Chemistry Update

Newsletter 327, 27 November 2020

Inside this Issue

Possible drug treatment on horizon for SARS-CoV-2 virus 2

Chemistry academic awarded prestigious Royal Society Industry 3

York scientist part of team awarded £8m to unravel breakdown of carbohydrates 4-5

Undergraduate project leads to publication success 6

SAQN Collaboration Building Workshop held online 7

New starters

Chemistry Graduate School Student Reps 8

Chemistree

Message from Professor Caroline Dessent, Chair of the Equality & Diversity Group 9

ChemYork Magazine - Autumn 2020

Calendar of Events

Inorganic Seminar
Speakers: Dr Sam Furfari, University of York &
Dr Deanna D'Alessandro, University of Sydney
Date: Wednesday 2 December
Time: 10am—11.30am
Location: Virtual

Chemistry All Staff Meeting
Date: Wednesday 9 December
Time: 2pm—4pm
Location: Virtual

BPSI Winter Research Symposium
Date: Friday 18 December
Time: 2pm—4pm
Location: Virtual

Date of Next Issue:
18 December 2020

Possible drug treatment on horizon for SARS-CoV-2 virus

Researchers from the Universities of York and Melbourne have shed new light on how viruses like hepatitis B, dengue and SARS-CoV-2 hijack a cell paving the way for potential anti-viral drugs to stop the virus in its tracks.

Like products on a factory assembly line, all proteins pass through 'quality control' checkpoints where they are inspected before they are transported to their destination to carry out their functions. The researchers showed that some viruses could hijack this manufacturing and distribution process in the cell.

The virus can use the cell's machinery to copy their DNA or RNA and produce the proteins they need to make copies of themselves and take-over their host.

Research demonstrated that viruses tend to harness a step in this process where sugar molecules coat newly assembled proteins. The team was able to develop inhibitors to block an enzyme that trims, checks, and modifies the sugar coating process, which can disrupt the viruses' ability to hijack the pathway.

Key target

When tested in human cells, these inhibitors where shown to reduce infection in dengue fever.

Professor Gideon Davies, from the Department of Chemistry, said: "The trimming process is a crucial quality-control step and when it does not occur, proteins are marked for degradation. The enzyme we have identified represents a key target for broad spectrum drug development against certain viruses, as inhibitors will trigger the destruction of their proteins.

"Targeting the sugar coat of viruses is a really exciting route to novel antiviral agents, especially in these challenging times. We hope to be extending this concept to SARS-Cov2 in the near future"

The findings have been published in the journal, PNAS, and are an important step in developing broad-spectrum antiviral agents.

Future viruses

Professor Spencer Williams, from the School of Chemistry at the University of Melbourne, said: "One approach to treating viral infections is to make a new drug for each virus that comes along. But it is slow.

"An alternative and attractive approach is to make a drug against a human target that viruses need to replicate. The same drug can then be used and reused against many different viruses, even ones that have yet to emerge."

Professor Davies said: "It has been fantastic to work with the Melbourne group, and with specialist virologists in Warwick and Oxford. It was a real team effort"

Chemistry academic awarded prestigious Royal Society Industry Fellowship

Professor Ian Fairlamb of the Department of Chemistry has been awarded a four-year Royal Society Industry Fellowship to work in collaboration with Johnson Matthey, on a project that will enable more efficient use of the planet's natural resources.

The fellowship, to the value £187,000, will allow Professor Fairlamb to spend 50% of his time working collaboratively with Johnson Matthey, a global leader in sustainable technologies. The collaboration will focus on precious metal palladium catalysts, which are embedded within the production of many important commercial products including advanced materials, devices and medicines, and on making their use more sustainable. A primary aim of the fellowship is to identify methods for the sustainable deployment and recovery of palladium catalysts.

Palladium (pre)catalysts are widely applied in cross-coupling reactions, including those that are in the top-10 reactions used globally within the pharmaceutical sector. The work will involve understanding how palladium precatalysts are activated under varying reaction conditions to deliver the active catalyst form. Catalyst changes, speciation and deactivation will be further examined, enabling lower catalyst loadings (towards sub-10 parts per million palladium catalyst) to be more routinely employed in appropriate reaction chemistries. For palladium to be sustainable we need to use less but recover and recycle more.

