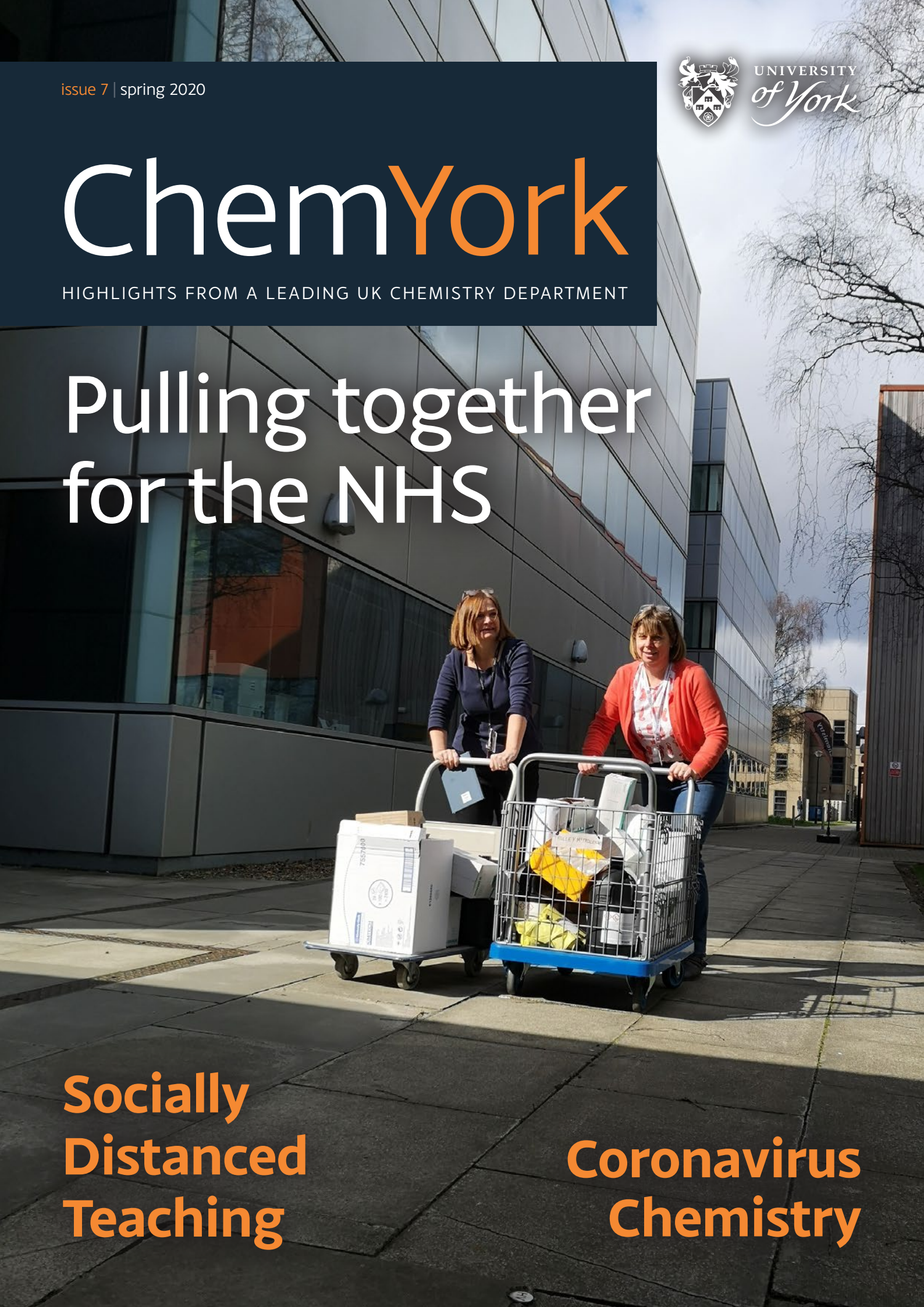
issue 7 | spring 2020

UNIVERSITY of York

ChemYork

HIGHLIGHTS FROM A LEADING UK CHEMISTRY DEPARTMENT

Pulling together for the NHS



Socially Distanced Teaching

Coronavirus Chemistry

Welcome

PROFESSOR DUNCAN BRUCE, HEAD OF DEPARTMENT, INTRODUCES THE SPRING EDITION OF CHEMYORK.

Let me start this introduction to the Spring 2020 edition of ChemYork by saying that I hope all of you reading this, your families and friends have been able to stay safe in these most difficult of times and that you are finding ingenious ways to manage lockdown.

In this edition as in others, you will read about the exploits of our colleagues and students, their successes and recognition, their advances in research and teaching and some of the wider activities of the Department. However, one difference will be the common theme that underpins several of these stories – COVID-19. You will read about the different responses in the Department – from the research work that is part of a national effort to understand the virus and to understand its effects, to the fantastic response in providing PPE to the local NHS, to the ways we have had to change our teaching.

