being diagnosed with glioblastoma; you can read our tribute on page 11. Paul was a remarkable personality, with a passion for organic chemistry, his research group and enjoying the very best of life. We miss him very much.

I hope you enjoy this edition of the magazine. There have been some changes in the 'Editorial Board' with Professor Dave Smith stepping down and Professor Duncan Bruce taking up the role of compiler. Dave did an outstanding job in this role, and I'd like to take this opportunity to say thank you to him for all his work in making ChemYork the success it is. He reflects on his experiences on page 12. I'd also like to put in a special mention for the articles on pages 8 and 9, which showcase some of our recent, high-profile research. These include a report on work led by Dr Terry Dillon from the Wolfson Atmospheric Chemistry Laboratory on detecting volatile organic chemicals, a group of chemical pollutants that can be generated indoors from cooking and cleaning products, and an article on Dr Seishi Shimizu's outstanding research on sorption isotherms.

Front cover image: *Guests from Kharkiv visiting local firm Croda's Widnes plant*

Compiled by *Duncan Bruce*

Designed by *Cookie Graphic Design*

Department Awards

Joy Parvin awarded the SCI Science for Society Award

Joy Parvin, Director of the Centre for Industry Education Collaboration (CIEC) was awarded the 2023 Science for Society Award of the Society of Chemical Industry. The award recognises her work, over many years, to combat science stereotypes and to help children from a wide range of backgrounds understand that a career in science is possible.

With a background in chemical engineering and primary teaching, Joy joined CIEC in 1992. Since then she has worked with scientists in industry to help them to explain their science to young people and to develop activities that make credible links between the science that happens on industrial sites and the primary science curriculum. She has also supported primary teachers to deliver engaging and relevant science lessons that capture the interest of young scientists and open their eyes to a wide range of STEM careers.

Her work has been driven by a belief that many children were being disadvantaged due to fixed ideas about who could, and could not, study science, with many children feeling that it wasn't a career open to 'people like me'. She also realised that science-based industries were missing out on a large pool of talent as potential scientists opted out at an early age by choosing non-STEM subjects at secondary school.

As director of CIEC since 2008, Joy has led a growing team of advisory teachers in Yorkshire, Humber, the Northwest, the East of England and beyond to continue the work which, evidence shows continues to have a lasting impact on the lives of the young people it touches. As a result of Joy's work, many children who would not traditionally have considered studying STEM subjects have gone on to have a career in science.

European Geosciences Union Award for Lucy Carpenter

Congratulations to Professor Lucy Carpenter FRS on being awarded the 2024 Vilhelm Bjerknes Medal of the European Geosciences Union (EGU). This prestigious international award is given by the EGU for distinguished research in atmospheric sciences, and recognises, in particular, Lucy's work in establishing a critical link between atmospheric chemistry, climate change and the production of trace gases in and over the oceans. It is further testament to Lucy's outstanding research achievements and international reputation.

International Prize awarded to Duncan Bruce

Professor Duncan Bruce has been awarded an International Cooperation Prize of the Petrochemical Foundation of China in recognition of his collaborative work with Professor Yafei Wang of the School of Materials Science and Engineering at Changzhou University in China.

Duncan and Yafei have been collaborating for some ten years since Yafei was a Marie Curie Fellow in the then group of Etienne Baranoff in Birmingham. Yafei is an expert in emissive materials and in the fabrication of organic light emitting diodes (OLEDs) and, like Duncan, was interested in how liquid crystal emitters might be used in OLEDs. Their collaboration continued after Yafei's return to China and together they have published some eleven papers and a review in the last seven years taking advantage of their complementary expertise around their shared interest.

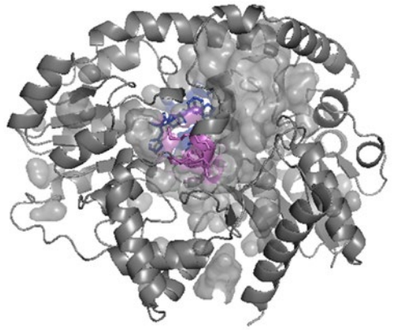
Numerous York postgraduates and postdoctoral fellows have been involved with the work, but of particular note are: Professor Jason Lynam with whom they collaborated on the design of some gold emitters; former PhD student Dr Rachel Parker who spent two weeks in Wang's laboratory fabricating OLED devices that used these gold complexes, and Dr Stephen Cowling who has done a good deal of the hands-on experimental work using polarising microscopy and small-angle X-ray scattering.

Their joint programme has been supported by the National Natural Sciences Foundation of China and the UK Royal Society, which has allowed visits in both directions as well as Rachel's stay in Changzhou.

Duncan said "It is a real honour to have received this award, which recognises the very productive collaboration that Yafei and I enjoy."

New enzyme discovered in bacteria makes unusual sugar linkages

RESEARCHERS IN THE DEPARTMENTS OF CHEMISTRY AND BIOLOGY HAVE DISCOVERED A NEW CLASS OF ENZYME, INVOLVED IN THE ASSEMBLY OF A SUGAR ON THE SURFACE OF A PATHOGENIC BACTERIA THAT TARGETS VULNERABLE PATIENTS IN HOSPITAL.



