Robot chemists
Automated synthesis could revolutionise healthcare

Fine China
Strengthening our international network

Inner space
Using virtual reality in the lab is helping students gain a deeper understanding of chemistry
I’m delighted to welcome you to this latest edition of Chemistry Explored, which happens to coincide with me being welcomed to the University of Bristol as the new Head of School.

I certainly feel that it’s an exciting time to be here, which I think you’ll agree judging by the projects, travels and innovations underway.

One of Bristol’s many strengths is the collaborative approach that underpins much of what we do, from the interdisciplinary research projects that give undergraduates the chance to work with leading academics to the use of new digital technologies in the lab.

As you’ll see, virtual reality experimentation has now been added to our winning portfolio of e-learning platforms. While in another revolutionary step, synthetic chemists are exploring how the molecular assembly of organic compounds used in the defence against disease could be automated, paving the way for improved healthcare.

On the international stage, our community of students continues to grow thanks to our expanding networks across China.

There’s so much to discover. I for one, am looking forward to what lies ahead.

Emma Raven, Head of the School of Chemistry
How do you teach students about computational enzymology? By allowing them to step inside an enzyme using the latest in VR technology. That’s the solution devised by a team of University of Bristol scientists whose work has earned them an Innovation in Teaching award.

Computational chemistry is ordinarily taught in undergraduate labs using traditional 2D screens for visualisation. This tends to involve setting up fiddly text-based programs.

Not so in Bristol’s chemistry labs, where researchers Dr Simon Bennie, Dr Kara Ranaghan, Dr David Glowacki, Helen Deeks and Mike O’Connor decided to develop an entirely new approach, in the form of a new VR chemistry course and lab. This allows students to step inside an enzyme, interacting with the dynamic system in real time, and affording them an experience that is as educational as it is experiential. Students have already noted how much more effective this approach is, with some even saying it has inspired them to consider further work in computational sciences.

The use of VR technology allows students to directly manipulate the atoms of the molecule, and to model a chemical reaction ‘by hand’, rather than through the use of standard computational chemistry software. As Dr Bennie says: “This is a much more intuitive process than learning the correct syntax for an input file. This work places Bristol at the forefront of chemical education – no other institution I know of offers real-time molecular VR on an undergraduate course. It’s a prime example of how research-driven teaching can improve the student experience.”

The research team, based in Bristol’s Centre for Computational Chemistry, has been awarded the 2018 University of Bristol Innovation in Teaching award for its work. Dr Bennie and his colleagues are also working on an academic paper profiling the results of using VR in the classroom.

Above The team implementing VR in chemistry at Bristol, picking up their Innovation in Teaching Award
Bristol's first ever conference aimed at encouraging greater take-up of science, technology, engineering and maths (STEM) among historically under-represented groups, proved a resounding success.

The conference was held in March and organised by Fusion, the School's Undergraduate Society, and a number of other STEM societies from across the University.

The event attracted undergraduate and postgraduate students from STEM departments in Bristol, as well as sixth-form college students who self-identify as from an under-represented group – women; black, Asian and minority ethnic (BAME); lesbian, gay, bisexual and trans (LGBT); and disabled.

One of the key subjects discussed during the conference, and addressed by speakers and students alike, was the need to tackle the lack of diversity in STEM subjects. This led to a call for more active methods to encourage more widespread interest and engagement from the community.

College students had the chance to meet with Bristol's current undergraduate cohort, outreach teachers and academic staff to discuss the opportunities opened by studying one of the STEM subjects. As well as addressing queries about the educational and academic career pathways for students, the conference provided a space for industry representatives, academics and students to discuss STEM careers outside academia.

Bristol’s record spin-out success

The University of Bristol created a record number of scientific spin-out companies last year. This was thanks to its thriving network, including a partnership with the Bristol-based innovation centre Unit DX, home to five of the seven companies set up in 2017.

Focusing on a range of new technologies, from detecting methane gas leaks using drones to developing vaccine candidates for emerging infectious disease, success has been facilitated by the University’s expertise in research, commercialisation and enterprise development.

Bristol alumnus Dr Harry Destecroix is Director of Unit DX and co-founder of University spin-out Ziylo, which is exploring how a new family of synthetic sugar receptors could help people with diabetes. He said: “Without lab space and a community, it is really difficult to start science companies. The huge increase is the result of a lot of talented people coming together.”
An award-winning event that aims to inspire the next generation of female scientists celebrated 10 years of consistent success this June, with the help of a strong Bristol contingent.

