Chemistry Update

Newsletter 321, 29 May 2020

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Calendar of Events

York Festival of Ideas 2020 online

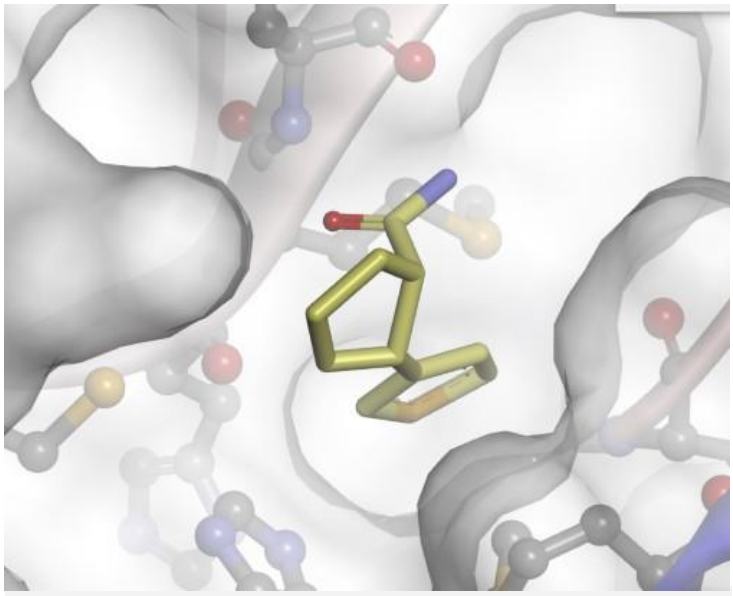
York Festival of Ideas 2020 launches on Tuesday 2 June, with a journey of discovery that will educate, entertain and inspire you from the comfort of your own home. There will be a diverse programme of talks, music, activities and community trails.

Date of Next Issue:
26 June 2020

Compounds synthesised in York could provide clue in the hunt for new treatments against Coronavirus

Researchers at the University of York have synthesised compounds that can bind to one of the key proteins in the COVID-19 virus. The discovery could pave the way for new drug treatments to fight the virus.

The team - led by Professor Peter O'Brien from the Department of Chemistry - made the discovery as part of their research programme synthesising 3-dimensional molecular 'fragments' for use in drug discovery.



York fragment bound to COVID-19 protein; Credit: Rod Hubbard

Therapeutics

More than 100 of the research programme's 'fragments' are part of a national library which was recently screened by a scientific team trying to find starting points to develop therapeutics in the fight against the current COVID -19 outbreak.

The team of researchers, working at UK's national synchrotron science facility, were able to identify around 60 compounds that could bind to a key protein in the COVID 19 virus. Two of the fragments were synthesised by PhD students, Tom Downes and Paul Jones, in Professor O'Brien's research team.

Emerge

Professor O'Brien said "It was great to see our 3-dimensional fragments turn up as hits in this screen, not least as this is the culmination of several years of synthetic work.

"It was especially exciting given their potential to ultimately generate new therapeutics targeting COVID-19 or other Coronaviruses that may emerge in the future."

Fragment

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. This would be the next step in the development of potential therapeutics.

Online Department suggestion box

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

Online chemistry course proves highly effective

A free online course developed by the Department of Chemistry has been shown to have excellent educational outcomes, with positive student attitudes, high levels of learner engagement and a significant impact on students making the transition to university.

The four runs of the Exploring Everyday Chemistry (eeDc) course, have attracted over 15,000 students from a wide range of backgrounds. Students visited around 232,000 steps, completed almost 203,000 of them and posted over 10,000 comments.

Evaluation of the four course runs demonstrated very positive student feedback, as evidenced by weekly learner experience ratings. Distinctively, the study also analysed the impact of the course on university applications to study Chemistry at York. In 2018, over 20% of applicants mentioned the online course in their UCAS applications, as a way of demonstrating evidence of commitment beyond the standard pre-university curriculum.

