UNIVERSITY of York

Chemistry Update

Newsletter 272, 29th April 2016

Inside this Issue

Calendar of Events

Royal Society Rosalind Franklin Award Lecture
Title: The Atmosphere and Oceans: A Changing Relationship?
Speaker: Prof Lucy Carpenter & Prof Mat Evans
Date: Tuesday 3 May
Time: 6pm—7pm
Location: A101

Atmospheric Seminar
Speaker: Dr Christa Fittschen, CNRS Universite Lille 1
Date: Friday 6 May
Time: 10.30am—11.30am
Location: WACL Seminar Room

Inorganic Seminar
Speaker: Dr Sebastien Bontemps, University of Toulouse
Date: Friday 6 May
Time: 1pm—2pm
Location: A122

Organic Chemistry Research Seminar
Speaker: Dr John Bower, University of Bristol
Date: Wednesday 11 May
Time: 4pm—5pm
Location: A122
Talk at 4pm, followed by drinks reception at 5pm

Inorganic Seminar
Speaker: Dr Phil Dyer, Durham University
Date: Monday 16 May
Time: 11am—12pm
Location: A122

STEM Communications Skills Workshop
Date: Wednesday 18 May
Time: 9.30am – 1pm; followed by lunch

Physical and Atmospheric Chemistry Seminar
Speaker: Dr Vas Stavros, University of Warwick
Date: Friday 20 May
Time: 2pm—3pm
Location: F106

RSC Award Symposium
Speaker: Prof Vivian Yam University of Hong Kong
Date: Wednesday 25 May
Time: 1pm—2pm
Location: A101

Green Chemistry Seminar
Speaker: Prof Shicheng Zhang, Fudan University
Date: Thursday 26 May
Time: 11.30am—12.30pm
Location: F106

Date of Next Issue:
27th May 2016

Discovering the Science that Helps Us Access Nature

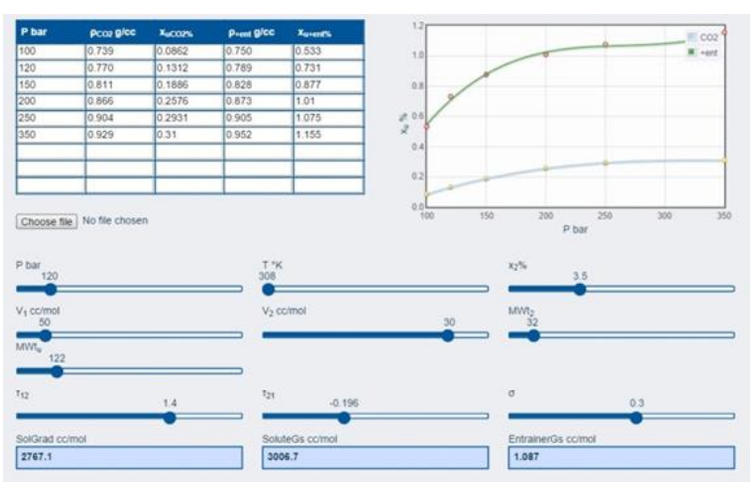
Dr Seishi Shimizu's research shows how fundamental scientific theory can unlock access to natural products and ingredients, and improve industrial processes.

From food and drink to dietary supplements and cosmetics, consumers favour "natural" products. But it can be a challenge to find the best processes for extracting key natural substances from plant matter, either to use as ingredients – such as naturally occurring anti-oxidants, flavours or colours – or to remove them, as in the decaffeination of coffee.

The use of chemical solvents is increasingly seen as undesirable. So there has been a trend towards using carbon dioxide, in its special "supercritical" fluid form, as a natural solvent for these extractions. But unfortunately, supercritical CO_2 ($scCO_2$) is often a poor solvent for many interesting natural substances, and its solvency has to be boosted with an "entrainer" – a small amount of another solvent such as water or ethanol, which can dramatically increase the solubility.

