Chemistry Update

Newsletter 277, 30th September 2016

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Calendar of Events

Research Seminar
Speaker: Dr Elizabeth New, University of Sydney
Date: Monday 3 October
Time: 1pm—2pm
Location: A122

KMS Prize Seminar and Year 2 Poster Session
Speakers: Hope Adamson, Naomi Farren & Michael James
Date: Wednesday 5 October
Time: 2pm—5pm
Location: A101 / A102

UCAS Days
Date: 11, 18, 20, 27 & 31 October
Time: 12.30pm—4pm

Research Seminar
Speaker: Dr Sophie Benjamin, Nottingham Trent University
Date: Wednesday 19 October
Time: 1pm—2pm
Location: A122

Postdoc Poster Competition Winners
Speakers: Rachel Dunmore, John Liddon & Pete Richardson
Date: Friday 21 October
Time: 3pm—5pm
Location: B102

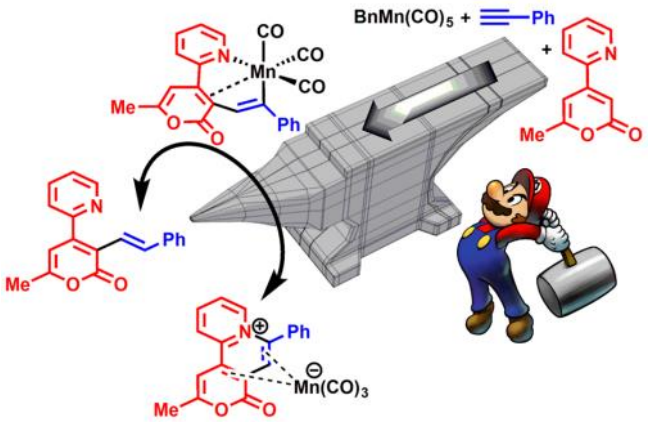
Research Seminar
Speaker: Dr Robin Bon, University of Leeds
Date: Wednesday 26 October
Time: 1pm—2pm
Location: A122

Anniversary Lecture
Speaker: Prof. Paul Dyson, EPFL, Switzerland
Date: Thursday 27 October
Time: 6.15pm—7.30pm
Location: A101

Date of Next Issue:
26th October 2016

Mn-Catalysed C-H Activation Breakthrough

A significant breakthrough in understanding the mechanisms involved in manganese-catalysed C-H bond activation.



Working collaboratively, the research groups of Duckett, Fairlamb and Lynam, have investigated the mechanism of C-H bond activation in organic substrates involving manganese(I) carbonyl species (*Angewandte Chemie International Edition* 2016, DOI: 10.1002/anie.201606236).

Direct web link: http://onlinelibrary.wiley.com/doi/10.1002/anie.201606236/epdf

Using a combined computational and experimental approach the team have been able to identify and characterise a highly reactive intermediate 7-membered manganacycle which acts as an anvil point to either reductive elimination or protonation, delivering different organic products (see figure).

The team have been able to understand the origin of the organic product selectivity by working with 2-pyrone derivatives, which possess a unique reactivity profile in the experimental mechanistic study. Furthermore, a highly unusual Mn-mediated Diels-Alder cycloaddition reaction and fragmentation process on a 2-pyridyl moiety was identified, when running reactions in neat terminal acetylene. Generally, Diels-Alder reactions of 2-pyridines are quite rare, and thus the findings offer much potential and scope for future studies.

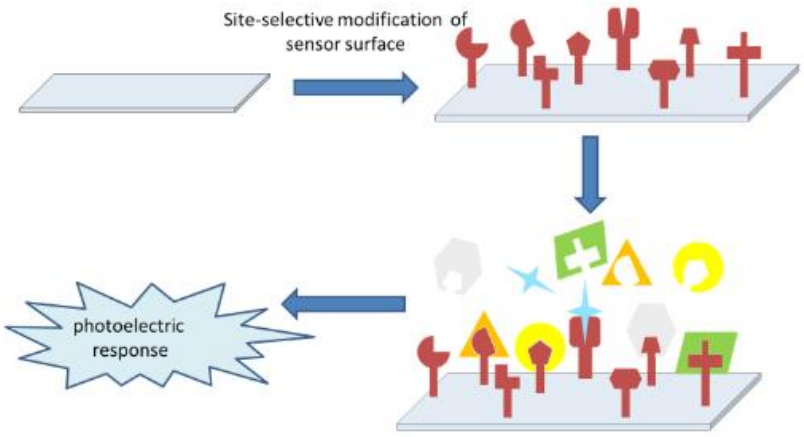
The most pleasing element of the study was that so many students contributed: Nasiru Yahaya (an overseas student from Nigeria, recently graduated) and Kate Appleby (a former graduate student and now a PDRA with Simon Duckett), supported by a key discovery from an undergraduate (Magdalene Teh), Erasmus exchange students (Conrad Wagner, Erik Troschke), and other PhD students playing a supporting role in the laboratory (Jonathan Ward, Joshua Bray and Lars 'Anders' Hammarback). We also gratefully acknowledge the X-ray crystallographic work done by Adrian Whitwood, Natalie Pridmore and Jessica Milani.

The paper was jointly dedicated to Professor Michael Bruce of the University of Adelaide and Professor Robin Perutz of the University of York. Professor Bruce pioneered the Mn-carbonyl C-H bond activation chemistry in the year Ian Fairlamb was born (1975), an interesting coincidence. Prof Perutz has been a pioneer in studying organometallic photochemical processes and when we needed to employ photochemical methods and NMR for the characterisation of the highly reactive manganacycle intermediate, it presented a warm and timely opportunity to recognise his significant contributions to the field.

A New Sensor for Multiple Disease Biomarkers

A new type of device has been developed that can monitor multiple disease biomarkers in parallel using electrophotonic technology.

A new type of sensor has been described in a recent *Nature Communications* paper (DOI: 0.1038/ncomms12769). This work was the result of a collaboration between the University of York's Departments of Physics, Electronics and Chemistry. Dr Alison Parkin, who uses electrochemical methods to probe the mechanism of proteins in her research, together with colleagues from electronics and physics were able to demonstrate that a silicon sensor could be used to generate a photoelectric response i.e. responses that are both optical and electrical.



This combination of sensing responses allows for a more in-depth analysis of smaller biological samples, which could result in speeding up the process by testing for multiple disease biomarkers at once. Rapid testing using such a device could allow for the testing of resistance of a patient's bacterial infection to antibiotic, enabling the most effective antibiotic to be more quickly used for treatment.