The course, developed by Professor Andy Parsons, highlights the application of chemistry in perfumes, antibiotics, brewing and sport, making it attractive to a wide range of online learners. The course is designed to help chemistry students make the transition to university by providing examples of university-level teaching and research.

The course is an exemplar of how interactive online learning can be delivered, a topic of increasing interest given the way COVID-19 has interrupted more traditional approaches to education. By combining bite-sized videos, text, polls, quizzes and practical activities with weekly competitions, in over 80 learning steps, the course provides excellent learner engagement.

There are opportunities for students to post comments and upload the results of their practical work. Some York undergraduate chemistry students have helped facilitate the course.

The course includes some recent research initiatives by our Green Chemistry and Atmospheric Chemistry groups. It also provides an insight into what a chemistry degree can lead to, by highlighting career opportunities in the perfume industry, drug discovery, food chemistry and materials science.

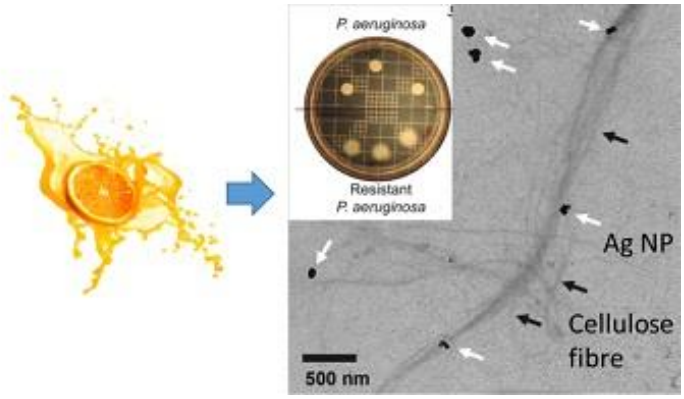
Iain Barr, who oversees the development of Massive Open Online Courses (MOOCs) at York, said: "Exploring Everyday Chemistry was our first ever MOOC to launch, and has set the standard for all future provision at York. Through showcasing our research strengths, encouraging learner contributions in home experiments and supporting the transition to higher education for numerous students, it remains an exemplar for how to engage large audiences effectively."

The free online course starts again on 29 June 2020. It is ideally suited to Year 13 students wanting to make the transition to university learning, as well as Year 12 students, particularly given they have experienced significant disruption to their school or college studies as a result of COVID-19.

The educational study of Professor Parsons' MOOC is published in *Journal of Chemical Education* and in an *ACS LiveSlide*.

Squeezing more than just orange juice: antimicrobial sustainable cellulose

Researchers in Green Chemistry have developed antimicrobial applications for waste citrus peel, potentially enabling the greater use of this resource in a circular economy.



Since the discovery of penicillin, pharmaceutical companies have produced antibiotics on a large scale to fight bacterial infections. Unfortunately, the misuse of these antimicrobial compounds has created a selective pressure in favour of antibiotic -resistant bacteria, leading to an overall increase of antimicrobial resistance (AMR). The World Health Organization (WHO) have campaigned against the threat of AMR with numerous initiatives, and the search for new or alternative antimicrobial agents is a global grand challenge.

In research just published in *Nature Scientific Reports*, Dr Avtar Matharu, Dr Tom Dugmore and Dr Eduardo de Melo from the Green Chemistry Centre of Excellence (GCCE), together with colleagues from Universidad Autónoma de Nuevo León (UANL) in Mexico, reported a novel nano-silver biocomposite derived from waste orange peel. This material shows antimicrobial activity against clinical multidrug-resistant strains, with stronger antimicrobial activity against Gram negative than Gram positive bacteria.

Cellulose is the most abundant biopolymer on earth – naturally-derived and biodegradable. Furthermore, food supply chains have unavoidable waste, such as citrus peel, which is often simply discarded, yet can be an excellent source of cellulose. Importantly, cellulose is also an interesting scaffold for antimicrobial agents. Using waste as a resource enables the development of a circular economy, and aligns with UN Sustainable Development Goals.