Until now, the way in which these entrainers boost solubility with $scCO_2$ has only been partially understood, which has made it difficult for food scientists to know how to select the perfect entrainer for any given foodstuff, or the optimal conditions (e.g. temperature, pressure) for the process.

A new paper published online on 11th April by Dr Seishi Shimizu of the York Structural Biology Laboratory (YSBL), Department of Chemistry, uses fundamental thermodynamic theory to solve this problem. Dr Shimizu disproves two of the common hypotheses regarding the behaviour of entrainers in $scCO_2$ extraction processes, concluding that it is molecular-level affinity between the entrainer and the solute (e.g. caffeine) which determines efficacy. The more the entrainer likes to associate with the substance being extracted, the stronger the effect.



[image shows app screenshot]

But these conclusions do not remain in the realm of dry theory. With collaborator Professor Steven Abbott of industrial process consultancy TNCF Ltd, Dr Shimizu has created a free, open-source app that runs on phones, tablets and laptops. The paper, published in the *Journal of Physical Chemistry*, focuses on the scientific theory, but it also encourages readers to go to the app and play with all the factors involved in the process.

The beauty of this approach is that it does not involve any complicated analytical equipment. It simply uses the data that the $scCO_2$ community regularly gathers – solubilities and densities at various temperatures and pressures. The app can read the data directly and do all the calculations to reveal which elements of the process (such as entrainer-solute interactions) are the most important.

Prof. Steven Abbott, TNCF Ltd

Both guiding theory and app will be welcomed by a wide range of industrial scientists looking to optimise their extraction processes.

Shimizu, S & Abbott, S 2016, 'How Entrainers Enhance Solubility in Supercritical Carbon Dioxide' *Journal of Physical Chemistry B*., (advance online press http://pubs.acs.org/doi/abs/10.1021/acs.jpcb.6b01380)

York Research Features on Radio 4's Inside Science

Research from the Wolfson Atmospheric Chemistry Laboratories (WACL) was featured on BBC Radio 4's Inside Science this month, with an interview held at the Faraday Discussions meeting on Urban Atmospheric Chemistry:

http://www.bbc.co.uk/programmes/b075mdy9

York contributed full papers on air pollution sensors, NOx and diesel emissions and the impacts of bioethanol on air quality.

Suggestion Box

Reminder: There is a 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.

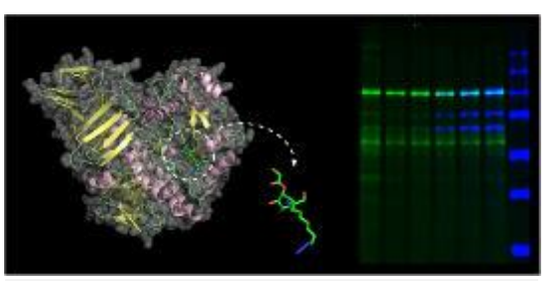
Breakthrough in the Treatment of Inherited Genetic Disease

Scientists at the Universities of York and Leiden have made a significant breakthrough in the treatment of an inherited genetic disorder which damages muscle and nerve cells in the body.

Pompe disease is caused by a defective gene that results in a deficiency of an enzyme called acid alpha-glucosidase (GAA) which causes progressive muscle weakness in people of all ages.

The crippling disease came to wider public attention through the 2010 film *Extraordinary Measures* starring Harrison Ford.

But the new research, which included a team from Leiden University in the Netherlands, has led to the synthesis of fluorescent chemical 'probes' which can be applied for medical diagnosis. These tools allow scientists to measure the level of the GAA enzyme in human cell extracts, allowing rapid detection of enzyme levels.



Left: 3D structure of an alpha glucosidase enzyme bound to probe, with close-up of probe structure. Right: Fluorescent labelling of enzymes in cell extracts

The researchers say the compounds will help inform more effective treatments, eventually allowing for better therapies and personalised medicine. Similar diagnostic approaches have already improved medical treatment for other inherited conditions.