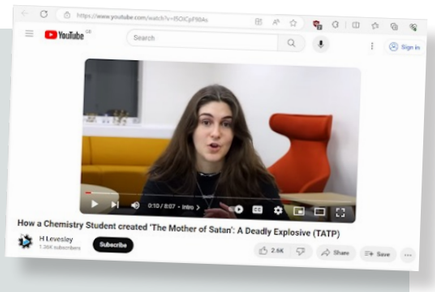
Human cells are covered in sticky layer of sugars called sialic acids which can act like a barcode to be read by the immune system, helping the body differentiate between human cells and pathogenic invaders. However, some pathogenic bacteria are able to mimic these sugars in order to trick the immune system. One such sugar is pseudaminic acid. It is an 'evil twin' of human sialic acid, present on the surface of a number of multidrug-resistant pathogenic bacteria including Acinetobacter baumannii, which causes hospital-acquired infections around the world.

Although the structures of the sticky coat on the surface of the bacteria were already known to include a pseudaminic acid sugar, how this was all assembled by the bug was unknown. Research led by PhD student Abby Walklett in the laboratory of Dr Martin Fascione from Chemistry, in collaboration with Professor Gavin Thomas from Biology, has now shown that this pseudaminic acid sugar is installed using a previously unreported class of glycosyltransferase enzymes, that are specific for pseudaminic acid and build an unusual linkage through a novel enzymatic mechanism.

This enzyme has several unique features and so, given that the bacteria are likely to use these sugars to camouflage themselves from the human immune system, it follows that an increased understanding of this enzyme class and the way in which they work will ultimately allow the design of chemical tools and inhibitors that could pave the way to new antibiotics for these pathogens.

This research has been published in *Angewandte Chemie International Edition*, 2024, **63**, e2023185.

Student video is bang on



The ability to communicate and contextualise our subject are key and valuable skills, and finding new and imaginative ways to do this is one of the possibilities on offer to BSc students undertaking their final-year project. One such student, Helen Levesley, created a video for her project that has turned out to be a YouTube success story, attracting more than 54,000 views, with over 2,600 likes and 150 positive comments.

The video, called 'How a Chemistry Student created 'The Mother of Satan': A Deadly Explosive (TATP)', describes the student's accidental synthesis of triacetone triperoxide, a very powerful explosive and looks at its reactivity drawing on first-year courses on organic reaction mechanisms.

Helen sought advice from fellow students on a suitable eye-catching topic, and then filmed and edited a short 8-minute video. Helen explains that 'feedback from students indicated there was a particular interest in understanding why certain compounds, including peroxides, are highly unstable'. This feedback inspired the selection of peroxides in the starring role, with Markovnikov's rule, homolysis, radicals, electrophilic addition and regioselectivity, all being featured in the clip. Feedback from Year 1 students, as well as comments published on YouTube, have shown that the clip explains some challenging aspects of organic mechanisms in a clear, engaging, and impactful way. Viewers from across the globe have appreciated how Helen described this 'explosive' topic sensitively and thoughtfully.

The project was supervised by Professor Andy Parsons, who commented that 'the Department offers a broad range of BSc projects to students, including in Chemical Communication, which allows them to explore new and effective methods to teach chemistry. The opportunity to create educational YouTube videos is one way that they can develop valuable communication and digital literacy skills.'

The video can be watched at: https://www.youtube.com/watch?v=l5OICpF90As.

Kharkiv-York partnership to tackle the environmental impact of the war in Ukraine

ORIGINATING IN A UK-WIDE TWINNING INITIATIVE TO OFFER SUPPORT TO ACADEMICS, STUDENTS AND UNIVERSITY LEADERS IN UKRAINE DURING THE CONFLICT THERE, THE DEPARTMENTS OF CHEMISTRY AND OF ENVIRONMENT AND GEOGRAPHY HAVE ESTABLISHED A NEW PARTNERSHIP WITH COLLEAGUES FROM KARAZIN KHARKIV NATIONAL UNIVERSITY AS PART OF A WIDER, UNIVERSITY-LEVEL COLLABORATION.

Following a nine-week introductory course in which there was much sharing of background information, about a dozen academics, PhD students and postdoctoral researchers from the Ukraine have spent eight weeks with research teams across the University. During the visit they gained hands-on experience of different research methods in ecotoxicology, environmental fate assessment and green chemistry and, while in the department, they were able to access cutting edge facilities and expertise.

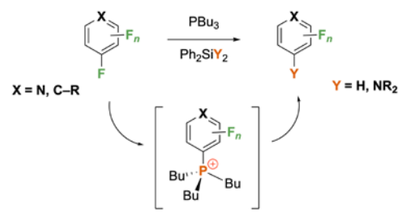
The programme aimed to provide the visitors with much needed respite, as well as building links for future collaboration and a programme of visits to local industry and sites of interest was arranged. Then, having gained experience of available local facilities, the visitors dispersed into the Department that best matched their expertise.

