

Chemistry Update

Newsletter 314, 25 October 2019

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Calendar of Events

UCAS Visit Days

Date: 28 & 31 October; 7, 11, 14, 18, 21, 25, 26 & 28 November
Time: 12pm—4pm

Physical Seminar

Speaker: Dr Olof Johansson,
University of Edinburgh
Date: Wednesday 6 November
Time: 1pm—2pm
Location: C/B101

Solvents Day

Date: Monday 18 November
Time: 10am—5pm
Location: C/F106

RSC Corday-Morgan Award Lecture

Speaker: Prof Igor Larrosa,
University of Manchester
Date: Wednesday 20 November
Time: 1pm—2pm
Location: TBC

Chemical Interactions talk

“Doing science from the intersection of colourblindness, autism and gender ambiguity”
Speaker: Prof Kevin Cowtan
Date: Tuesday 3 December
Time: 1pm—2pm
Location: C/B101

Departmental Christmas Party

Date: Thursday 12 December
Location: Marriott Hotel, York
Further details to follow about menus and tickets

Date of Next Issue:
29 November 2019

Learning about green pharmaceutical synthesis

A recent educational study from the Department outlines an innovative approach to teaching students about environmentally-friendly methods of pharmaceutical synthesis.



This project, developed by [Professor Andy Parsons](#) and [Dr Graeme McAllister](#) gives students the opportunity to prepare a blockbuster medicine in an authentic context. It has motivated and enthused students and is further enhanced through collaboration with AstraZeneca chemists.

Working in teams of 8–12 people, students synthesise the antiulcer medicine esomeprazole. To provide insight into the modern process chemistry industry, they have to propose, and then perform, environmentally-friendly modifications to the asymmetric oxidation synthetic step.

To function on a large scale, drug syntheses should be simple, safe and straightforward, as well as causing limited environmental impact. The development of such understanding and skills is of vital importance to the pharmaceutical industry.

Evaluation of the projects demonstrated very positive student feedback, and consistently showed that the project provided students with the key tools to develop 'greener' syntheses. The contextual approach of learning about such skills applied to an important drug helps cement the key learning goals. By the end of the project, each team achieved reproducible yields of esomeprazole of over 70%, in an enantiomeric purity of at least 70%.

In addition to giving the students creative input into their experimental work, the project also offers students the opportunity to develop valuable communication and team working skills. As part of the project, students have a final review meeting with a chemist from AstraZeneca, where they present a poster, focus on aspects of personal interest and reflect on their learning.

Reflecting on the success of the project, Professor Parsons said:

“It is very rare to have an industrial collaboration lasting over 10 years and this has helped us introduce an authentic context into our teaching programme, that has been shown to motivate and enthuse over 100 of our students. Our most recent AstraZeneca collaborator, Alex, is a Process Chemist, who completed an MChem degree at York and actually selected to do this project during the third year of his degree!”

The Department of Chemistry is committed to delivering high quality, innovative teaching, as reflected in its exceptional scores in the [National Student Survey](#) and the high rankings of the Department in [university league tables](#). Practical teaching in York is very innovative and focuses on developing students practical skills in a high-quality [laboratory environment](#).

Professor Parsons and Dr McAllister's educational study is published in [Journal of Chemical Education](#).



Our 2019 cohort of students, with framed copies of their posters, together with Alex from AstraZeneca.

Clarke group news

On the weekend of 20-21 September, the Clarke group celebrated its 20th anniversary. Former and current group members got together for a series of activities which included a trip to the York Beer Festival, a historic walking tour of York and a celebration dinner. Former group members travelled from as far away as Sweden, Italy, Portugal and Leeds to join in the fun.

The group welcomes Chloe Howman and Lee Duff, who are starting PhD and MSc(Res) projects respectively.



Grant award for project to tackle air pollution in West African cities

Environmental and atmospheric scientists at the University of York and Stockholm Environment Institute (SEI) have been awarded £674,000 for a research project which aims to measure air pollution in some of West Africa's fastest growing cities.



The project will create an online, open source platform to share designs for low cost air quality monitors developed at York in collaboration with academic institutions and agencies in West Africa.

Using the new platform, partners will be able to access technical information and diagrams to help them build their own monitors. The monitoring units can then be installed at key locations to give accurate air quality readings in cities across the region where atmospheric pollution is a growing problem.