And then there are the things that are less visible. Our undergraduates and taught postgraduates, at different stages of their degree, are now finishing the academic year via remote learning with tutorials and seminars held using Google Meet, Zoom or Blackboard and exams and other assessments conducted online. Our postgraduate research students, whose projects are on hold, are writing parts of their thesis where they can and researching the literature while all the time hoping to get back into the lab. Our postdoctoral fellows are in a similar position – writing papers where they can and wondering how they can make up the lost time. And underpinning much of this, the academic, technical and administrative staff of the Department who are silently somehow keeping all of this on the rails.

> "Times like this can bring out the very best in people and frankly I am overwhelmed with pride in the way that all members of the Department have risen to the multitude of challenges they are facing."

In all of these groups, people face their own challenges in both doing their work and coping with isolation. Many are living in households where the needs of young and even very young children have to come first. Some will be working with poor internet connections or with shared IT capability which limits all they might like to do. And some are in households that have been visited by COVID-19 and who have coped with the illness, anxiety and exhaustion that can follow infection. And some have lost loved ones.

But one of the things I know about my colleagues and our students, is the way they will go several extra miles to support one another. This is something that you will find evident in reading this edition. Times like this can bring out the very best in people and frankly I am overwhelmed with pride in the way that all members of the Department have risen to the multitude of challenges they are facing. For example, we now run our research seminars online so we can keep the collective research culture going. I am therefore delighted that we are able to record some of these successes in this issue. Our colleagues deserve this recognition. From ground-breaking research, to grants and awards that reflect advances in both teaching and research, to innovative approaches to teaching at a distance, there is much of which we can and should be very proud.

Virus researchers, Dorothy Hawkins, Oliver Bayfield and De-Sheng Ker (left to right) discuss progress.

Front cover image:
Christina Surdhar

Compiled by David Smith and Christina Surdhar

Designed by Cookie Graphic Design

Award winners

By royal appointment – Queen's Anniversary Prize for YSBL

The pioneering work of the University of York's Structural Biology Laboratory (YSBL) in the Department of Chemistry has received royal recognition.

The prize, the highest national honour awarded in UK Further and Higher Education, is for the work of the YSBL in studying proteins. The ceremony at Buckingham Palace was carried out by HRH The Prince of Wales and HRH The Duchess of Cornwall.

YSBL researchers study proteins: developing methods for determining what they look like and how they work, and exploiting this knowledge. The methods developed in York are used by thousands of scientists around the world.

Studies of individual proteins in YSBL have revolutionised fundamental understanding of living processes. These vital insights have directly contributed to the development of new medicines, such as modified insulins for treating diabetes, and been used in industrial processes to improve sustainability and food security. The Laboratory continues to evolve with new initiatives in advanced imaging methods and a reputation for studying the sugar molecules that are vital to living organisms.

Professor Tony Wilkinson, head of YSBL, explained: "YSBL works at the intersection of many different disciplines, harnessing the synergy of physics, computing and chemistry to answer questions about biological processes. This prize recognises the quality of the work of the many hundreds of scientists who have passed through the Laboratory and benefitted from our collaborative and flexible culture."

VIce Chancellor of the University, Professor Jeffery, who received the award alongside Professor Wilkinson added: "This award is a fantastic achievement and richly deserved. It recognises the excellence and dedication of the YSBL team over more than 40 years."

Dr Penkman wins major award

Dr Kirsty Penkman was recognised by the prestigious Blavatnik Family Foundation and New York Academy of Sciences for her pioneering work in fossil dating. She is the Foundation's 2020 Chemistry Laureate, receiving an award of £75,000. The Blavatnik Awards for Young Scientists recognise the pioneering work of academics under the age of 42.

Dr Penkman's work has led to improvements in the accuracy of dating fossils from the last three million years, leading to new insights into human evolution and climate change. Her research focuses on the analysis of fossil biomolecules: their pathways of degradation, methods for their detection, and explores the information these molecules can provide about an organism's history.

Professor Deborah Smith, Pro-Vice-Chancellor for Research, said: "Dr Kirsty Penkman's ground-breaking work has brought new insight into our understanding of how ancient events impact on the world today. The award of this prestigious prize is richly deserved and will inspire others who follow in her pioneering footsteps."

Professor Duckett wins Gunther Laukien Prize

Professor Simon Duckett was a recipient of this year's Gunther Laukien Prize – awarded annually for cutting-edge nuclear magnetic resonance (NMR) research. He was recognised for his pioneering research on developing methods that are expected to dramatically improve the quality of medical imaging, helping to fight diseases like cancer. Researchers hope that in the future, doctors will be able to accurately make diagnoses in minutes from advanced MRI scans. Currently this takes days, weeks and sometimes months to implement.

The underpinning technique, known as Signal Amplification by Reversible Exchange (SABRE), has been developed by scientists in York since their first report in the journal Science in 2009. It works by magnetically labelling drugs or substances that occur naturally in the body, without changing their molecular structure, making the method very safe and versatile.

Professor Duckett, was a joint winner of the prize along with Konstantin Ivanov (Novosibirsk State University) and Warren S. Warren (Duke University). The prize carries a monetary award of $20,000 to be divided equally among the awardees and was officially presented to Professor Duckett at the Experimental Nuclear Magnetic Resonance Conference in Baltimore in March.