Staff and students from the School of Chemistry have been taking part in Skirting Science for the past five years. This year involved the largest Chemistry team to date, including 12 contributors from the EPSRC Centre for Doctoral Training in Chemical Synthesis, who engaged with more than 100 girls from schools in North Somerset and Bristol via workshops on everything from perfume blending to detecting acids and bases with a cabbage indicator.

Dr Natalie Fey said: “This is a great event, allowing us to meet and enthuse girls from local schools about chemistry, and taking the time to talk to them about careers in chemistry.”

Inspiring girls about science for a decade

From science enthusiast to research fellow

A chemistry researcher inspired to study science during her school years will see a lifetime’s ambition come true this year, thanks to a Royal Society University Research Fellowship.

Beatrice Collins was first inspired to take up chemistry at secondary school and went on to study organic chemistry at undergraduate and PhD level at Cambridge University.

“Having spent my PhD learning how to make molecules, I knew I wanted to be able to control their motion and behaviour,” says Beatrice, who carried out a postdoctoral stay in the Netherlands, working in the field of molecular machines under Professor Ben Feringa. She then came to Bristol to take up a postdoctoral research associate post in the group of Chemistry’s Professor Varinder Aggarwal, working to develop new methods for introducing boron into organic molecules.

This year, Beatrice takes the helm of her own independent research group, which will explore how to use transition metals to control the motion of organic molecules, making molecules ‘walk’ along a molecular track or rotate in one direction.

“I couldn’t be more excited,” adds Beatrice, “to engage with colleagues in the department and to inspire students in their own research.”
New digital tools make for smarter lab work

Here in the School of Chemistry, we have a reputation for leading the way in digital education, using the latest findings from our research to help shape how students learn.

In 2007, the undergraduate teaching laboratories were completely overhauled to provide a state-of-the-art environment. This development was coupled with the simultaneous introduction of innovative e-learning software, in the form of our famous Dynamic Lab Manual (DLM), an online, fully interactive tool that features videos, virtual instrumentation and equipment, as well as inbuilt e-assessments.

As of this year, the DLM has gone one step further to include ‘smart worksheets’. This allows students to input their own experimental results, which provides personalised feedback based entirely on their own work.

Dr Chris Adams, Teaching Laboratory Fellow, says: “This means that when students process their lab data in an Excel spreadsheet, for example, they know they’re doing it correctly. This marks a really important difference with most digital worksheets, which ask set questions using example data.”

As part of his final year research project, third year student Monty Eayrs reviewed how effective the smart worksheets are and found that not only do students find them extremely beneficial, the personalised nature means there is less chance of students copying each other’s work.

Monty was also tasked with coming up with a plan to embed virtual reality into lab work, building on the award-winning research of theoretical chemist Dr David Glowacki, whose work with computational chemists and other colleagues in Chemistry has led to several innovative approaches combining science and technology.

Monty was inspired to create new resources that show students how to conduct an experiment in VR, using gaming-style hand-held controllers to move benzylamine molecules around to react with benzoyl chloride. Thanks to Dr Glowacki lending the lab some VR equipment, new first year students will be able to do the experiment twice, side-by-side – once in the real world and once in a virtual world.

New digital tools make for smarter lab work
Thanks to an outstanding portfolio of people and facilities, the University has provided the springboard for many of history’s major scientific discoveries and developments. One of the cornerstones of our teaching and research is interdisciplinary collaboration. This gives students the chance to work with academics from different academic specialisms, so as to provide a fresh and innovative perspective on new ideas. These joint projects are also a major catalyst for new avenues of experimentation and exploration.

For undergraduates, we offer around 20 research internships each year, which take place over eight weeks during the summer. These are open to all undergraduates across the University. This year, three Chemistry students successfully applied for one of these Interdisciplinary Research Projects (IRPs). Here we take a look at their ideas and what they hope to achieve...

