

Chemistry Newsletter

 Autumn 2022
 

Inside your Newsletter:

- 1 Important Dates
Graduation
- 2 Graduation and Awards
- 3 Refurbished Common Room
- 4 Celebrations and Congratulations
- 6 Research Updates
- 7 RSC President 2022-2024
- 8 Chemistry Outreach 2022
- 9 Enterprise in Chemistry:
Sam Munday
- 10 Enterprise in Chemistry:
Tom Carew
- 11 Chemistry Student activities
- 12 Chemistry Poster Prizes 2022
- 13 Beyond Chemistry
Useful Information
- 14 Chemistry Code of Conduct

Chemistry Graduation



Super Graduation 2022 at St Mary's Stadium

Important Dates

2022 Term Dates:

Welcome week: Mon 26 Sept 2022 to
Sun 2 Oct 2022

Autumn: Mon 3 Oct 2022 to Sat 17 Dec
2022

Spring: Mon 9 Jan 2023 to Sat 25 Mar
2023

Summer: Mon 24 Apr 2023 to Sat 17
June 2023

Semester 1: Mon 26 Sept 2022 to Sat
28 Jan 2023

Semester 2: Mon 30 Jan 2023 to Sat 17
June 2023

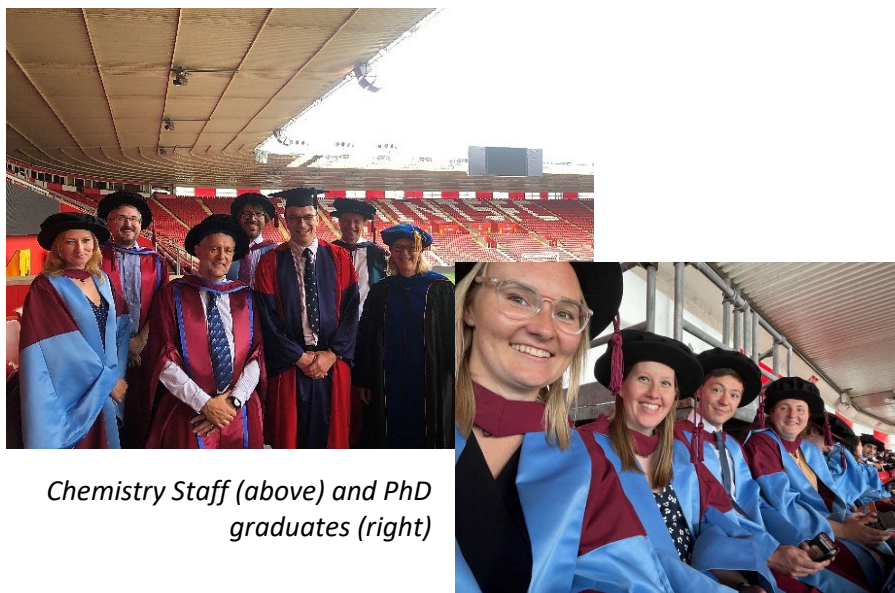
Student Vacation: Sun 18 Dec 2022 to
Sun 8 Jan 2023

University Closure days:

Closure day Fri 23rd Dec 2022 and Wed
– Fri 28-30th Dec

Public holidays Mon-Tues 26-27th Dec
2022 and Mon 2nd Jan 2023

This was a unique year for Graduation since the 2020 and 2021 ceremonies were cancelled due to the Covid pandemic. Instead of the normal campus graduations, St Mary's stadium was used for a Super Graduation, celebrating graduates from the classes of 2020, 2021 and 2022.



*Chemistry Staff (above) and PhD
graduates (right)*

The School of Chemistry would like to congratulate all those who graduated in 2022 and to our graduates from 2020 and 2021 who had the chance to attend a ceremony this year.



2015 Silver Award Winners - Chemistry at Southampton

Do you have an article you wish to contribute to a future edition?

Please email Julie Herniman J.M.Herniman@soton.ac.uk or Dawn Dunlop D.Dunlop@soton.ac.uk

Graduations and Awards

Congratulations to all our Undergraduate students who graduated in the Summer of 2022, and further congratulations to the prize winners below:

Toby Lindup - John Mellor Prize;

Outstanding project in Organic Chemistry or related field for a Y4 MChem project

Urvaashi Heramun - Alan Carrington Prize;

Outstanding project in Physical Chemistry or a related field for a Y4 MChem project

Naadrah Hussain - Judith Corker Prize

Outstanding project in Inorganic Chemistry or related field for a Y4 MChem project

George Armstrong - Progression Award;

Academic development award across contributory part of degree

Jessica Slough - A E Clarence Smith prize;

Outstanding performance by a student graduating from a BSc degree

Toby Lindup - David Runciman Boyd prize;

Outstanding performance by a student graduating from a MChem degree

Jacob Venn - Outstanding Research Placement Project;

Outstanding research placement project

Hannah Shotter - R E Parker Project prize;

Best BSc Project

Toby Lindup - Roger Parsons Prize;