From soup to cells: a potential role for gels in the chemistry of life

A STUDY BY PROFESSORS DAVID SMITH AND PAUL CLARKE CASTS NEW LIGHT ON THE ROLE OF GELS IN THE EVOLUTION OF LIFE.

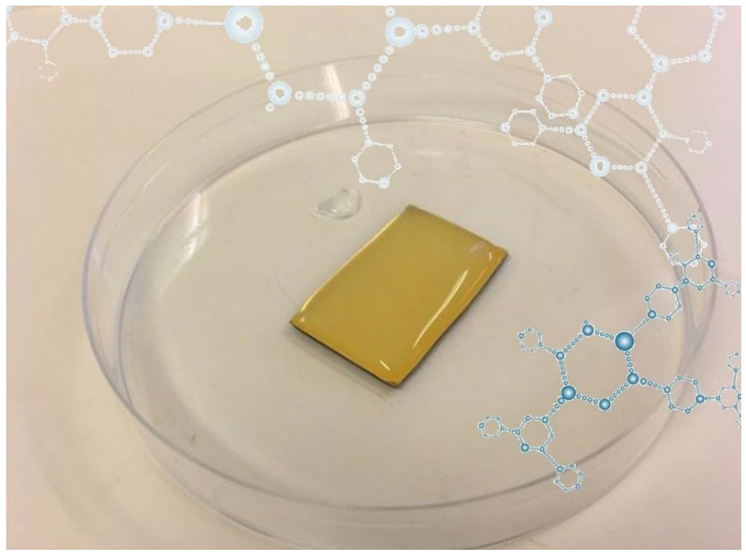
Professors David Smith and Paul Clarke from York's Department of Chemistry investigated the role of gels in the formation of simple cell-like structures drawn from the chemicals present in the early Earth's 'primordial soup' - where life is thought to have begun. As part of her PhD studies in their labs, Kirsten Hawkins discovered a new gel that could spontaneously assemble from component parts that may have been present in the primordial soup (Journal of the American Chemical Society, 2020, 142, 4379).

The team then demonstrated that the gel could be useful in a prebiotic worldby catalysing an important sugar-forming reaction in water, with good yield and selectivity. Making sugars with defined chirality is an important step in prebiotic chemical evolution. Most excitingly, the catalyst was only active when it was self-assembled as a gel. If it was added in non-assembled form, the reaction did not proceed.

The researchers argue that their hypothesis that gels could have played an important role in the evolution of simple cells will go on to influence others working to understand how life first emerged.

New way to test for drug resistant infections

A TEAM OF SCIENTISTS ACROSS THE UNIVERSITY, INCLUDING PROFESSOR ANNE DUHME-KLAIR AND DR LISA MILLER, HAS DEVELOPED A METHOD TO TEST WHETHER AN INFECTION IS RESISTANT TO COMMON ANTIBIOTICS.



Antimicrobial resistance (AMR) is a major global threat accelerated by the inappropriate use of antibiotics. Beta-lactam antibiotics (such as penicillin) are one of the most important classes of antibiotics, but resistance to them has grown to such an extent that doctors often avoid prescribing them in favour of stronger drugs.

Corresponding author on the paper, Dr Lisa Miller, a postdoctoral researcher working in the team of Professor Anne Duhme-Klair, modified an antibiotic from the beta-lactam family so it can be attached to a sensor, enabling the detection of bacteria resistant to treatment.

The new method, published in ACS Appl. Mater. Interfaces, 2019, 11, 32599, could lead to clinicians being able to rapidly detect whether an infection is treatable with common antibiotics, reserving stronger alternatives for the patients that need them most. The research team are now working with clinicians at York Teaching Hospital NHS Foundation Trust to integrate their system into a rapid diagnostic test for antimicrobial resistance in urinary tract infections.

Synthesis of an 'impossible' complex

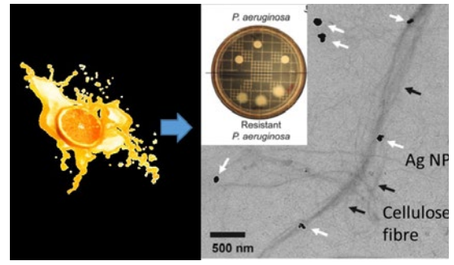
PROFESSOR ANDREW WELLER AND HIS RESEARCH TEAM, LED BY PHD STUDENT TIM BOYD, HAVE SYNTHESISED A FASCINATING NEW COBALT COMPLEX PREVIOUSLY CONSIDERED TOO REACTIVE TO MAKE.

They achieved the synthesis of a highly unstable, paramagnetic, cobalt(I) alkane complex using a single-crystal to single-crystal conversion in the solid phase driven by simple addition of hydrogen gas. This allows a stable precursor to be converted into the desired complex in the solid-state. This approach is needed because the weakness of the metal-alkane bond means such species would not survive using traditional solution techniques. A key aspect of the stabilisation in the solid-state comes from a surrounding anion microenvironment, which forms a protective cage around the highly-reactive metal cation. The paper was published in Angewandte Chemie, 2020, 59, 6177, with the 'impossible complex' being highlighted in the journal's cover art.