The project is a joint initiative between the University's Wolfson Atmospheric Chemistry Laboratories (WACL), the SEI and the Department of Environment and Geography who will work with partners in Cote d'Ivoire, Ghana and Togo. The award, from UK Research and Innovation (UKRI) and the Global Challenges Research Fund (GCRF), will help develop the new online resource to support West African partners in the building of their own air pollution monitoring equipment which will be used to support urban air quality policy.

Scalable solution

York is one of 18 international partnerships to win a share of £14.8m awarded to deliver scalable solutions for issues faced by low and middle-income countries.

[Dr Pete Edwards](#) from WACL said that commercial air quality monitors are available, but they are expensive to run and maintain. Many are also prone to faults caused by fluctuating power supplies and have high energy demands making them unsuitable for use in some developing countries.

"We've created a monitor made up of clusters of low cost components that are widely available - but can be assembled in different ways to suit the conditions and requirements for cities in West Africa," he said.

"There are multiple components in each unit which means there are back-up components if one fails. And because they are low cost and widely available, it is easy for partners to maintain the units and replace faulty parts."

Online community

As well as sharing technical information and training guides, the planned new web platform will support an online community where project partners can share information, technical support and advice.

Emissions from industry, cars and diesel powered generators in expanding urban areas all contribute to air quality problems in West Africa. The conditions cause major health problems and damage the lives and livelihoods of millions of people across the continent.

Progress in tackling the problem has been hindered by a lack of reliable and robust monitoring data. The project will help to overcome this by providing detailed analysis on pollution hot spots.

The data gathered by the monitors will also help cities develop different ways to improve air quality with the help of a modelling tool developed by the SEI. The modelling tool - Long-range Energy Alternatives Planning Integrated Benefits Calculator ([LEAP-IBC](#)) - will help governments develop policies to reduce pollution.

Collaboration

[Dr Johan Kuylenstierna](#), SEI Research Leader, said: “By combining the ability to monitor and model air pollution, cities will be provided with the necessary tools to support strategy development that will reduce the large impacts on human health. This will be the first time these cities will have access to these affordable tools and equipment that they can develop and maintain themselves.”

[Dr Chris Malley](#) from SEI said collaboration is the key to the project: “Rather than imposing a solution we will continue to work closely with partners in West Africa to co-design technology and approaches that are suited to the requirements and conditions found in the region.

“We have developed monitors that generate high quality data while being simple, reliable and easily repaired while having minimal demands on time and electrical power. The LEAP modelling will also help to inform government environmental policy and decision making.

“The GCRF award will help us translate this sustainable low cost technology from the labs to the streets of West Africa where it has the potential to make a major contribution to tackling a growing health crisis.”

The project has been funded as part of UKRI’s GCRF Innovation and Commercialisation Programme, developed to fast track promising research findings into real-world solutions.

Dr Jon Agirre appointed to the editorial board of *Acta Crystallographica Section F*

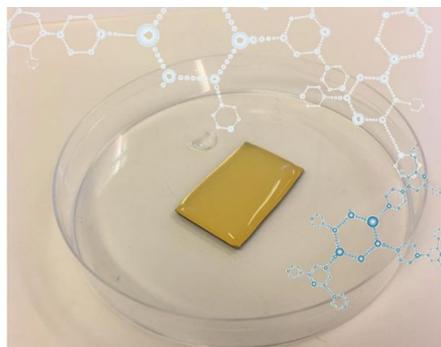


After guest-editing a successful special issue on structural studies of glycoproteins and protein carbohydrate complexes for [Acta Crystallographica Section F: Structural Biology Communications](#), [Dr Jon Agirre](#) – currently a Royal Society Olga Kennard Research Fellow in YSBL – has been taken up a position as permanent co-editor of that journal.

Dr Agirre will primarily handle short methodological communications, as well as longer submissions dealing with protein-carbohydrate complex structures. The news comes at the end of a successful year in which Dr Agirre has also been involved in the organisation of the forthcoming CCP4 Study Weekend, to be held 7-9 January 2020 in Nottingham.

New way to test for drug resistant infections

Scientists from across the University, including researchers from the Department of Chemistry, have developed a method to test whether an infection is resistant to common antibiotics.



The research team are now working with clinicians at York Teaching Hospital NHS Foundation Trust to integrate their system into a rapid diagnostic test for antimicrobial resistance in urinary tract infections.

