Chemistry Update

Newsletter 344, 27 May 2022

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Calendar of Events

Inorganic seminar
Speaker: Prof Fiona Meldrum, University of Leeds
Date: Wednesday 1 June
Time: 1pm—2pm
Location: C/A/101

Organic seminar
Speaker: Dr Sarah Barry, King's College London
Date: Wednesday 8 June
Time: 1pm—2pm
Location: C/A/101

Mechanism & Measurement Mini Symposium
Speakers: Prof Scott McIndoe, University of Victoria, Canada; Neda Jeddi, Dr Claire Brodie, Dr Barbara Procacci, University of York
Date: Monday 6 June
Time: 3pm—5pm
followed by drinks reception
Location: C/A/101

Education seminar
Speaker: Dr Iain Smellie, University of St Andrews
Date: Wednesday 15 June
Time: 1pm—2pm
Location: C/F/106

Professorial Inaugural Lecture
Speakers: Prof Avtar Matharu & Prof Andrew Weller
Date: Wednesday 15 June
Time: 4pm—5pm
Location: C/A/101

Date of Next Issue:
24 June 2022

The York Chemistry Approach to Research Excellence

The outstanding results of REF2021 have indicated that research in the Department of Chemistry at York is in the Top 10 UK Chemistry departments, as ranked by Times Higher Education, with the majority of its research activity being scored as world-leading (4*). Importantly, the Department has taken a uniquely inclusive approach to achieving this research excellence.

The REF2021 assessment of the Department of Chemistry assessed more than half (52%) of its research outputs as world-leading (4*) with all of the rest being internationally excellent (3*). Furthermore, 70% of the research impacts, ranging from atmospheric science to drug discovery were rated as world leading, and the research environment achieved a 4* world-leading ranking of 87.5%.

These outstanding REF results propelled the Department of Chemistry into the Top 10 in the UK (9th) as ranked by Times Higher Education with a grade point average (GPA) of 3.60. This is an improvement on the REF 2014 results and very significantly above the national average for chemistry departments (median score 3.35). Furthermore, the University of York as a whole also moved into the Top 10 universities in the UK as ranked by Times Higher Education analysis of the REF results.

Research across boundaries

The guiding principle of Chemistry research at York is that it aims to achieve the highest international quality, whilst having a unique reach across traditional disciplinary boundaries, facilitating genuine impacts on society wherever possible. Furthermore, it aims to do all this while placing a focus on inclusion and diversity, allowing individuals to thrive.

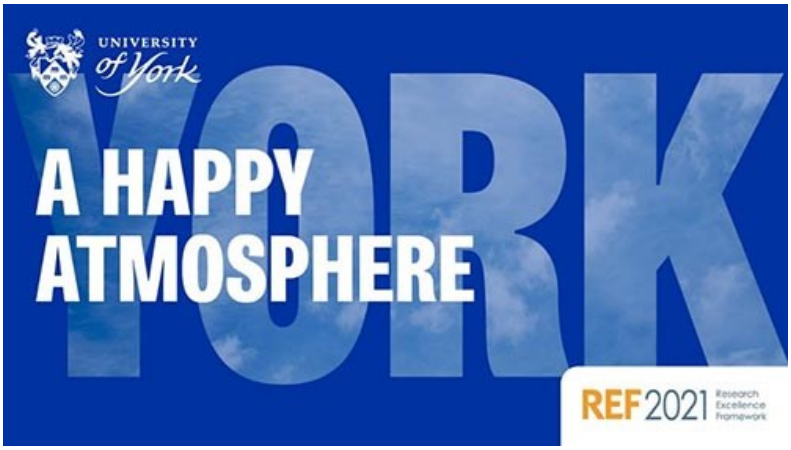
The breadth of research in York is unusual for a chemistry department, with research themes that reach out from core chemistry to fields as diverse as archaeology, biology, environmental science, medicine and sustainable development. All of this diverse research activity is an integral part of the Department of Chemistry, and also plays a key role in contributing to the education of our Chemistry undergraduate students.

Across these diverse research themes, York researchers are producing work of the highest quality, funded by over £10M per year. As indicated in the REF2021 results, this contributes to a vibrant environment in which research is well-supported and able to thrive at the highest level.