The interaction between Professor Fairlamb and Johnson Matthey will enable exchange of knowledge about complex reaction mechanisms (academic insight) to be translated to an industrial setting. Professor Fairlamb will benefit from exposure to the real-world challenges involved in large-scale industrial processes, including palladium catalyst manufacture.

Professor Fairlamb said: "The Industry Fellowship represents a fantastic opportunity. Our academic studies and findings are increasingly becoming important to industrialists, especially in Process Chemistry, where understanding about what is going on within a catalytic reaction mixture very much matters."

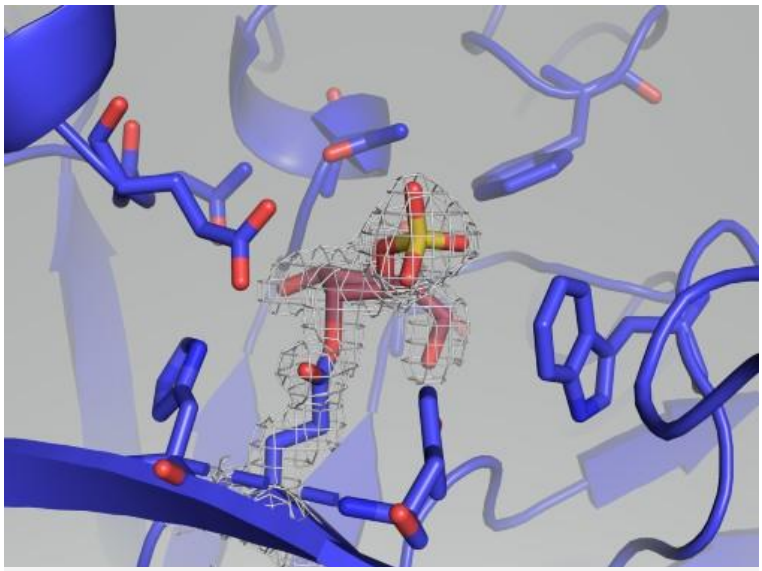
Professor Fairlamb's collaborative work with Johnson Matthey adds to existing strong links between Johnson Matthey and the Department of Chemistry, from individual research collaborations across a range of topics.

Professor Fairlamb is the Department's second recipient in the past two years of the Royal Society Industry Fellowship; in 2019 Professor Peter O'Brien was awarded a three-year fellowship to work in collaboration with the Fragment Chemistry Group in AstraZeneca, Cambridge. The award of two industrial fellowships in consecutive years highlights that industrially-aligned academic research is vibrant within the Organic Chemistry section.

The Industry Fellowship is part of the Royal Society's Science and Industry Programme which aims to connect science, industry and government. It enables the mobility of talented scientists and engineers from industry and academia in order to move between the sectors.

York scientist part of team awarded £8m to unravel breakdown of carbohydrates

A team of scientists - including an academic from the University of York - has been awarded more than £8m (9.1m euros) for a major research programme into how enzymes work on complex sugars.



3D structure of an activity-based probe. Credit: Dr Nicholas McGregor

The research – funded by the European Research Council (ERC) is expected to have major implications for improving human health in the fight against diseases and finding green solutions to energy production.

Professor Gideon Davies from the Department of Chemistry will work with Dr Carme Rovira from the University of Barcelona and Professor Hermen Overkleeft from the University of Leiden to form the "Carbocentre" synergy team.

Biomedicine

They will develop novel chemical entities to study the enzymes involved in the synthesis and breakdown of carbohydrates and design compounds that inhibit and visualize each of the glycol-processing enzymes - eventually applying them in the areas of biomedicine and biotechnology.

Many viruses, including influenza and Covid-19, use carbohydrates (glycans) for cellular entry and as part of their structure.

Professor Davies said: "Carbohydrates (glycans) have mind-boggling chemical diversity. They are the most abundant and diverse class of biomolecules on Earth.

"It's a great honour to obtain this European funding, especially at this time. Our collaborative work will provide truly disruptive technologies for health (cancer, genetic disease and viral invasion) as well as allowing the discovery and characterization of enzymes for biomass degradation leading to green energy solutions."