The combination of York's ability to produce 'sustainable cellulose' using microwave technology with skills of Professor Ruben Morones-Ramirez and colleagues at UANL to incorporate nanoscale silver produced a novel biocomposite with exceptional antimicrobial activity. In this way, the researchers manage to squeeze more out of an orange than just orange juice.

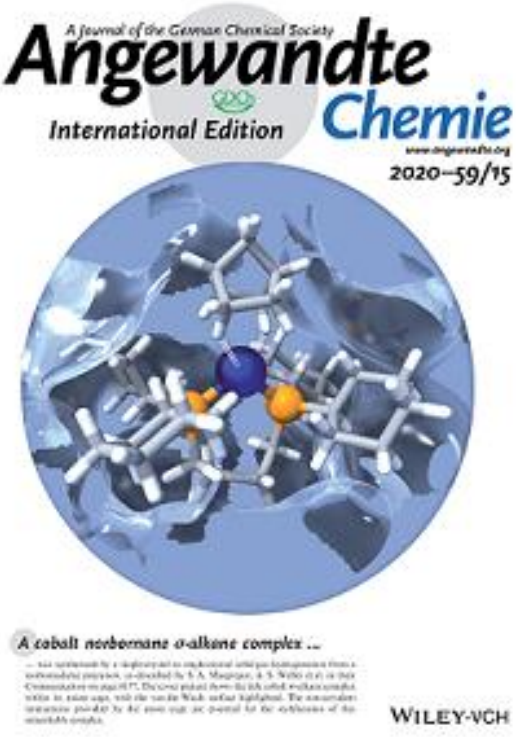
Dr Avtar Matharu said, "This is an exciting collaboration for us with colleagues at UANL and demonstrates the power of networking. It is great to see materials investigated by Eduardo during his PhD studies at Science without Borders making an impact. Our composite has interesting potential healthcare applications and we are delighted to be doing our part to combat antimicrobial resistance."

Dr Tom Dugmore added, "We've spent a lot of time on reducing the environmental footprint on production of these materials from food waste, but a question always remains about how well they will ultimately perform. It was great to get positive results, particularly in such an important field."

"Antimicrobial activity of a silver-microfibrillated cellulose biocomposite against susceptible and resistant bacteria" is published open access in *Scientific Reports*

Synthesis of an ‘impossible’ complex

A research team from the Department of Chemistry has synthesised a fascinating new cobalt complex previously considered too reactive to make.



Professor Andrew Weller and his team, led by PhD student Tim Boyd, have synthesised an example of a highly unstable, paramagnetic, cobalt(I) alkane complex with a unique mode of stabilisation.

They achieved this using a single-crystal to single-crystal conversion in the solid phase driven by simple addition of hydrogen, which 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. This is shown in the cover art highlighted in *Angewandte Chemie*.

Such metal-alkane complexes are key intermediates in C−H activation reactions: processes that turn simple hydrocarbons, which currently are just burned for heat, into valuable feedstocks in the chemical's 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.