The research team included Dr Liang Wu and Professor Gideon Davies of the Structural Biology Laboratory, Department of Chemistry, at York.

Professor Davies said, "These tools allow scientists to measure levels of enzyme in healthy and sick people. Imaging active enzyme levels will help assess disease severity and also help inform more effective treatments."

Dr Wu added "It is an exciting breakthrough, made possible by the power of European collaboration. We believe that this technology will have widespread application beyond genetic disease and into cancer therapies."

The work, funded by the European Research Council, is reported in the journal *ACS Central Science.*

The paper can be found here: http://pubs.acs.org/doi/abs/10.1021/acscentsci.6b00057

York Chemistry in UK Top 5

The excellence of the Department of Chemistry at York has been recognised by the 2017 Complete University Guide, which sees York entering the Top 5 for Chemistry, achieving an outstanding 4th place.

This independent and trusted league table rates departments for **Research Quality, Student Satisfaction, Graduate Prospects and Entry Standards**, with the department gaining high scores across the board.

The Department has a unique ethos of supporting all of its staff and students, enabling them to succeed in a **collegiate** and **caring** environment, as recognised by the recent renewal of its Athena SWAN Gold status. In terms of teaching, the Department listens carefully to student feedback and responds pro-actively in order to make improvements to the student experience.

With outstanding new research buildings and teaching laboratories, the department is well-placed to build on this success, and aims to continue improving both research and teaching yet further in the coming years.

I am delighted to see this outstanding recognition for the Department. Our staff work very hard to ensure that, against the backdrop of high-quality, world class research, their innovative approaches to teaching and learning provide an excellent experience for our undergraduates, equipping our students for the next stage in their lives and careers.

- Professor Duncan Bruce, Head of Department

YSBL PhD Graduate Invited to SET for Britain Exhibition

Dr Wayne Paes (recently of YSBL, Brzozowski Group) had his work on chlamydia selected to be presented at the House of Commons on Monday 7th March, in the Biological and Biomedical Session of the SET for Britain 2016 Poster Competition.

The **SET for Britain** exhibition offers early career researchers a unique opportunity to communicate the impact of their research to Members of Parliament at the House of Commons. This impressive forum also provides a platform for MPs to engage with scientists and discuss the socio-economic benefits of current research in relation to lobbying for a broader set of political objectives. This is of particular importance ahead of the UK's impending EU referendum, and in the context of allocation of government funding to specific industrial and scientific sectors, from biofuels to drug development. For instance, the scientific community within the UK gains much value from EU membership, with Marie Skłodowska-Curie Fellowships and Training Networks benefitting individuals who gain new technical and employability skills abroad, and a large amount of funding coming in from the European Research Council and Erasmus exchange programmes. The SET exhibition raises the profile of science in Parliament, and gives MPs the chance to take ideas back into parliamentary debates surrounding key issues such as the EU referendum.

