



# Chemistry Update

Newsletter 253, 26<sup>th</sup> September 2014

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## Calendar of Events

### iDTC Launch

Date: Wednesday 1 October

Time: 4pm—6pm

Location: DS/008

*All PhD students and supervisors invited*

Please sign up to attend:

<https://uniofyork.doodle.com/eruqtvmtsh6zur8b>

### Departmental Seminar

Speaker: Professor Antony Williams

Date: Thursday 2 October

Time: 1pm

Location: A101

### Building Sustainability into your Business:

#### The Case for Bio-Based Chemicals

Speaker: Various

Date: Monday 6 October

Time: 9.30am—5pm

Location: GCCE, First Floor F-Block

### KMS Prize Winners' Seminar and Poster Session

Date: Wednesday 8 October

Time: 2.30pm

Location: A101

### YorCat End of Year 2 Talks

Date: Friday 10 October

Time: 9.30am—5pm

Location: A122

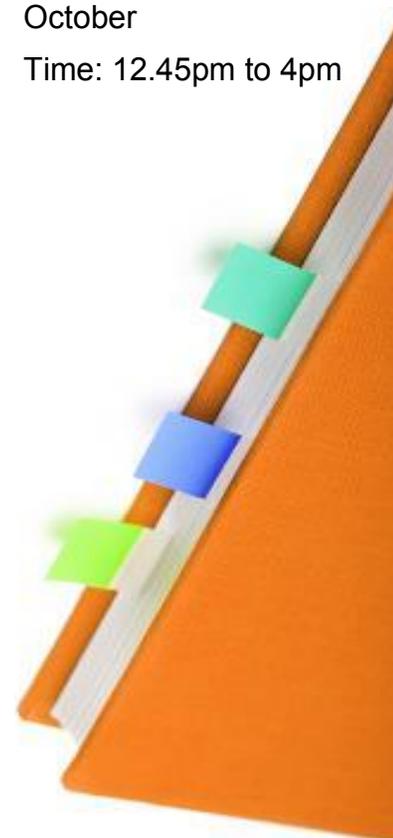
### UCAS Interview

#### Afternoons

Date: 14, 23, 28 & 30 October

Time: 12.45pm to 4pm

**Date of Next Issue:  
31<sup>st</sup> October 2014**



## 50-Year Anniversary Celebration & the Official Opening of Block F

### The opening of our latest new building coincides with our anniversary and the launch of our York Chemistry 50 Fund

To celebrate the success of the Department, on our golden anniversary, we invited our Chemistry alumni to join us for the opening of our latest new building over the weekend of 5-7 September 2014. The opening of Block F, which houses our Green Chemistry Centre of Excellence and our undergraduate teaching laboratories, is the latest development arising from a £29 million investment in Chemistry at York.

Our celebrations started with opening ceremonies for the two parts of the new development. Dame Ellen MacArthur opened the Green Chemistry Centre of Excellence's new research facilities while the teaching labs were opened by the first female President of the Royal Society of Chemistry, Professor Lesley Yellowlees, of Edinburgh University and by Professor Sir John Holman, Senior Education Advisor to the Wellcome Trust, who also presented a demonstration lecture on "Teaching Science the Practical Way" in the National Science Learning Centre.

**Over 200 guests** attended Professor Holman's talk, which was followed by an exhibition, highlighting some of our recent teaching innovations, with participation by the Royal Society of Chemistry and Alfa Aesar. Finally, Professors David Smith and James Clark joined Professors Yellowlees and Holman, to take part in a panel Q&A session on the challenges and opportunities facing chemists in teaching and research.

On Saturday, over **100 of our alumni** enjoyed a packed programme of events starting with a welcome reception, sponsored by the Royal Society of Chemistry, featuring a periodic table-themed cake. Our guests enjoyed a panel session that focussed on the early days of the Department, with reminiscences from Professors David Waddington, Eleanor Dodson, and Bruce Gilbert, along with Dr Roger Mawby and former student Chris Boon.