Highest level of academic achievement in the graduating cohort

Congratulations to the following students on their Awards since our last newsletter:

Masters of Philosophy:

Nicola Yaxley - Biochemical and Structural Studies of the Radical SAM Enzyme HydG

PhD awards:

Maria De Lourdes Gonzalez Juarez -

Thermoelectric Properties of Semiconducting Metal-Organic Framework Thin Films and Composites

Stephen Barnes - The Role of Subject Matter Knowledge in Teaching A level Chemistry

Fred Robinson - Precursor Synthesis, Chemical Vapour Deposition and Thermoelectric Measurements of Group (14) and (15) Chalcogenide Thin Films

Shiyue Yang - Development of Methods for Structure Prediction and Characterising the Lattice Energy Surfaces of Organic Molecular Crystals

Theerapoom Boonprab - Towards the Development and Coordination Chemistry of Rotaxane- and Catenane-based Ligands

Hannah Felstead - The Design and Synthesis of Fluorinated Model Compounds to Investigate the Influence of Fluorination on Lipophilicity and Hydrogen Bonding

George Tierney - Investigating Nanoscale Catalysts from Primary Growth to Catalytic Activity

Mariana Manso - Synthesis of substituted bicyclo[1.1.1]pentane scaffolds

Gabriela Hoffman - Synthesis of Atomic and Molecular Endohedral Fullerenes

Luke Wilding-Steele - The Development of Flow Photochemical Methods for the Synthesis of Phenanthrenes, Helicenes and Benzochromenes

Diego Collin - Synthesis of Novel Cubane Scaffolds

Jack Youngs - Understanding Bubble Dynamics in Sonicated Edible Lipids to Improve their Physicochemical Properties

Joseph Stephenson Clarke - Exploring Protein Stabilization as an Approach to Drug Discovery

Simon Holland - The Synthesis of Fluorinated Obeticholic Acid Derivatives

Briony Downes-Ward - Generation of XUV Photons and their Application in Time-Resolved Photoelectron Spectroscopy

Ryan Bennett - The Discovery and Investigation of Novel Rearrangements of Cyclobutenediones Triggered by Nucleophilic Addition

Peter Johnson - Development of Multiphoton Label-Free Super-Resolution Microscopy Techniques for Biomedical Imaging

Chi Cheng - Computational Screening of Small-Molecule Organic Semiconductors

Daniel Irving - A Total Scattering Study of Aqueous Magnesium Sulfate

Mabel Wong - The Role of Hydration and Flexibility in Computational Antibody Design

Iona Doig - Synthesis of Thin Film Metal Organic Frameworks Using Aerosol Assisted Chemical Vapour Deposition

Gabriel Bramley - Developing and Evaluating Implicit Solvent Models for Catalytic Metallic Surfaces

Li Shao - Templated Electrodeposition of Nanoscale Materials

Miroslav Suruzhon - Evaluating and Improving the Robustness of Alchemical Binding Free Energy Calculations Using Adaptive Enhance Sampling Methods

Julie Herniman - *Applications and Implementation of Modern Ultrahigh-Performance Supercritical Fluid Chromatography-Mass Spectrometry*

Rhys King - *Coordination Chemistry of Group 14 with Pnictine Ligands and the Development of Precursors for the Electrodeposition of Antimony Chalcogenides*

James Pearce - *Development of a Flow Electrochemical Method for Effecting Reductive Radical and Radical-Polar Crossover Reactions with Non-Sacrificial Electrodes*

Khaled Abdel Maksoud - *Conformational Enhanced Sampling - The Study and Development of Accelerated Sampling Algorithms for Classical Biomolecular Dynamics*

Federica Rizzi - *Interlocked Molecules with Unusual Properties: Luminescent Rotaxanes and Mechanically Chiral Catenanes*



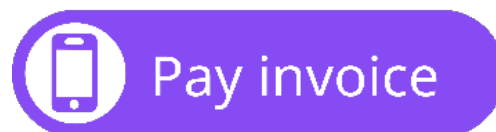
The coffee room is staffed by Genny and managed by Sally. They are always willing to listen to suggestions for different snacks or ideas to promote the facility.

Refurbished Chemistry Common Room



As many of you will have noticed, the Chemistry coffee room was refurbished over the summer. It is a great place to meet colleagues informally and there is also some space for more formal meetings with the addition of enhanced AV equipment. The coffee room is open between 9 am and 12.45 pm every day for hot and cold drinks, biscuits and snacks, all at reasonable prices.

The facility is cashless so you will need to set up an on-line account following the link below or scan this QR code:



<https://soton.ac.uk/teams/SchoolofChemistry/SitePages/Chemistry-Coffee-Shop-Payments.aspx>



Chemistry Common Room - Payment for Coffee Shop Items



Amount (£)

Description

Pay for your coffee shop items quickly and securely online here.

Please enter the amount from your invoice by overwriting the amount in the field above.

Celebrations and Congratulations

Congratulations to Nikolay Zhelev on the birth of their daughter Indie who was born on the 12th of January this year. “One of the things we’ve been looking forward to is sharing our love for the outdoors with her.