Green Chemistry hosted a Chemistry PhD student from Kharkiv, who undertook a project considering the nature of pollutants likely to be present after the war and looking at bio-derived sorbents for pollution remediation. The project aims to equip the Ukrainian researchers with the skills and knowledge needed to tackle the inevitable clean up of the country's natural environment and it is hoped that in due course, this will develop into a more extensive collaboration. Indeed, the chemical industry in Ukraine accounted for around 9% of its exports before the war began.

Professor Helen Sneddon, Director of the Green Chemistry Centre of Excellence noted, 'We were keen to help in any way we can in the hope of a tangible benefit to Ukraine and in the hope that it would facilitate future projects helping monitor the damage, facilitate the clean-up, and ultimately 'build back better'. We are keen to learn from our Ukrainian colleagues – and see how best we can collaborate in future.'

Anything you can do...

Phosphorus as a transition metal mimic



Catalysts play an important role in the synthesis of many of the key compounds essential to our daily lives such as polymers, pharmaceuticals and agrochemicals. Catalysts based on transition metals are amongst the most important and widely used and central to this success is the ability of the metals to shuttle around electrons, that is change their oxidation state. Despite their importance in catalysis, many transition metals are scarce and expensive (such as rhodium and palladium) and so there is great interest in finding cheaper alternatives.

As part of an EU-funded Marie-Curie Network Grant, a team formed between the University of York and the Laboratory of Coordination Chemistry in Toulouse, France, have discovered a way to make simple, cheap and readily available phosphorus compounds mimic the flexible oxidation state behaviour of transition metal catalysts.

Working under the supervision of Jason Lynam and John Slattery in York, and Christian Lorber and Antoine Simmoneau in Toulouse, PhD student Sara Bonfante demonstrated for the first time that a simple phosphine-based catalyst can promote the functionalisation of C-F bonds in fluoroaromatic compounds. Such reactions are important for the preparation of industrially relevant fluorine-containing molecules.

Importantly, her work demonstrated that the phosphine was acting in a similar way to a transition metal, in changing oxidation state to promote the key steps in the reaction mechanism. As all the reagents involved were cheap and readily available, this discovery represents a cheaper and potentially more sustainable method, replacing transition metal compounds, for the synthesis of some chemicals. The work has been published in the *Journal of the American Chemical Society*, 2024, **146**, 2005.

STOP PRESS

CDT Success

The Department has been successful in being a partner in the award of two new Centres for Doctoral Training funded by UKRI, namely The Chemical Synthesis for a Healthy Planet (CSHP) CDT (with the University of Oxford) and The Process Industries: Net Zero (PINZ) CDT (with Newcastle University). The York lead on both is Professor Helen Sneddon, Director of the Green Chemistry Centre of Excellence. The CDTs will result in more than 27 PhD studentships in the Department over eight years and will involve more than 40 companies, from large multinationals to SMEs. A full story will appear in the next issue.

STOP PRESS

Marking Ten Years of Manganese Photochemistry

Some ten years after beginning to work together on photoinduced catalysis using complexes of manganese(I), Ian Fairlamb and Jason Lynam have pulled all of this beautiful work together in a review article in the prestigious journal *Accounts of Chemical Research*.

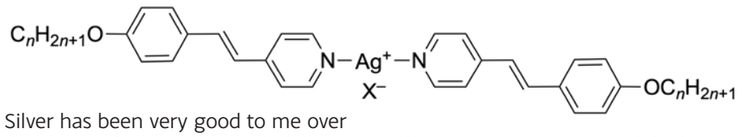
The work has been a real team effort with extensive collaboration with colleagues at the Central Laser Facility and those in industry, not to mention some in York. It was also recognised by a Horizon Prize from the Royal Society of Chemistry.

A full story will be found in the next edition.

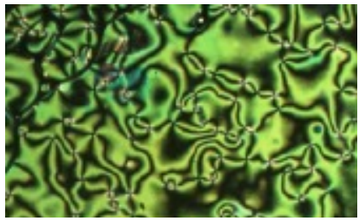
In My Element
Silver

^{47}Ag

IN A NEW FEATURE, PEOPLE ARE INVITED TO NOMINATE A FAVOURITE ELEMENT FROM THEIR WORK. DUNCAN BRUCE KICKS US OFF...



Silver has been very good to me over the years. I first used it as a halide-abstracting reagent during my PhD studies of platinum complexes (*J. Chem. Soc., Dalton Trans.*, 1984, 2249), but it was when we began preparing liquid-crystalline complexes with silver at the heart of things that my relationship with it blossomed. The first complexes studied are shown in the diagram and in fact at the time, the struggle was in preparing the ligand (although we are now very much better at that). Two anions (X^-) in particular proved interesting, namely $CF_3SO_3^-$ (OTf) and $C_{12}H_{25}OSO_3^-$ (dodecyl sulfate or DOS).



We learned a great deal of liquid crystal science from these materials over several years. For example, both the OTf^- and the DOS^- salts above were the first examples of ionic materials showing a nematic phase. Six of the DOS^- salts showed a cubic phase, which at the time was half of those known anywhere, and using both these complexes and those related by having two terminal alkoxy chains on each ligand, we were able not only to provide great insight into the transition between columnar and cubic phases, but also annunciate structural principles common to materials forming the mysterious cubic phase. Much of this is captured in two publications (*J. Mater. Chem*., 2001, **11**, 2852 and *Acc. Chem. Res.*, 2000, **33**, 831). From our first publication (in Nature!) in 1986 to our most recent in 2022, silver has lasted a (professional) lifetime and I think it still has more to give.