Site-selective modifications of the sensor's surface using electrochemical grafting allowed for multiple groups to be added which are selective for different biomarkers, allowing for control of their position on a micrometre scale so that a high density of the detecting chemical groups could be achieved.

Alison Parkin said "We are delighted to have demonstrated that silicon, the cheap and readily available material which underpins the electronics industry, can be modified in such a way to allow highly selective and sensitive monitoring of DNA binding. I hope that this invention will underpin future developments in affordable diagnostic devices to improve healthcare."

Suggestion Box

Reminder: There is an online anonymous suggestion box for staff under the Equality and Diversity section of the intranet: http://www.york.ac.uk/chemistry/internal/ and a physical suggestion box located outside Room K167 for YSBL staff. Suggestions from staff are most welcome. All suggestions are discussed by the appropriate departmental committee.

Government Advisers Look to York Experts for Insight Into Bio-Waste

A delegation of top Government officials visited the Biorenewables Development Centre (BDC), a University of York subsidiary, this week to investigate how waste can be converted into valuable products to benefit the UK economy.

The Government's Chief Scientific Adviser, Sir Mark Walport; Chief Scientific Adviser to the Department of Environment, Food and Rural Affairs (DEFRA), Professor Ian Boyd; and Mark Turner, of the Department for Business, Energy and Industrial Strategy (BEIS) were on a fact finding mission to explore how a waste-based bio-economy might help the UK thrive.

The Green Investment Bank has estimated there could be an investment opportunity of £5 billion in the UK waste market by 2020. Organisations across Yorkshire are working together to make the most out of this opportunity by turning unavoidable bio-wastes including, household and food processing waste into products, such as antibiotics, anti-fungal compounds, and biofuels.

Director of the BDC, Dr Joe Ross, said: "We currently rely heavily on fossil resources, but these are finite and cannot meet the demand for future generations. The BDC focuses on harnessing developments in industrial biotechnology and green chemistry to support the transition to a low-carbon economy, which will ultimately replace oil refineries with biorefineries."

Scale-up

The delegation visited the BDC's Research and Development facilities at York Science Park and Dunnington to meet clients, including local company, Wilson Bio-Chemical, who are working with the BDC to scale-up their technology for turning household waste into biofuels and high-value products. They also discussed research collaboration with GSK, and Veolia to convert food by-products into antibiotics.

Sir Mark Walport said: "It is great to see first-hand how the chemistry and biology science base at the University of York is working with industry to solve some of the major challenges they face.

"Organisations like the Biorenewables Development Centre (BDC) and their partners who are doing pioneering work to turn municipal waste into reusable products such as biofuels and chemicals will help make UK businesses more sustainable and more competitive."

Add value

The Steering Group for local innovation cluster, BioVale, which is composed of leading industries working in the bioeconomy as well as academics and policy makers, demonstrated how to add value to bio-waste and what the Government can do to help develop a waste-based bioeconomy.

The York, North Yorkshire and East Riding Local Enterprise Partnership (YNYER LEP) Chair, Barry Dodd, also announced a new £10 million bioeconomy Growth Fund to boost local bio-based innovations.

Barry Dodd said: “This is about creating a future economy based on renewable resources rather than finite, fossil fuels. With our area’s growing strengths in the biorenewables industry plus our excellent research organisations, this will enable our area to become a global leader in the sector.”

Selective Synthesis Rules Uncovered

York chemists uncover rules for the selective synthesis of medicinally important structures.

Many natural molecules with promising biological activity contain structural units in which functional groups can be arranged in one of two possible ways. One of the challenges in synthesising these molecules is to control this arrangement of functional groups relative to each other; as often current methods lead to mixtures of both possible arrangements. This lack of control can be likened to the molecules in the reaction coming to a fork in the road. Some molecules take the left fork and have one arrangement of atoms (trans), while others take the right fork which gives a different arrangement (cis). The challenge is to make sure all the molecules go the same way, so that only one of the possible arrangement of atoms results. The Clarke group in the Department of Chemistry at the University of York has discovered a method to direct the reaction down only one of these paths, leading to a large excess of one product.

The group used a combination of experimental and computational chemistry to understand the factors that control which reaction path the molecules take, and hence they have been able to control the direction of the reaction. This has enabled them to devise a set of general rules to enable the selective synthesis of these molecules. The utility of the rules have been demonstrated as they have been applied to the synthesis of both diospongin A and B, natural products with anti-osteoporotic activity.

This research is published in *Chemical Science* **2016**, DOI: 10.1039/C6SC03478K.

Protein Sequences Bound to Mineral Surfaces Persist Into Deep Time

An international study involving researchers in the Department of Chemistry at York have unlocked a key to obtaining ancient protein sequences much older than was previously thought possible, thanks to the help of ancient ostrich eggshells.

An interdisciplinary study, published in the journal *ELife*, suggests that analysis of ancient fossil proteins in a 3.8 million year-old ostrich eggshell could provide genetic information almost 50 times older than previously thought. Crucially, the findings provide archaeologists and palaeontologists with the ability to be more targeted in which fossils they select for deeper analysis.

Ostrich eggshells are a common find at fossil sites in Africa and are packed full of proteins which regulate the shell's growth. With the expertise of the Department of Chemistry (NEaar lab, Centre of Excellence in Mass Spectrometry and Wolfson Atmospheric Chemistry Laboratories) and using state of the art proteomics (by mass spectrometry), chiral amino acids and volatile organic compound analysis, the York researchers tracked older and older fossils from very well-dated sites in Tanzania and South Africa, spanning the last 3.8 million years. They observed the eggshell proteins degrading into building blocks, the amino acids, and ultimately leaving little more than a bad smell.

Dr Beatrice Demarchi, the first author of the study and who worked on the project through two postdocs, first in Chemistry and then in Archaeology, explains "Evidence had been growing that unstable regions of proteins are the ones promoting and regulating mineral growth in biominerals, but being unstable we would not suspect them to survive." However as the York team examined older and older eggshells, and with the help of Professor Jane Thomas-Oates with her trusty calculator doing the *de novo* sequencing, it was the more unstable regions which survived the best. Could there be a link?

Dr Kirsty Penkman, who led the chiral amino acid and volatile organics work at York, said "The remarkable thing is that for the first time we can prove that these fossil sequences are authentic, because of the overwhelming combination of multiple lines of evidence. The characteristic patterns of protein breakdown and the preservation of highly volatile compounds in >2 million year eggshell shows that these minerals can trap and preserve biomolecules for much longer timescales and in much harsher environments than was thought possible." Chris Mortimer, formerly in workshops, ingeniously invented an in-line crusher that enabled the "bad smell" to be characterised as a suite of thiols and thioethers by the GC/Q-TOFMS in WACL with the help of Dr Martyn Ward and Dr Jacqui Hamilton.

