Chemistry Update

Newsletter 346, 22 July 2022

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Calendar of Events

Seminar: "From Yeast labs to Seaweed Start-ups: the Meandering Pathway to Impact"
Speaker: Professor Christopher Chuck, University of Bath
Date: Thursday 28 July
Time: 2.30pm—3.30pm
Location: C/F/106

Seminar: "Creating opportunities for resource development, networking and shared learning through the new Green Chemistry Teaching and Learning Community (GCTLC)"
Speaker: Dr Jonathon Moir, Beyond Benign (USA)
Date: Wednesday 17 August
Time: 1pm—2pm
Location: C/F/106 & Zoom

Date of Next Issue:
26 August 2022

Understanding how reducing particle pollution can increase photochemical smog

Researchers from the Department of Chemistry have discovered why reducing particle pollution is actually increasing surface ozone pollution in some emerging economies, negatively impacting health, ecosystems and agriculture.

A Smog in New Delhi. Image credit: Professor Jacqueline Hamilton, University of York.

Surface ozone is the main component of "smog" and is created by chemical reactions between oxides of nitrogen (NOx) and volatile organic compounds (VOC). This happens when pollutants emitted by cars, power plants, industrial boilers, refineries, chemical plants, and other sources react in the presence of sunlight.

In the last decade, when countries such as China improved air quality by reducing particle pollution – which is emitted from burning coal, steel making, vehicles, and fires – the scientific community was surprised to see ozone pollution increase. This new study, published in *Nature Geoscience*, has provided an insight into the relationship between these two pollutants.

Policymakers have historically considered ozone and particles as separate problems, but the researchers have shown that in some regions they are closely linked. Some short-lived components necessary to make ozone (peroxy radicals) stick to particle pollution, preventing them from going on to form ozone. As the number of particles decreases, the peroxy radicals become available for reactions and ozone increases.

The study modelled the effects of reducing particle pollution and found that it could cause an increase in ozone of 20-30% in some highly populated areas of India and China. If left unmanaged, this would have a significant negative impact on ecosystems and crop yield.

The researchers are calling for new strategies that take this interaction between pollutants into account. The problem can be overcome by targeting reductions in a wider range of pollutants, particularly (VOCs) from chemicals and fuels and NOx from combustion.

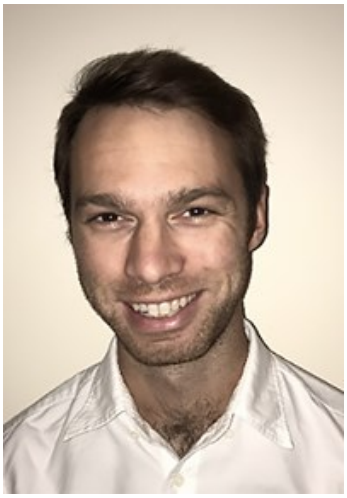
Co-lead author of the study, Professor Mathew Evans said: "Particle pollution and ozone pollution have been viewed by policy makers around the world as separate issues, but our study emphasises the need to look at them together. For 40 years we have thought that ozone depended only on volatile organic compounds and nitrogen oxides and it's only now that we are putting the pieces of the puzzle together and seeing this relationship with particle pollution."

The WHO estimates that 4.2 million die prematurely every year as the result of exposure to outdoor air pollution. Developing countries such as India and China are among the worst affected.

Professor Alastair Lewis from the National Centre for Atmospheric Science, co-lead author, added:

“Policy now needs to be adapted to this new knowledge. This study highlights the complex choices facing governments in how they invest to manage air pollution. For example, there has been dramatic improvement in particle pollution in China over recent years, but emphasis only on particles can lead to unintended consequences. Action to accelerate the reduction in emissions of NOx and VOCs is now essential to keep ozone pollution in check.”

Major Wellcome Trust Career Development Grant



Early career academic in the Department of Chemistry, Dr Chris Spicer, has been awarded a prestigious Wellcome Trust Career Development Grant worth £990,000.

Dr Chris Spicer was appointed as a Lecturer in the Department of Chemistry in 2018. He has been developing a reputation for his innovative research, combining chemical biology with molecular materials science with the goal of creating biomaterials for tissue engineering.