Such metal-alkane complexes are key intermediates in C–H activation reactions: processes that turn simple hydrocarbons, which are currently just burned for heat, into valuable feedstocks in the chemicals supply chain. Isolating and understanding the properties of such species can therefore lead to improved, lower energy and more selective methods in synthesis and catalysis.

Innovative Antibacterial Materials

TWO RESEARCH GROUPS IN THE DEPARTMENT HAVE REPORTED INNOVATIVE APPROACHES TO MATERIALS THAT MAY HAVE POTENTIAL BIOMEDICAL APPLICATIONS AS A RESULT OF THEIR ACTIVITY AGAINST RESISTANT BACTERIA.



The rise of antibiotic-resistant bacteria means that antibacterial materials are of key importance. Incorporating silver nanoparticles into materials is an effective way of endowing them with antibacterial properties.

Postdoctoral researcher Dr Carmen Piras, working in the research team of Professor David Smith, has developed well-defined gel beads loaded with silver nanoparticles. As described in Chemistry A European Journal 2020, doi 10.1002/chem.202001349, these beads were created by combining two different gelators, a robust polymer gel to form the shell, and a self-assembling gel that is capable of generating silver nanoparticles in situ as the core.

Dr Clare Mahon demonstrated that these beads were active against drug-resistant bacteria, in particular, *vancomycin resistant enterococcus faecium* and *pseudomonas aeruginosa*, both of which are highly problematic hospital-acquired infections.

Dr Piras explained: "These gel beads are very easy to make and manipulate. They would be straightforward for surgeons to apply into wounds during orthopaedic surgery, and their antibacterial properties could potentially make them valuable for patients during the healing process."

Working in Green Chemistry, Eduardo de Melo, a PhD student in the research teams of Dr Avtar Matharu and Dr Tom Dugmore took a sustainable approach to antibacterial materials. In Scientific Reports 2020, 10, 7281, these researchers reported a novel nano-silver biocomposite derived from cellulose extracted from waste orange peel by microwave methods. Using waste as a resource enables the development of a circular economy, and aligns with UN Sustainable Development Goals.

Working with colleagues from Universidad Autónoma de Nuevo León (UANL) in Mexico, they demonstrated this material shows antimicrobial activity against clinical multidrug-resistant strains, with stronger antimicrobial activity against Gram-negative than Gram-positive bacteria.

Dr Tom Dugmore added, "We've spent a lot of time reducing the environmental footprint on production of these materials from food waste, and it was great to get positive results for their performance in such an important field."

Pulling together in a crisis

DEPARTMENT HELPS COORDINATE THE DONATION OF MEDICAL EQUIPMENT TO SUPPORT THE NHS

On the last day before lockdown, the Department of Chemistry helped coordinate a university-wide collection of medical equipment and PPE to support the NHS. It was an extraordinary day where staff pulled together as the Department became a central hub for donations. We take a look back at some of the events of the day.

The collection was initiated by Archaeology PhD Student Andy Langley, who first got in touch with York Teaching Hospital. The Chief Nurse for the York Pandemic Operations Group provided a list of items that would be useful and a first load of donations from Archaeology and Environment was delivered to the hospital. Head of Archaeology Professor Nicky Milner then contacted the Vice Chancellor, who advised that efforts should be expanded to the rest of the university. When the communication arrived in Chemistry, Operations Manager, Simon Breeden, volunteered the Department as the central collection point.

By 9.00am on Friday 20th March, donations had started to arrive. The call had gone out to research groups in the Department as well as to labs across campus. First arrivals were directed to Chemistry Stores, where Steve Hau and Mike Keogh began to get them ready to ship out. By late morning however, it was becoming apparent that more space would be needed.

With Chemistry's technical team leading the efforts, one of the Department's larger seminar rooms, C/B/102, was transformed into a temporary 'warehouse', which soon began to fill up. Chemistry's Teaching Labs and research groups were now sending across boxes full of donations and more items were pouring in from across campus.

"I think everyone was overwhelmed at the response," said Chemistry's Experimental Officer Graeme McAllister. "At one point it was coming in so fast, it was hard to keep track of who was bringing it. Donations came from Archaeology, Environment & Geography, Chemistry, Biology, Physics, Electronic Engineering, and the Library & Archives, who also provided a van and driver."

By the end of the day, the spacious seminar room was full with donated items. The campus-wide effort had resulted in the collection of 1000 boxes of disposable gloves, 150 sharps bins, 200 boxes each of syringes and needles, over 100 lab coats and over 100 pairs of safety glasses, disposable clothing including aprons, sleeve protectors, boilersuits, overshoes and surgical masks, waste bags, anti-bacterial foaming soap and dispensers, blue roll, tissues and much more, even boxes of tea and coffee for staff.

"Because we pooled items from many departments, we managed to get a large delivery," said Dr David Pugh, Associate Lecturer in Laboratory Teaching. "Departments I wouldn't even have associated with having PPE, such as the library, supplied boxes of disposable gloves which they use to handle items in the archives. We contacted the hospital and said we would hold on to the stuff until they needed it, but they replied within the hour and asked us to send it immediately.