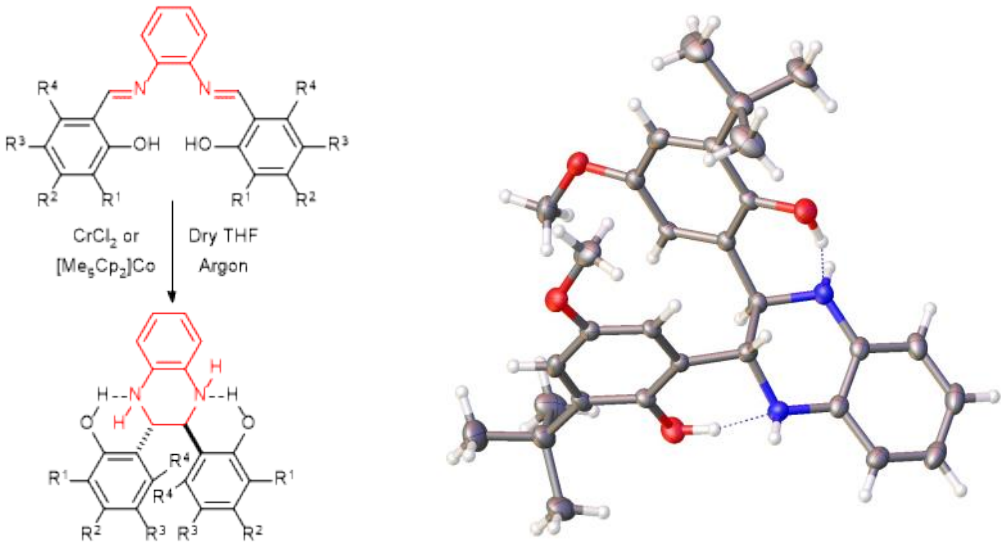
This research is published in *Angewandte Chemie*, with the cover art prepared by Dr Karl Harrison (University of Oxford). The work was funded, in part, by the EPSRC and SCG Chemicals.

Yoga Sessions

The yoga sessions which usually run in the Department have continued to run virtually. The instructor, Jo Merlin has recorded sessions and released YouTube links to those who have signed up. There are 2 yoga (75 min) and 1 grounding class (30 min) each week and payment depends on how many classes you sign up for. If interested, please contact Jo directly for details: joannemerliniyoga@gmail.com.

Unprecedented research during unprecedented times: GCCE researchers publish novel research just before lockdown

Researchers from the Green Chemistry Centre of Excellence (GCCE) have recently published a paper in *Chemical Communications*, detailing a previously unreported and novel synthetic route to the formation of tetrahydroquinoxalines, compounds used in many bioactive molecules and in drugs used for HIV infection treatment. However, this publication almost didn't happen, due to the current closure of most research labs at the University of York following the outbreak of coronavirus in the UK.



Dr Katie Lamb, a current Postdoctoral Research Associate with Professor Michael North at the GCCE, carried out this research. She said: "I feel extremely lucky that this publication ever happened. This paper was the result of many years of hard work and it all began due to an unpredicted discovery during my PhD research at the University of York. We submitted our manuscript to *Chemical Communications* and were pleased to hear that this paper would be accepted after some corrections, and if we could address certain questions raised by the reviewers by performing some more experiments in the lab. Two weeks later, and the week before the GCCE research lab closed for lockdown, time was running out for us to address these comments. On top of that, I was advised to go into self-isolation due to being an asthma sufferer, and stopping going into work the final week the GCCE lab was open. Thanks to the help of Rafael Alarcon, a visiting PhD student from Brazil in the Mike North research group, who was able to finish off reactions for me which I had left running in the lab, and obtained the last pieces of data that we needed, even on the final day the lab was open. Thankfully, the reviewers accepted our comments and experimental results and the paper was accepted for publication shortly after the UK went into lockdown. I therefore must give my sincere thanks not only to all the co-authors on the paper, but especially to Rafael, as undoubtedly this publication would not have happened without him. I wish Rafael the very best for the future, as due to going into isolation and Brazil opening their borders for Brazilian nationals again, I did not get the chance to thank him in person. Obrigada Rafael".