There was the opportunity to 'go back in the lab', with our alumni analysing inks and painkillers, together with a Chemistry-at-York quiz, followed by a tour of our new teaching laboratories.

Our alumni also heard about some recent developments in our teaching and research, with talks by Professor David Smith, recent graduate Lizzie Wilcock, Dr Avtar Matharu and postgraduate student Kirsty Davey.

Finally, the Vice Chancellor joined us for our official 50th anniversary dinner and reunion, with an after dinner speech by Professor Paul Walton on the Chemistry of Chocolate.



We enjoyed meeting old friends, rekindling old memories and launching our [YorkChemistry 50 Fund](#), established to support our students and researchers - helping to ensure we continue to be the Department of choice for talented chemists.

Chemistry graduate Dr Anthony H. Wild (a major supporter of the Department's investment into laboratory and teaching space) has initiated a matching challenge to help encourage fellow alumni to support the York Chemistry 50 Fund. Between September 2014 and December 2015 graduates will be asked to support the appeal and **all donations will be matched £1 for £1**. Gifts over £500 will be matched £2 for every £1 given.

To celebrate our anniversary we have produced a [booklet](#) highlighting some of our notable events and key achievements.

Also, a number of former members of staff, together with the Head of Department, are in the process of compiling a book that charts the first fifty years of Chemistry at York.

If you would like to receive further information on the book, please [contact Professor Richard Taylor](#).



We look forward to keeping in touch with our alumni – there are a number of ways they can [interact with the Department](#). This includes:

- Attending a Chemistry seminar and/or Open Day;
- Talking about their career at an undergraduate or postgraduate careers event;
- Writing an article for [Chemistry Review](#).

## Suggestion Box



Reminder: there is a Suggestion Box located next to the pigeon holes in the foyer of A Block and one outside Room K167 for YSBL staff. Suggestions from staff are most welcome. All suggestions are discussed at the departmental communications meeting.

## York's Major Role in Scientific Assessment of Ozone Depletion



Professor Lucy Carpenter, from the Department of Chemistry has played a key role in a major new scientific assessment of the ozone layer which will inform government policies across the globe. She acted as a Chapter Lead Author for the Scientific Assessment of Ozone Depletion: 2014. The Assessment for Decision-Makers, a summary document of the assessment, is published this week.

The assessment is conducted under the auspices of the World Meteorological Organization (WMO) and the United Nations Environment Programme (UNEP), and co-sponsored by NASA, the National Oceanic and Atmospheric Administration (NOAA) and the European Commission. It is written and reviewed by leading experts in the international atmospheric sciences community at the request of the Parties to the U.N. Montreal Protocol and contains the most up-to-date understanding of ozone depletion. The assessment will guide policymakers as they strengthen the original provisions of the Montreal Protocol.

The 2014 assessment concludes that actions taken under the Montreal Protocol have led to decreases in the atmospheric abundance of controlled ozone-depleting substances (ODSs), with expected return of the ozone layer toward 1980 levels by mid century in midlatitudes and the Arctic, and somewhat later in the Antarctic. It also finds that, whilst the Montreal Protocol and its Amendments and adjustments have made large contributions toward reducing global greenhouse gas emissions, these could be significantly offset in the future by projected emissions of hydrofluorocarbons (HFCs) currently used as ODS replacements

Professor Carpenter said: “The report – the first comprehensive update in four years - analyses the impact on the Earth’s protective ozone layer of concerted international action since the adoption of the Montreal Protocol in 1987. It also assesses the implications of the phase out of ozone-depleting substances on efforts to address climate change.”

Professor Carpenter’s chapter of the report concentrated on ozone-depleting substances and other gases of interest to the Montreal Protocol. Some of the work cited in this section of the assessment was carried out by researchers based at York.