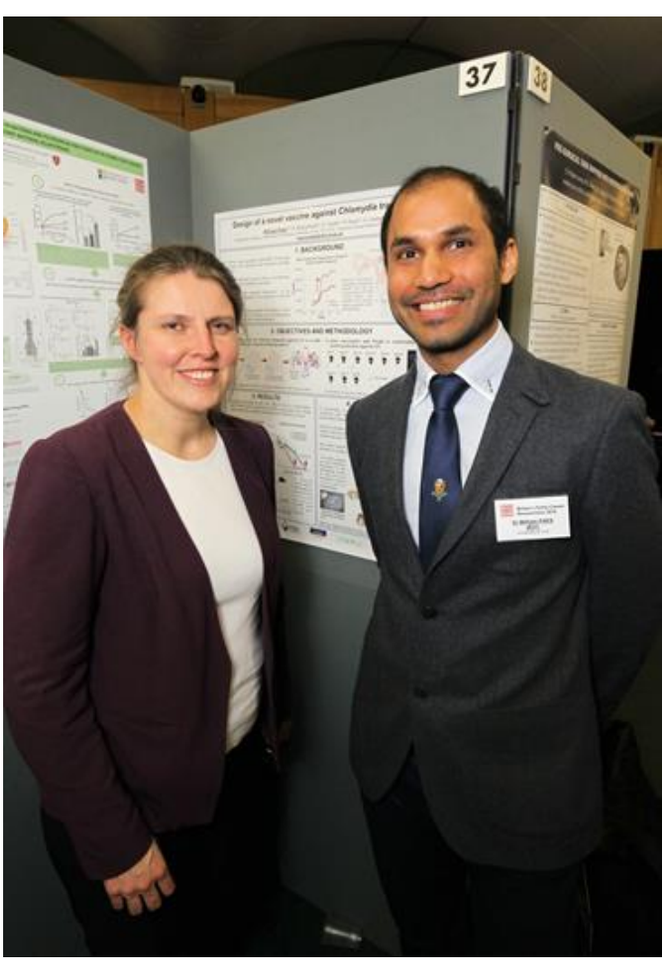


Image copyright John Deehan Photography Ltd

During the event, I met with my local and workplace MPs from York - Rachael Maskell and Julian Sturdy. Both were extremely interested in discussing the future impact of a vaccine for sexually transmitted *Chlamydia trachomatis* infections, but they were also keen on understanding more about the key issues surrounding vaccine development and antibiotic resistance in a broader context. Thus, it is a good opportunity for us as scientists to take a step back from the microscope and question and observe the bigger societal picture.

Finally, the event was a fantastic opportunity to gain further insight on cutting edge research taking place at a wide range of other institutions, and for networking (for example, enabling me to meet people who work down the road from my current research institute in Oxford.)

Research Summary

Worldwide, *Chlamydia trachomatis* (*Ct*) is the most common sexually transmitted bacterial pathogen, responsible for ~90 million new cases of disease each year. If left untreated, asymptomatic infections often lead to pelvic inflammatory disease and infertility in women. While antibiotics can resolve initial infections, they are not effective at preventing reinfection, which impacts adversely on disease outcome. Furthermore, 'seek and treat' approaches in public health clinics across the UK cost ~£100 million between 2003-2009, and ~$2 billion per annum in the U.S. However, *Ct* is still highly prevalent within the global community. Thus, development of a vaccine is likely to be the most effective means of eradicating or controlling the spread of disease. We have developed a novel preclinical vaccine that elicits robust protection against sexually transmitted chlamydial infection in mice. Overall, our research has the potential to enable significant progress towards improvement of the reproductive health of men and women worldwide, and future work now aims to conduct vaccine efficacy trials to assess the immune response to the vaccine in humans. Importantly, protection against infection from human papilloma virus, a causative agent of cervical cancer in women, illustrates the feasibility of successful vaccine development against sexually transmitted pathogens.

Science Week at Wilberfoss Primary School

At the end of March, PhD student Dan Cornwell from the research group of Professor David Smith was invited to Wilberfoss Primary School to deliver a practical activity as part of the school's Science Week. Dan took along the popular demonstration of alginate gels, which were to be made by dropping small amounts of sodium alginate solution into calcium chloride solution to produce small jelly spheres. However, many of the pupils soon found out that pouring in larger quantities of alginate resulted in bigger blobs of "slime", much to their amusement - and to the slight annoyance of the teachers who had not appreciated how messy the practical would get! Dan also gave a short talk to the Key Stage 2 students about high-tech gel research from the Smith group, including using gels to remove pollution from water. There was plenty of time for questions at the end – the most frequent of which was "why do you wear a white coat?" and the most vexing of which was "who was the first scientist?" (answers on a postcard please). Hopefully some future scientists were inspired!