The Wellcome Trust Career Development Grants target researchers who have the potential to be international research leaders, helping them to develop their research capabilities, drive innovative programmes of work and deliver significant shifts in understanding that could improve human life, health and wellbeing. This award will allow Dr Spicer to accelerate his research programme over the next six years by supporting four postdoctoral research fellows to work within his team.

Dr Spicer’s research aims to create materials that can mimic the complex biological stimuli that nature relies on to control the growth of tissues within the body. By combining cutting-edge tools in bioconjugation, biomaterial functionalisation, and dynamic covalent chemistry, these materials can then be used to support the growth of human cells, and the formation of *in vitro* tissue models.

These tissue models have exciting applications helping us to understand and develop treatments for disease, allowing researchers to study tissue biology and the activity of new pharmaceutical agents under controlled, lab conditions, and reducing the need for animal testing.

Speaking about the award, Chris said: “I’m very grateful to the Wellcome Trust for supporting our research and excited to get started. This Award will allow us to build on the early results my group have obtained since I joined York, targeting one of the most important challenges in biomedical research – how we can grow synthetic tissues in the lab that recreate some of the complex biology of actual human tissues. Support from the Wellcome Trust will allow us to bring together a highly interdisciplinary and international team of researchers and collaborators to achieve our goals, and we look forward to using our chemistries to answer real-world questions in tissue biology."

Dr Spicer is part of the Molecular Materials research grouping in the Department of Chemistry - MolMatYork.

CARE-ful Synthesis of Cyclic Compounds

A new synthetic method developed in York, conjugate addition/ring expansion (CARE), enables the simple synthesis of a wide range of cyclic compounds that can incorporate many different functional groups.

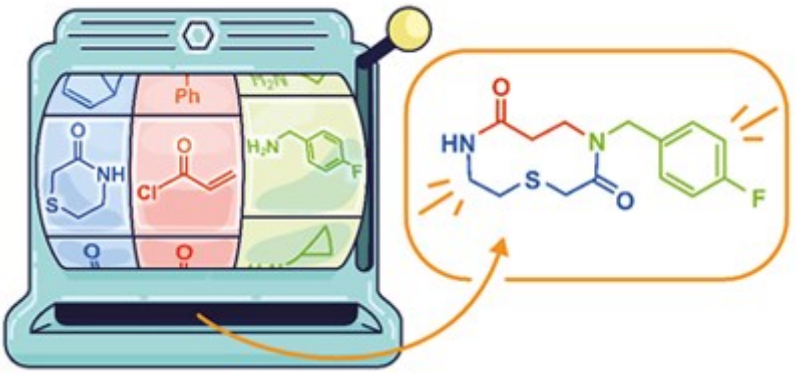


Image credit: Claudia Flandoli

Compounds containing medium-sized rings have biological relevance and potential applications in the development of new drugs. Dr Will Unsworth and his research team have great interest in the development of new and improved synthetic routes to make this type of compound. With this synthetic target in mind, they combined two different reactions – conjugate addition and ring expansion (CARE) – into a single step.

Cascade reactions, which combine multiple reaction steps into a single operation are highly desirable in organic synthesis. They bring benefits in terms of making synthesis quick and easy, and avoiding the need to handle or isolate potentially toxic intermediates. In this work, Kleopas Palate, a PhD student in Dr Unsworth's lab, combined conjugate addition and ring expansion into a single reaction step.

As shown in the Figure, this enables medium-sized ring and macrocyclic bis-lactams to be prepared from cyclic imides (blue), a,b-unsaturated carbonyls (red), and primary amines (green). The reactions are simple to perform, generally high yielding, and very broad in scope, especially with respect to the primary amine component. By varying the components used in the reaction it is possible to 'program in' a wide range of different functionalities – indeed a library of around 50 different cyclic compounds was prepared using this approach.

Talking about the research Dr Unsworth said: 'Our research team have been working on the development of ring expansion reactions for several years, but our previous methods have tended to be quite time-consuming. With the discovery of CARE, we can make the molecules we're interested in much more quickly and easily, using a 'greener', more environmentally sound approach. This should dramatically increase the attractiveness of our synthetic methods for macrocycles in various applications – most notably the discovery of new pharmaceuticals and agrochemicals.'

This work is published in *RSC Chemical Biology*.

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.

High-quality Teaching

The high-quality teaching in the Department of Chemistry has been recognised in the latest National Student Survey (NSS) results.