Chemical

The scientists will harness computational and structural analyses of how enzymes work and use that to inform chemical synthesis of activity-based probes that allow the detection, imaging and isolation of these enzymes in living systems.

Professor Overkleeft said: "Carbohydrates and glycans are all around us. They are the language of cells, our cellular bar-codes, but they are also incredibly complex. Once we have the tools to decipher nature's glyco-codes we can begin to unlock their biology for societal benefit. It is fabulous to be working with two world class groups in this major endeavour."

Insight

Dr Rovira, who will lead the computational strand, said: “The three teams have incredible synergy. It will be wonderful to see how computation, structure and organic chemistry can come together for major biological insight. ”

Collaborative ‘ERC Synergy’ grants are amongst the most prestigious European grants for curiosity-driven research and are only awarded to teams of world-class researchers coming together to tackle major scientific challenges.

York academic is runner-up for prestigious award

An atmospheric chemist from the University of York is runner-up for a major award by a leading science journal.

Dr Pete Edwards from the Department of Chemistry was one of eight leading researchers nominated for the Nature Research Awards for Driving Global Impact.

The award acknowledges his work in the Wolfson Atmospheric Chemistry Labs to understand the chemical processes controlling global challenges such as air pollution and climate.

Dr Edward’s current research develops novel measurement techniques to reduce uncertainties in the models used to inform air quality and climate policy.

After being named runner-up, Dr Edwards said: “It is an honour to be recognised in these research impact awards alongside such eminent researchers in their respective fields, and is a huge tribute to my team and collaborators past and present.

“This award acknowledges the global importance of atmospheric chemistry research, and will allow me and my team to further our work investigating key atmospheric processes.”

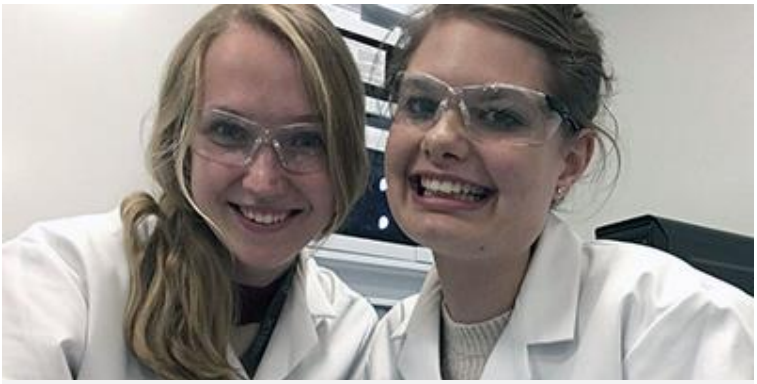
Professor Duncan Bruce, Head of the Department of Chemistry said: "I am absolutely delighted to see this recognition for the work that Pete has devised and led. His approach is truly holistic from design of sensitive instruments and testing their function in the lab, to deploying them in real-world situations to collect data and then using computational approaches to process those data. These are the marks of a true polymath and Pete is applying his expertise in an area of real global significance, showing the positive impact that Chemistry has in tackling environmental issues."

You can find out more about this year's winner and runners up via the Nature Research Awards website.

Undergraduate project leads to publication success

Groundbreaking work which began as a Laidlaw summer project in the Department of Chemistry results in publication for two graduating students.

Laura Berga (MChem 2020) and Isobel Bruce (MChem 2020) achieved publication of their project work in the international journal *Cellulose* in the September following their graduation.



Laura Berga (left) and Isobel Bruce (right)

Laura began work on the project in 2017 as a first-year undergraduate student, when she was awarded a prestigious Laidlaw Scholarship to explore the use of ionic liquids as solvents for biomass processing, with Dr Seishi Shimizu.

Cellulose is a key component of biomass but utilising it is a challenge. Strong hydrogen bonding makes it insoluble in many solvents. Ionic liquids can readily dissolve cellulose, but there are many challenges with using them, such as their high costs, sensitivity to water and difficulty to regenerate the solvents after their use.

The project, which addressed these challenges, attracted the interest of Worn Again Technologies, a start-up company developing a novel solvent-based technology for textile recycling. In addition, Bioniqs Ltd, another start-up company, and the Japan Agency for Marine-Earth Science and Technology joined the collaboration. Worn Again Technologies sponsored both Laura (2018 and 2019) and a second York Chemistry undergraduate, Isobel Bruce (2019), to continue the work in their research laboratory at Nottingham during the summer, where Dr Joshua Reid supervised the project towards completion.