Delivery to the hospital

At around 6.00pm, Simon Breeden spoke to the team about the first delivery, which was to go out to the hospital that evening. ITV Calendar reporter Matt Price also arrived to film a live clip from C/B/102 for the local evening news, as posts on Chemistry's Instagram and Twitter feeds throughout the day had communicated the events far and wide. While waiting to be filmed, Chemistry's technicians passed boxes to one another down the outside steps from C/B/102 to load the van. The first delivery was taken to York Teaching Hospital by David Pugh and Tom Borgia from IT Services, where it was gratefully received. Subsequent deliveries were taken to the hospital on Monday 23rd.

Dr Simon Breeden said: "This was very much led and delivered by technicians across the campus, working in a multitude of academic departments and professional services."

Professor Duncan Bruce, Head of the Department of Chemistry, said: "It has been fantastic to be able to help out. This shows what can be done when people are prepared to pull together - supporting the NHS and all those charged with caring for us is so important. Well done to all who made this possible."

Technicians join effort to make Coronavirus face shields

TECHNICIANS FROM THE UNIVERSITY OF YORK HAVE BEEN PRODUCING PERSONAL PROTECTIVE EQUIPMENT (PPE) FOR FRONTLINE WORKERS AS PART OF THE NATIONAL RESPONSE TO COVID-19.

Working alongside staff from the Departments of Biology and Archaeology, technicians in the Department of Chemistry have helped to produce hundreds of face shields using laser-cut recyclable plastic.

The 2D laser-cut safety visor utilises a design which is being used effectively across the world in the fight against Coronavirus. The design is freely available and may be redistributed and modified.

The initiative was led by Biology Research Workshop Manager Mark Bentley who called on colleagues in Chemistry for help when he realised numbers were increasing after the first batch. "Chemistry has two larger bed laser cutters like Biology, so they were perfect to help," he said. "Mark Roper and Abby Mortimer came in first to start preparing A4 acetate materials for the visors, then I supplied Mark and Stuart Murray with materials for the laser cutting."

"First we prepared acetate sheets to be attached to the headbands, which were going to be cut later," explained Mark Roper, Chemistry Workshops Manager. "I then picked up the remaining stock from Biology - 1000 sheets of A4 acetate. These were hole punched in precise locations to be affixed to headbands, cleaned with isopropanol, and bagged up into batches of 100. Abby did great work here, working in a hugely efficient manner to get the majority of these cleaned and bagged in a timely fashion."

Mark and Stuart then worked on laser-cutting mask component parts from polypropylene while in Biology, Mark Bentley was doing the same. "He cut front bands while we cut the rear bands, so we worked together to get the largest amount of shields made as quickly as possible."

Mark added, "I was only too happy to help. Using our technical skills to help deliver potentially life-saving equipment was really fulfilling."

Abby Mortimer said, "Mark Bentley did an excellent job of coordinating the face shield production, but it was a fantastic team effort from everyone that was involved, both in Biology and Chemistry, which resulted in an amazing 5545 face shields being produced overall. I'm glad I could help out in some way."

The visors have been distributed free of charge through a York collective that has also recruited additional manufacturers and raised funds to support the effort. They are offered to anyone in the York area who is required to work with the public during the pandemic.

Socially distanced teaching and learning

AS WE GO TO PRESS, ALL UNIVERSITY TEACHING IS BEING DELIVERED 'AT A DISTANCE' BECAUSE OF COVID-19. CHAIR OF BOARD OF STUDIES, DR DEREK WANN, AND CHAIR OF TEACHING COMMITTEE, DR NIGEL LOWE, TELL US MORE.

How are Summer term lectures being delivered?
All lectures are online. This was all arranged very quickly and it was not possible to do this with the level of detail that we would if we were planning an online course from scratch. In many cases, lectures recorded from previous years have been made available. However, on some occasions content has been delivered for the first time. (Derek points out that he had to learn how to record himself delivering a lecture from his dining room table!)

How are Summer term tutorials and workshops being delivered?
Nick Wood has done amazing work to help prepare us for online tutorials using Google Meet and Zoom. We were adamant we wanted these to be true to the small-group teaching that we pride ourselves on delivering in York Chemistry. The innovative use of cornflakes boxes, mobile phones and Lego to create devices to capture sketches during online tutorials has been amazing. Student feedback has been positive and attendance excellent. Workshops (normally delivered to 20-25 students) were more challenging. These are being delivered by recording new video content and making problems and answers available. Students can contact their tutor for follow-up questions, and some tutors are offering 'office hours' through Google Meet.

How are Summer term labs being delivered?
David Pugh, Nick Wood, Victor Chechik and Moray Stark worked really hard to deliver lab content true to the learning outcomes. Model data is used alongside in-depth video briefings from the Graduate Teaching Assistants (GTAs) ahead of the 'lab sessions'. Our GTAs have also provided real-time feedback to students using Google Meet while they analyse their data. Integrated Chemistry Group Practicals will also be delivered online, but will incorporate key elements of experiment design by releasing data only in accord with requests from the student groups, meaning that they must plan carefully how to 'collect' their data.