The National Student Survey (NSS) 2022 results indicate that York Chemistry students are particularly happy with the teaching on their course and the learning opportunities available. The NSS gathers students opinions on the quality of their courses and reports the data in a standardised form.

92% of York Chemistry students indicated overall satisfaction with the 'Teaching on the Course', the second highest score for any Russell Group chemistry department and well above the average score of 80% for these departments. In particular, 99% of students agreed that 'the course is intellectually stimulating'.

In terms of learning opportunities, an overall score of 87% saw York as the highest placed chemistry department in the Russell Group – 10% above the average. In particular, over 90% of students agreed the course was structured to 'bring together information and ideas from different topics'.

When students were asked about their overall satisfaction with the degree, the Department was once again well-placed, with a score that was 7% above the average for Russell Group chemistry departments.

Head of Department, Professor Caroline Dessent said: "The Department of Chemistry is proud of the quality of its teaching, the opportunities it provides to its students, and will continue to develop and further enhance our degree programme so that it produces the best equipped Chemistry graduates."

PYROSTAR – a new collaborative project in the GCCE

Dr Duncan Macquarrie was part of a team who recently won Innovate UK Smart funding for a one-year project to develop a highly controllable pyrolysis method for the production of Starbon®, a material invented in the GCCE and now commercially available via Starbon Ltd.

Starbon® is a highly mesoporous carbonaceous material with tunable surface properties, and the ability to selectively adsorb a range of species, ranging from toxic gases to dissolved metals to bioactive materials. Its preparation is a three-step route involving expansion of polysaccharides via hydrogel formation, freeze drying to avoid pore collapse and carbonisation via pyrolysis. The first two stages were successfully scaled up during an earlier project, but the final pyrolysis step is still challenging due to the insulating properties of the material, which makes even heating difficult, and also re-condensation and polymerisation of some of the volatiles, blocking the pores.

The new PYROSTAR project aims to solve these issues by working with Starbon Ltd and with ICMEA, a Sheffield-based engineering company who specialise in Fluidised Bed Pyrolysis. We are hoping that the research will harness the outstanding heat and mass transport performance of fluidised beds to give far better pyrolysis performance and better materials.

Dr Glenn Hurst in the United States

In June, Dr Hurst travelled to the United States to initially present work at the 50th American Chemical Society (ACS) Middle Atlantic Regional Meeting (MARM) at the College of New Jersey in Ewing, New Jersey. Dr Hurst presented three talks as part of the conference based on his work on systems-inspired design of transferrable interventions for green chemistry education. One of the talks, in collaboration with Dr David Laviska (Seton Hall University (South Orange, New Jersey)) involved outlining a large-scale international project aspiring to transform the global green chemistry education community from one of practice to transformation. Through working with Beyond Benign and the ACS Green Chemistry Institute, this $250,000 project will result in the development of a new online community space for green chemistry resource sharing, learning, collaboration, networking, and mentorship: the Green Chemistry Teaching and Learning Community (GCTLC). Dr Hurst leads on how the GCTLC will nurture the development and provide the highest quality green chemistry education resources at all levels. In conjunction with Dr Laviska, he also works as part of the Diversity, Equality, Belonging and Respect working group, which functions to ensure that these four principles form the foundation of the platform.

After ACS MARM, Dr Hurst had the opportunity to go to New York City for the first time where he participated in a meeting at the United Nations Headquarters. One facet of this visit was as part of the work that Dr Hurst is doing in conjunction with the United Nations Environment Programme (UNEP). Through his experience in integrating green chemistry into curricula, Dr Hurst was asked by the Chemicals and Health Branch of UNEP to work in collaboration to prepare a specialised manual on green and sustainable chemistry education that can be implemented globally. This manual will be used as a framework to integrate green chemistry across the globe into all types of education, in both formal and informal learning environments such as community and spiritual centres.