Professor Carpenter said: “Research at the University of York has contributed to the assessment by determining trends and abundances of ODSs and their substitutes in the atmosphere and by assessing the contributions of natural compounds to ozone depletion”

## Fairlamb Group News

Professor Ian Fairlamb presented at an EPSRC Dial-a-Molecule meeting "Computational Prediction of Reaction Outcomes and Optimum Synthetic Routes", which was held 10<sup>th</sup> & 11<sup>th</sup> September 2014 at Weetwood Hall (Leeds). His lecture on "Intelligent Synthesis" was warmly received - the approach was discussed more broadly in the workshop sessions. The meeting also focused on innovative approaches utilising computation (including DFT calculations) for the improvement of chemical synthesis.

There was an interesting discussion about how one represents organometallic species in chemical search databases, like Scifinder, Reaxsy and related. One interesting synthetic equivalent discussed was the highly reactive molecule, cyclobutadiene, and Rowland Pettit's stable and isolable eta-4-cyclobutadienyl iron(0) tricarbonyl complex (a synthetic equivalent). There are many other systems like this, where a seemingly elusive organic intermediate can be stabilised by a metal complex, but where there is currently no mechanism for searching for it in the chemical literature. As the meeting was attended by several companies developing new chemical databases, the hope is that this problem will be addressed in coming years, which will hopefully inspire chemical syntheses in the future.

In August, Ian delivered an invited lecture at the Chiretech Technology Centre (Dr Reddies Laboratories) in Cambridge. His lecture was titled "Improving Pd catalysed cross-coupling through mechanistic interrogation and synthetic applications". He discussed the role played by both homogeneous and heterogeneous Pd species in cross-coupling reactions. Recent results from the PhD projects of Tom Ronson and Alan Reay were presented, in addition to work from past PhD students (Sara de Ornellas, Thomas Storr and Thomas Williams). Sara is now a post-doctoral scientist at the University of Oxford, working with Prof. Tom Brown. Tom Storr is working as a post-doctoral scientist with Prof. Christopher Moody at the University of Nottingham, and Tom Williams is working as a post-doctoral scientist at the University of Manchester with Prof. Mike Greaney.

Congratulations to Jonathan Ward who has recently secured a post-doctoral research associate position with Prof. Martin Bryce at Durham University. Jonathan worked on an interdisciplinary project funded by the BBSRC working on therapeutic CO-releasing molecules, co-supervised by Jason Lynam and James Moir (Department of Biology). Jonathan fully-embraced the interdisciplinary nature of his project, which involved chemical synthesis, drug design, physical measurements and microbiology work. His recent work on a promising CO-releasing molecule, called TryptoCORM, has been accepted for publication in Chemistry A European Journal.

Congratulations to Dr Margot Wenzel, a post-doctoral scientist in the group (IMI-4, Chem21 project - collaboration with Green Chemistry), for securing a new post-doctoral position at Imperial College (London) working with Dr James Wilton-Ely. Margot has worked very hard over the last year and her efforts have been greatly appreciated.

## Chemistry Bake Off 2014

The Chemistry Department Bake Off 2014 was a great success. There were 22 baked items, all scrupulously analysed by Jason Lynam and Katrina Sayer. Sherry Chan of YSBL claimed the presentation award, Danielle Jowett of Inorganic Chemistry claimed the taste award and Amy Ruddlesden of CHYM claimed the overall enjoyment factor award.

£180 was raised for York Food Bank. We delivered the cash, which will go towards the fuel needed for delivery of food to vulnerable people in our community.

Chris Unsworth and Ellis Wilde would like to thank to all who attended, baked and donated!



## Atmospheric Chemistry Group News



This month saw the first of three intensive measurement periods at the Manchester Aerosol Chamber to study the oxidation of diesel emissions. This NERC funded work, part of the COM-PART project, brings together researchers from the Universities of Manchester, York and Birmingham. Kelly Pereira and Rachel Holmes took York's comprehensive two-dimensional gas chromatograph (GC×GC) to study the complex mixture of organics that are emitted from a typical diesel engine.