Solar energy to power air pollution research

A solar energy system has been installed to power the laboratories of the Department's Wolfson Atmospheric Chemistry Laboratories.

Championed by WACL's Professor James Lee and funded by the Natural Environment Research Council, the new system covers 500 m^2 of roof space, and is expected to generate around 35,000 kWh of electricity annually.

Recognising that scientific activities have environmental impacts, the air quality research site in York is now using solar energy to reduce greenhouse gas emissions by 7245 kg CO_2e and provide 12% of the building's total yearly power usage.

Eleanor and Guy Dodson Building formally opened

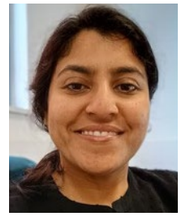
It was a delight to see the formal opening of the Eleanor and Guy Dodson Building by Nobel Laureate Dr Richard Henderson of the MRC Laboratory of Molecular Biology in Cambridge. Described as probably the highest-specification building on campus, it houses the Department's state-of-the-art capability in electron cryo-microscopy, as well as facilities for X-ray structure determination, protein crystallisation and high-field, cryo-probe NMR spectroscopy. Its construction was paid for by a generous grant from the Wolfson Foundation and by the University of York, while the equipment was funded by the Wellcome Trust, Biotechnology and Biological Sciences Research Council, and Dr Anthony H Wild, an early York Chemistry graduate and generous benefactor to the Department.

The building's name pays tribute to the pivotal role played by Eleanor and the late Guy Dodson in establishing the world-renowned York Structural Biology Laboratory (YSBL) within the Department of Chemistry. It is fitting that the opening was performed by Richard Henderson, a long-standing friend of YSBL, whose 2017 Chemistry Nobel Prize recognised his part in developing electron cryo-microscopy.

The technique has revolutionised the study and understanding of biomacromolecules as it allows their structures to be determined without the need for perfect single crystals. It also enables the structural characterisation of proteins too large for existing X-ray methods and, in addition, has the facility to allow tomographic imaging of very much larger features in cells.

The day, which included an outreach event for local schools, culminated in a packed public event with lectures by Richard Henderson and Dr Jamie Blaza, the academic lead on the new facility.

Dr Purba Mukherjee joins YSBL



DR PURBA MUKHERJEE, AN EARLY CAREER ACADEMIC, JOINED THE YORK STRUCTURAL BIOLOGY LABORATORY (YSBL) IN THE DEPARTMENT IN FEBRUARY HAVING BEEN AWARDED A £1.7M EPSRC OPEN FELLOWSHIP TO DEVELOP SUSTAINABLE, ENZYMATIC ROUTES TO MAKING NUCLEIC ACIDS AND THEIR CONJUGATES.

After her first degree at the West Bengal Institute of Technology, Purba moved to the State University of New York at Albany to complete her PhD, studying mechanism and fidelity in replicative and repair DNA polymerases. She continued her research with postdoctoral positions at Harvard Medical School in Boston studying DNA replication in Herpes Simplex Virus and at the Scripps Research Institute in La Jolla working on mechanisms of coagulation and thrombolysis. She then returned to her native India setting up a research group in Kolkata before moving to York. She writes:

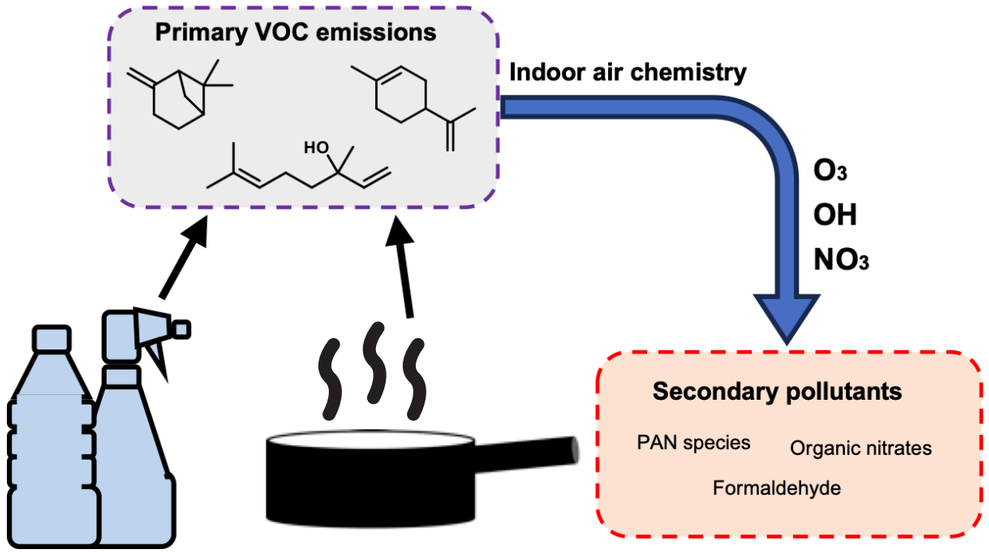
'Since the introduction of insulin, an array of therapeutic biomolecules have gained relevance as effective medicines. A recent addition to this group are nucleic acids and their analogues, including chemical hybrids made from nucleic acids and other types of biomolecules, such as the protein/peptide-nucleic acid conjugates (PNCs). These have joined the repertoire of next-generation therapeutics and are providing targeted approaches for treatment of rare, hereditary diseases – such as Duchenne muscular dystrophy and spinal muscular atrophy, that are highly debilitating and frequently lethal in childhood.