Professor Matthew Collins, from the University of York's Department of Archaeology, had been intrigued about the presence of a stable fraction of proteins since the mid 1990s. "We had known for many years that the protein decay in eggshells was unusual, when compared to other fossil materials, but until now we have not really known why." In collaboration with computational materials scientists, simulations showed the regions that should be chemically unstable were the strongest binders to the mineral. Only one peptide sequence survived consistently in samples dated beyond 1 million years, the same one identified theoretically by the Sheffield team. Remarkably, in the oldest eggshell in the study - from the famous Australopithecus footprints site of Laetoli in Tanzania (3.8 million years) - the peptide was still there.

Eggs are an excellent target for ancient protein studies: fragments of ostrich eggshells are abundant in Africa, and often found at archaeological and palaeontological sites. They were exploited by the earliest modern humans as raw materials to make art, jewellery and useful objects (for example, they make excellent water carriers). The shell is very thick, hardwearing and therefore survives under many different environmental conditions, so the longevity of its entrapped proteins opens up an exciting new avenue for palaeontological research.

The research, "Protein sequences bound to mineral surfaces persist into deep time" was published on 27 September in the journal *ELife* (https://elifesciences.org/content/5/e17092). The work in Chemistry was funded with the support of NERC and the Leverhulme Trust. This collaborative study included researchers from the University of Sheffield, University of Copenhagen, University of Oxford, Bangor University, Arizona State University, Nelson Mandela Metropolitan University, University of Cape Town, New York University, Complutense University of Madrid, American Museum of Natural History, National Museum of Tanzania, The Hebrew University, University of Toronto, and the University of the Witwatersrand.

New Starters

Dr Fadi Ahwal, PDRA Engineering Solutions working with SBD
Room: CHM/114; Extension: 8893; Email: fadi.ahwal@york.ac.uk

Dr Kirsty High, NERC Knowledge Exchange Fellow, working with KP
Room: D024; Extension: 4772; Email: kirsty.high@york.ac.uk

Cat Dunn, Communications Officer
Room: A133; Extension: 3056; Email: catherine.dunn@york.ac.uk

Suzanne Mennie, Advisory Teacher CIEC
Email: suzanne.mennie@york.ac.uk

New Pilot-Scale Facility Opens to Create High-Value Products from Municipal Waste

Wilson Bio-Chemical have opened their Micro Autoclave Fibre Production Plant for turning municipal solid waste (MSW) into biomass fibre that can be converted into a range of useful products. The facility has been developed with the help of the University of York subsidiary, the Biorenewables Development Centre (BDC) and is based at the BDC's site just outside York. This new technology aims to divert substantial amounts of mixed waste from landfill and produce a range of chemicals and fuels to replace the use of fossil-resource-based products.

An estimated 47 million tonnes of municipal solid waste (MSW) is produced in the UK every year, around 40% of which is sent to landfill. Wilson Bio-Chemical have developed and installed a specialised, rotating autoclave which can treat the biological portion of MSW (mainly food waste, garden waste, paper and cardboard) with steam and high pressure and convert it into a sterile fibre (Wilson Fibre®). Biorefinery specialists, the BDC, have provided support and expertise in the development of the new production plant, which at full commercial scale can process 150,000 tonnes of waste per year.

Wilson is now working with the BDC and with the Centre for Novel Agricultural Products (CNAP) at the University of York on a variety of projects to test the fermentation process as well as the feasibility for use in bioenergy. They are also collaborating on an EU-funded research project aiming to effectively turn this fibre into biofuel as well as high-value chemicals (e.g. butanol, hydrogen, acetone and ethanol).

"The Micro Autoclave Fibre Production Plant is an important step in the continuing development of what we believe is a game-changing technology, diverting unsorted MSW from landfill and producing valuable feedstock from a renewable source for the biofuel and biochemical markets," says Tom Wilson, Managing Director and Principal Engineer of Wilson Bio-Chemical.

"We are pleased to be working with Wilson Bio-Chemical on their innovative technology and also pleased that they have chosen to site their new pilot-scale plant at the BDC, in order to benefit from our biorefining expertise and facilities," says Dr Joe Ross, Director of the BDC.

The plant was formally opened by Barry Dodd CBE, Chair of the York, North York and East Riding Local Enterprise Partnership. The BDC receives funding from the European Regional Development Fund (ERDF) and the Higher Education Funding Council for England (HEFCE).

Wilson Bio-Chemical have won a series of competitively-funded projects to develop applications for their product, including ERDF funding for the Micro Autoclave; Innovate UK and BESTF2 funding for the development of the technology.

Eleanor Dodson Fellowship

The celebration of 50 years of Chemistry at York and the generous donations of our alumni have led to the creation of 'The Eleanor Dodson Fellowship Fund'.

We are seeking to appoint to an Eleanor Dodson Fellowship for an individual researching any branch of chemistry. The aim of the Fellowship is to:

- Launch talented researchers into independent research/ academic careers
- Support scientific excellence in any area of chemistry
- Provide these opportunities for someone requiring flexible work patterns

You must be able to demonstrate a current need for flexible support due to personal circumstances at the time of application. This can include current parenting or caring responsibilities (such as raising children or looking after ageing or seriously ill family members), clinically diagnosed health issues or other personal circumstances that create a need for a flexible working pattern. You will already have an excellent track record at PhD and postdoctoral research, and will now be aiming for an independent research career.

This Fellowship celebrates the achievements of Professor Eleanor Dodson FRS, a researcher in York from 1976 until her formal retirement in 2005 and now a Professor Emerita. Professor Dodson is famous for her innovation in methods of determining structures of proteins from X-ray data to which she brought new mathematical and computational solutions. She represented the inclusive values of the Department with her non-traditional qualifications and by working part time.

To apply for the fellowship, visit https://jobs.york.ac.uk/wd/plsql/wd_portal.show_job?p_web_site_id=3885&p_web_page_id=276416

Gideon Davies Awarded Royal Society Research Professorship

Professor Gideon Davies has been awarded the prestigious Royal Society Ken Murray Research Professorship.

He is one of six scientists to be honoured by the Society in a post that will run for an initial period of five years. The award provides long-term support for internationally recognised work in areas such as biochemistry, genetics, chemistry, developmental biology and physics.