**Aidan McFord**  
With Professor M. Carmen Galan (Organic and Biological Chemistry) and Dr Jim Spencer (Microbiology)  
"Thanks to being awarded a bursary, I will be working on bio-inspired probes for the development of antimicrobials. We hope to use catalytic methods to produce rare or unusual glycosides in a stereoselective manner. Combining these sugar molecules and fluorescent nanomaterials, we are aiming to make nanoprobe to detect specific bacterial strains and counter antibacterial resistance."

**Izzie Scott Douglas**  
With Professor Charl Faul (Materials Chemistry) and Professor Jonathan Rossiter (Robotics)  
"I am developing a material for use as a current collector in flexible supercapacitors. I’m working with researchers from the Bristol Centre for Functional Nanomaterials and the Robotics labs who are developing a flexible supercapacitor and intend to develop a fully 3D printable device. My research involves combining various materials and then 3D printing them, before assessing the physical and electrical characteristics of the composite materials."

**Henry Caldora**  
With Dr Alastair Lennox (Physical Organic Chemistry) and Dr Adam Perriman (Hybrid Biomolecular Systems)  
"I am collaborating with researchers to develop an electrochemical defluorination reaction and using 3D printing to aid in the optimisation of the reaction set-up. The reaction should be a useful method to efficiently synthesise molecules that can be incorporated into drug scaffolds. This bursary has given me the opportunity to work alongside and learn from amazing academics and PhD students in a project that will hopefully lead to the discovery of new and sustainable synthetic methods."
Generations of our graduates testify to a learning environment where students thrive, both during their time with us and after they move on. Here we look at where a Bristol Chemistry degree can lead.
Stefan Fidlschuster
Graduated in 2017 with an MSci Chemistry with Industrial Experience

Three months after I graduated from Bristol I started on the Business Leadership Graduate Scheme at Severn Trent. The scheme consists of three placements of nine months. I have completed my first placement as a GIS (Geographic Information Systems) Technical Expert, where the analytical skills I picked up during my degree proved useful in facilitating and owning a data improvement project. I have now moved on to be a Waste Water Treatment Process Advisor, where I need to solve real-world problems quickly using my knowledge of Chemistry and Biochemistry to prevent plant failures and large scale pollution incidents.

Sally Tam
Graduated in 2017 with an MSci in Chemistry

After graduating from Bristol in 2017 with an MSci in Chemistry, I joined PwC (PricewaterhouseCoopers) as an auditor and have started studying towards the ACA (Association of Chartered Accountants) qualification. I have already worked with a wide range of interesting clients in financial services and also helped organise multiple charity events for non-profit organisations. From acquiring the skills that are valuable for a career in professional services, to gaining the confidence I needed for interviews, my degree has certainly helped me secure this fantastic role and will continue to prove useful in the future.

Dan O’Flynn
Graduated in 2018 with a PhD in Chemical Synthesis

Having completed my PhD in Chemical Synthesis via the CDT programme in 2018, I began employment as a medicinal chemist at Sygnature Discovery (BioCity, Nottingham). We provide experienced drug discovery support to international clients on projects spanning from oncology and inflammation to anti-infectives and diabetes. The job is multidisciplinary, dynamic, interesting, challenging and, most importantly, enjoyable. For me, it’s great to apply the skills and techniques I developed at Bristol to real-world drug discovery projects where the eventual result may help cure a disease and greatly improve a person’s quality of life.

In numbers

85% of our 2017 graduates were in graduate roles six months after graduation

1,300+

Different firms employed University of Bristol graduates across all sectors

(source Destinations of Leavers from Higher Education survey, 2018)
Below Professor Charl Faul (left) from the School of Chemistry is greeted by Prof Yang Bin, Vice-President and Provost of Tsinghua University, Beijing. Professor Faul regularly visits China to build connections with its scientific institutions.
Bristol in China

The strong ties between the University of Bristol and China’s academic community have already garnered success, and new partnerships are set to open up even more opportunities for students to achieve academic excellence.

Here at Bristol, we’re proud to have a long history of attracting people from across the world. This is especially the case in the School of Chemistry and in the Faculty of Science overall, where our innovative approaches to teaching and research are enriched by a strong international community of both students and researchers.

We’ve long enjoyed close ties with schools, colleges and universities in China. Currently, the University is home to more than 2,000 Chinese undergraduates and postgraduate students, while our alumni community in China already includes 8,000 members.