Nucleic acids and PNCs are being developed for myriad other applications including as sustainable biomaterials, drug delivery systems, vaccines and data storage solutions, to name a few. This breadth of potential uses is in part because chemical hybrids synergise the properties of their individual molecular parts and open up new possibilities. A major roadblock, however, lies in making such large chemically diverse molecules by simple synthetic processes which, consequently, has influenced downstream translation.

In the next five years, our group will build nature-inspired nanomachines from repurposed enzymes to reduce the synthesis process of PNCs to a one-pot reaction. DNA polymerases are enzymes involved in making copies of nucleic acids present in organisms, be it humans, bacteria or viruses. Group members will focus on studying and designing specialised DNA polymerases capable of performing unique reactions with nucleic acids.'

Reflecting on this Purba said, "Bringing enzymes into the picture can help reduce intermediate steps of purification when making PNCs and nucleic acids. Ultimately, this should make processes more cost effective, making access to these beneficial molecules much easier in underdeveloped nations across the world. I am very excited to start implementing my ideas to achieve our bigger aim of developing greener means to make large biomolecules. This funding from UKRI will allow me to make complex biologicals with real world implications."

Tony Wilkinson, who currently heads YSBL added, "We are delighted to have Purba join our grouping with her ambitious research programme that sits well alongside our traditional and growing strengths in structural and chemical biology."



The enemy within – what's cooking (and cleaning) at your place?

VOLATILE ORGANIC COMPOUNDS (VOCs) ARE AN IMPORTANT GROUP OF AIR POLLUTANTS, WHICH ARE EMITTED BY A HUGE RANGE OF DOMESTIC PRODUCTS, SUCH AS CANDLES, AIR FRESHENERS, BUILDING MATERIALS, SOFT FURNISHINGS AND CLEANING PRODUCTS, AS WELL AS BY ACTIVITIES SUCH AS COOKING AND CLEANING. DOMESTIC COOKING AND CLEANING IN HOMES ARE LARGE SOURCES OF VOCs.

In developed countries, people spend approximately 90% of their time indoors and so understanding the VOCs inhaled is important, for while many are harmless, some react with other compounds found in indoor air to form secondary products that are more harmful.

A research team led by Professor Nicola Carslaw in the Department of Environment and Geography and Dr Terry Dillon from the Wolfson Atmospheric Chemistry Laboratories (WACL), Department of Chemistry and funded by the EPSRC, recently published results from such studies.

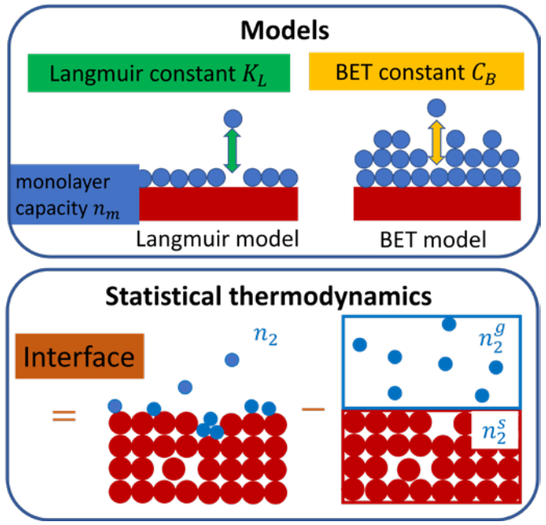
In one study led by postdoctoral fellow Dr Helen Davies, the WACL research team investigated the types of VOCs that are emitted from cooking a typical meal. A stir-fry was cooked multiple times whilst the air was sampled and the use of Selected-Ion Flow-Tube Mass Spectrometry (SIFT-MS) allowed for real-time VOC monitoring. The results, published in *Environmental Science: Processes & Impacts* (2023, **25**, 1532), showed that: frying with oils resulted in large amounts of harmful aldehydes being emitted, vegetables produced alcohols and cooking spices yields high concentrations of reactive monoterpenes (naturally occurring fragrance compounds).

This same technique was then used in the laboratory in combination with another high-resolution mass spectrometry technique to measure the VOCs emitted directly from a range of regular and green cleaning products. In reporting the results, which were also published in *Environmental Science: Processes & Impacts* (2024, **26**, 436), PhD student Ellen Harding-Smith showed that these reactive monoterpenes were also found in both regular and 'green' fragranced cleaning products. Indeed, the 'green' cleaning products were found to emit more monoterpenes compared to regular cleaners, while non-fragranced products (green and regular) emitted much less.