This is a photo of our family doing the Old Man of Coniston in the Lakes. A hike she’s actually done twice now, but this time on the outside with better views.”



Congratulations to Nuno Bimbo on the arrival of José Maria in June. “José is having a great time, and he’s a pretty chilled and quiet baby (so far!). His big sister Teresa, who is 3 years old, is also doing a great job taking care of him.”



Congratulations to Sami Kanza on receiving a VC Award 2022.

Sami was awarded for her outstanding contribution to the University in the award category of “Bringing the Triple Helix to Life”. She has played a major role in setting up skills training, with website and YouTube channel as well and developing a significant research profile, and all of this is achieved with a most generous and tactful style.



Dr Samantha Kanza

Samantha excels in all aspects of her 'triple-helix' work life. She coordinates two EPSRC networks: having grown the AI Network to over 1,600 academic and industrial members, she is now developing the EPSRC New Blood Testing Network, deploying the full range of enterprise, management, and media skills for the new hybrid world.

She has excellent supervision skills, navigating difficult times with a Knowledge Transfer Partnership (KTP) project, ensuring the associate was well looked after and continued to advance his career prospects. She set up digital skills training (www.ai4science.network, YouTube channel and summer school), a major contribution to skills and training. Samantha has a significant research profile, leading a task group on AI Ethics and Food, with publications in this area, Semantic Web and electronic laboratory notebooks.

Samantha is a rare genuine example of the intersection of social and physical sciences. She has immense and unwavering dedication to all her work. She is hugely popular with everyone she works with and extremely effective at getting things done, and this is always achieved with a most generous and tactful style that ensures commitment and reflects excellently on the reputation of the University.

Congratulations to Sally Dady celebrating 30 years' service, working in Chemistry at the University of Southampton. HoS Jon Essex was pleased to present these flowers to Sally at a recent Chemistry staff meeting.



Congratulations to Curve Therapeutics who earlier this year signed a US\$1.7 billion deal with multinational pharmaceutical company MSD, the trade name of Merck & Co., Inc., Kenilworth, NJ USA.

The deal will see the two companies collaborate on research using Curve Therapeutics' pioneering and potentially game-changing drug discovery platform. The platform enables the direct discovery of functionally active molecules against difficult-to-drug targets – enabling new ways to treat complex diseases.

Simon Kerry, Chief Executive Officer of Curve, said: "This collaboration is a major milestone for Curve and an important endorsement of our ground-breaking drug discovery platform. Working with MSD on selected therapeutic targets will complement Curve's in-house drug discovery and development programmes."

Curve Therapeutics grew out of the world-leading research of the group of Professor Ali Tavassoli.

Chemistry researchers recognised with international prize

A multidisciplinary team, led by former Southampton Chemistry student Dr James Eills, and including current Southampton Chemistry staff Professor Malcolm Levitt and Dr Laurynas Dagys, has developed a new "hyperpolarization technique" that enhances the signals from an MRI instrument and enables it to capture the metabolic biochemical reactions within the body. This could pave the way for more targeted cancer treatments.

The team, which includes chemists, physicists, engineers and biologists from England, Germany, Italy and the USA, has been awarded the **Erwin Schrödinger Prize** - Science Prize of the Stifterverband, by the Hermann von Helmholtz Association of German Research Centres.

The research originated in a project James undertook during his undergraduate degree at Southampton and later his PhD, which he also carried out at Southampton under the supervision of Malcolm, which showed new ways to achieve hyperpolarization with parahydrogen in order to increase the sensitivity of NMR and MRI.



James joined the University of Southampton in 2011 and says: "I really enjoyed my time in Southampton – I came back to Southampton in 2015 for my PhD for the opportunity to work with Professor Levitt. He is a world-renowned professor in the field of magnetic resonance, and Southampton is perhaps the best place to carry out research in this field. This is in large part thanks to the opportunities to collaborate with other scientists both internally and externally.

"The research project developed quickly and seemed to work, to our surprise, at every step of the way. I'm really proud and somewhat surprised that I was able to continue what I started in Southampton, and it's now been recognised in this way."

Malcolm says: "This was a particularly difficult challenge to deal with. But through the interdisciplinary nature of the research team, we were able to combine our expertise and develop the process that would remove the toxins and therefore could eventually be used in patients.

"We are very proud to have received the "Erwin Schrödinger Prize - Science Prize of the Stifterverband" – this team shows what can be achieved when we work together across disciplines and national borders."

Research updates



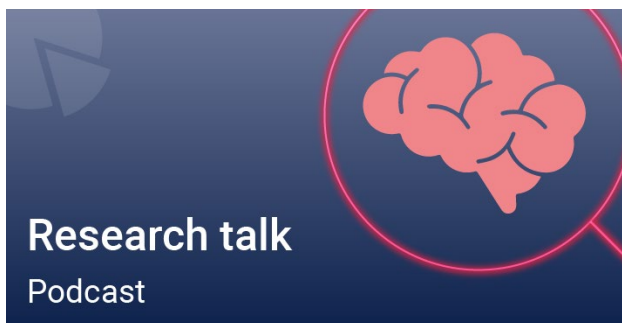
In REF2021 results Chemistry performed exceptionally well, with 97 per cent of its overall submission judged as world-leading or internationally excellent. 100 per cent of its research publications were assessed as world-leading or internationally excellent.