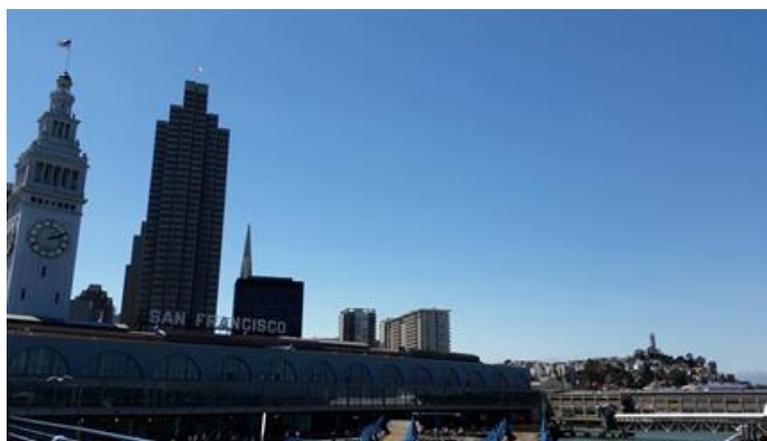
After some “teething” issues, the instrument was used to test the emissions under a range of different operating conditions. This information will allow us to map the emissions in terms of their volatility, polarity and reactivity in order to assess their impact on air quality.

In September, Dr Jacqui Hamilton travelled to the International Aerosol Conference in Busan, South Korea to give a presentation on “Investigating Aerosol Chemistry One Molecule at a Time”. This large conference only runs every four years and it was a great opportunity to catch up with recent work and enjoy the local kimchi and soju.

In August, Dr Andrew Rickard travelled to the American Chemical Society meeting in San Francisco to give an invited talk on “Mechanistic Insights into the Tropospheric Ozonolysis of Alkenes”. This year's meeting had two dedicated symposia on the “Fundamentals of Atmospheric Chemistry” and “Chemistry of Atmospheric Nitrogen-Containing Compounds”.



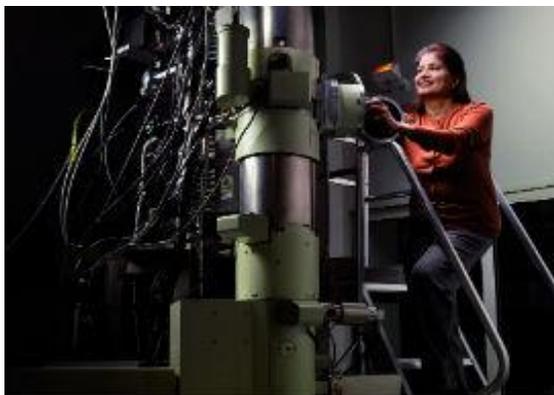
Jacqui with Dr John Wenger, University College Cork and Dr Rob Healy, University of Toronto in Busan market.



Strolling down to the Ferry Building in San Francisco to sample some artisan cheese and wine

## Pratibha Gai Wins Royal Academy of Engineering Recognition

Professor Pratibha Gai, Chair of Electron Microscopy, was one of 59 new Fellows announced by the Royal Academy of Engineering. The Royal Academy of Engineering is the National Academy of Engineering of the United Kingdom.



She is head of the York JEOL Nanocentre, a major long-term collaboration between the University's Departments of Chemistry, Physics and Electronics, the European Union, Yorkshire Forward and leading electron optics manufacturer JEOL.

Professor Gai said: "I am extremely pleased to be elected a Fellow of the Royal Academy of Engineering. It is humbling that my work has been recognised by my academic colleagues. It will be an honour to join a group of such outstanding scientists and engineers."

Professor Gai attended the University of Cambridge after initial education in India. She graduated with a PhD in Physics from the Cavendish Laboratory, specialising in electron microscopy, before establishing and leading the Surface Reactions and Catalysis group at the University of Oxford.

After senior research positions with DuPont, USA and concurrently as adjunct Professor at the University of Delaware, she came to York in 2007 as the Founding JEOL Professor of Electron Microscopy, with Chairs in the Departments of Chemistry and Physics. She is a Fellow of several scientific societies and was awarded the Gabor Medal and Prize of the Institute of Physics, UK in 2010.