Research for Public Good

The wide-ranging departmental research ensures we are well-positioned to deliver societal impacts from atmospheric science to drug discovery. To achieve this, the Department has developed a unique approach to translating research, in which it co-locates external researchers to work alongside and within its research themes. This enables proper integration of academic research outputs into an applied setting as indicated by the fact that 70% of the department's impacts were ranked as world-leading in REF2021.

For instance, the Wolfson Atmospheric Chemistry Laboratories (WACL) houses staff from the National Centre for Atmospheric Science, and has joint academic appointments with DEFRA and industry. Key external organisations were therefore fostered as partners, and as a result, York atmospheric chemists regularly advise UK Government Select Committees and the United Nations.



An inclusive culture

Crucially, the York research environment is about more than just excellent funding, outputs and impacts. The Department of Chemistry is a beacon of good practice for Equality, Diversity and Inclusion and has a focus on people at the heart of its approach.

A 2020 culture survey revealed that many felt that the Department is a 'great place to work' (87% of academic, research and professional support staff), with the vast majority of staff and postgraduate researchers understanding the Department's policies in relation to equality; underlining the emphasis on a supportive, fair and sustainable culture.

The Departmental focus on inclusion is exemplified by figures showing female and male appointment rates for research positions are equivalent, and at the time of the REF2021 submission had a balanced gender 'pipeline' amongst academic staff - 25% of professors were female with 28% of all academic staff being female.

The Department has also used The Wild Fund to improve the representation of ethnic minority researchers. This has focussed on supporting overseas students, many from developing countries, to come and carry out PhD research here in York.

Supporting people

A key part of creating the research culture has been building a 'pipeline' and trying to ensure a diverse range of chemists can excel. This has been achieved through enhanced support for early career independent researchers with grant writing, matching funding and mentoring. The Department has an excellent record of helping independent research fellows secure permanent lectureships (>90%).

Postdoctoral researchers also receive mentoring and are supported by an academic post-doc 'champion'. For career development, they are offered opportunities to sit on committees, co-supervise junior research students, and deliver a small number of tutorials/workshops.

Postgraduate research students all have mentors from the research student community and benefit from an academic Independent Panel Member (IPM), who provides an additional point of support.

The Department also runs the EPSRC DTP Mobility Training Pilot which fits the theme of inclusivity, being designed to help UK businesses up-skill their current employees and attract applicants from non-traditional backgrounds.

A Collaborative Ethos

The focus on people and inclusion has yielded a strong ethos of collaboration. For example, The Green Chemistry Centre of Excellence (GCCE), working with organic chemists from the Synthesis, Catalysis and Mechanism theme, participated in Europe's largest public-private partnership (CHEM21) dedicated to making pharmaceutical manufacture more sustainable.

Over one third of the Department's REF2021 outputs had two or more co-authors from departmental academic staff, and 80% had at least one non-York author. Moreover, over 60% of all publications included at least one international author. Recently, members of the Department have been particularly successful in receiving Royal Society of Chemistry (RSC) 'Horizon Awards' which recognise collaborative research.

Creative and successful

The overarching themes of interdisciplinary and collaborative working, alongside a commitment to equality, have borne fruit in terms of helping Chemistry at York develop world-leading areas of research. This has led to greater citation rates, increased collaborations, growing grant income, international research awards and genuine societal impact - as recognised by the outstanding REF2021 results. Most importantly, this has been achieved while developing and supporting the people involved, helping them to be as creative and successful as possible.

New arrival

Dr Tom Dugmore (Green Chemistry Associate Lecturer) and wife GiGi are delighted to announce the birth of their new baby girl, Elise. She was born on 29th April weighing in at 3.98 kg.

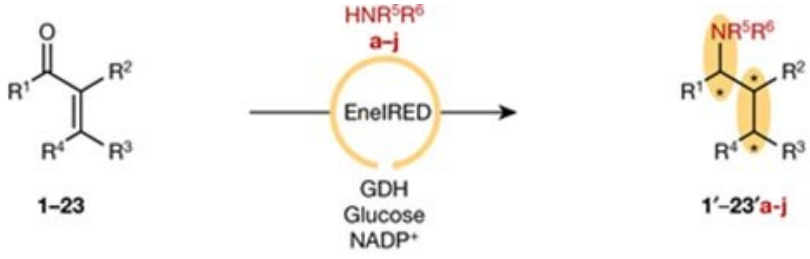
GiGi and Tom are both doing well and we pass on our congratulations and best wishes to the family.