The subsequently-published paper, "Cellulose dissolution and regeneration using a non-aqueous, non-stoichiometric protic ionic liquid system" shows how the challenges of cellulose dissolution were addressed by demonstrating a novel approach to using protic ionic liquids, which are more cost effective than traditional ionic liquids and can simplify the solvent regeneration process.

Project Supervisor at the University of York, Dr Seishi Shimizu said: "Laura's outstanding drive, determination and resilience made all this possible. Isobel's important contribution came when it was badly needed. Josh, my former PhD student, led the team with his expertise. We are grateful to the Laidlaw Scholarship for this opportunity."

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.

SAQN Collaboration Building Workshop held online

Facilitator Christine Bell celebrating the end of the workshop with a homemade mocktail'

The STFC Air Quality Network (SAQN) held their first Collaboration Building Workshop in November. Collaboration Building Workshops bring air quality scientists together with STFC staff to find innovative solutions to air quality challenges using STFC capabilities. The workshops include the opportunity to apply for Scoping Study funds to develop ideas beyond the workshop.

The event was originally planned to be a two day residential workshop in June, but COVID restrictions prevented this. The network worked with the Centre for Facilitation to convert the workshop to an online experience, with the same opportunities to make new connections and apply for funding. Feedback from the participants was very positive, any many said that they felt that holding it online was in some ways better than in person, as they made more connections with other participants, and were able to fit sessions around caring responsibilities and other commitments. One person said, " The format was brilliant, and in many ways actually better than an in-person workshop as it gave time for us to step away from the ideas and let them slowly develop."

Six projects were pitched to the funding panel at the end of the workshop, and five were successful, whilst the sixth project team were given an opportunity to re-submit. The funding panel were impressed by the quality of the proposals and praised the participants for their spirit of collaboration not competition.

Details of the funded projects will be shared with network members over the coming months, and a second Collaboration Building Workshop will be held in 2021. To receive the latest information, become an SAQN member for free on our website.

New starters

Soheila Kharratian, Research Associate in ultrafast 2D-infrared spectroscopy
Room: C/A057 & P/C104; Ext: 4525 (2699 Physics); Email: soheila.kharratian@york.ac.uk

Dr Xiao Wu, Green Chemistry PDRA
Room: C/F119; Email: xiao.wu@york.ac.uk

Fazeelah Munir, Marie Skłodowska-Curie Early Stage Researcher
Room: C/D026; Ext: 4472; Email: fazeelah.munir@york.ac.uk

Thomas Christian Stephens, Associate Lecturer
Room: C/A126; Ext: 2537; Email: thomas.stephens@york.ac.uk

Chemistry Graduate School Student Reps

Following the elections that took place in Week 7, the **Chemistry Graduate School Student Reps 2020/21** are:

- Year 1 PhD and MSc by research rep - Magdalini Alexiadou (ma1563@york.ac.uk)
- Year 2 PhD rep - Giuseppina Barile (gb857@york.ac.uk)
- Year 3 PhD rep - Ryan Barker (reb576@york.ac.uk)
- Year 4 PhD rep - Rhianna Rowland (rjr519@york.ac.uk)
- GTA rep - Ryan Barker (reb576@york.ac.uk)
- YSBL rep - Rhianna Rowland (rjr519@york.ac.uk)