Two years ago, Professor Gai was named the Laureate for Europe in the L'OREAL-UNESCO Women in Science Awards for 2013.

## Quadrennial International Microscopy Congress

The Quadrennial International Microscopy Congress (IMC-18) was held in Prague during 7-12 September 2014. Invited keynote presentation was made by the Nanocentre Directors Professor Pratibha Gai and Professor Ed Boyes, with their co-workers Dr Leonardo Lari, Michael Ward, Tom Martin, Ian Wright and Dr Kenta Yoshida. There were contributed papers and posters by Nanocentre researchers, including by Dr Leonardo Lari, Tom Martin, Michael Ward, Daniel Gilks with Dr Vlado Lazarov et al. The Congress attendance was very high (in the few thousands) and the quality of papers was excellent. Katrina Bakker from Professor John Goodby's group also attended the Congress.

## Pratibha Gai's Friday Evening Discourse at the Royal Institution

Professor Pratibha Gai presented Friday Evening Discourse at the Royal Institution (Ri) of Great Britain on 27<sup>th</sup> June.



Nanocentre researchers in the above photograph are L-R: As.Prof. Kenta Yoshida, Dr Michael Ward, Prof. Pratibha Gai, Prof. Ed Boyes and Tom Martin

## KMS Prize Winners' Seminar and Year 2 Poster Presentation

**Wednesday 8<sup>th</sup> October**

**2pm in A101**

Winners of the KMS prize will present their work to the Department:

**Kate Horner:** Off-Nucleus NMR: Poking Molecules with a Magnetic Shielding Stick

**Babatunde Okesola:** Supramolecular Envirogel: A 21st Century Nanosorbent for Water Purification

**Kirsty Davey:** Nematic polymer and elastomer particles

There will also be a poster session in A102 during the tea break where Year 2 PhD students will be displaying a poster about the first year of their work

All Welcome

## Promotions

The following promotions were given formal approval at Senate on 16<sup>th</sup> July 2014.

Personal Chair: Dr Gideon Grogan

Readerships: Dr Paul Clarke, Dr Duncan Macquarrie and Dr Julie Wilson

Senior Lectureships: Dr Jacqui Hamilton and Dr John Slattery

Research Grade 7: Dr Vitaliy Budarin

Many congratulations to all on their well-deserved promotions.



## 5<sup>th</sup> EuCheMS Chemistry Congress 2014

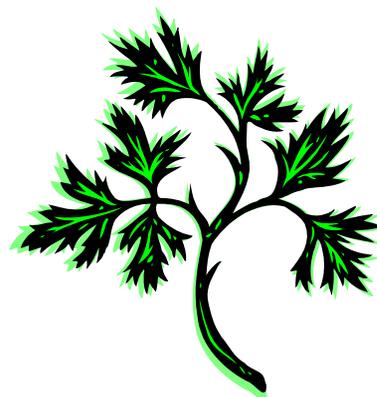


From the 30<sup>th</sup> August to 5<sup>th</sup> September, Dr Jose Castro-Osma and Dr Xiao Wu from Professor Mike North's group attended the 5<sup>th</sup> EuCheMS Chemistry Congress held in Istanbul, Turkey. At the conference, Jose gave an oral presentation on "Unprecedented halide-free aluminium catalyst for the synthesis of cyclic carbonates from epoxides and carbon dioxide", and Xiao obtained the RSC travel grant and presented a poster on "Synthesis of Cyclic Carbonates from Polyols and Carbon Dioxide over Zinc-Based Catalysts". Jose and Xiao have not only attended talks presented by renowned scientists such as Sir Venki Ramakrishnan and Professor Barry Trost, they have also visited the historic Blue Mosque.

## Edible Plants in the Quad

The barrels in the Chemistry Quad have: Lovage; Lettuce; Thyme; Ginger Mint; Rosemary; Coriander; and Marjoram. There is also a small amount of Basil and Mixed Salad.

Please help yourself.