New enzymes synthesise amines with multiple chiral centres

Recent work performed in collaboration between the Universities of Manchester and York, with input from industrial partners, has uncovered a novel and powerful enzyme capable of synthesising amines with multiple chiral centres.

Chiral amines are ubiquitous in pharmaceuticals and agrochemicals, yet their preparation often relies on multi-step synthetic procedures which sometimes only proceed with difficulty. Furthermore, these valuable compounds must be manufactured asymmetrically, with control over each chiral centre, as biochemical properties can differ based on the chirality of the molecule. Each additional chiral centre in the molecule introduces significant complexity to this process.

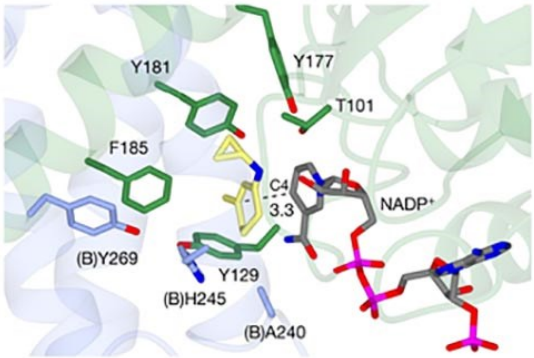
Previously, this team of researchers led by Professor Nicholas Turner in Manchester have worked on imine reductase (IRED) enzymes capable of control over a single chiral centre during amine synthesis. However, in this new work, they have discovered an enzyme capable of also controlling two additional chiral centres.



Reaction between α,β-unsaturated carbonyl compounds (left) and amines (red) catalysed by EneIRED to give the controlled synthesis of amines with three chiral centres.

The enzyme (EneIRED), identified from a panel of enzymes provided by Prozomix Ltd, can reductively couple a broad selection of α,β-unsaturated carbonyls with amines (see reaction scheme). In this way, not only is the chirality of the new amine group controlled, but also the chirality of the reduced alkene. This yields chiral amine products bearing three chiral centres (marked with asterisks in scheme).

Mechanistic and structural studies have been carried out to probe the catalytic process. Led by Professor Gideon Grogan in the Department of Chemistry, the team in York performed crystallographic and docking studies to understand the enzyme in molecular-level detail, giving insight into how the stereochemistry of both alkene and imine reduction could be governed by the enzyme active site. The predictions from the modelling mapped onto the experimentally observed outcomes for these reactions.



Active site of EneIRED complexed with co-factor $NADP^+$ (grey). The X-ray structure has been used to model interactions with the reaction intermediate (yellow) in order to understand the chirality control of the reaction.

Reflecting on the work, Professor Grogan said: 'These EneIRED enzymes possess broad scope, being able to convert many different precursors into valuable amines with multiple chiral centres in a one-pot, single-catalyst approach. We anticipate that further optimisation of the enzyme will enhance its practical utility, and look forward to working with our industrial partners, Prozomix and Pfizer, to develop industrial applications of this technology.'

This research has been published in *Nature*.

University researchers produce comic about green research for York school children

Researchers have created a comic about green and sustainable chemistry research which will be given to all of York's primary schools.

Developed by academics at the Department of Chemistry, University of York and Teesside University, "Green Kid" aims to boost enthusiasm about science in children aged between 9 and 12.

Green Kid artwork. Image credit: University of York and Teesside University.

The project is funded by the Royal Society of Chemistry and will ensure every primary school in York will be given 30 copies along with a teacher pack with extra learning materials.

Climate change

The comic, set in 2064, sees the character Green Kid go back in time to the 2020s where they meet their inventor Summer as a child to see how scientific research to create green solutions and a circular economy could save the world from the ravages of climate change.

The comic, which also includes educational games and puzzles, focuses on the sustainable solvent Cyrene™ - which was discovered by York researchers in 2014. The bio-based chemical can be used to sustainably manufacture a range of products from lithium batteries and carbon fibre bicycles to medicines.