Results from both studies were then used to simulate virtual cooking and cleaning experiments using computer models developed in the Department of Environment and Geography. The modelling demonstrated that monoterpenes from cooking and cleaning were the main driver of formaldehyde production. Formaldehyde is a known carcinogen at high enough concentrations. The identity of the monoterpenes in the cleaning products was important as some monoterpenes are much more reactive than others, and so can produce larger quantities of the harmful secondary products. While green cleaners emitted more monoterpenes overall, it was the regular cleaning products that emitted the most reactive species and thus were responsible for more harmful secondary products.

Re-writing Isotherm theory – Dr Seishi Shimizu's success in Langmuir

AN ACADEMIC IN THE DEPARTMENT OF CHEMISTRY HAS HAD OUTSTANDING SUCCESS WITH HIS RECENT PAPERS AMONG THE 'MOST READ' ARTICLES IN LANGMUIR, A LEADING INTERNATIONAL JOURNAL DEALING WITH SURFACE AND COLLOID CHEMISTRY PUBLISHED BY THE AMERICAN CHEMICAL SOCIETY.



Dr Seishi Shimizu's recent research papers, which focus on sorption isotherms, have proved popular with the Langmuir readers.

Sorption isotherms are important in a range of disciplines and applications, such as how food moisture content and cement paste change with humidity, measurement of the porosity and surface area of materials, and the characterisation of battery electrodes. The use of isotherms in these areas is very well established and many of us are very familiar with the most popular isotherm models such as Langmuir, BET, and GAB. However, working with Professor Nobuyuki Matubayasi of Osaka University in Japan, Seishi realised that there were some fundamental flaws in the way many of these analyses are carried out.

Rather than add yet another model to sort it all out, the two researchers addressed the problem starting from fundamental principles of statistical thermodynamics. Literally using pen and paper, they developed:

- universal basic equations for sorption isotherms (valid for any surface shape and geometry, incorporating adsorption and absorption)
- a universal method to derive isotherms *via* differential equations
- the capacity to model all six IUPAC isotherm types by the combination of only two statistical thermodynamic isotherms

Seishi then extended his theory further to sorption from solution, where the simplistic adaptation of the gas adsorption model precluded clarity for decades.

Now, many of his theories have been made interactive by long-term collaborator Professor Steven Abbott, and are therefore usable for practitioners with their own data.

Towards the end of 2023, four papers from the collaboration were featured in the 20 'Most Read' articles in Langmuir in the period of a month and now two of them appear in the most read articles of the last 12 months out of more than 550 published in 2023.

As any researcher will tell you, when you start to suggest that well-regarded and much-loved theories need an update, then choppy water can lie ahead. It is testament to the rigorous application of theory by the two collaborators that the work has attracted so much attention.

The four papers, all authored by Shimuzu and Matubayasi, that made it in the '20 Most Read Articles (30 days), are given below, with the first two being those that still feature in the Most Read Articles of the last 12 months.

- *Surface Area Estimation: Replacing the Brunauer–Emmett–Teller Model with the Statistical Thermodynamic Fluctuation Theory, Langmuir,* 2022, **38**, 7989.
- *Understanding Sorption Mechanisms Directly from Isotherms, Langmuir,* 2023, **39**, 6113.
- *Sorption from Solution: A Statistical Thermodynamic Fluctuation Theory, Langmuir,* 2023, **39**, 12987.
- *Cooperativity in Sorption Isotherms, Langmuir,* 2023, **39**, 13820.

From 2-D to 3-D in fragment-based drug discovery

PROFESSOR PETER O'BRIEN REFLECTS ON THE SUCCESSES AND LEGACIES ARISING FROM HIS ROYAL SOCIETY INDUSTRY FELLOWSHIP WITH ASTRAZENECA, HELD IN THE PERIOD 2019-2023.

The idea behind this fellowship was the two-way exchange of know-how and expertise between myself and the fragment group at AstraZeneca. As it happened, my main contact was an ex-York undergraduate for whom I had been the supervisor for their final-year MChem Year in Industry project – it's a small world!

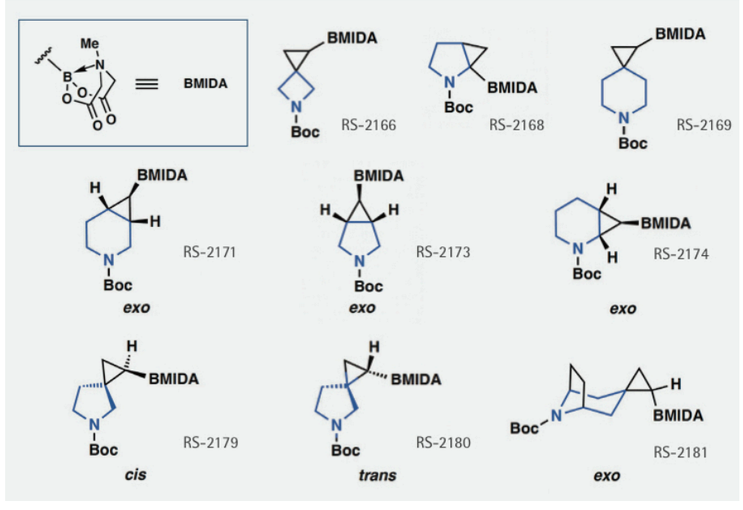
Much of the beginning of the fellowship was during the Covid-19 pandemic and so many of these early meetings were on-line, although this did enable the easy participation of AstraZeneca staff from other sites in the UK as well as in Sweden and the USA. There were weekly Hit Discovery meetings and three-monthly Oncology Scale-up meetings in which I could participate, feeding in ideas to ongoing projects. Pleasingly, after the Covid restrictions at AstraZeneca were eased, I was then able to have two very productive research visits to Cambridge, aided by an extension to the original timescale of the grant.