Professor Davies has made discoveries relating to the role of specific parts of an enzyme's structure in the catalysis of carbohydrate synthesis, modification and breakdown reactions. His insights mean that molecules can be designed to mimic or interfere with these reactions, offering potential new treatments for conditions such as Alzheimer's disease and cancer.

Commenting on the appointment, Professor Davies, said: "It is a great honour to have been awarded the Royal Society Ken Murray Research Professorship.

"This award will allow me to work on challenging targets in glyco-science; studying the complex roles carbohydrates play in human health and disease.

"I hope to inspire a new generation of chemical biologists to tackle the scientific challenges where chemistry can aid discovery in the biological sciences."

Scientists from the Universities of Glasgow, Cambridge, Manchester, and University College London have also been honoured by the Society.

John Skehel, Biological secretary and a Vice President of the Royal Society, said: "The scientists awarded the 2016 Research Professorships are amongst the world's most distinguished.

"All six have already made outstanding contributions to science and society and we hope that the professorships will support their current projects, as well as opening up new opportunities to enable them to continue their exceptional work."

For more information about the Royal Society Research Professorship, please visit: https://royalsociety.org/grants-schemes-awards/grants/research-professorship/

Departmental Chromatography Service: New Laboratory

Departmental Chromatography Service
Location: D127, E110 (Office);
Email chem-chroma@york.ac.uk

The DCS has recently moved to B130. Both 6890 GCs, the analytical HPLC and the prep HPLC made the journey from D Block with only very minor incident – the antique leaky compressed air fitting in B130 needed some encouragement before it could be connected to the GCs.

D127 with the Shimadzu ready to go; Paul and Neil (KRSS engineers) carefully moving the Varian across the paving stones.

The prep-LCMS survived both the move and the power cut, although it now requires recalibration after switching off the entire system. It now has a dedicated Work Station, with solvent preparation shelves, a flexible monitor and most importantly, a quiet box for the Edwards pump!

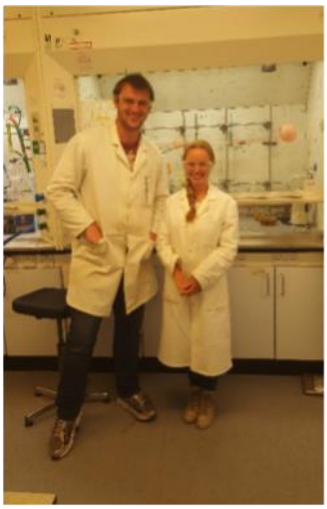
B130 – the chaos!

The Service is open on a restricted basis until resuming full service on Monday 3 October. Please use the Bookings system if you wish to use an instrument, or contact Amanda Dixon via email: chem-chroma@york.ac.uk

B130 – the new LCMS work station, and the 'Chromatography Wall'.

The CHN service will also be relocating to B130 at some stage – details to follow.

Summer Vacation Bursary Researchers: Holly Bonfield and Barbara Hadrys



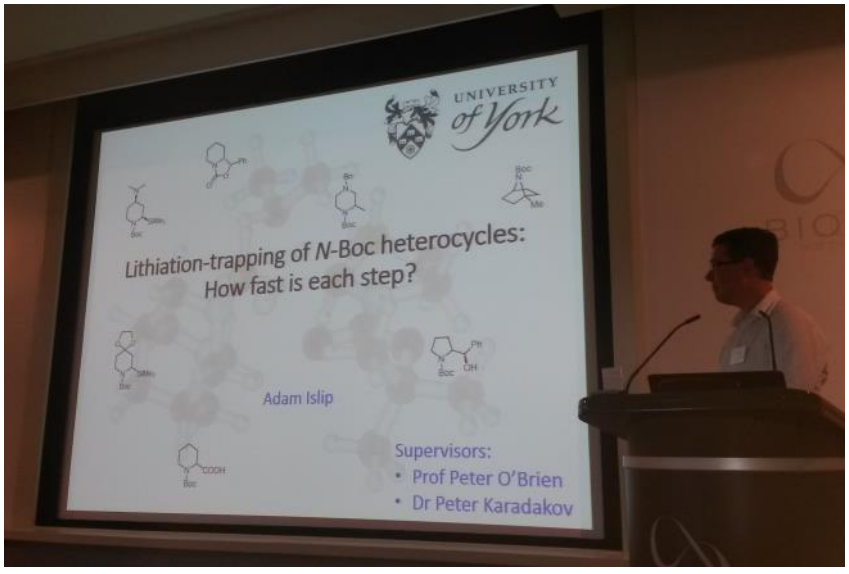
Barbara and Tom on the last day

This summer, two second-year York undergraduates, Holly Bonfield and Barbara Hadrys, got the chance to work in the O'Brien group labs on the group's fragment-based drug discovery project. The two students were tasked with making novel fragments with the supervision and help of two PhD students in the group: Paul Jones and Tom Downes. Both students made good progress with the work and will no doubt be excited to find out the screening results for these fragments when they are finished.

The project gave both students an opportunity to build upon the practical skills they had learned in their first two years and no doubt will stand them in excellent stead for their third year practicals! The group are grateful for the hard work of both Holly and Barbara and the experience was enjoyed by both the students and the supervisors alike.

31st Postgraduate Symposium, RSC Heterocyclic and Synthesis Group Sygnature Discovery, BioCity, Nottingham, 20th September 2016

Peter and five members of the group recently attended this postgraduate meeting in Nottingham. Adam Islip (co-supervised by Peter Karadakov) gave a warmly-received talk on his research work entitled "Lithiation-trapping of N-Boc Heterocycles: How Fast is Each Step?" whilst Tom Downes and Paul Jones presented a poster on their 3D Fragments PhD project.



Adam in action!

It was also good to catch up with ex - group member Giorgio Carbone who works for Sygnature (who are obviously on a recruitment drive as they tried to sign up most of the post-graduate participants!) and ex-York undergraduate, Hannah Dexter, who also gave a very good talk.

Peter's First Marathon – Born to Run?

As some of you might have heard… Peter has been training quite a bit for his first marathon… On Sunday 9 October, he will run from the University to the University (via the Minster and Stamford Bridge!) as he participates in the Yorkshire Marathon. The route is mostly flat apart from the challenge of getting up Green Dykes Lane in the last few hundred metres of the race – whoever thought that would be a good idea?

Peter hopes to do it within the 4-hour mark – he is raising money for MacMillan Cancer Support and would welcome any sponsorship.

His JustGiving page is:

http://www.justgiving.com/Peter-O-Brien7

Thanks for any sponsorship – it is much appreciated.