How will Summer term assessment be carried out?
The University took an early decision to cancel Year 1 exams. We will provide study aids to allow these students to assess their own strengths and weaknesses, and guide self-study over the summer. For years 2-4, we have run exams in 24 hour 'open book' form following some adaptations. The University has implemented a 'safety net', helping protect a student's overall mark in the current year based on their previous performance. Perhaps the biggest effect is on our final year MChem students who will not do the normal oral exam with a research talk and questions from academic staff. Students will instead prepare a voice-over for their talk and submit it online. Combined with the cancellation of graduation ceremonies, this will be a rather sad end to 4 years of study.

How have the students been coping with the changes?
Based on the online supervision meetings with our students at the start of Summer term, we were impressed with how many of them were taking the "new normal" in their stride. However, we are aware of students who find working from home very hard. Some students have said how much they miss attending

lectures and the personal interaction this provides. We have hosted e-coffee meetings with each cohort of students, so they could ask questions and get answers from the senior management team. This highlighted problems we had not necessarily considered. We are already learning and will, for example, enhance our online lectures.

How have staff been coping with the changes?
Everyone has been adapting working practices to their new circumstances but there have been extreme challenges for many. It has been amazing to see some colleagues take on a huge amount of extra childcare and still maintain some university work. Our impression is that the wheels of the Chemistry machine are turning with the usual collegiality and goodwill, and we have redistributed workload to alleviate some of the problems.

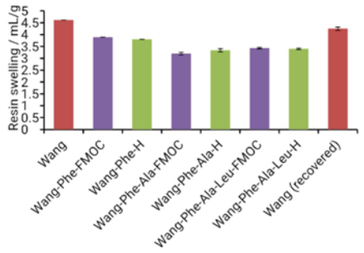
Do you think the Covid shutdown will change our teaching methods in the future?
We think it is likely. Many of the changes we have implemented have made us think about what we teach and why we teach in the ways we do. Some colleagues might now find themselves suggesting a quick online meeting to resolve an issue rather than arranging an office visit. Equally, some of the new resources will live on to support our course. As we turn our thoughts to students arriving and returning in September, we are considering how we can cope with students and staff still working from home, or perhaps a hybrid model where some students attend sessions but in a way that allows social distancing. It will be a challenge, but there is no doubt that we will continue to try and give our students the best possible educational experience in the circumstances.

York Chemistry undergraduates publish world-leading research paper

Research carried out by eight University of York Chemistry undergraduates has been published in an international open access chemistry journal (ChemistryOpen, 2020, 9, 431). The students, led by Professor Michael North and Dr Anne Routledge, investigated how physical and chemical characteristics associated with polymeric resins affect their ability to interact with 15 sustainable solvents.

Understanding how polymers interact with solvents - especially with new, environmentally-friendly and sustainable solvents - is a major challenge, with applications to areas as diverse as pharmaceutical synthesis, polymer synthesis, graffiti removal and plastic recycling.

The results of the students' work indicated that the chemical properties of the polymer had a larger influence on the solvent interaction than the physical properties. This is particularly important for the solid phase-supported multi-step synthesis of pharmaceuticals (e.g. antiviral drugs) because the chemical properties of the polymer will change as the synthesis proceeds. The results show that the optimal solvent may be different for each step of the synthesis. By understanding how the solvents and polymer interact, it becomes possible to choose a single solvent (or solvent mixture) which performs well for every step of the synthesis.



The students involved were Chidi Amadi-Kamalu, Holly Clarke, Matthew McRobie, James Mortimer, Dani Sibbald, Matthew Tickias, Kai Tse, Helen Willway and Yanrui Ran; they carried out the work for various projects, such as BSc group projects, Year 4 MChem projects and summer projects. In addition to contributing to the research, the students gained experience of working as a team and statistically analysing their experimental results for reproducibility.

Professor Michael North said: "This work is an example of how we embed cutting-edge research into the undergraduate curriculum. It is not unique, but is unusual in having involved such a large number of undergraduates."

American Chemical Society education award

Dr Glenn Hurst has been recognised with one of the 2020 American Chemical Society's Committee on Environmental Improvement awards. The award program recognizes individuals and organizations that have made exemplary contributions to the incorporation of sustainability into chemical education.

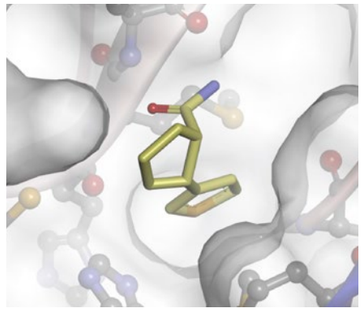
Dr Glenn Hurst was recognised for his work "Systems thinking approaches to teaching green and sustainable chemistry in alignment with the United Nations Sustainable Development Goals". 'Systems thinking' enables students to study the interdependence of components in dynamic systems allowing them to transition from a fragmented knowledge of subject matter to a more integrated and lateral understanding of concepts, resulting in deeper learning.

Dr Hurst explained: "Green chemistry is well suited to a systems thinking approach as the 12 fundamental principles

all depend on the reliance of reactions and processes on each other and with both local and global systems."