The fellowship had at its heart a growing project in my group in the area of fragment-based drug discovery. In particular, we wanted to develop a new modular synthetic platform that could allow the elaboration of small-molecule, 2-D fragment hits in drug discovery programmes into 3-D lead compounds for further development. We were able to transfer some of the compounds synthesised in York to AstraZeneca for 'Wave 1 analysis', which measures or generates computationally a range of medicinal chemistry-relevant properties. Combined with biochemical assay data on some of our compounds, we generated a really elegant proof-of-concept case study for our 3-D fragment elaboration concept and we are just in the final stages of putting together a paper to present these exciting results.

Another aspect enabled by the fellowship project was commercialisation of the 3-D building blocks central to the synthetic methodology, which we started with the SME Redbrick Molecular and which continued through Key Organics who now sell around 20 of our 3-D building blocks (some are shown in the image below).

While the original project started with cyclopropanes, it is now being extended to cyclobutanes through a co-funded PhD project supported by the Department and AstraZeneca, which will extend our collaboration into 2026 and hopefully beyond. However, perhaps the most unexpected development that the Fellowship made possible was a completely new project focused on a fragment-based approach to inhibitors of the Nsp3 Macrodomain (Mac1) found in SARS-CoV-2. This was a direct result of the pandemic and the fact that, in early 2020, collaborators at Oxford and Diamond were screening compounds from their libraries against some of the proteins found in SARS-CoV-2; this included around 100 York 3-D fragments from a pre-Fellowship project. Our compounds featured in publications that reported hits against two of the SARS-CoV-2 proteins, one of which has led to the new project.

During the Fellowship, I was also able to see directly the wide range of diverse and talented researchers at AstraZeneca in action, trying to develop the drugs of the future. The company has a strong and impressive commitment to championing inclusivity and diversity, and it was a privilege to see this first hand. Overall, it was a very productive and exciting period for both myself and the group as we were able to do things that would not have been possible without AstraZeneca's support.



Professor Paul Andrew Clarke

(25 October 1970 - 22 November 2023)

IT IS WITH GREAT SADNESS THAT WE REPORT THE PASSING OF OUR FRIEND, COLLEAGUE AND MENTOR PAUL CLARKE, WHO DIED ON 22 NOVEMBER 2023 AFTER A YEAR-LONG ILLNESS.

Paul grew up in Plymouth, and began his Chemistry career at the University of Bath where he obtained his BSc(Hons) in 1993. He remained at Bath for his PhD under the supervision of Professor Alan Armstrong, studying intramolecular dioxirane epoxidation reactions. In 1996, he moved to Florida State University where he spent two years working with Professor Robert Holton on the synthesis and functionalisation of taxane ring systems, before returning to the UK as a postdoctoral researcher with Professor Chris Moody at Exeter. He got his first academic job in 1999 at the University of Nottingham and then in January 2006, Paul moved to York as a Senior Lecturer, being subsequently promoted to Reader and then Professor. He was admitted as a Fellow of the Royal Society of Chemistry in 2009.

Paul carried out high-quality research in organic chemistry, ranging from natural product synthesis with a focus on oxygen-containing heterocycles, through to studies of potentially prebiotic reaction processes and was an outstanding mentor to the many scientists who spent time in his research team. He was a much-valued colleague who made many contributions to improve student training. For example, he thought through and led on the revised structure for practicals in the teaching laboratory, which saved the day when in 2010 we ended up taking around 50% more students than we had envisaged. Then during his tenure as Chair of the Department's Graduate School between 2013 and 2015, he did much to re-imagine graduate training with the establishment of the Department's bespoke *i*DTC. He cared deeply about external speakers, running a contemporary organic chemistry seminar series for many years, hosting visitors from around the UK and the world – always with panache and a twinkle in his eye. He was also an integral member of the Department's coffee club, where he would regularly swap stories with colleagues about the night before and share opinions on life, the universe and everything in between.

Beyond York, Paul was an active member of the UK and international Chemistry communities. He was a visiting academic at Universidad Complutense, Madrid, Spain in 2010 and 2011, and at the Research School of Chemistry at the Australian National University, Canberra in 2018. He was also an alumnus of the Apeldoorn (NL-UK: North Sea Neighbours) 2012 Conference 'Higher Education at the Heart of Growth'. From 2013-2017, he was a member of the Editorial Board of the international open-access journal *Advances in Chemistry* and also served on the Editorial Boards of *Life* and *Science of Synthesis*. Paul was an active member of the Society for Chemical Industry (SCI) and recently completed a period as Chair of the Yorkshire and Humber SCI Regional Committee. He was also very well known for organising the Gregynog conference for early career chemists.