Professor Jonathan Essex, Head of Chemistry, said: "I am absolutely delighted with the REF result for Chemistry at Southampton. The Research Excellence Framework assesses the work of all our academic staff, and our results truly reflect the excellence across our School. I am extremely proud of our academic staff; the result confirms that Southampton is among the best institutions in the UK for Chemistry."

Have you seen (or heard)

Research Talk: Digital research infrastructure: with Prof Jeremy Frey

During this episode of the Research Talk, Helen Clare was joined by Professor of Physical Chemistry and Head of Computational Systems Chemistry at the University of Southampton, Jeremy Frey.



As well as conducting his own experimental research he is investigating how e-Science infrastructure helps make an intelligent laboratory; he is an enthusiastic supporter of interdisciplinary research and the PI of the EPSRC Network+ on Artificial Intelligence and Automated Scientific Discovery.

Together they discuss digital research infrastructure, how the current systems and tools need to change to better support research and the opportunities that could be realised with these advancements.

https://www.jisc.ac.uk/podcasts/research-talk-digital-research-infrastructure-07-sept-22?utm_medium=jeremy-frey&utm_source=guest&utm_campaign=research-talk

Grant successes in Chemistry

Congratulations to the following staff and their co-investigators on their recent research grant awards.

Characterisation and Analytics

- **Simon Coles:** *X-Ray Crystallography National Facility*
- **Simon Coles:** *An integrated workbench environment for quantum crystallography*
- **Simon Coles:** *Physical Sciences Data Infrastructure (PSDI)*
- **John Langley:** *South-West Region Centre of Excellence (CoE) for two-dimensional liquid chromatography (2D-LC) with high resolution ion mobility mass spectrometry (IMMS)*

Chemical Biology, Diagnostics and Therapeutics

- **Seung Lee:** *Caught in the act: Aptablotting for decoding the signals by two component systems*

Computational Systems Chemistry

- **Chris Skylaris:** *Particles at Exascale on HPC (PAX-HPC)*
- **Chris Skylaris:** *Supporting research communities with large-scale DFT in the next decade and beyond*

Electrochemistry

- **Peter Birkin:** *In Situ high-speed electrochemical sensing of surface cleaning*
- **Nuria Garcia-Araez:** *Gas evolution on polycrystalline and single crystal cathodes electrodes as a function of temperature for Li-ion batteries*

Functional Inorganic, Materials and Supramolecular Chemistry

- **Stephen Goldup:** *Controlled synthesis of carbon nanotubes through mechanically interlocked carbon nanobelts*
- **Stephen Goldup:** *New applications for interlocked molecules: materials synthesis and MRI imaging*
- **Robert Raja:** *High throughput identification of electrocatalysts*

Magnetic Resonance

- **Marina Carravetta:** *Understanding structure-property relationships in defect-free nanosized zeolites using advanced solid-state NMR spectroscopy*
- **Marcel Utz:** *paraQchip - Parahydrogen-Induced Hyperpolarisation on a chip for microfluidic perfusion culture*

RSC President 2022-2024: Prof Gill Reid



I was extremely honoured to take up the role of President of the Royal Society of Chemistry (RSC) in July this year. Having been a member of the RSC since my student days, I've seen at first-hand the huge range of work that the staff and our ~50,000 members are engaged in to advance the chemical science, supporting the global chemistry community, helping individuals to fulfil their potential and to make the world a better place. This ranges from dissemination of knowledge through the journals portfolio, to influencing policy, supporting teachers, recognising excellence through the prizes and awards, degree accreditation, increasing professional standards and encouraging young people to study chemistry.

Following our immediate past-president Tom Welton's great advocacy for sustainability, I'm very keen to continue to take this work forward, with a particular emphasis on linking sustainability to education. Through our research we heard an overwhelming message that young people want to learn more about the strong connections between sustainability and chemistry and that this would make it a more purposeful, relevant and engaging curriculum. I strongly believe that this sort of engagement is essential to attract more young and talented people from diverse backgrounds into our subject. We will therefore be advocating for a greater focus on sustainability within the school/college curriculum.

Moreover, our education mission in the RSC is to *"empower communities to offer an excellent chemistry education to all, driving diversity and improving skills in the chemical sciences"*. This really resonates with me - in particular working to improve our impact with disadvantaged and underrepresented groups. I had the pleasure of meeting with the first cohort of young people from underrepresented groups attending the *Broadening Horizons* event with industry leaders in early September at Burlington House.

It was inspiring for me to witness the level of engagement and enthusiasm from all parties, and I really hope programmes like these are effective in helping individuals to transition successfully through the different training and career choices in chemistry. This in turn will help to influence the future make up of our community and also to increase the general public's perception of the value and importance of chemistry in a modern society.