If you are watching on the day, look out for him in his bright green MacMillan t-shirt.

Professor James Clark in China and Sweden

James Clark spent three days in September teaching at Fudan University as their Visiting Professor. Fudan is over 100 years old, and is one of China's top three universities. It has recently moved to 51st in the world QS rankings with physical sciences in the top 100 of all the major tables. We have signed an agreement with Fudan that will include our hosting some of their (top) graduate students. One of their growing research areas is biomass chemistry giving us a good reason to collaborate!

During a recent visit to Umea in the north of Sweden (where it was starting to freeze in August!) for an update meeting on the York-Umea FORMAS wood biorefinery project, James gave an Honorary Doctorate lecture at Umea University in Sweden ahead of the actual award (in Uppsala in October).

International Conference on Carbon Dioxide Utilisation 2016

The 14th ICCDU was held between 11-15 September 2016 at the University of Sheffield with Professors Michael North (GCCE) and Peter Styring (Sheffield) as co-chairs. This was the first time the ICCDU had been held in the UK and was also the first time that the conference had been held on an annual rather than biannual basis, the previous meeting having been in Singapore in July 2015. The 14th ICCDU was a financial and scientific success, attracting 250 delegates from 31 different countries. York chemistry was well represented with five people from GCCE attending and all presenting lectures. In addition, three of the overseas speakers (from Norway, Germany and Brazil) gave lectures on the work that they have been doing in collaboration with the GCCE.

From the GCCE, Michael North gave a keynote lecture on the recently published work on CO_2 capture using mesoporous carbonaceous materials. Dr Xiao Wu and Dr Paul Reiss gave talks on homogeneous and heterogeneous catalysts for cyclic carbonate synthesis from CO_2 respectively, both covering work carried out within the CyclicCO2R project. Dr James Comerford gave a talk on the use of room temperature, atmospheric pressure plasma to convert CO_2 into CO and the subsequent use of the stream of dilute CO in palladium catalysed reactions. Final year PhD student Katie Lamb gave a lecture on her work on electrochemical CO_2 mineralisation. The York participants found the conference stimulating and are already receiving enquiries and interest about the unpublished work on CO_2 electrochemistry and recently published work on CO_2 capture we presented at the conference.

The UoY delegation at ICCDU14

Organising and running a major international conference on this scale was a significant undertaking, not least as the eventual venue had not been built when our bid to host the conference was accepted in 2013. The formal conference dinner was held at Cutlers Hall, the headquarters of the Guild of Cutlers in central Sheffield where the accompanying photo was taken. Unfortunately the photographer had already had too many glasses of champagne, hence the slightly blurred picture.

Looking forward, the next ICCDU is only 10 months away and continuing the theme of being hosted by cities starting with an S, will be held in Shanghai in July 2017. Somewhat closer to home, preparations are already underway for another major international conference, the third EUChems green and sustainable chemistry symposium which will be held in York in September 2017.

York Educators Attend VICE-PHEC

The annual Variety in Chemical Education & Physics Higher Education Conference took place at the University of Southampton this year. York sent three representatives (Dave Smith, Glenn Hurst and David Pugh) who were joined by around 100 other delegates including a number of past staff and students from the organic section at York who have moved into teaching roles at other institutions. Attendees with ties to York included previous Taylor group members Mike Edwards (Keele) and Russ Kitson (Warwick); previous Smith group members Stephen Bromfield (Bath) and Daniel Cornwell (King's College); and previous Clarke group then teaching fellow Nimesh Mistry (Leeds).

The conference featured keynote lectures from both chemistry and physics including "ChemTube3D", "Opening the Lab" and "Taking Higher Education into the Classroom", plus a number of other presentations, oral bytes, workshops and poster sessions. Glenn delivered two talks; one on "Graduate Teaching Assistant Training" and the second on "Greener Reagents" and "Sustainable Processes (GRASP)" in the undergraduate curriculum. A particular highlight was the NMR workshop from Keele using team based learning and a scoring system using scratchcards. Some rivalry was to be had with both of Dave Smith's ex-students being assigned into a team against their old supervisor! Dave has already ordered his scratch cards and team based learning will be coming to a DKS workshop soon…

David Pugh and Glenn Hurst would like to thank the Department for providing funding to attend this event.

The University of York Solar System

The University of York AstroSoc society, chaired by first year PhD student Mathew Hawkridge, are building a scale model of the solar system across campus. The Mechanical workshops in Chemistry have designed and are building the plinths that the planets will stand on, along with the mechanical workshops in Biology.

The solar system will be shrunk down approximately 3.6 billion times, with the distances between the planets staying to scale, allowing people walk between each planet and gain an understanding of just how large the solar system is. Beginning with the Sun at the Physics Department's Astrocampus near James College, the planets will spread across campus, finishing with the planetoid Pluto at Constantine College on Heslington East. The planets themselves are being individually hand sculpted in clay, before being cast in fibreglass resin that is mounted to the plinths made in Chemistry and Biology. The hope of this project is to create a permanent, educational art installation that spans both campuses, increasing astronomical awareness for both students and the general public.

Construction is well underway with completion coinciding with Tim Peake's visit to the University of York for the UK Space Agency's Schools Conference being held on November 5th. AstroSoc are crowd funding to help raise funds for this project, which can be found here: https://yustart.hubbub.net/p/solarsystem

This project would not have been able to happen without the help of the Department of Chemistry's Mechanical Workshops, specifically Chris Mortimer who designed the plinth, and Mark Bentley from Biology who is now overseeing the project.

Left: Mounting pole designed and made in Chemistry (Chris Mortimer and Stuart Murray) with plain planet mold mounted

Right: Clay sculpting and texturing of Earth and Neptune

Left: Mounting system.

Right: Poles the plinths will sit on (Both made in Biology workshops—Mark Bentley)

Presidential Lecture at BA Festival of Science

Dr Avtar Matharu, Deputy Director of the Green Chemistry of Excellence gave the prestigious Chemistry Section Presidential Address on 9th September in Swansea at the 2016 British Association Festival of Science.

His address, “Chemistry: a circular sustainable future” explored chemistry’s role in achieving the UN Sustainable Development Goals. Avtar highlighted how the European chemical manufacturing industry must adapt to ensure sustainable consumption through optimising resources, reducing waste generation and engaging the public. He discussed the demand to train sustainable-thinking scientists to keep pace with the latest developments and transition from ‘brown’ to ‘green’ chemistry.

https://www.britishsciencefestival.org/event/chemistry-a-circular-sustainable-future/

30th European Crystallographic Meeting (ECM30)

Despite their title suggesting a narrowly-focused meeting, modern crystallography congresses offer an increasingly diverse menu: 'Diffraction of X-rays from crystals' has evolved over the years to 'whatever interference we can get from using any kind of radiation on samples in any degree of disorder'. Name your substitution! Diffraction of electrons from flash-frozen hydrated samples? Sounds like a session on electron cryo-microscopy! Fortunately it would seem that, no matter how many new topics are introduced, this meeting will always feel like home to YSBL scientists, who have made sustained, stand-out contributions over the years.