Made from sawdust, Cyrene™ is safe, sustainable, recyclable and does not harm the environment. A company called Circa is building a plant in France to produce Cyrene™ and will sell it to manufacturers to replace toxic solvents.

Exciting

Dr Rob McElroy, from the Green Chemistry Centre of Excellence (GCCE), is one of the researchers behind the comic and a co-inventor of Cyrene™ .

He said: "I have a love of comics and visual arts and have wanted to use them to help get across the exciting world of Green Chemistry for a long time. When I met Julian Lawrence from Teesside University, we talked about how he wanted to use his art to help inform the public about scientific research and we realised we could work together.

"We really wanted to show kids that science isn't boring and the comic gets across some exciting scientific concepts, that aren't usually introduced until degree level, in a simple way.

“The plot is centred around the climate crisis, but with a hopeful message that scientists are working hard to come up with solutions like Cyrene™. Through the characters, we also wanted to reflect the fact that Chemistry at York is a diverse place, with an equal number of women and men undertaking a PhD, and with researchers from all over the world.”

Enthuse

Co-creator of the comic, Julian Lawrence, Senior Lecturer in Comics, Graphic Novels and Sequential Arts at Teesside University, added: “Comics and illustrations are always a great way to engage, enthuse and educate a young audience on an important issue or topic.

“This has been a really interesting project to be involved with – showcasing the expertise here at Teesside University and the impact comics can have. I am delighted to see that this will be distributed to primary schools in York and hope it helps get the message across.”

The researchers have tested what children and their teachers think about the comic at two schools in York - Acomb Primary Academy and All Saints. Teachers read the comic with their classes and did a lesson around its key themes including an experiment with sugar, starch and cellulose to demonstrate the power of solvents. Feedback from the schools suggests that pupils had an increased understanding of words like sustainable and solvent after this session.

Engaged

Alice Hurd from All Saints RC School said: “The pupils really enjoyed having something slightly different in their science lessons. We spent a few lessons working with the comic, including doing some practical work related to the topics covered, which the students really engaged with. As a teacher, it was fantastic to be able to do something off the curriculum and was timed really nicely that when we did work with the comic it was during science week, so could make links to that as well.”

Tom Dennis from Acomb Primary Academy added: “The comic had a real impact on the children’s subject knowledge and confidence when discussing key issues in relation to climate change. Not only did the comic engage them, with the approachable character Green Kid, but was informative also, sharing key statistics such as the increase of global temperature and how processes, such as the production of Cyrene™, can help improve the situation.

“When asked after finishing the comic what could be improved, all children were unanimous - they wanted another one! A real, ringing endorsement and this was mirrored in the work they produced. We are delighted to have been involved in the project and look forward (hopefully) to further editions to come”.

The researchers are now seeking further funding for another two issues of the comic.

Major research grant to transform MRI

More than £2m has been awarded to Professor Simon Duckett to develop a new method that ultimately aims to improve the effectiveness of MRI scanners to detect diseases.

The battery will magnify nuclear magnetic resonance (NMR) signals to make diseases more visible to MRI scanners. Image credit: A

Magnetic resonance imaging plays a key role in modern medicine, enabling the early detection and diagnosis of disease. However, there are a number of drawbacks with the method, including expensive equipment and limitations on the quality of the images that can be obtained.

Over a number of years, Professor Simon Duckett and his interdisciplinary team have been pioneering research methods to dramatically improve the quality of pictures associated with medical imaging, in order to help fight diseases like cancer. He has now been awarded £2.2m from the prestigious Advanced Grant Fund of the European Research Council (ERC) to use molecular catalysis to develop a 'hyperpolarisation battery'.

The project - called Magnify - will seek to make chemicals more visible to MRI scanners, enhancing image quality and allowing new types of imaging to be achieved. Professor Duckett and his team will develop this method using Nuclear Magnetic Resonance (NMR) spectrometers (the chemist's version of an MRI scanner) in their laboratories, which will also allow the approach to be applied in a chemical setting.