As a scientific organisation I would also like to see us continue to gather robust data to make well informed decisions within our work, across the board, not just in education. That allows robust monitoring to ensure we're making progress, as we have done on campaigns across sustainability and Diversity & Inclusion in the recent past – these activities have also elevated the RSC's profile and influence inside and outside the scientific community, as well as internationally.



Equality, Diversity and Inclusion

ED&I is central to the ethos in Chemistry, and we have a committed team that works hard to build a positive environment for all members of our School to be able to develop and succeed. As a school we have been involved in the [Athena SWAN charter](#) for the advancement and career progression of women in science for many years and its principles run through all we do.

Chemistry holds a Silver Athena SWAN Award, the first department at the University of Southampton to achieve this status twice.

If you would like to know more about our work, there is lots of useful information on our website which also includes our Early Career Support Hub.

<https://www.southampton.ac.uk/chemistry/about/Equality/index.page>

For more information about ED&I or to raise any issues or concerns please contact Dr Paul Duckmanton or Dr Julie Herniman

Chemistry Outreach activities 2022

Thanks to the Covid pandemic, and the teaching laboratory refurbishment that preceded it, we had been unable to run our annual series of 'twilight' practical sessions for Year 12 students since January 2018. As normal service had started to resume during 2022, we were keen to restart in-person outreach activity and we took the opportunity to run sessions in a new June/July slot.

Over 300 students from 24 schools and colleges took the opportunity to join us in the new laboratories to undertake the extraction of trimyristin from nutmeg. Every year, we ask ourselves if it is time for a new practical, but the positive feedback from students and teachers alike convinces us to stick with the tried and tested formula; students experience a wide range of practical techniques and typically isolate a good yield of colourless crystalline trimyristin from supermarket-sourced nutmeg.



We took the opportunity to evaluate the activity, with 2/3 of responding teachers indicating that they felt students were highly inspired by their visit. A recurring theme was that the demonstrators, 14 of whom contributed over the series of events, were excellent role models who provided visitors with valuable insight into what studying chemistry was really about. Comments included:

'Very well organised and a fantastic ratio of demonstrators: students. Good introduction to new techniques and really piqued students' interest in Higher education.'

'A really good atmosphere that allowed students to experience the university lab.'

'Outstanding and well-equipped laboratory. Very relevant practical work and techniques used, in line with current learning. Very welcoming atmosphere and well organised. Brilliant experience. Thank you.'

'It was a well-planned positive event. Students enjoyed the whole session and found it very inspirational.'

A key finding was that running the sessions in the summer actually worked better for the visitors, given their increased knowledge of chemistry and practical techniques in comparison to the traditional January window. In future, we will continue to run events for state schools and colleges in the summer, with January sessions potentially targeted at private schools.

We also reintroduced work shadowing at the end of July, led by Dr Seung Lee, in which we hosted 36 Year 12 students over two days. A number of the visitors had also attended the twilight sessions, giving them further exposure to the great things that Chemistry at Southampton has to offer. We know that work shadowing is quite demanding on research groups and the postgrads and postdocs who host the students, and we are extremely grateful for the hard work that goes into providing an excellent experience for the visitors. Once again, we evaluated the activity and comments included:

'The equipment and labs were very impressive, so I feel very lucky to have got the opportunity to spend time in them.'

'It was really helpful to see how PhD students work to give an insight into what being a research chemist is like.'

'The chemists I were shadowing were absolutely fantastic, showed me everything, went through a variety of different scientific instruments alongside detailed explanations. They were great to get along with as well, 10/10 experience!!'

Additionally, we have continued to run webinars for Year 12 students that put exciting research at UoS into the context of the global challenges that chemistry can contribute to solving, reaching hundreds of students across the country. Overall, it has been a successful summer for our outreach programme, and we look forward to expanding the programme further over the coming years.



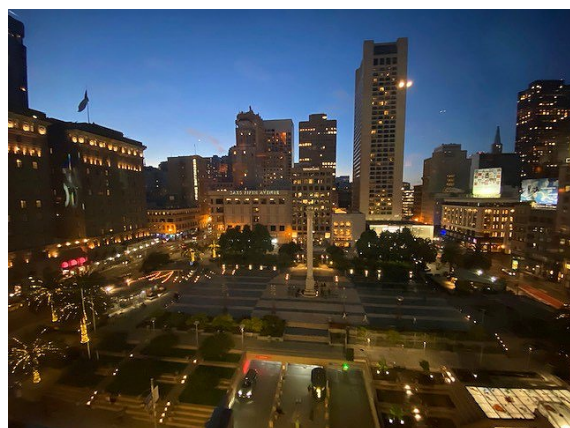
Enterprise in Chemistry: Update on Data Revival - Sam Munday

A lot has happened with Data Revival since we wrote into the newsletter last year. We've been through the absolutely amazing Future Worlds Founders Cohort 2022, have successfully started on the Southampton Science Parks Catalyst programme, are about to complete the Student Enterprise Foundership programme and have secured a grant from the Innovate UK Young Innovators 2022/23 award. On top of all of this success, we have run successful trials with Allnex (\$2.1B revenue), are in talks with a very large pharmaceutical company and are running a pilot to digitise and extract all the data from the Chemistry department's lab books. It's been a whirlwind of a journey that continually validates Data Revival's core proposition that there is value in the untapped resources of scientific research.