Antimicrobial resistance (AMR) is a major global threat accelerated by the inappropriate use of antibiotics. Beta-lactam antibiotics (such as penicillin) are one of the most important classes of antibiotics, but resistance to them has grown to such an extent that doctors often avoid prescribing them in favour of stronger drugs.

Corresponding author Dr Lisa Miller, a postdoctoral researcher working in the team of [Professor Anne Duhme-Klair](#), modified an antibiotic from the beta-lactam family so that it can be attached to a sensor, enabling the detection of bacteria resistant to treatment.

The new method could lead to clinicians being able to rapidly detect whether an infection is treatable with common antibiotics, reserving stronger alternatives for the patients that need them most.

One of the major ways in which bacteria become resistant to treatment is through the production of enzymes that can break down beta-lactam antibiotics, rendering them ineffective. The researchers were able to test for the presence of these resistance enzymes by attaching the modified antibiotic to a sensor surface, which enabled them to see whether or not the drug was broken down.

Dr Lisa Miller said: "Our results provide important insights into the development of surface-based tests for drug resistance, helping the advancement of much needed fast diagnostics."

[Dr Steven Johnson](#), Reader in the University's [Department of Electronic Engineering](#), said: "This important study is the result of a close collaboration between physical, chemical and biological scientists at the University and lays the foundation for a new diagnostic test for drug resistant infections. We are now working with clinicians at York Teaching Hospital NHS Foundation Trust to integrate this modified antibiotic into a rapid diagnostic test for antimicrobial resistance in urinary tract infections."

The work was supported by a research council funded [Healthcare Impact Partnership](#), led by [Professor Thomas Krauss](#) in the Department of Physics.

The research is published in [ACS Applied Materials and Interfaces](#).

Online Department suggestion box



The online Equality and Diversity suggestion box has been extended to be a suggestion box for the whole Department. You can submit your thoughts/suggestions/ideas for general Departmental matters as well as matters relating to Equality and Diversity. You can find the Google form on the intranet homepage or at this [link](#).

New NERC-funded project on dating teeth

This autumn, [Dr Kirsty Penkman](#)'s new three-year NERC-funded project "Wisdom teeth: refining our understanding of mammalian evolution through dating dental enamel" started, which combines biomineral chemistry and physics to develop the technology development needed to date tooth enamel over the last four million years.



An example of the type of tooth (in this case from a mammoth) sampled for detailed analysis of both the organic and inorganic fractions in order to date it.

Directly dating mammal fossils older than the limit of carbon dating (~50,000 years) is very challenging, but this narrow time window is extremely limiting if we aim to understand the effects of climate change on land-based organisms, or unpick our own evolutionary history. The patterns of human evolution are far more complex than previously believed. The lack of chronology means that we are hard-pressed to pinpoint the major evolutionary drivers for both humans and other mammals, and to compare patterns across the African continent.

Working alongside Kirsty, Dr Marc Dickinson (the Wisdom Teeth PDRA) has made a methodological breakthrough

which enables amino acid dating to be undertaken on tooth enamel. Dating enamel has the enormous advantage of providing a direct date on mammal teeth (critical fossils of interest), and the technique is now ripe for expansion to a range of mammalian species and additional geographic regions.

Collaborating with Manchester Metropolitan University, Oxford, Cambridge and an international group of project partners, this project will address the three areas of technology development needed, and the time frame it opens up will enable a significant shift in the range of research questions answerable regarding the environmental forces on mammalian evolution, including that of humans. The three strands of technological advance are:

- 1) a microfluidics ("lab-on-a-chip") approach, which will enable both a significant decrease in the physical sample size needed, as well as preparation / analyses to be undertaken outside specialist labs;
- 2) combining analysis and imaging of both the organic and inorganic fractions to understand their structure, function and any impact on the protein breakdown; and
- 3) using advanced chemical models to understand the breakdown reactions.

The team will then apply these methods to two regions of Africa of particular evolutionary interest: east Africa (including the Rift Valley) and southern Africa (including the 'Cradle of Humankind'). The developed chronology will enable models of human-environment interaction to be tested, providing a breakthrough in our understanding of our evolutionary past.

KMS Winners' Seminar and Year 2 Poster Session

The popular KMS Winners' seminar took place on Wednesday 9 October, combined with a poster session from our Year 2 research students. This combined event provides a great opportunity to showcase the different research taking place in the Department, and with the arrival of our new PG students just the week before, it gave everyone a chance to chat and mix with staff and students from different groups.