## Departmental Seminar

### Professor Antony Williams, Creator of ChemSpider

Thursday 2 October, A101, 1pm

#### **Beyond the paper CV and developing a scientific profile through social media, altmetrics and micropublication**

Many of us nowadays invest significant amounts of time in sharing our activities and opinions with friends and family via social networking tools. However, despite the availability of many platforms for scientists to connect and share with their peers in the scientific community the majority do not make use of these tools, despite their promise and potential impact and influence on our future careers. We are being indexed and exposed on the internet via our publications, presentations and data. We also have many more ways to contribute to science, to annotate and curate data, to “publish” in new ways, and many of these activities are as part of a growing crowdsourcing network. This presentation will provide an overview of the various types of networking and collaborative sites available to scientists and ways to expose your scientific activities online. Many of these can ultimately contribute to the developing measures of you as a scientist as identified in the new world of alternative metrics. Participating offers a great opportunity to develop a scientific profile within the community and may ultimately be very beneficial, especially to scientists early in their career.

All Welcome

## Jason Lynam Visit to the University of Western Australia



Dr Jason Lynam visited the University of Western Australia for two weeks in August. The trip was funded by a Royal Society of Chemistry Journal Grant and allowed him to develop his collaboration with Professor Paul Low. This work is focused on developing an understanding of the mechanistic process involved in the formation of ruthenium vinylidene and alkynyl complexes. Jason gave a seminar “Understanding the role of vinylidene ligands in catalytic transformations” which discussed how experimental methods may be combined with Density Functional Theory (performed by John Slattery) may be used to elucidate key steps in ruthenium-catalysed reactions. In addition to writing papers and visiting vineyards, Jason and Paul even got time to go in the lab and develop some new routes to the key building blocks used in this area.

## Green Chemists in South Africa

This August was a busy and eventful month for a number of Green Chemistry Centre of Excellence (GCCE) members of staff and PhD students, who headed to Durban, South Africa, to attend the 5<sup>th</sup> International IUPAC Conference on Green Chemistry held on 17-21 August.



At the event, Lucie Pfaltzgraff, Thomas Attard, Dr Helen Parker, Dr Andrew Hunt and Prof Mike North (pictured above left) gave talks on the exciting recent research carried out at the GCCE, including utilization of waste orange peel, extraction of valuable chemicals with supercritical CO<sub>2</sub>, exploitation of plants for metal remediation of contaminated soil, development of greener solvents and use of CO<sub>2</sub> as a chemical feedstock.



Prof Mike North was presented with the RSC Green Chemistry Award, and GCCE visiting academic, Prof Vania Zuin (Federal University of São Carlos in São Carlos, Brazil; pictured below left) was awarded the CHEMRAWN VII Prize for Atmospheric and Green Chemistry.

The IUPAC conference received tremendous support from the Organization for the Prohibition of Chemical Weapons (OPCW), an international NGO and winner of the 2013 Nobel Peace Prize. According to OPCW, safer, non-toxic chemicals and chemical processes can ensure that the manufacturing of chemical weapons is easier to spot through routine audits under the Chemical Weapons Convention, which is why they actively support green chemistry research. Overall, an incredible diversity of research subjects was presented at the conference, emphasising the versatility and widespread appreciation of the principles of green chemistry.

Moving away from the shore of the Indian Ocean to the more familiar Atlantic, GCCE members headed to the second annual meeting of the Global Green Chemistry Centres (G2C2) held in Cape Town on 25-27 August. The GCCE team was joined by Prof James Clark and Dr Avtar Matharu, and the meeting was hosted by Dr Anwar Jardine and his team from the University of Cape Town's Department of Chemistry.

The G2C2 is a [Green Chemistry Network](http://www.greenchemistrynetwork.org/g2c2/) initiative that aims to unite green chemistry centres worldwide to promote research and collaboration, and to provide developing GC centres with access to the advice and expertise of more experienced members. To date the number of centres in the G2C2 network has reached 20, and it shows every sign of continuing to grow (See all members here <http://www.greenchemistrynetwork.org/g2c2/>).