The Future Worlds Founders Cohort was a bit of an inflection point for Data Revival. It enabled us to transform from an interesting research project to a potential spin out with a lot of the skills, tools and contacts to become a success. We applied for the Founders Cohort Bootcamp starting back in February and were lucky enough to get selected for the 3 day event. After a weekend of learning the fundamentals of what it takes to launch an idea, and hearing from some of the amazing alumni, we pitched to the room and secured one of the 10 places available.



From here it was an intense 3 months of training, mentoring, pitching, and meeting investors culminating in a transformational trip to Silicon Valley to see how the best in the world operate. Whilst there we had a jam-packed schedule, visiting some of the biggest start-ups on the planet, pitching to investors and learning how accelerators such as Y-Combinator and SkyDeck help businesses like ours to become world beaters. The key take away for Data Revival was that even though Southampton feels a million miles away from the Valley, the skills we have and the innovations we've made are on a par with those on show in America. Future Worlds has really created a wonderful initiative that sets the foundations for success, and it's brilliant that so many projects from Chemistry have found their way onto it.



If you'd like to find out more about Data Revival you can find us at www.data-revival.com, and if you have any lab books/COSHH forms that can be added to the 2000 we are currently processing from the department please reach out!

Enterprise in Chemistry: Tom Carew

Tom is a 1st year PhD student in Dr Seung Lees' lab, with his project focusing on developing next-gen antimicrobial compounds to combat the rise of antibiotic-resistant gram-negative "super bug" bacterial species. His project will combine data-driven *in silico* and wet lab *in vitro* approaches, identifying novel bacterial metabolites that can be used as biomarkers of pathogenicity, in parallel with developing a machine learning model for predicting the efficacy of antimicrobial drug candidates. Before joining the department, Tom was working at Scripps Research institute in California, working as part of a research team developing a vaccine against HIV and CoV-SARS-2.



Tom Carew in the UoS Wind Tunnel

Alongside his studies, Tom is also part of the International Institute for Astronautical Sciences (IIAS) Scientist-Astronaut program, which was founded by former NASA astronaut candidates to train the next generation of scientist to conduct spaceflight research on the new commercial space vehicles, such as Virgin Galactic, Blue Origin and SpaceX. Interlinking this research focus with his PhD project, Tom is keen to probe the effect(s) of microgravity and deep space cosmic radiation on antibiotic resistance in both commensal and pathogenic bacterial species.



With the IIAS, Tom has trained in high G-force acrobatic flights, tested intravehicular activity (IVA) suits and orbital mechanics, under the guidance of several NASA alumni, including retired astronaut Captain Winston Scott. Tom is also set to partake in a parabolic (zero-G) flight early next year in Canada, where he will be testing a device prototype, he designed for transporting biological sample to the International Space Station (ISS).



Tom was recently selected for an upcoming analogue astronaut research mission at the LunAres Space habit in Poland, where he and the rest of the crew will test prototype technologies to be used in future spaceflight missions.

Outside of his studies and extracurricular activities, Tom's hobbies include gymnastics, eskrima, diving and nature.

Chemistry Student activities

Chemistry Publications: UG contributions to research papers

Important research outcomes are the result of work carried out by undergraduate project students and summer placement students. Recent examples include:

Bowen Liu, Andrew L. Hector, **Weronika O. Razmus** and Richard G. A. Wills,
Temperature dependence of hard carbon performance in sodium half-cells with 1 M NaClO₄ in EC/DEC electrolyte,
Batteries, 8, 2022, 108
DOI:10.3390/batteries8090108

Michael A. McCoy, **Dominique Spicer**, Neil Wells, Kurt Hoogewijs, Marc Fiedler, and Matthias G. J. Baud,
Biophysical Survey of Small-Molecule β -Catenin Inhibitors: A Cautionary Tale
Journal of Medicinal Chemistry 2022 65 (10), 7246-7261
DOI: 10.1021/acs.jmedchem.2c00228

PGR: Pizza social event – 13th July 2022 Nikita Rank, PGR Committee

First, we would like to thank the Doctoral College for their financial support, which allowed us to host The Pizza Social for PGRs on 13th July 2022.

As this was the first social event after the COVID pandemic and new members joined the Chemistry PGR committee, our goal was to give PGRs a chance to socialise and to introduce the committee to the PGR community.



This event was held in the Chemistry fire assembly point and around 40-50 PGRs attended the event. We kept all the possible dietary options in mind when we plan the gathering to avoid any exclusion. Everyone enjoyed the break and the sunny weather together.