BEM Award Ceremony for Adrian Whitwood

On Wednesday 20th April, I went to County Hall, Northallerton to receive my British Empire Medal (BEM) accompanied by my wife, Amanda, my two children and my mother. We arrived in the early afternoon on a lovely sunny day and took a few pictures outside before moving inside for the ceremony. After a few minutes, we were ushered into The Grand Meeting Room and into our seats. I was sat at the front with the 6 other recipients of the BEM. Then the Lord Lieutenant for North Yorkshire, Mr Barry Dodd, entered accompanied by the Vice Lord Lieutenant, Major Peter Scrope, the leading Navy and Army cadets for the region plus two local councillors. After a brief introduction and welcome, the ceremony started with the full nomination of the medal winner being read out by the Vice Lord Lieutenant followed by the presentation of the certificate by the Lord Lieutenant with the medal being pinned on, somewhat nervously, by one of the cadets; there was then an official photograph in front of a picture of the Queen. True to form, I was the last of the 7 - frequently the case when your surname begins with a W. My nerves settled a bit after this and we went out into the Spring sunshine for more official and unofficial photographs.

Photos completed, we returned to The Grand Meeting Room for afternoon tea. What was really nice was that the dignitaries moved from table to table chatting with each group. When the Lord Lieutenant was sitting with us, my daughter Lizzie asked him what the medal was around his neck. The answer was a CBE to which Lizzie replied that she'd have to get one as it matched her nail varnish! Towards the end, we were all asked to say a little about why we'd been awarded the medal. After a slightly hesitant start, Chris, my son, said that once I got onto talking about crystallography I became more confident and enthusiastic. It's quite fun explaining complex science to people without a strong scientific background. It was a wonderful day with a great mix of formal and informal and it was great to have all my immediate family with me.

- Adrian Whitwood BEM!

Left: With the family, feeling slightly nervous before the ceremony

Mum takes a better photo and I'd relaxed enough to smile!

After the presentation!

New Starters

Dr Ryan Hossaini, Eleanor Dodson Fellow
Room: G/C116; Extension: 4755; Email: ryan.hossaini@york.ac.uk

Dr Gillian Higgins, YSBL PDRA
Room: K266; Extension: 8276; Email: gillian.higgins@york.ac.uk

Kate Appleby, CHyM PDRA
Room: CHYM108; Extension: 8890; Email: kate.appleby@york.ac.uk

Tom Frankland, CIEC Administrator
Room: B016; Extension: 2523; Email: tom.frankland@york.ac.uk

Dr Liz Dickinson, Daphne Jackson Fellow
Room: D015; Extension: 4230; Email: liz.dickinson@york.ac.uk

Sarah Henshaw, NMR Technician
Room: NMR Lab; Extension: 8892; Email: sarah.henshaw@york.ac.uk

Clarke Group News

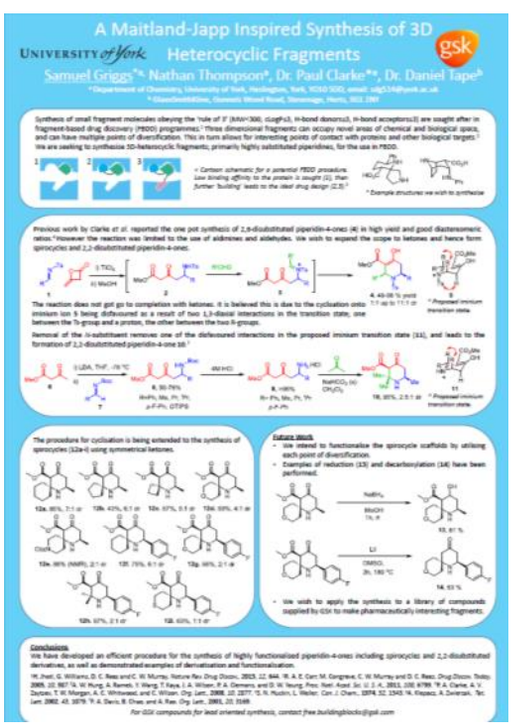
It's been a busy month for the Clarke group.