This year's 30th European Crystallographic Meeting (ECM30) took place in Basel (Switzerland), a city that is within walking distance of France and Germany. Accommodation was scarce and spread across all three countries: this had an inconvenient geographical scattering effect on YSBL lodgers. Nevertheless, Basel's outstanding tram service more than made up for it. The conference centre was well equipped, but offered a highly asymmetrical distribution of room space: with around 900 participants, many popular sessions outgrew their available space, whereas some others looked absolutely desolated in oversized rooms.

YSBL again had a phenomenal participation, increasing their presence from last year's meeting in Croatia: Eleanor Dodson co-chaired (with Prof Randy Read FRS, from the University of Cambridge) once again a methods session (MS.04: New developments in phasing and refinement), and Jon Agirre co-chaired (with Dr Gerlind Sulzenbacher, from AFMB in Marseille) for the first time a session on structural glycobiology (MS.07: Protein and glycobiology structure determination). Also, three talks were delivered by YSBL scientists Jon Agirre, Huw Jenkins and Saioa Urresti, and a poster was presented by Christian Roth.

The University of York, the Department of Chemistry and YSBL, all pride themselves on their reputation for promoting work and family life reconciliation; this once again became evident during ECM30, when Jon Agirre and Saioa Urresti - who are married and have a 6 year-old daughter, Iraia - were scheduled to take part in the same session: the rest of the YSBL fellowship (Eleanor, Huw and Christian) took proper care of Iraia, who quietly sat in the back benches, playing games on a tablet computer. This was Iraia's third crystallographic meeting, and many of the exhibitors (with a special mention to the European Protein Data Bank's charming lot) know her already and give her all kinds of treats.

The conference gala dinner took place in the City of Basel Zoo. A guided tour set the scene to a delicious - and expensive (~£90) - dinner. As the sun set, the time to go back to the hotel approached fast and some of us decided to venture into the darkness, only to find that our way out had been signalled using fire torches! A fantastic experience indeed.

The next ECM, which will skip 2017 as the International Union of Crystallography is scheduled to meet up in Hyderabad (India), will take place in Oviedo (Spain) in 2018, and it is being publicised as a child-friendly conference, with activities for children, a built-in nursery in the conference centre and even encouraging parents to bring their children to the sessions. Something is changing… exciting!

Session MS.07: Protein and glycobiology structure determination, co-chaired by Jon Agirre (YSBL) and Gerlind Sulzenbacher (AFMB, Marseille).

Dinner at the Zoo. In the picture, YSBL crew (including Iraia and her inseparable tablet computer) share a table with several eminent crystallographers. The restaurant kindly provided child-friendly food, free of charge.

Organic Plenary Session

On Monday 26 September, the organic chemists in the Department were treated to an afternoon of top quality research presentations as four final year PhD students took the floor and showcased their PhD research with the professionalism and flair you might expect from some of the most experienced researchers.

Andrew Grantham (Chechik / Rickard groups) kicked things off with a fantastic talk that highlighted his efforts towards the design and development of portable chemosensors for applications in the detection of atmospheric radicals. This was followed by Adam Islip (O'Brien/ Karadakov groups) who presented work that made significant strides in understanding mechanistic aspects of lithiation-trapping of N-Boc heterocycles and the behaviour of these species in solution as well as in silico. Jorge Ruiz-Olles (Smith group) then gave a compelling lecture on the dynamic processes that occur within supramolecular gels and emphasised the enormous impact these gels could have in real-world applications. Finally, Andrew Steer (Clarke/ Smith groups) ended the session with a thought-provoking lecture on the prebiotic synthesis of 2-deoxy-D-ribose as he took us on a journey through time and delved into his endeavours on understanding the origins of life and prebiotic chemistry.

The high level of research presented was reflected by the audience's engagement as each talk sparked riveting discussions that spilled over into the tea and coffee session that followed, and created a perfect end to the afternoon.

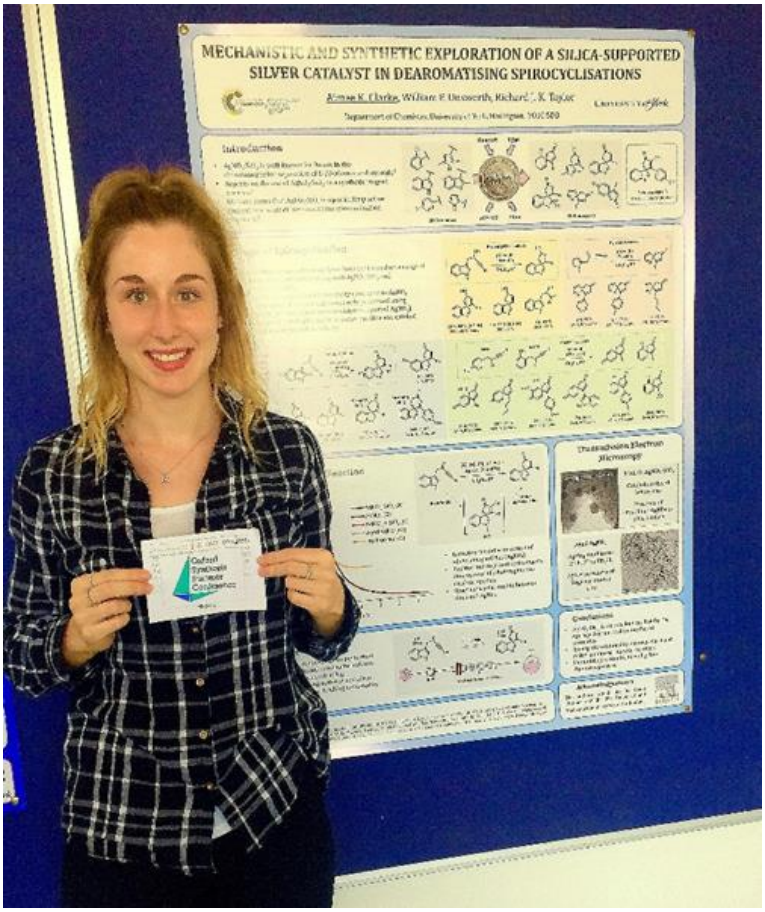
We wish these four PhD students well for the coming months leading up to their vivas and future careers. They are indeed proof that the University of York continues to produce top quality research and even better research students. All the best guys!