Our KMS Winners this year were:

Nick Yates (AP/MAF): *Bio-orthogonal conjugation for "wiring" redox active proteins to any conducting surface*

Kirsten Hawkins (PAC/DKS): *Potentially prebiotic catalytic hydrogels*

Jenny Lewis (SBD): *SABRE and SABRE-Relay*

Yann Lie (DJM/TJF): *The production of fine and platform molecules from microalgae: The "Chemicalgal" Plant*

Tom Stephens (WPU/MAF/PAOB) was also a winner, but was not available for the seminar

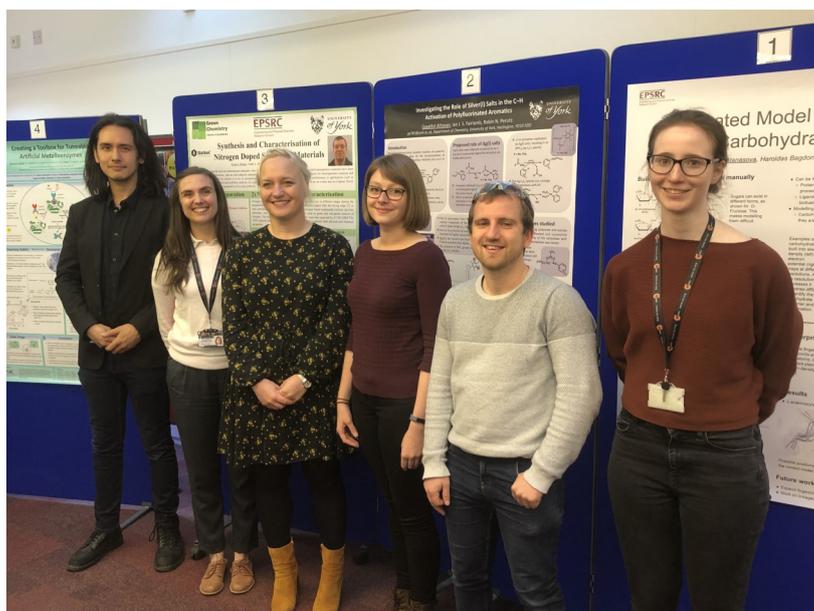
The KMS Panel also wanted to recognise those shortlisted for interview:

Freya Squires (JDL/JFH)

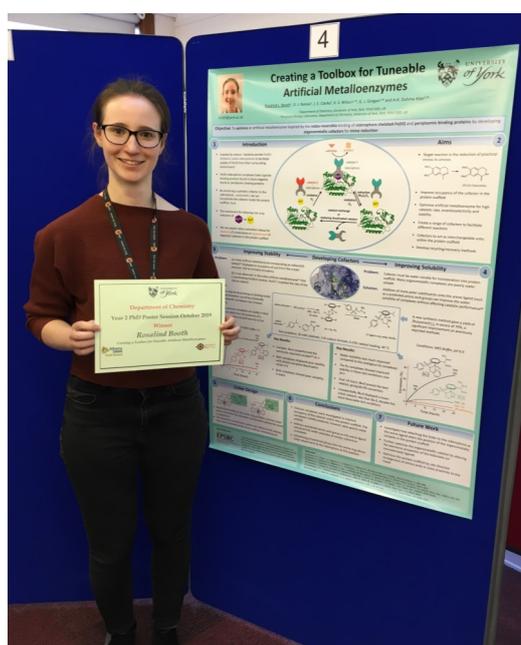
Neil Scott (IJSF)

James Rossi Ashton (RJKT/WPU)

Mark Dowsett (AP/MN)



L-R: Yann Lie, Jenny Lewis, Alison Parkin, Kirsten Hawkins, Nick Yates, Rosalind Booth



Rosalind Booth with her winning poster

Half way through our KMS talks there was a break for refreshments and chance for everyone to view the 38 fantastic posters from our research students. We had a wide range of posters on display, generating plenty of interest and discussion around the room. An informal competition took place with people being asked to vote for their favourite. The winner was **Rosalind Booth** (AKD/KSW/GJG) with her poster entitled *Creating a toolbox for tuneable artificial metalloenzymes*.

Congratulations to our winners and well done to all nominees and shortlisted candidates. Thanks to the KMS Panel chaired by Alison Parkin with Aneurin Kennerley, Terry Dillon and Anne Duhme-Klair.

Next year, Aneurin Kennerley will take over as Chair of the Panel so we would like to say a big thank you to Alison for all her work on the KMS Panel over the last four years.