Dr Hurst delivering a lecture at the ACS GC&E

Dr Hurst then travelled to Reston, Virginia for the 26th ACS Annual Green Chemistry & Engineering Conference of which he works on the advisory board for. During this conference, Dr Hurst delivered two talks on directly assessing systems thinking competencies within green chemistry through the design of a first generation biorefinery. This was in conjunction with Alex Ridley (former MSc student in Green Chemistry and Sustainable Industrial Technology), Dr Tom Dugmore and Dr Michael Wentzel (Augsburg University, Minneapolis). The second talk was focused on the outputs of the work in conjunction with undergraduate MChem students in 21/22 in collaboration with Dr James Sherwood. Additionally, Dr Hurst served as a symposium co-organiser on a lively session on highlighting diversity, equity, inclusion, and respect as key components of chemistry and engineering curricula. Some highlights included Dr Juliana Vidal (McGill University) sharing how women are agents of change from several leading green chemistry researchers together with Mary Kate Lane (Yale University) presenting on ‘what to expect

when expecting in the lab'. Mary's talk offered an array of helpful resources, as pregnant women (and their unborn children) face unique risks in the lab and as a result, pregnant women have historically had to make choices that can adversely impact their careers.

A team of green chemistry educators at the ACS GC&E

Finally, Dr Hurst visited Washington DC and met up with Lori Brown (formerly Senior Manager for Global Outreach at the ACS). Dr Hurst had first met Lori in 2016 at Belem (Brazil) as part of an ACS Global Innovation Imperative to incorporate green chemistry experiments in remote locations (including the Amazon Rainforest). Following the production of a White Paper with associated recommendations for integration, it was heartening to be able to come full circle and re-visit the progress made since 2016. Coincidentally, a colleague in Rio de Janeiro with whom Dr Hurst has worked closely with got in touch on the journey home to the UK to provide an update on the state of green chemistry education in Brazil and how further collaborative work can be done to enhance provisions further.

Dr Hurst wishes to acknowledge JoVE for substantially funding this trip as part of receiving the JoVE 2021 Innovation in Instruction Award.

Kathleen Mary Stott Prize Winners

PhD students in Year 3 are eligible for consideration for the Kathleen Mary Stott Prize. Endowed in 1965, the KMS Prize provides a monetary prize for students demonstrating excellence in scientific research. Nominations are invited from eligible students and their supervisors, and shortlisted candidates are invited to an interview with an academic panel: Terry Dillon (Chair of interview panel), Megan Halse, and Chris Spicer who listen to a presentation from candidates and then ask them questions about their research and wider chemistry. Jamie Blaza was Chair of the panel during the shortlisting process but was unable to attend the interviews due to Covid. This year we received ten nominations, of whom seven were selected for interview.

Congratulations to this year's winners who will present their work at the KMS Winners' Seminar on Wednesday 5 October:

- **Pooja Gupta** - Jamie Blaza, Tony Wilkinson
- **Amelia Gilio** - Gideon Grogan
- **Becky Wagner** - David Carslaw, Marvin Shaw

Demonstrator Award Winners

The Roger J Mawby Demonstrating Prize is awarded to 5-6 students annually at a value of £150 per prize, to reflect Roger's passion for student learning.

Roger was one of the founding academic staff members of the Department of Chemistry and was an inspirational teacher, giving detailed and engaging lectures, frequently using chemical demonstrations to illustrate important concepts in transition metal chemistry and catalysis. In addition, he gave stimulating and challenging tutorials that allowed students to develop and build their understanding of chemistry.

The Awards were held earlier month, in person for the first time since 2019. This was a chance to thank all our demonstrators for their effort throughout the year, and to award prizes thanks to the generous fund in memory of Roger Mawby.

L-R - Giordaina, Ryan, Theo, Nat, Saikran, Richard D as chair of awards panel. Jonathan, not pictured.

Our winners this year were Nat Baranska, Ryan Barker, Jonathan Churchill, Giordaina Hartley, Saikiran Ravi and Theo Tanner who were presented with a beautiful glass trophy thanks to our talented glass-blower, Abby Mortimer. Each winner will also receive a prize of £150.

Further details of the Roger J Mawby Awards.

Back in the game: The RSC Dalton Division Northern Regional Meeting

By Dr Luke A. Wilkinson

The RSC Dalton Division Northern Regional Meeting (last hosted at York in 2019) is an annual one-day conference that brings together inorganic chemists in the broadest sense from across the region. From Lancaster and Liverpool, right across to Hull. This year, on 24 June, the conference was hosted by the University of Huddersfield and organised by Dr Paul Scattergood. Due to the pandemic, this was the first time the conference was able to go ahead in two years and for many students, this was the first ever in-person conference they had been able to attend, so naturally there was a healthy mix of excitement and nerves leading up to the event.