Covid-19 Research

Towards novel COVID-19 therapeutics



Professor Peter O'Brien and his research team have synthesised compounds that can bind to one of the key proteins in the COVID-19 virus. Professor O'Brien has an active research programme synthesising 3-dimensional molecular 'fragments' for use in drug discovery. Around 100 of his fragments are part of a national library that was recently screened for binding to the SARS-CoV-2 main protease (MPro), which is part of the COVID-19 virus.

By screening the binding of this library to the main protease enzyme, the team of researchers working at Diamond was able to identify around 60 compounds that were bound to this target. Two of these compounds were fragments synthesised by PhD students Tom Downes and Paul Jones in the O'Brien research team. Their PhD research was funded by a consortium of industrial partners from around the world (Asahi Kasei, Astex, AstraZeneca, Lilly, Pfizer, Vernalis).

One of the fragments was bound in the active site of the protein (see Figure). The fragment, together with the other bound fragments from the screen, could provide a starting point for the development of better binding compounds by applying the techniques of fragment-based drug discovery - the next step in the development of potential therapeutics targeting COVID-19 or other Coronaviruses that may emerge in the future.

Atmospheric monitoring during the Coronavirus shutdown

Research from the Wolfson Atmospheric Chemistry Laboratory (WACL) in the Department of Chemistry has shown that air pollution levels in some UK cities have dropped to levels lower than the average of the previous five years as the coronavirus pandemic disrupts travel and work.

Researchers from WACL, including PhD researcher Will Drysdale, processed data from roadside monitoring sites from 100 cities across the UK to reveal the significant reduction. They used data from the London Air Quality Network and UK Automatic Urban and Rural Network which monitors nitrogen dioxide (NO_2) and particulate Matter (PM2.5) levels. Air pollution causes an estimated 40,000 early deaths in the UK each year. It is linked to health problems including stroke, heart disease, lung cancer and disease, and respiratory diseases and infections, as well as stunting the growth of children's lungs.

The data showed that levels of nitrogen dioxide are down by over 40% in some large cities, including Leeds, Newcastle, Cardiff and Glasgow. Nitrogen dioxide is primarily emitted from vehicle

exhausts, so this reduction is likely to be caused by lower levels of traffic in the cities.

Professor James Lee said: "From our analysis, pollution levels are clearly lower than the average of the previous five years. I would expect them to drop even further over the coming weeks."

Also working within the team in WACL, Professor David Carslaw, who is an expert in urban air pollution, analysed data from local traffic monitoring sites and found that air quality in York has improved by 30 percent in terms of nitrogen dioxide concentrations.

Dr Carslaw said: "Although satellite measurements have been especially compelling, we do of course, have hundreds of ground-based continuous air pollution monitors across the UK that can be investigated to better understand the changes in air pollution at a very local level.

The most significant drop across the city was a 43 percent reduction in nitrogen dioxide concentrations in Fishergate, with a 28 percent reduction in Fulford Road and a 29 percent reduction in both Gillygate and Lawrence Street.

Building on this monitoring work, Professor Alastair Lewis is leading a national scientific advisory group calling for scientists and researchers to share their data on air pollution during the Coronavirus pandemic. He is Chair of the UK Government independent science advisory group on air pollution, who will use the data to inform future air quality management.

Professor Lewis said: "Evidence and insight into possible changes to the factors that control air pollution will help us to refine and improve how we deliver the best possible air quality for the UK. In order to provide more accurate assessment of the potential impacts of air pollution in the coming months, better estimates of UK emissions, concentrations and exposure during COVID-19 are needed."

Inclusive and Sustainable Science

Beacon Equality and Diversity Lecture 2020

DR JESS WADE GAVE THE DEPARTMENT OF CHEMISTRY'S ANNUAL BEACON EQUALITY AND DIVERSITY LECTURE, INSPIRING A PACKED AUDIENCE WITH HER THOUGHTS ON EQUALITY IN SCIENCE. THIS YEAR'S LECTURE COINCIDED WITH INTERNATIONAL WOMEN'S DAY ON 9 MARCH

Jess is a physicist at Imperial College London, where she researches polymer-based organic light-emitting diodes. She is widely known for the work she does on public engagement in science, and her campaigning work to promote women in science and engineering. She is particularly well-known for her work tackling gender bias across Wikipedia, and has written over 900 biographies about leading female scientists on Wikipedia. Her work has been acknowledged by a 2019 Order of British Empire medal, and by being one of Nature's 2018 top 10 people who matter in science.

Jess gave an inspiring and entertaining talk that included examples of how attitudes towards women's education as chemists have changed over time. She encouraged us to use scientifically-tested approaches to inform our approach to Equality and Diversity, and suggested a number of practical areas to focus on, including provision of clear guidance for reporting sexual harassment, encouraging lecturers to use diverse examples of scienists to illustrate their teaching, and lobbying funding organisations and high-impact scientific journals to make their practices more gender neutral.

Dr Caroline Dessent, Chair of the Department's Equality & Diversity group said "This was an amazing talk. I think everyone came away thinking how important it is to celebrate the achievements of diverse scientists of all types."