Sustainable Metrics Symposium



On 11 September 2019, Dr Kadambari Lokesh and Dr Katie Lamb from the Green Chemistry Centre of Excellence (GCCE) held a one-day symposium titled “*Sustainability Metrics: Tracking, Measuring and Reporting Responsible Innovation*”, at the GCCE. This was the second “Sustainability Metrics” symposium to be held at the University of York, following the successful event run last year by Dr Lokesh, and was sponsored by the EU Horizon 2020 research project, STAR-ProBio. The aim of the symposium was to give researchers the opportunity to discuss their use of green chemistry metrics and other toolkits, to assess the sustainability of their research, and to encourage discussions and future collaborations between academic and industrial researchers. A total of 25 delegates from academia and industry across the UK and Europe, attended the event with speakers from the University of Sheffield, University of York, Drax, Croda, CO2Chem, OWS Limited, Pré Sustainability and Novamont in attendance. Dr Lokesh and Dr Lamb thoroughly enjoyed running the symposium this year and are hoping to run the event again next year.



Left: Dr Kadambari Lokesh and Dr Katie Lamb at the end of the symposium; Right: The symposium included oral presentations from academic and industrial researchers. Dr Julia Creasey (pictured) discussed how Croda are using different metric toolkits to assess the greenness and sustainability of their research.

Green chemists attend 4th EuCheMS Conference on Green and Sustainable Chemistry in Tarragona, Spain



Professor Michael North delivering his keynote presentation on sustainable solvents



Dr Ale Pellis giving his presentation on sustainable polymer formation



Dr Katie Lamb presenting her work on metal catalysed carbon dioxide utilisation

4th EuCheMS Conference on Green and Sustainable Chemistry

TARRAGONA, 22-25 SEPTEMBER 2019

Following the successful 3rd EuCheMS Conference on Green and Sustainable Chemistry at the University of York in 2017, the 4th EuCheMS Conference was held at the Institute of Chemical Research of Catalonia (Institut Català d'Investigació Química, or ICIQ) in Tarragona, Spain on 22-25 September. The overall aim of the symposium was to *"offer opportunities to discuss the latest developments in green and sustainable chemistry, create new partnerships and amplify existing networks between academia and industry."*

Many members of the Green Chemistry Centre of Excellence (GCCE) attended this conference and gave a mixture of oral and poster presentations. [Professor Michael North](#) gave an invited keynote lecture at the symposium on *"Sustainable Solvents for Organic Synthesis"*. Postdoctoral Research Associates Dr Ale Pellis and Dr Katie Lamb also gave talks on their research, entitled *"Enzymes: Powerful Catalysts for the Synthesis of Functional Polymers"* and *"Using Metal Salen and Salophen Complexes for the Green Synthesis of Cyclic Carbonates from Epoxides and Carbon Dioxide"*, respectively. Green Chemistry PhD student Roxana Milescu also presented a poster on her work entitled *"Fabrication of PES/PVP Water Filtration Membranes Using Cyrene[®], a Safer Bio-Based Polar Aprotic Solvent"*. Ale, Katie, Mike and Roxana all thoroughly enjoyed the symposium and are already looking forward to the 5th EuCheMS symposium, which will be held in Greece in 2021.



Roxana Milescu with her poster and deep in conversation with Professor David J. Cole-Hamilton from the University of St. Andrews and Professor Michael North



Group photo of the participants and organising committee for the 4th EuCheMS conference on Green and Sustainable Chemistry at the ICIQ

ReSolve solvents project stakeholder workshop

On 30 September, attendees from industry, universities and research institutes gathered at a workshop in Brussels. The half-day workshop, held as a pre-conference event to EFIB 2019, provided the latest results from the ReSolve project, alongside external perspectives of solvent substitution from Merck and The Dutch National Institute for Public Health and the Environment (RIVM). Further information about the event, including copies of the presentations, is available from the [ReSolve project website](#).



ReSolve, coordinated by the GCCE, is a three year research project funded by the [BBI-JU](#), a public private partnership comprising the European Union and the Bio-based Industries Consortium. It aims to deliver high-performing, safer alternatives to replace the hazardous solvents NMP and toluene. During the project, the lead NMP-replacement candidate,

Cyrene™, which was developed in conjunction with the GCCE, has obtained REACH Annex VIII registration, allowing ReSolve partner Circa Sustainable Chemicals Limited to manufacture or import Cyrene at volumes of between 10 and 100 tonnes/year. A collaboration with Merck has resulted in the official launch of Cyrene on 24th April 2019 and it is currently being evaluated by over 400 organisations as a suitable replacement for NMP. Dr Jane Murray from Merck and Dr Fabien Deswarte from Circa attended the workshop to share their experiences of bringing a bio-based solvent to market.