This annual conference typically consists of a series of talks from PhD students who have been nominated by their department, and a busy poster session with MRes, PhD students and PDRAs presenting their work. After an open competition within the Inorganic Section at York, we put forward Alice Jane McEllin (Bruce Group) and Rajat Sharma (Chechik Group) to give talks entitled

"*An Investigation into the Mercuration and Auration of C^N^C Pincer Ligands and the Photophysical and Liquid Crystal Properties of their Complexes with Gold(III)*"

and

"*Magnetically - triggered protein release using iron oxide core - PNIPMAM shell nanoparticles*"

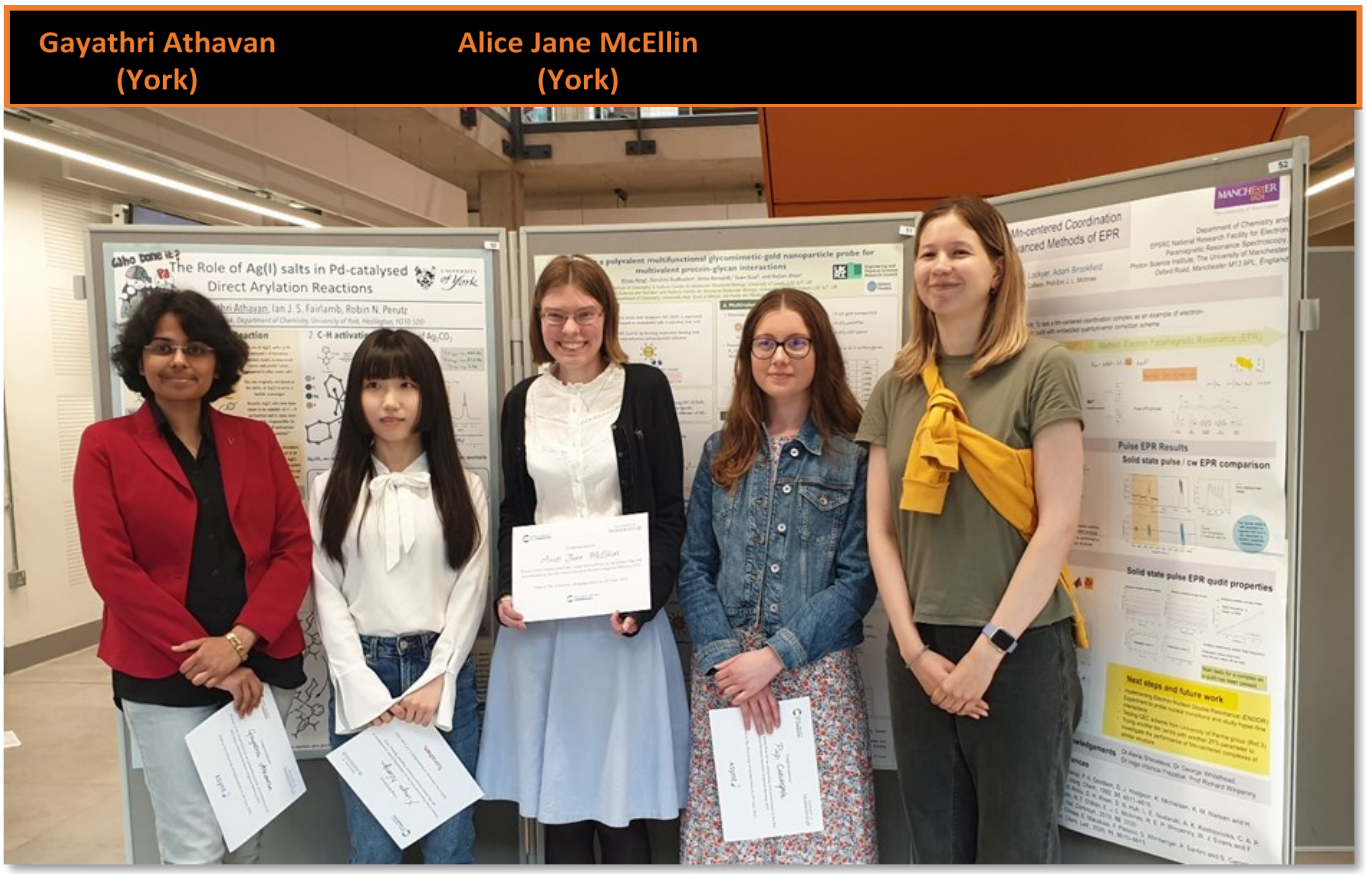
respectively. Both Alice and Rajat delivered a fantastic talk which sparked plenty of questions from the audience. The poster session was equally successful with a strong turn-out from our department in York. The chemistry on display truly was world class and it was fantastic to see York staff and students mingling with inorganic chemists from other departments across the region after so long apart.