During this event we also asked people to share their reviews about the committee and share ideas for future social events they would like to attend. Going back to in person events, it was a great occasion to get in touch with the PGRs in Chemistry.

Moreover, during a PhD, research projects do not always work out the way it is expected, and this can be very frustrating. These social events are very helpful and valuable for researchers to have discussions, to share their experiences with others and to seek advice.

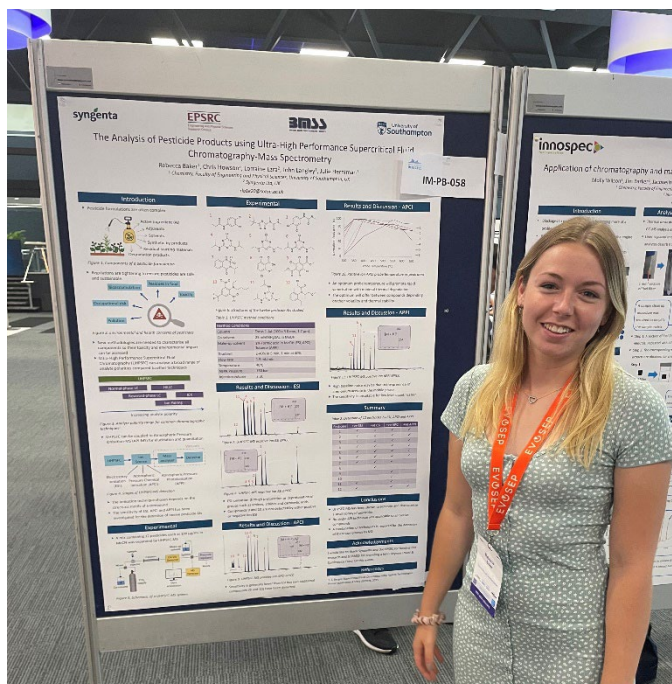
Having the chance to build up a wide scientific network and getting the ability to be involved in interdisciplinary discussions will greatly contribute to the development of each ECR, personally and professionally.



We are very thankful and appreciate the support provided by the Doctoral College for this event. We would also like to personally thank Catherine Howe for her guidance.

Chemistry Poster Prizes 2022

Three PhD students from the Characterisation and Analytics research section have been awarded prizes for their research presentations at recent conferences.



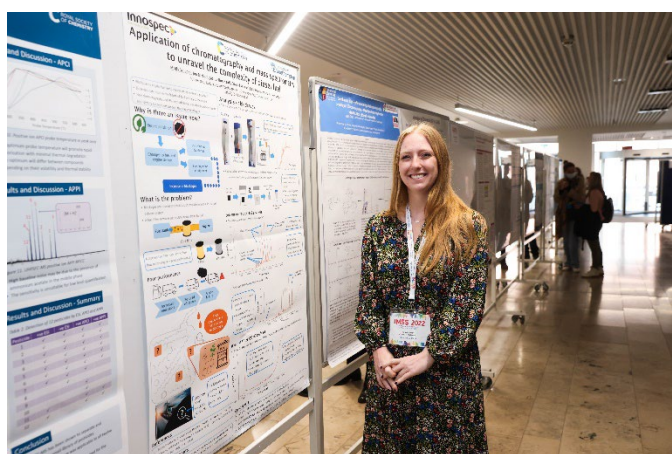
In early March, Rebecca Baker was awarded second place #RSCAnalytical prize at the Royal Society of Chemistry's 2022 #RSCPoster Twitter Conference. **This year's event took place over a 24-hour period** with around 900 posters from 69 countries, and 8,000 tweets. Her poster focussed on her research on the use of Supercritical Fluid Chromatography-Mass Spectrometry (SFC-MS) for the analysis of pesticides.

Rebecca's project is funded by EPSRC, and Syngenta and Molly received a University Presidential scholarship to work with Innospec. Both are supervised by Professor John Langley and Julie Herniman.



Rob Carroll's poster entitled "Developing the Application of the Crystalline Sponge Method" described his work using crystalline MOFs to encapsulate molecules, to get single crystal structures for compounds that have never been suitable for crystallography before. This earned him a poster prize at the British Crystallographic Association Spring Meeting in Leeds.

Rob is supervised by Professor Simon Coles and works closely with Dr James Horton from the UK National Crystallography Service.



In April, Molly Wilson took first prize for her talk at the 5th International Mass Spectrometry Summer School in Belfast. 50 early career researchers presented posters and based on her abstract Molly was selected to present a 20-minute talk along with 7 others. Her presentation described the application of chromatography and mass spectrometry to unravel the complexity of diesel fuel.

Do you have an article you wish to contribute to a future edition? We also welcome your feedback on the newsletter.

Please email Julie Herniman J.M.Herniman@soton.ac.uk or Dawn Dunlop D.Dunlop@soton.ac.uk

Beyond Chemistry

Making Amaro with Jacek Dziedzic- Senior Research Fellow

Amaro simply means “bitter” in Italian. However, *amari* are different from bitters (where only a few drops are added to a cocktail) – they are mild enough to drink straight. They are very aromatic, bittersweet, herbal liqueurs served as a digestif after a meal, usually drunk straight or on ice. Jägermeister (which is too sweet for an amaro) would be their distant relative, and so would be Angostura (which is not normally drunk straight). Fernet is a well-known example.