Professor Charl Faul has visited China more than 35 times in little over 10 years, helping to expand the connections between Bristol and institutions including the Chinese Academy of Science, where he was a visiting professor at the National Centre for Nanoscience and Technology.

“China is a fascinating place, the science in China is equally impressive,” says Professor Faul, who also holds an adjunct position at Tsinghua University in Beijing.

“We are fortunate to benefit from the huge investment in science in China, with its large number of world-class universities and funding that comes from the Natural Science Foundation of China, as well as the ministries of Education, and Science and Technology. Over the years, we’ve been lucky to attract a steady stream of undergraduate, masters’ and PhD students, and many post-doctoral researchers who contribute hugely to Chemistry’s success. For many, their time at Bristol has helped them to launch successful careers in academia and elsewhere in China on their return.”

Strength to strength

Building on this history of success, the School of Chemistry is working with the University’s Partnerships team in the International Office to further develop its network in China. We are currently in the process of finalising partnerships with Jilin University’s College of Chemistry (in Changchun), the University of the Chinese Academy of Science, Tsinghua University (Beijing), Zhejiang University (Hangzhou), Shandong University (Jinan), and the Beijing Institute of Technology (Beijing).

The University is also increasing the number of scholarships on offer, thanks to a collaboration with the China Scholarship Council. Together they have introduced the China Scholarships Council – University of Bristol Joint Scholarship PhD Programme. As a result, 40 new high-calibre Chinese students will begin their PhD studies at Bristol in 2018, with this number expected to increase by 20 places each year.

Working together

Xiaoyu Li and Yang Gao

Husband-and-wife team Xiaoyu and Yang came to Bristol in 2013 to join Ian Manners’ research group as postdoctoral research fellows. “Those were some of the best two years in our lives so far,” says Xiaoyu. “Doing fancy and funny experiments together, making many wonderful friends – and the best bit: we ended up writing some really nice science papers.” Xiaoyu has since obtained a Thousand Talents Program award, and an academic position at the Beijing Institute of Technology back in China, while Yang has moved into academic publishing.

Yan Qiao

Yan worked as a postdoc in Steve Mann’s protolife research group between 2014 and 2017. She has now secured an independent position within the Chinese Academy of Science, after obtaining a Thousand Talent Program award in 2018: “I was drawn to the world-famous colloid research group at Bristol because my doctoral and first period of postdoc research was about self-assembled functional colloids. My research now is primarily focused on the use of artificial cells in terms of the origin of life and soft robotic devices. My career was helped enormously by my time at Bristol.”

Celebrating in Shanghai

Graduation ceremonies are a milestone in the lives of all students. In April 2018, we again held a dedicated ceremony for students in China. The Shanghai event attracted over a thousand graduates, alumni and their families. The celebration also reached more than two million viewers online, who were able to tune into the graduation via a mobile platform-based video campaign organised by our UoB China Representative Office: the first of its kind by any UK university.
Robots and revolutions

New methods of creating organic molecules using an automated system will revolutionise the delivery of healthcare products, and may not require experts
Imagine a world in which the creation of complex molecules could be fully automated, simply by inputting a set of commands into a machine. It’s a bold move that could dramatically transform our ability to improve pharmaceutical drugs for the sake of better healthcare.

This is precisely the vision that underpins the work of synthetic chemists at the University of Bristol.

Their work focuses on polyketides, a vast family of organic compounds that represent the single most successful family of compounds that have been harvested for the promotion of human health. They form the basis of natural products which are particularly rich in biological activity, and so are useful agents of defence against many illnesses – from cancer to autoimmune diseases, and bacterial and viral infections.

However, their highly complex structure means that it can be extremely challenging to make medicines with the desired pharmacological results. And while modifications of the natural product might have the optimum features for pharmacological purposes, the limited chemical modifications that can be done make the process and the results less than ideal.

Take the drug eribulin, a synthetic analogue of the complex natural marine product, helicodrin B, which was approved for the treatment of metastatic breast cancer in 2010. Helicodrin B could not be harvested from the marine organism in sufficient quantities and so the analogue that became the drug, eribulin, had to be made from scratch. This proved to be a daunting task, requiring 59 synthetic steps in a highly labour-intensive process.

Mass production
Varinder Aggarwal, Professor in Synthetic Chemistry, is working on what promises to be a new, easier approach to organic synthesis that would make polyketide analogues more accessible for testing and development. This would involve growing carbon chains one atom at a time in a manner akin to a molecular assembly line.