The attendees also learned more about 2,2,5,5-tetramethyloxolane (TMO), an alternative safer alternative to toluene. Building on the initial research completed at the GCCE, ReSolve is aiming to produce a large enough volume of TMO in order to test it as a replacement to toluene in an industrial setting. The outcome of this testing will be available by the end of the project in May 2020.



Attendees were interested to learn more about the toxicity testing completed during the project to ensure that the alternative solvents were safer than the existing ones. A question and answer discussion session completed the event, after which attendees could join the EFIB 2019 welcome reception.

Professor James Clark (top) and Dr Fergal Byrne (bottom) giving presentations at the workshop.

GCCE attendees were [Professor James Clark](#) (speaker), Dr Fergal Byrne (speaker), [Dr Tom Farmer](#) (workshop chair) and Janice Lofthouse (ReSolve project manager - event co-organiser).

10th Eurasian Meeting on Heterocyclic Chemistry



The 10th edition of the Eurasian Meeting on Heterocyclic Chemistry (EAMHC) was held in Milano Marritima, Italy on the 15-19 September. The 10th edition of the meeting was organised by Italian Chemical Society, with Professor Domenico Spinnelli of University of Bologna and Professor Giovanni Petrillo of University of Genoa as the main organisers. York was invited and represented by [Professor Richard Taylor](#), [Dr William Unsworth](#), and Dr Hon Eong Ho (RJKT/WPU/POAB). The conference gathered delegates across the Europe and Asia and featured a series of excellent research talks with heterocyclic chemistry as the main theme. All the talks from York were well-received, including Professor Richard Taylor's plenary lecture entitled 'From Natural Products to Organic Diversity', Dr Will Unsworth's insightful talk on macrocycles' synthesis, and Dr Ho's research talk on making spirocycles using palladium catalysis. On a special note, it was good to see former group member, Angela, who spent six months in RJKT/WPU groups as part of her ERASMUS exchange

programme. There were plenty of in-depth scientific arguments and discussions on possible future scientific collaborations. On the last day of the conference, the group attended the conference tour in the ancient city of Ravenna which nicely summed up the warm hospitality (with exceptionally good food and wine!) and sunny weather in Italy. The next EAMHC meeting will be held in Tbilisi, Georgia.

- Dr Hon E. Ho

New starters

Jordan Herod, Research Associate and Associate Lecturer (line managed by DWB & DAW)
Room: C/B123d; Ext: 5896; Email: jordan.herod@york.ac.uk

Alexandra Males, Postdoctoral Research Associate (line managed by GJD)
Room: B/K267 and B/K266; Ext: 8276; Email: alexandra.males@york.ac.uk

Matthew Rowlinson, NCAS Research Associate in Tropospheric Composition (line managed by LJC)
Room: C/G116; Ext: 4755; Email: matthew.rowlinson@york.ac.uk

Katy Holmes, HR Administrator (line managed by MAB)
Room: C/A121; Ext: 2716; Email: katy.holmes@york.ac.uk / chem-admin@york.a.c.uk

Sri (Sari) Hapsari Budisulistiorini, Postdoctoral Research Associate (line managed by JFH)
Room: C/G116, Ext: 4178; Email: sari.budisulistiorini@york.ac.uk



Solvents Day

Advances in Solvent Based Technologies



Monday 18th November 2019, 10am—5pm

Green Chemistry Centre of Excellence, Department of Chemistry, University of York

A free symposium for producers, users and recyclers of solvents

- **Learn** about the policies that are changing solvent use and availability
- **Discover** alternative solvents that are safe and sustainable
- **Hear** from the industries developing new solvent technologies with Sensient, Circa Group, Chrysalix Technologies, and Worn Again
- **Discuss** new solvents with the Universities of York, Leeds, and Liverpool
- **Participate** in networking and knowledge transfer activities

Who Should Attend?

This symposium would be of interest to academic and industry personnel working in all solvent applications, including:

- Synthesis
- Formulation
- Extraction
- Cleaning
- Analysis

Register your place by Monday 11 November 2019 at solventsday2019.eventbrite.co.uk