Professor Duckett, who is the Director of York's Centre for Hyperpolarisation in Magnetic Resonance said: "Although both NMR and MRI are very powerful methods, they are also very costly and suffer from low sensitivity. In this new project, we will use molecular catalysis to develop a hyperpolarisation battery in order to power dramatic improvements in their operation. By improving our ability to analyse chemical systems via NMR we will create opportunities to optimise chemical transformations and thereby create more environmentally friendly outcomes, whilst simultaneously creating MRI methods that improve our ability to diagnose disease."

ERC Advanced Grants are awarded to exceptional leaders in terms of originality and significance of their research contributions, in order to support high-risk, potentially ground-breaking new projects over a five-year period.

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 at this link.

Chemistry PhD student invited as a speaker at ChemUK

Maria Garcia Flores is a PhD student at the Green Chemistry Centre of Excellence (GCCE) with Professor Avtar Matharu. She is one of the five students currently undertaking the EPSRC DTP mobility pilot programme. This programme explores new, inclusive and flexible pathways to doctoral training by enabling individuals working in industry to move from companies back to academia.

Maria graduated from the National University of Ireland (Galway) in 2011 with an BSc in Chemistry. After graduation, she moved to The Netherlands to study an MSc in Molecular design, synthesis and catalysis. Because of her interest in carrying out research in industry, she was selected to become part of the prestigious TI-COAST ATLAS programme which allows talented students to further develop their abilities and knowledge in analytical techniques used in modern research. She then worked in a variety of industry roles ranging from novel drug design and synthesis to material development in big companies. In 2018, she moved to the UK where she gained experience working as a scientist for different start-ups within the field of green chemistry and circular economy.

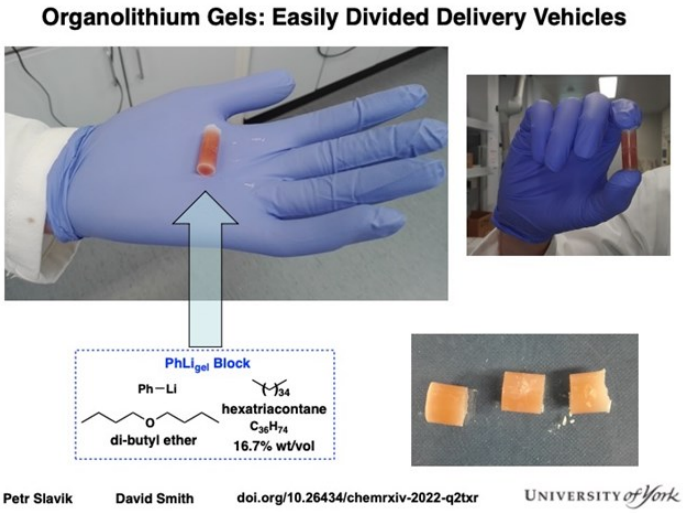
Maria enjoys working on her research project at the GCCE and balances her PhD with her job at Bindethics Ltd. Recently, she was asked to participate as a speaker and to talk about her research in the field of bio-adhesives at the only major expo for the UK chemical industries, ChemUK.

The two-day event brings together attendee groups from all segments of the industrial chemicals, formulated products, pharma and biochemical & process industries. The RSC is heavily involved in the show and this year RSC President-Elect, Professor Gill Reid, was the keynote on Wednesday 11 May. The Sustainability Stage of the event hosted panel sessions and featured presentations embracing critical themes such as chemical recycling and sustainable chemical processing, together with green chemistry innovation and transition to bio-based products.

Dr Anna Zhenova, CEO at Green Rose and University of York PhD graduate, hosted the 'Innovation in bio-based chemicals flash talk' session in cooperation with BioVale. Eight SMEs, including BindEthics, Startbons, Nuspec Oil and MORFS, presented a range of sustainable, low-carbon, novel and drop-in bio-based products, processes, and services.

Maria said: "It was a very busy couple of days but I got to meet very interesting people, make important connections and have a good time. I highly recommend students to attend at least one conference a year. It is a good platform to hear about career opportunities, be updated on the latest scientific community news and expand your network."