Amari are very common in Italy, and it is there that I first got to know them and fell in love with the concept. It was not love at first taste – it’s an acquired taste, and the first couple of times they all resemble peppermint drops. It takes a while to discover individual notes and their combinations.

Drinking alcohol, however fancy, is not really a hobby. My hobby is preparing my own. This started just before the pandemic. I was visiting friends who had an old bottle of *genziana*, a very simple amaro made with only one bittering agent – gentian root. It was home-made by someone in Italy, and it tasted fabulous. And so I thought – what’s stopping me from making a bottle or two of my own? I googled a recipe, bought a few ingredients online and a few months later the product turned out to be respectable. For Christmas my wife gave me a book with some tried recipes for more involved amari. With some knowledge on how to properly macerate different herbs, how to clarify and age the intermediate product, and having sourced a few fancier botanicals (like zedoary, quassia or devil’s club), I was ready to make my own.

The results turned out quite tasty, to the point where we now prefer our produce to most store-bought alternatives. My friends seem to enjoy them too, particularly after a large meal, as the bitter alkaloids aid digestion. During lockdown, I delved deeper into the art, and my collection of botanicals grew to several dozen small jars, and I’m now exploring original recipes in Italian that date back to the 1920s. Weighing out and mixing herbs and roots feels a little like alchemy, but some basic chemical principles can be applied in the production too. Patience is a major requirement – it takes about five months from start to completion, but it’s definitely worth the wait.



New Academic Year: useful info

School of Chemistry Email Etiquette

Email etiquette: In regard to email and other similar electronic communications, members of the faculty:

- should not be expected to read and reply to emails outside of their normal working hours. While each individual is free to read and send emails at any time suitable to their own working pattern and/or preference, this does not put the onus or expectation on recipient(s) to do likewise. We encourage the use of the ‘Send Later’ feature in (e.g.) Outlook where appropriate.
- are not expected to have their email on at all times and are not expected to read/respond to email immediately. The concept of replying “by return” should not be used. When an email requires a response, it should be sent, wherever possible, with a long enough lead time to allow those on part-time or flexible arrangements (or indeed on any working pattern different to that of the sender) a chance to respond.
- are encouraged to set up an out-of-office message if they are likely to be away from the office and out of email contact for extended periods.

School of Chemistry Carer’s Out-of-Hours Fund

The School of Chemistry recognises that attendance open-days and UCAS days out of hours can pose difficulties for those with caring responsibilities. With this in mind the School has established a small fund, to which those with caring responsibilities can apply, to cover additional costs incurred by attending out-of-hours activities.

Application information and process:

There is a limited budget available each year which will be administered by the School of Chemistry’s Equality, Diversity and Inclusion Committee until it is used.

Applications should be submitted via the form found here:

<https://www.southampton.ac.uk/chemistry/about/Equality/guidelinesandcommittee.page>

and submitted to Julie Herniman (co-Chair of the ED&I Committee, jmh7@soton.ac.uk); receipts may be required.

Code of Conduct

School of Chemistry

- We are resolute in our commitment to provide a supportive environment in which we value differences, respect diversity and treat each other with equity and respect.
 - We ensure individuals are treated equitably regardless of gender and gender identity/ expression, ethnicity, religion, nationality, sexual orientation, race, physical appearance, age or disability.
 - We do not condone or tolerate intimidating behaviour, including harassment (verbal, non-verbal or physical), bullying or victimisation.
 - We collaboratively preserve a community in which positive working relationships are forged and everyone feels valued, encouraged and supported.
 - We strive to maintain an environment free of inappropriate or offensive language or behaviour, where individuals consider their own behaviour and the impact that this can have on others.
 - We are dedicated to fostering a culture that empowers all members of our community to act promptly to challenge unacceptable behaviour.
 - We provide support to staff, students and visitors who feel they have been subjected to, or have witnessed, harassment, bullying or victimisation.
 - We ensure that allegations of harassment, bullying or victimisation are addressed fairly, with respect for the rights and dignity of all those involved.
 - Every member of the community is committed to playing an active role in creating and maintaining an environment that does not tolerate harassment, bullying and victimisation.
- Together we can continue to ensure Chemistry is an outstanding and inclusive place to work and study.

“The time is always right to do what is right.”

Martin Luther King, Jr

➤ **If you have experienced or witnessed abuse, bullying, or harassment at work or study, the university Harassment Contacts can offer support, and guidance for further action:**
www.southampton.ac.uk/hc

For further information please read the University Dignity and Work and Study policy, Embedding Collegiality and Whistleblower policy.



Chemistry Code of Conduct PDF can be found on the Sharepoint here:

<https://www.southampton.ac.uk/~assets/doc/Chemistry/code-of-conduct-chemistry.pdf>