On 6th April, we went to the RSC NE regional meeting in Newcastle. At this meeting Andy Steer, Sam Griggs, Yin-Ting Hsiao and Nadiah Nasir all presented posters. Despite stiff competition from fellow York chemists and those from other regional universities, Sam won the best poster prize, for his poster: "A Maitland-Japp Inspired Synthesis of 3D-Heterocyclic Fragments". At the same meeting Paul gave the opening lecture on Andy's project: "The Prebiotic Synthesis of Carbohydrates".

On the 14th April, the group went to Huddersfield to support Andy give a talk on his PhD research "The Prebiotic Synthesis of 2-Deoxy-D-Ribose" at the SCI Postgraduate Research Symposium, Northern Section. Andy was one of 10 students selected to speak at this event.

On 18th April, Paul and Sam visited GSK, Stevenage to discuss some of Sam's exciting results in the area of "The Synthesis of 3D-Spirocyclic Piperidines". Interest in this project from GSK is high and there was much discussion of how to take the project to the next level and apply it to industrial drug discovery.

Paul is attending an EU ORIGINS COST meeting on The Origins of Life in Vilnius, Lithuania 23-30th April and will give a lecture "The Prebiotic Synthesis of Carbohydrates".



Sam's winning poster

Sam being presented his poster prize

Organic Group News

SCI Post-graduate Symposium, University of Huddersfield

On Tuesday 14th April, the SCI held its annual postgraduate symposium (North!) on Novel Organic Chemistry at the University of Huddersfield. I think that York has had a speaker selected to present each year for the last 20 years! This year, the event attracted speakers from all around the region including Manchester, Leeds, Lincoln, Sheffield, Lancaster, Nottingham and Newcastle. However, York was the only department to have two speakers presenting their research! Andy Steer from the Clarke group gave an excellent and entertaining lecture on his work towards developing new prebiotic routes to carbohydrates and Sarah Chambers (Taylor/O'Brien groups) gave a great lecture on her indole spirocyclisation chemistry. Around 20 people from the dept (academic staff, post-docs and PhD students) attended the meeting and were delighted to see Sarah winning the £100 runners-up prize. Congratulations!

- Peter O'Brien

Equality and Diversity Seminar and Discussion with Professor Lesley Yellowlees

We were delighted when Professor Lesley Yellowlees CBE BSc PhD FRSC FRSE accepted our invitation to give a diversity seminar. Lesley is currently Vice Principal and Head of the College of Science and Engineering at the University of Edinburgh. She has worked with the Royal Society of Chemistry for many years and became their first female President in July 2012.

Lesley is a champion for the promotion of women in science and in 2011 was honoured by the IUPAC as a Distinguished Woman in Chemistry for her scientific contributions to the global chemistry community. She was the first female graduate in Chemical Physics from Edinburgh and her research interests include inorganic electrochemistry and spectroelectrochemistry, epr spectroscopy, solar energy and CO_2 conversion.

She was awarded an MBE in 2005 for services to science, a CBE in 2014 for services to chemistry, and was elected as a Fellow of the Royal Society of Edinburgh in 2012. She has honorary degrees from both Heriot-Watt and the Open Universities. Lesley is married to Peter and they have two children, Sarah and Mark.

The large audience who assembled in B101 on 25th April were not disappointed as Lesley's enthusiasm and energy were very evident throughout her presentation "Promotion of Diversity in Chemistry". Her presentation started with her quote about running out of patience and having to take action to make a difference:

"I've often heard myself say we have to be patient, but there comes a time when you have to run out of patience, because if we don't run out of patience and we don't start demanding more from the system, demanding that culture change to happen faster than it's happening at present, then I think we not only do ourselves a disservice, but we do the generations both past and the ones to come a huge disservice as well."

Lesley discussed her personal journey as an academic and her long involvement with the work of the RSC and stressed how important it is to never stop with actions and initiatives that promote diversity and inclusivity, as you can quickly lose any ground you have gained without continued effort. We should not underestimate the wealth of knowledge, skills, expertise and different view-

points we are missing out on by not including individuals from diverse backgrounds in all of our teams.