This publication is now available to read on the *Chemical Communications* journal website:
Katie J. Lamb, Mark R. Dowsett, Michael North, Rachel R. Parker and Adrian C. Whitwood, "Unprecedented Reductive Cyclisation of Salophen Ligands to Tetrahydroquinoxalines during Metal Complex Formation", *Chem. Commun.*, 2020, 56, 4844-4847, DOI: 10.1039/D0CC01192D

Co-ordinating Research Action: Air Quality & CV-19 Online Workshop, Wednesday 20 May

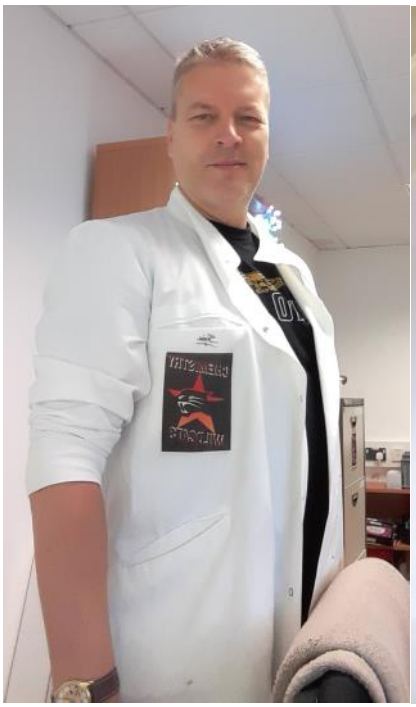
Over 170 people attended the Air Quality & CV-19 workshop, which was organised by the STFC Air Quality Network (SAQN), based in the Wolfson Atmospheric Chemistry Laboratory at the University of York. The event was delivered in collaboration with the UK Indoor Environment Group (UKIEG) and Air Quality Network UK (AQNUK). It was designed to bring together air quality, virology, aerosol, meteorology, climate, health and built environment researchers to determine the current state of knowledge on the possible interactions between air quality and COVID-19, ambient environmental conditions indoors and out, establish evidence gaps and make recommendations for a necessary rapid response and longer term research agenda.

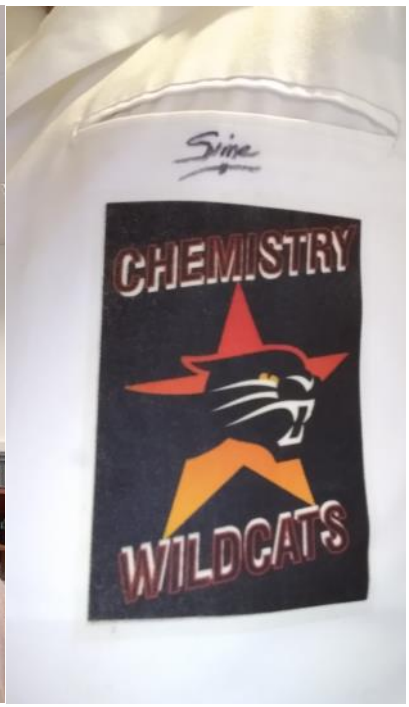
Speakers included the UKRI Air Quality Champions, representatives from Public Health England, the Met Office, the Committee on the Medical Effects of Air Pollution (COMEAP) and the SAGE government advisory group. Prof Ally Lewis (WACL) presented the initial findings from the evidence submission to Defra's Air Quality Expert Group (AQEG). Participants contributed to online discussion boards to identify critical knowledge gaps and shared ideas for research action. The content of the discussions will form the basis of a report to be published by SAQN in the coming weeks.

The event was extremely popular, with over 220 people registering to attend the live event or to participate afterwards. It was a useful learning experience in managing large scale online events (something that is becoming more prevalent and is likely to remain so), as well as an excellent starting point for future interdisciplinary research on this important topic.

The agenda of the event can be found on the SAQN website.

Chemistry Wildcats





In the run up to closing the University, Simon Breeden coined the term "Wildcats", to refer to the Chemistry Technicians. The first Wildcats rota was drawn up on 23 March and communication began on a Chemistry Wildcats chat channel on Slack. Wildcats is a name used in popular American culture to refer to people who are early responders to emergency situations, giving front-line cover to stop the emergency spreading e.g. Wildcat firefighters. This month Simon Grist in YSBL (pictured) and Adrian Whitwood worked on a team logo and transfers for lab coats. It looks like the "Wildcats" are here to stay!