- Wade Petersen, Post-doc in the Taylor group, Chairperson on the day

Oxford Synthesis Summer Conference

York's Department of Chemistry was well represented at the first Oxford Synthesis Summer Conference (11-12 August 2016) by several Taylor, Unsworth and O'Brien group members including: Aimee Clarke (RJKT), James Rossi Ashton (WPU/RJKT), Tom Downes (PAOB), John Liddon (RJKT), Wade Petersen (RJKT) and James Donald (RJKT). This newly established conference, was a national forum aimed at engaging young researchers considering a career in academia and was organised by a student committee at the University of Oxford.

The innovative two-day conference programme featured some impressive rapid-fire talks and an engaging poster session alongside a fantastic line-up of internationally renowned speakers: Jonathan Clayden, Ben Feringa, Veronique Gouverneur, Amir Hoveyda and Dirk Trauner. The Taylor group was represented by John Liddon with an excellent rapid-fire talk on his 'Catalyst-Driven Scaffold Diversity' work. John and Aimee Clarke (RJKT) both presented posters of their research and Aimee was awarded a prize for her poster 'Mechanistic and Synthetic Exploration of Dearomatising Spirocyclisations Using Silica-Supported Silver Catalysis' in a highly competitive field of 75 entrants.



The conference concluded with an unorthodox but enlightening panel discussion, which provided students with the opportunity to ask speakers (Ben Feringa, Dirk Trauner and Amir Hoveyda) questions on a range of topics relating to a career in organic chemistry and life as an academic. All in all this was a very inspiring conference and was also a great opportunity to network with other students and established career academics. This conference was widely regarded as being very well-organised by the student committee and will be an event to look forward to in future years.

RSC Joliot Curie Conference 2016, 6-7 Sept, York

The RSC Joliot Curie Conference 2016, was jointly hosted by the RSC and Department of Chemistry here in York. This fantastic annual conference aims to support the aspirations of Early Career Researchers, particularly women and those who are under-represented in academia. This year's focus was on advice and support for PDRAs who aspire to establish an independent career in academia. To encourage participation and to demonstrate the value we place in our research staff, Chemistry PDRAs were invited to apply for departmental funding to attend.

There was a terrific line up of speakers and significant participation from members of the department, with Duncan Bruce opening the conference and Paul Walton chairing the first day. Sue Gibson OBE FRSC gave a fantastic Keynote address highlighting the tenacity of role models such as Irene Joliot-Curie and giving many wise words of advice "We need to do a better job of putting ourselves higher on our own 'to do' list".

During the first panel discussion on *Multiple Pathways to Success,* Lucy Carpenter reminded us that "Science is a marathon not a sprint" and talked very candidly about her career, this nicely captured the atmosphere at the conference which was very open and supportive. Stephen Wells from Bath gave a humorous insight in to his personal experiences of the 'Two Body Problem' using a double pendulum to illustrate the difficulties for academic couples trying to find suitable work and live together.

Dave Smith talked in the second session about *Standing Out From The Crowd*:

"Be Brilliant, Be Yourself and Network."

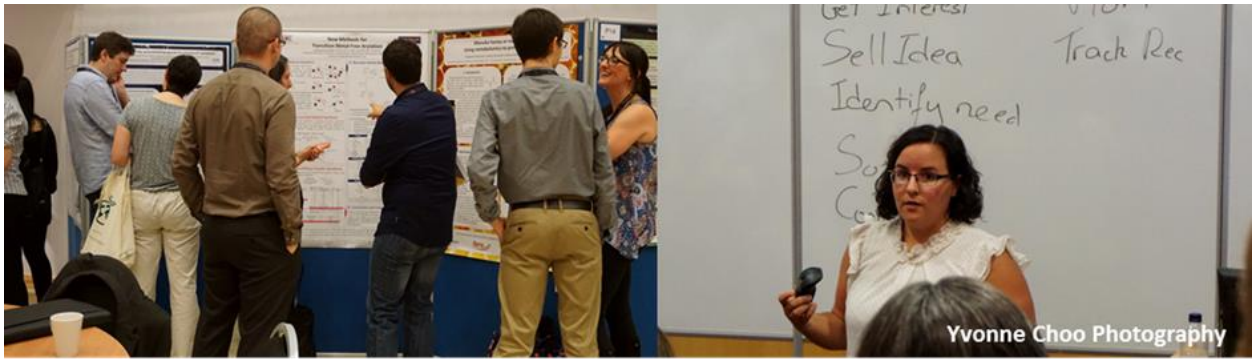
Mary Babcock RSC Publishing Deputy Editor provided some great tips on getting published. There were lively discussions of the use of social media (tweeting your paper gets you more citations) and Brexit where the audience shared their worries about the impact on research funding in particular.

During the pre-dinner session, Paul summed up the day and showed The Royal Society's video

on *Understanding Unconscious Bias* which provided food for thought: https://youtu.be/dVp9Z5k0dEE.

The dinner was hosted by Sir John Holman and after a great meal, our after dinner speaker, Tom Welton from Imperial College talked about the myths around "*The Magic Carpet Ride to Success*", picking up on the recurring theme of 'imposter syndrome' (which even the most successful academics suffer from at times). Tom highlighted the importance of having a supportive network around you at these times.

Day two, focusing on *Funding Your Research*, was chaired by Clare Viney FRSC and included a group exercise where delegates peer reviewed one another's research proposals and provided feedback. Leonie Jones and Paul Walton helped facilitate the session and Derek Wann, along with many of the speakers, met with PDRAs who had requested a mentoring session to discuss their career development.



The final panel discussion focused on *The Practicalities of Applying for Grants* and included expert advice and tips from speakers with experience in obtaining funding including Alison Rodger FRSC, University of Warwick, Hazel Philips, University of Bristol, Cecilia Fenech Brincat, Cranfield University and York alumni Dr Renée van de Locht from EPSRC.

The conference was really well attended, with a fantastic buzz. In total we had at least 22 York attendees (14 PDRAs) and the feedback has been extremely positive.

> Fantastic time at #JoliotCurie2016 Thank you @RoySocChem Invaluable advice - a must for postdocs/fellows/early career researchers next year

Many thanks to the RSC, all the speakers and everyone else who contributed, including Yvonne Choo from Newcastle who kindly allowed us to use her excellent photographs of the conference. A full list of speakers can be found here:

http://www.rsc.org/events/detail/21600/joliot-curie-conference-2016

- Leonie Jones

Green Impact

Discounted Bus Tickets!