Lesley showed how the drop off points for females which vary in different subjects but in all cases there is a drop off with the percentage of women reaching the highest grades being very low; one of the highest rates of drop-off being in Chemistry.

Many of the audience were very envious when Lesley showed a photo of the new nursery at Edinburgh, just one of the areas where Lesley has convinced the University of Edinburgh to make an investment. They are looking at after school care provision, funding for parents to have family and friends look after their children at home so that they can attend conferences away from home and have recently begun working towards a Race Equality Charter Mark.

Following Lesley's talk, a Q&A session was held with PDRAs and PGR students invited to meet with Lesley over tea and cake. Leonie Jones, the employability and diversity officer for chemistry, chaired a lively discussion about issues affecting underrepresented groups in academia. In particular, the reasons for the drop off in the proportion of females at higher levels, the impact of short contracts and moving around on individuals with partners and families, and the importance of support and encouragement in the form of mentoring relationships. It was great to see representation from across the groups and I think that everyone found the session both interesting and enjoyable. Many thanks to everyone involved.

- Helen Coombs and Leonie Jones

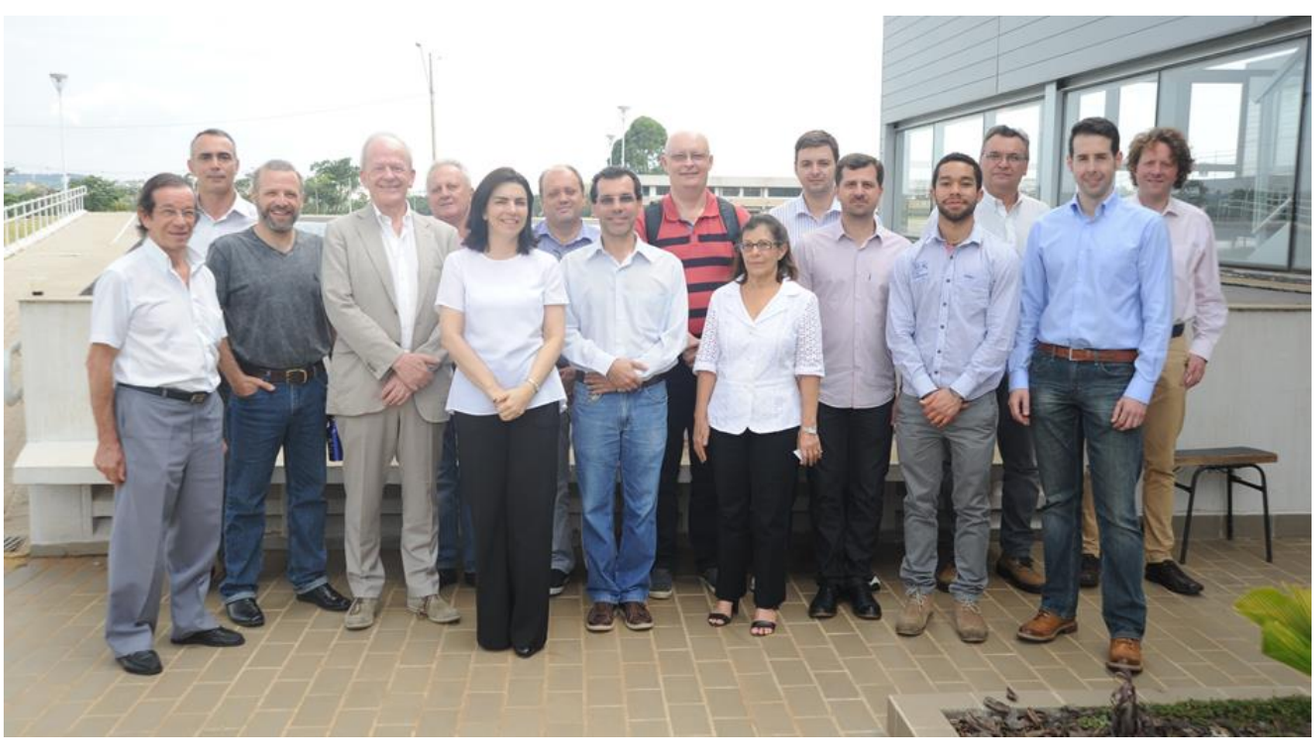
Professor Lesley Yellowlees and Leonie Jones meeting PDRAs and PGR students