One factor that really stood out was the attendance. Despite challenges associated with a national rail strike, the number of delegates from York was fantastic and this highlights, not only the quantity of excellent students/PDRAs we have in York, but also the sense of camaraderie. To overcome the

challenges of the rail strike, the Inorganic section clubbed together to organise car pools and make sure that as many people who wanted to go, could go, which was so great to see!

So not only did we turn up in large numbers and deliver world-class science. Two of our students were also awarded prizes for their work and delivery! **Alice McEllin** won a prize for her talk and **Gayathri Athavan** (Fairlamb and Perutz groups) was awarded a poster prize for her work exploring "*The Role of Ag(I) salts in the Pd-catalysed Direct Arylation Reactions*." **If you would like to see the poster in all its glory, it can be found in the E1 corridor next to the E110 office**.

A huge congratulations to both our winners and to everyone else who did an exceptional job of representing York Inorganic Chemistry.



A little bit about our prize winners…

Alice Jane McEllin

"*I am a fourth year PhD student, with Professor Duncan Bruce, who has spent the last few years investigating the mercuration and auration of C^N^C pincer ligands and the liquid crystalline and photophysical properties of the resulting gold(III) alkynyl complexes and porphyrin dyads. Notably, we have isolated and characterised pure monomercury and dimercury cyclometallated complexes in high yield. I graduated from the University of York in 2018 with a MChem (Distinction), spending my last year studying liquid crystals in the Liquid Crystals Group in the Chemistry Department. I was the winner of the 2017 John Twycross Prize, the 2018 Whinfield Medal for best overall MChem performance and a recipient of one of the 2018 Salters' Graduate Prizes. I have since joined the Salters' Company as an Apprentice. Previously, I have also built a mircolight plane as part of the Schools' Build a Plane project. Outside of the lab I enjoy playing the violin, singing and walking, being a highly active member and walk leader for the Outdoor Society*."

Gayathri Athavan

"I am currently a 4th year PhD student and just managed to successfully complete my PhD defence (Yay!). I am co-supervised by Ian Fairlamb and Robin Perutz. My PhD project was about the role of Ag(I) salts in Pd-catalysed direct arylation reactions. Typically, in C–H activation reactions, Ag(I) salts are common additives in C–H direct arylation reactions and were often thought to act as either the base or halide abstraction agent. However, publications since 2016 have shown that Ag(I) salts were both capable of and in some cases solely responsible for the C–H activation step in the reaction. Thus, my project was primarily focused on elucidating the mechanism of C–H activation by Ag in the catalytic cycle. In my spare time I really enjoy drawing and making silly noises in the lab."

Chemistry at York ranked 7th in the UK by the Complete University Guide

York's Department of Chemistry is the 7th strongest department in the UK, according to the latest Complete University Guide ranking (2023).

We have always been proud of the teaching and learning environment we foster at York, and of the community of staff and students that contribute to this.

Our expertise spans across chemical biology, medicinal chemistry, green chemistry, and chemistry of the atmosphere and environment. We are delighted to have the quality of our teaching and learning endorsed in this way.

York as a whole was ranked as one of the top 20 universities in the UK. A further eight departments are now ranked in the top 10 in the UK, including Archaeology, Biological Sciences, Theatre, Film, Television, and Interactive Media (TFTI), English and Related Literature, Language and Linguistic Science, and History.

Professor Caroline Dessent, Chemistry Head of Department said "I'm delighted that we've been ranked at 7th in the new CUG. We are extremely proud of the outstanding teaching and research York Chemistry conducts, alongside being a department that has diversity and inclusion as one of its core values."

The Complete University Guide (CUG) is an annual league table which ranks 150 universities throughout the UK. The main league table is based on criteria including entry standards, student satisfaction, research quality and graduate prospects. This prestigious league table is aimed at guiding prestigious students in their higher education decision making. The CUG has been running for 25 years and its website attracts 10 million visitors a year.