Students – travel on the 66 bus for only £99 for 12 months!

https://www.firstgroup.com/york/more/your-bus-66-and-university-services/buy-tickets?user=1201%3f

Staff – travel on the 66 bus for only £250 for 12 months!

https://www.firstgroup.com/york/more/your-bus-66-and-university-services/buy-tickets?user=1211%3f

Monthly Bike Doctor

Free repairs - The University monthly 'Bike Doctor' sessions ensure that your bike can receive routine maintenance checks completely free of charge. A special discount has been agreed if major work is required!

GET CYCLING

Arrive early to avoid disappointment due to limited slots - First come First served basis.

Get Cycling will also be selling discounted cycle equipment and Unibike!

2016 dates:

- 20th October – Berrick Saul Building, Vanbrugh
- 17th November – Ron Cooke Hub, Heslington East
- 15th December – Your Space, at The Student Centre, James College

2017 dates:

- 12th January – Your Space, at The Student Centre, James College
- 16th February – Your Space, at The Student Centre, James College
- 16th March – Ron Cooke Hub, Heslington East
- 13th April – Berrick Saul Building, Vanbrugh
- 18th May – Ron Cooke Hub, Heslington East
- 15th June – Berrick Saul Building, Vanbrugh
- 13th July – Ron Cooke Hub, Heslington East

Departmental Showers for Staff/Postgraduate Students

To all staff cyclists and pedestrians who travel to work by bike and on foot...

We have departmental showers in D Block located in the disabled toilets on the Ground, First and Second floors.

We also have a shower on the ground floor of D block, 'D016A', located by the E014 labs / lifts (just beyond the wet labs).

Further showers are located in WACL building (both ground and first floor) and the CHyM building (inside the main entrance, next to the disabled toilet (ie. before you need Kaba access to get through into CHyM).

When using the showers, it would be really helpful if you could be careful not to leave water on the floor - if so, please mop up. Many thanks.

Macmillian Coffee Morning

Hello everyone and thank you all so much for supporting the

2016 Macmillan Coffee Morning!

With cake sales in the biology and chemistry departments, we raised an amazing

£743.61

Many thanks to all the helping hands and of course the lovely bakers who created a broad variety of treats for us!
I especially want to thank Helen Burrell in chemistry for organising a sister event and generously contributing to our total!

Thank you all again
I hope to see you next year!
Tamara

Responses to Postgraduate Feedback

The Postgraduate Research Experience Survey (PRES) runs every two years. The survey targets all research students at the University of York. The results of the survey are shared with departments to discuss with staff and students. They help to inform improvements to services and facilities for research students. We are pleased that overall, the results of the survey tend to be positive in Chemistry, but there will always be some areas that need improvement. Provided below is a summary of some of the key areas raised in the PRES surveys from both 2012/13 and 2014/15 and how we have tried to address these. The next survey will take place in 2016/17.

Areas for consideration	**Action taken**
Students would like more guidance in relation to training requirements and identifying training and development needs	• Comprehensive revision of Graduate training programme and Handbooks as part of iDTC • Survey sent to students to gather feedback on first year of iDTC training, Results so far have been considered and training adapted. A full iDTC review will take place in Summer 2017
Students would like more opportunities for integration within student cohort and department and to discuss research with other students	• All new research students, including former York undergraduates are now allocated mentors. • Introduction of Core cohort based activities as part of iDTC • Introduction of Graduate Research Seminars • Introduction of informal poster session for students entering their second year as part of KMS seminar
Seminar programme provided by department	• Improved coordination of Departmental and Section Seminars and promotion to encourage attendance in a regular timeslot
Opportunities to become involved in wider research community beyond department	• Opportunities for graduates to have posters displayed at MChem industry meeting which is attended by industrial contacts. • Promotion of other events as they arise and we are notified
Institution to value and respond to feedback from research students	• All graduate students notified of each GSB meeting to raise matters through reps and sent minutes of meetings • Updates for Chemistry Update on how feedback is being addressed. Also posted on Graduate webpages

Opportunities to develop contacts or professional networks	• We will highlight networking opportunities at departmental and University events • Networking session ran in March 2016 and will be mandatory as part of iDTC core training
Managing own professional development during programme	• Promotion of Becoming an Effective Researcher Tutorial and Employability Tutorial – included in handbooks and covered during induction events
Support for publishing work, public engagement and career planning	• Introduction of core sessions as part of iDTC on: Employability and Professionalism, Preparing scientific papers, Preparing scientific posters, Oral presentation skills, Preparing grant proposals, CV and interview skills, Outreach opportunities plus the introduction of careers talks through Chemical *Inter*Actions
Opportunities for submitting a paper for publication in an academic journal or book	• Roll-out of core iDTC paper writing course to Year 2. Successful launch of revised writing course with additional feedback for students
Opportunities for taking part in a placement or internship	• Guidance on identifying and securing work placements will available on the graduate web pages in October
Confidence that research degree will be completed within the institution's expected timescales	• This is difficult to address in the short term as it has always been common for a Chemistry PhD to take nearly 4 years. However, core iDTC session now includes a brief introduction to expectations of thesis writing in Year 1 TAP report writing session and students are reminded to raise any concerns / request advice from Thesis Advisory Panel in relation to planned completion dates – particularly when limited funding is available
Provision of computing resources and facilities in department for postgraduate students	• This has been raised with Head of Dept and has been included in Departmental financial planning – we are awaiting further updates

Students are always welcome to provide feedback on graduate school issues. This can be done either by email to chemgrad@york.ac.uk, or via the student reps on the Graduate School Board.

RSC '175 Faces' Visit to York

The RSC 175 Faces of Chemistry visited the National STEM Learning Centre (NSLC) as part of the Joliot Curie Conference 2016. The exhibit and online database of case studies was developed to celebrate 175 years of the RSC and features a diverse range of inspirational chemistry role-models. It took a certain amount of logistics to fit the whole exhibit in the NSLC atrium but it looked fantastic and provided inspiration to delegates and those who visited. There are at least 10 'Faces' with a connection to York including staff and students past and present (see if you can find them all!). We hope to have the exhibit return to York sometime next year but in the meantime, have a look at the fantastic website:

http://www.rsc.org/diversity/175-faces/

Chemistry at York Now on Instagram

We have a brand new Instagram account!

Check it out at https://www.instagram.com/chemistryatyork