Newton Fund Visit to Brazil by GCCE

In mid-April, 5 members of the Green Chemistry Centre of Excellence (GCCE) travelled to Brazil to present at a number of meetings in São Carlos and Rio de Janeiro. The first workshop was held in the Federal University of São Carlos (UFSCar) impressive new Petrobras-funded Green Chemistry centre where members from the GCCE, UFSCar, University of São Paulo (USP) and the citrus company Agroterenas presented their work and looked to build further collaborations especially in the area of food waste valorisation. Of special note was the announcement from Agroterenas that with further adoption of green chemistry principles, what was their waste streams were now new product lines and were delivering almost as much income as their primary juicing business.

A well-attended workshop at SENAI Cetiqt in Rio de Janeiro offered a chance to showcase our research to like-minded colleagues from Federal University of Rio de Janeiro, the SENAI (National Service for Industrial Training – institutions designed as a learning environment to improve the education and welfare of the working class in Brazil in addition to acting as bridge between industry and academia) and industry. Built on the wealth of available biomass, the significant industrial companies including Braskem, Croda Brazil, Fibra, Oxiteno and Solvay all presented examples of their commercially successful application of sustainable chemistry. Again this event resulted in discussions around further future collaborations and shared goals.

Further meetings between the GCCE and representatives from a number of SENAIs resulted in the identification of potential research collaborations and exciting opportunities for expanding our training material. These included new green chemistry experiments for Brazilian high school teachers, our currently under-development online training courses and short courses, as well as the possibility of SENAI students taking parts of our undergraduate programme.



Careers Days Proved a Big Hit in York and Middlesbrough

Pupils from Middlesbrough working on the liquid crystal activity

The final two STEM careers days for this academic year were held in Middlesbrough and York on the 3rd and 10th March respectively.

These two sessions were for the younger age groups (11-14 year olds) – sessions for 14-16 year olds and A level students had already taken place.

Pupils at the YSOC facility taking part in the spectroscopy activity.

Students from Wetherby High School enjoyed the day and their teacher, Jenny McCartney said, I would like to thank you and your students for putting on the STEM day for our students yesterday, they were truly inspired and came back so eager to talk about what they had done and what they wish to do in the future. “We are definitely going to take triple science; we didn’t know that there were so many interesting jobs" which is fantastic to hear. And their body lotion smelt lovely!

Joy Parvin, CIEC Director, is already planning for a similar series of days for 2016-2017. The Careers Days this year were generously supported by Cogent and other, local, industries delivered the various workshops. CIEC hope to involve other industries in next year’s sessions.

Joy was delighted with the feedback from this year’s events “Many of the schools that have taken part have now been inspired to think about STEM careers. At a time when there is a serious skills shortage in the process industries this is very encouraging.”

CENTRE *for* INDUSTRY EDUCATION COLLABORATION

CIEC invite you to participate in a one day workshop that will increase your potential to offer exciting applied science across the community

STEM Communications skills workshop

Wednesday 18th May 2016, 9:30 – 13:00 followed by lunch

- Explore new and innovative ways to interact with schools
- Trial a range of exciting practical activities to motivate and inspire students of all ages
- Develop your understanding of the science support that schools need
- Gain access to an extensive bank of practical resources form over 50 project titles
- Assess the potential to use the **University YSOC laboratory** for STEM related outreach activity
- Lunch time networking with like-minded professionals with shared aims to promote scientific research

Contact Tom Frankland at ciec@york.ac.uk to book your place!

CENTRE *for* INDUSTRY EDUCATION COLLABORATION

YSOC

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