Paul was a gregarious individual and an inveterate traveller, with a particular love for Australia. He had a very wide circle of friends and his parties were the stuff of legend, especially when it came to marking Eurovision. His views on matters of the day were strong and sincerely held, and recently he led a local residents' campaign in opposition to the expansion of the National Railway Museum, which would restrict pedestrian and cycling access to the city for residents of the St Peter's Quarter where he lived.

Sadly, in October 2022, Paul was diagnosed with glioblastoma (a malignant brain tumour), but while he received the best possible treatment, the disease progressed. In November 2023, just over a year later, he passed away in the comfort of his own home, surrounded by friends, family and his husband and best friend, Szczepan.

Paul lived his best life to the end, holidaying at the Savoy with Szczepan during the summer and meeting friends for drinks whenever his health was up to it. He has left a significant hole in the Department and we have all noted how difficult it has been to walk past his empty office. Paul's popularity and the respect he engendered were demonstrated through the large turnout for his funeral at the start of December. Cremated in an outfit that would have looked great on any dancefloor and sent off with the congregation raising a shot of vodka and to the beat of Kylie's Your Disco Needs You, it was an opportunity for family, friends, colleagues and former students from York and beyond to say goodbye.

Head of Department Caroline Dessent summed up the feelings of many: "All in the Department were terribly saddened by Paul's death. He was a talented synthetic chemist, who was deeply respected for his independence of thought, and his honest and enthusiastic support of the students and academics with whom he worked. He will be very sorely missed by his friends and colleagues at York and across the wider Chemistry community."

Reflections from the editor's chair

AFTER COMPILING SOME THIRTEEN ISSUES OF CHEMYORK, PROFESSOR DAVE SMITH HAS HANDED THE BATON ON TO DUNCAN BRUCE, WHO NOW INVITES HIM TO REFLECT ON HIS TIME AT THE HELM.

What has been your approach when looking for stories to include in each edition?

I've always tried to reflect the full diversity of the Department's activities and uncover the most interesting stories. Some, such as those concerning research prizes and papers, or major teaching innovations, are easy to find out about. Others – for example, the amazing things our students or staff have achieved both inside and outside the Department – can be more difficult to track down. Ultimately, I wanted to reflect a Department that is academically vibrant, but also has a sense of community, with people at the heart of everything it does.

What have you learned about the Department in more than six years of compiling ChemYork?

I have learned that there are some remarkably talented people doing incredible things. Compiling a story about our many academic staff who won ERC Fellowship Grant Awards opened my eyes to some real research leadership, including from staff then only recently appointed. Meanwhile, writing a feature on Andy Parsons' fantastic Massive Open Online Course (MOOC), Exploring Everyday Chemistry, showed me how chemistry education could reach out from the Department and touch thousands of lives across the world. Putting together the magazine has been a joy, as I have got to see the very best of the Department, and help celebrate it.

Do you have a favourite story?

I think my favourite story, and one of the most impactful, was from early 2020, when with Covid-19 rapidly approaching, members of the Department worked together to collect PPE and donate it to local healthcare facilities. It was a time when many of us felt powerless, yet that sense of coming together before what we knew was going to be a difficult few years was exceptionally powerful in giving people a sense of meaning and community. Writing about that was a genuine privilege.

Handing this role on will hopefully give you a little more time to concentrate on your science among other things. What is your group working on at the present time?

My group works on supramolecular gels made from small molecule building blocks. On a fundamental level we try to understand how complex mixtures of molecules behave, trying to 'program them' with smart properties. We also engineer our gels by introducing dynamic shaping and patterning. Ultimately, we want our gels to be useful.

For example, we are using gels to stabilise highly reactive chemicals, so that they can be handled more safely and easily in the laboratory (image is of a gel-stabilised organolithium reagent). We have also been using gels for enhanced nasal delivery of active pharmaceuticals directly into the brain – with the potential to treat neurodegenerative diseases.

As well as communicating science to academic peers, you've given many schools and other lectures. What motivates you to do this?

Almost all of my family (parents, grandparents and great grandparents) were teachers – I think there is a gene for it! I love teaching at university level and, in particular, I enjoy trying to inspire students with 'context' – the applications of fundamental chemistry. I often speak at large events attended by many different schools, but reflected that pupils from disadvantaged backgrounds may not have the chance to attend. That was a driver in setting up a YouTube channel to talk about chemistry. In principle, anyone can watch it in their bedroom, making it accessible and inclusive.

You've also been a passionate advocate for EDI. How is that landscape changing?

In many ways, much progress has been made. Minority scientists have more visibility than ever before, and support systems in science are slowly improving. However, the current climate is proving a little more challenging and progress in some areas, such as institutional racism, would seem to have stalled. Hopefully, this is a blip, and progress towards greater inclusion will get back on a political track in the future. I'll certainly be working to try and achieve that.

> "Putting together the magazine has been a joy, as I have got to see the very best of the Department, and help celebrate it."