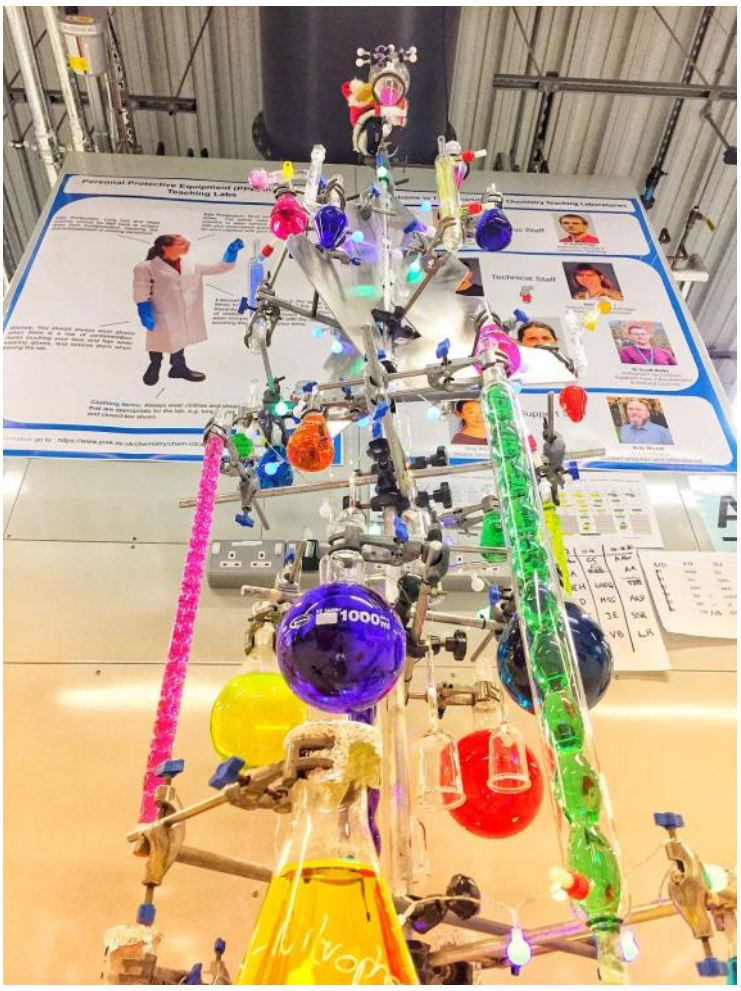
Your reps attend the Chemistry's Graduate School Board (GSB) to raise matters on your behalf. If you wish to raise a matter to be discussed by the Board, please do so by emailing your rep. Matters should be those that affect a group of students or the Chemistry postgraduate student body as a whole.

Chemistree

This year's tree is twice the usual size and celebrates 10 years of Chemistry at York chemistree .

Standing on an 8ft retort stand and showcasing some more unusual pieces of chemistry glassware such as coil condensers and fractional distillation columns, this year's chemistree celebrates 10 years of the Teaching Labs tradition. Chemistree 2020 was put together by Helen Burrell and the teaching labs team, with the giant retort stand specially made in our mechanical workshops. It is bringing some much needed colour and light to Lockdown 2 - as well as some fantastic glassware!

There will be more pictures to come of the Chemistree on our Instagram and Twitter.



Message from Professor Caroline Dessent, Chair of the Equality & Diversity Group

The issue of bullying in the workplace has been in the news over the last few days, providing an opportunity to think again about bullying in Chemistry. Bullying is unwanted, aggressive behaviour that involves a real or perceived power imbalance. The behaviour is repeated or has the potential to be repeated. Bullying actions include making threats, spreading rumours, attacking someone physically or verbally, and excluding someone from a group on purpose. A study published in the journal *Nature* in 2019 revealed that bullying in science is a worldwide problem, with 21% of PhD students surveyed reporting having been bullied. Incidences of bullying and harassment have been found to have a strongly negative impact on women's retention and progression in science, and on LGBTQ+ scientists experiences.

In response to this problem, the Royal Society of Chemistry launched a Bullying & Harassment Helpline at the end of last year. The service can be accessed by calling a confidential line on 0800 5200115 (Freephone in the UK) from 8am-8pm Monday-Friday. Bystanders can access the service as well, to provide support around reporting potential bullying that they witness.

York Chemistry stands strongly against bullying in all its forms, and will support any individual who comes forward to report bullying.

ChemYork Magazine - Autumn 2020

The lastest issue of ChemYork, the Department of Chemistry's twice-yearly glossy magazine is now live and available online.

In the latest issue you can find out:

- How Teaching Labs have been getting on with 'Covid-secure' teaching
- How some of our undergraduates did some 'Tik-Tok teaching' and ended up featured in Times Higher Education
- How the Department is looking to best support and understand the needs of BAME students
- How research from Gideon Davies' team may lead to new broad spectrum anti-viral drugs