As part of the Equality & Diversity day, Jess also met with a group of early career researchers for a question and answer session. Dr Leonie Jones, the Department's Employability and Diversity Officer, led the session and said "We had lively discussions about everything from short-term contracts to gendered Lego. It was fantastic for our PhD students and postdocs to meet with Jess and discuss how we can all help to make science more accessible".

York Green Chemists Meet for World Earth Day 2020

Students and Staff from the MSc course in Green Chemistry and Sustainable Industrial Technology met virtually during the Coronavirus shutdown to mark World Earth Day 2020.

The meeting was led by Course Director Dr Avtar Matharu, who invited participants to discuss what the day means to them, both personally and as practitioners of green and sustainable chemistry. A wide variety of home countries was represented, and students were given the opportunity to share their thoughts in their native languages.

Participants at the meeting spoke on themes of hope, listening to one another, the importance of small changes to our daily lives and in particular, the need to work collectively and internationally in order to solve the environmental issues we face.

Dr Matharu said: "This year is the 50th anniversary of World Earth Day, so it was very important to us as practitioners of green and sustainable chemistry, to mark the occasion. We're at a critical time in what we are doing, with a lot of the environmental

issues we face being man-made. As green chemists, we are passionate about protecting the planet, and about the United Nations Sustainable Development goals, and it is important to reflect on our shared values as we move towards the future."

Doing coronavirus research during a global pandemic

FOR OVER 15 YEARS, PROFESSOR FRED ANTSON AND HIS RESEARCH TEAM HAVE WORKED TO STUDY THE CHEMISTRY AND BIOLOGY OF VIRUSES USING STRUCTURAL BIOLOGY TECHNIQUES.

As COVID-19 began to sweep across the world, the team realised they were in an ideal position to gain insight into the virus. Their labs therefore stayed open - we got together with Fred, obviously with social distancing in place, who told us all about it.

How would you describe your particular area of expertise in virus chemistry?

Using X-ray crystallography and electron microscopy, we are trying to understand how virus particles assemble, in particular how viruses store their genetic material in their capsid shell and what happens to the capsids when they are being filled.

What are you trying to learn about the Novel Coronavirus SARS-CoV-2?

Globally, most researchers have been focussing on the spike proteins on the surface of the virus, but we are interested in understanding how the virus genome is stored and protected. Based on information available for other RNA viruses, it is expected that multiple subunits of a key SARS-CoV-2 protein (the 'nucleocapsid' protein) bind to the genomic RNA. They should form a long helix-like assembly that is condensed inside the virus particle, safeguarding it from degradation. Imaging of the virus carried out in York indeed shows this protein, highlighted in blue in the image.

Why is this information useful?

Obtaining a high resolution structure of the nucleocapsid protein assembly will inform our understanding of coronavirus assembly and replication. This could help in the development of antiviral drugs that disrupt protein-protein or protein-nucleic acid interactions that are critical for assembly of virus particles.

How might what you learn impact upon treatments of COVID-19?

In the long term, it may inform the development of novel antiviral drugs, not only against SARS-CoV-2, but also SARS-CoV and MERS-CoV. Even more importantly, such drugs may be valuable in treating related coronaviruses that could emerge in the future.

In the short term, the protein we have expressed is being used to develop testing procedures for COVID-19 in our collaborators' labs. The nucleocapsid protein produces a strong antibody response in infected people, making it an important component in tests.

How quickly did you start working with SARS-CoV-2?

We had the gene synthesised in early March, and started working on expression and characterisation of the protein using molecular biology techniques immediately upon its arrival - this was just as the UK was going into lockdown.

Who are the different members of your team?

The team is composed of postdoctoral researcher Oliver Bayfield and two PhD students, Dorothy Hawkins and De Sheng Ker. Beyond York, we are working with Becky Thompson, who is the cryo-EM facility manager and senior support scientist at Leeds. With Becky we are collecting data on the protein and protein-RNA complexes produced at York.

We have also been sending purified protein and the gene encoding several of the protein constructs produced in York, to labs at Sheffield, Oxford, and London, to help develop antibody tests for COVID-19.

Are there any particular challenges of working through the shutdown?

Once we had received clearance for this work to continue, we then had to look closely at how the team would work safely. The team have been working in shifts round the clock, so they can maximise progress and also follow social distancing guidelines

Shipping material between labs has also needed a bit more planning - if sending locally then it has been fastest to deliver in person.

We have had lots of essential support from colleagues in Chemistry and Biology. We are grateful to Peter O'Toole and the Biology Technology Facility staff who came in to help with sequencing and mass spectrometry, and to Lucy Hudson, operations manager in Biology, who provided organisational support.

Personally, how do you feel working on COVID-19?

The project started very quickly as a response to the growing need for more structural data on the virus. Since starting, we have been receiving a lot of messages and offers of support from colleagues across the University, and have been receiving enquiries about collaboration almost daily. This is something very positive for science emerging from this troubling time.

Nucleocapsid protein of SARS-CoV-2. Image: Jake Smith, Oliver Bayfield