At the meeting, representatives from 15 GC centres, including the ACS Green Chemistry Institute, the SynBioC of University of Ghent, the European Bioenergy Research Institute at Aston University, and the Centre for Green Chemistry at the University of Massachusetts gave talks on the research carried out at their institutions, and shared the state of GC in their countries.

The highlight of the meeting was four networking sessions on food waste, industrial collaboration, GC education, and public outreach. Attendees got to express their opinions, concerns and hopes about each topic, and share their experience, which highlighted just how different approaches to GC are in different institutions and countries. For full report on the G2C2 meeting please see the [GCN September Newsletters](#).



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For the second year in a row, the first prize in the International Solid Waste Association's international video competition has been awarded to GCCE green chemistry students Will Soutter (former MSc student) and Aleksandra Borisova (current PhD student).

The competition called for a creative approach to communicating the problems of waste in our society, using a short-form video. The winners partially attribute their success in the 2013 and 2014 competitions to the MSc in green chemistry, which broadened their understanding of environmental issues, encouraged big-picture thinking, and emphasized the importance of effective communication on scientific issues.

The winning video, titled "The Story of a Bottle", can be viewed here: <http://youtu.be/7j18NpQkcs8>

## Green Chemistry Centre Wins S-Lab Award

The Green Chemistry Centre of Excellence (GCCE) has been announced as one of 11 winners of the highly coveted S-Lab Awards for Laboratory Improvement and Innovation. The GCCE won the award in the Laboratory Based Teaching and Learning category, for training graduate and senior undergraduate students from all over the world and from a variety of backgrounds in practicing sustainability in modern chemistry laboratories.

The Awards are supported by many leading professional and higher education bodies. They were presented at a prestigious ceremony preceding the Supporting World Class Science conference at King's College, London on 2-3 September, which was attended by Professor James Clark, Dr Avtar Matharu and Dr Laurianne Moity. It provides a forum for science managers, estates and facilities, technical support, specialist services, suppliers and others to hear about the lab innovations and to network with a wider range of lab and facilities managers and designers.



## Katie Stott Running York Marathon

Katie Stott (covering maternity leave for Lyndsay Muschamp, the CHyM Administrator) is running in the York Marathon on 12 October 2014. Katie is very modest about her achievements and dedication but it would be great if the Department showed our support for Katie and raised some money for her charity: Sue Ryder hospices.

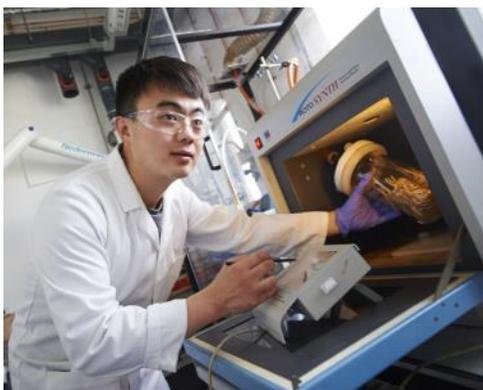


Katie says:

Here is my fundraising page for my first (and last) marathon attempt in October - raising money for Sue Ryder hospices. If anyone would like to sponsor me I would be very grateful.

<http://www.virginmoneygiving.com/katiestott>

## Building Sustainability into your Business: The Case for Bio-Based Chemicals



**Monday 6 October 2014, 9.30am to 5pm**

**Green Chemistry Centre of Excellence**

Speakers include David Calvert of iFormulate, Roland Arnison of Ricardo-AEA, Corrado Topi, SEI and Davide Di Maio, NNFCC

Included in the event is a buffet lunch and tours of our brand new research facilities.

Presentation Topics will Include:

- The benefits of using bio-based chemicals in business
- Sources of bio-based chemicals
- Issues to be resolved
- Research being undertaken at the University of York
- Technology for bio-based products - extraction / processing

Register to attend for free at <https://biobased-chemicals.eventbrite.co.uk>

All welcome.