O'Brien Group News



A brief update from the O'Brien group. First of all, it was great to get everyone together and take an up-to-date group photo. Then on 4 May, the group had an away day to Durham. In the morning, we took in some of the local historical sites, ably guided by our "local" tour guide Stuart. In the afternoon, we descended on Durham's chemistry department to attend the Musgrave Lecture symposium. The line-up included the Musgrave Lecture from Professor Paul Knochel (LMU, Munich) and local speaker Professor Patrick Steele. Peter also gave a lecture entitled "New Synthetic Chemistry for the Exploration of 3-D Pharmaceutical Space" which featured a "mystery guest" half way through – our collaborative work with Dave Smith's group on organolithium gels got its first public airing, now that the patent has been filed and our draft paper is on ChemRxiv.

We also recently welcomed two "new" post-docs into the group – Ben Trowse and Giordaina Hartley.

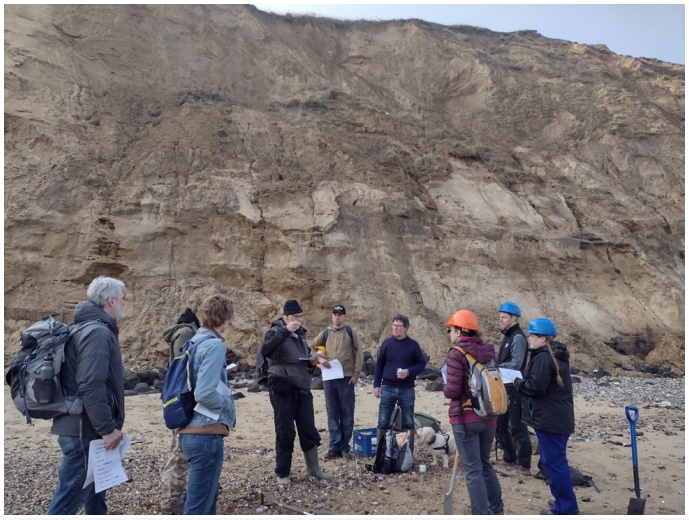
Poster Prize at the Annual Conference of the British Liquid Crystal Society in Bristol, 11-13 April

Giuseppina Barile receiving the Mark Warner Poster Prize from Prof Doug Cleaver, along with Conference Chair, Dr Susanne Klein.

Giuseppina Barile, a Year 3 PhD student working with Dr John Moore and Dr Stephen Cowling, was awarded the Mark Warner Poster Prize at the Annual Conference of the British Liquid Crystal Society held in Bristol on 11-13 April. Giuseppina's poster, entitled "Experimental and Computational Studies of the Effect of Molecular Design on Smectic A Liquid Crystal Phases", outlined some key aspects of her research on new molecular designs for liquid crystals and dyes that may be used in bistable guest-host devices.

EQuaTe project fieldwork along Norfolk Coast

York members of the ERC EQuaTe project (Ellie Nelson, Dustin White, Marc Dickinson & Kirsty Penkman) and colleagues from Aberystwyth University, University of Cambridge, Natural History Museum London and the Cromer Museum, recently conducted fieldwork along the Norfolk Coast. As part of the project's broader investigation of the palaeoclimate and early human occupation of Europe, the aim of this fieldwork was to collect new dating samples for amino acid and thermoluminescence geochronology, and undertake some cryptotephra analyses. Fieldwork over the first two years of this pan-European project have been rather hampered by the pandemic, to say the least! But handily nearby are some critical geological sections (Beeston Regis, Sidestrand, West Runton and Weybourne), which can be linked to key deposits in continental Europe, and therefore enable us to resolve their chronology. With the gradual easing of Covid travel restrictions, team members are planning several new field projects over the coming months, hopefully at some point leaving this island!



Photos left to right: Beeston Regis and Sidestrand

Wanted volunteers for York Pride outreach stall

The university is planning to have an outreach stall at this year's York Pride on the Knavesmire Saturday 18 June. Chemistry plans to have a table with some rainbow -themed chemistry activities. We are looking for a number of volunteers to help throughout the afternoon. Please let us know using this short Google Form. Contact derek.wann@york.ac.uk for more information.

New starters

Isabelle Pickles, PDRA in Chemical Biology of Polysaccharide Degrading Enzymes
Room: B/K266; Email: isabelle.pickles@york.ac.uk