He and his research team have already created a small set of building blocks that can be joined together in an iterative process without having to purify the intermediates created after each addition.

“This robust methodology is now ripe for automation as this will enable the preparation of libraries of these molecules much more rapidly,” says Professor Aggarwal. If the process can be automated, it will enable a greater variety of molecules to be made, simply by changing the order and nature of the building blocks that are added. With a greater variety of molecules tested, there is a greater chance that bioactive molecules will emerge.

Synthesis
The next stage involves the use of an automated workstation recently acquired by the School of Chemistry, which has the power to set up, run and operate up to 96 reactions at a time, and allows researchers to subject the end product to further modification with additional reactions.

“This could revolutionise the synthesis of organic molecules. By synthesising structurally complex molecules in a simple and ultimately automated way, we should be able to generate a vast array of highly functionalised, polyketide-like molecules, many of which are expected to display significant biological activity,” adds Professor Aggarwal.

“If successful, this process could transform and hasten the delivery of improved healthcare products. And it wouldn’t even require an expert to do it, because complex molecules could be prepared routinely using a fully automated system.”
You’d be hard-pressed to find a more quintessentially English summer tipple than a gin and tonic. But quinine, the core component of tonic water, has more depth to it than merely being the bitter accompaniment to a classic cocktail.

Quinine was first isolated from the bark of the cinchona tree in 1820. To this day, this remains the most reliable source and method of isolating this alkaloid. Quinine then became the first natural compound to be used as an antimalarial. Later in the 19th century it was purified into a powder and issued to British soldiers in India to ward off malaria. They agreed to take it when it was mixed with sugar to mask the bitter taste – and eventually blended this with gin to create the now famous concoction of a G&T.

Quinine continued to be used as an antimalarial until the 1940s, after which alternative treatments for malaria, with fewer side effects and better effectiveness, were introduced. Its colour is just as intriguing as its taste. When exposed to a lamp that emits UV light, tonic water – and any solution containing quinine – will glow a brilliant blue colour. This is caused by luminescence, where excitation by a photon in the UV range is followed by emission of a photon of slightly lower energy.

While the molecule is excited, it collides with other molecules and loses energy, dropping into lower vibrational energy levels. Eventually, as the molecule returns to its original state, a photon is re-emitted, but because of the energy loss from collisions, the energy is different and so is the wavelength. This produces a different colour emission to the light that was absorbed. Since the amount of light emitted by quinine is precisely known, quinine can be used as a yardstick for other luminescent compounds.

So the next time you come across a bottle of tonic water, consider the chemistry within.

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Quinine is one of many everyday substances whose chemistry is visualised on the University’s Picture It... blog. Read more at chempics.wordpress.com

Contributors: Huw Powers (former student, BSc Chemistry, 2016), Tom Young (PhD student, Theory and Modelling in Chemical Sciences Centre for Doctoral Training), Derek Durand (PhD student, Centre for Doctoral Training in Catalysis).
“Working in science has opened up opportunities I couldn’t have dreamed of”

Newly appointed Head of the School of Chemistry

Emma Raven talks heme proteins, the role of women in science and why she gets out of bed in the morning

Why did you choose to come to Bristol?
Because it is a great university and it has the best Chemistry department in the country. I’ve long been an admirer of Bristol Chemistry, and I am looking forward to learning more about all the amazing science that happens in the School.

What is your own area of specialism?
I work on heme proteins and their role in biology. The best-known heme proteins are hemoglobin, which carries oxygen in red blood cells, and myoglobin, which binds oxygen in muscle tissue. I worked on hemoglobin as an undergraduate, and myoglobin as a postdoc at the University of British Columbia in Vancouver, Canada. It was in Vancouver with Grant Mauk and Mike Smith that I learned how to apply site-directed mutagenesis to protein engineering. In my recent work at the University of Leicester – where I have been based since 1995 – I have used protein engineering to learn about how heme proteins function in biology.

Why do you think a chemistry degree is a good investment for undergraduates?
Chemistry is such a useful and versatile qualification for students – it can open doors into sectors such as finance, government, academia, chemical industry and biotechnology. I would say to students: do something that you enjoy and that you’re interested in, work hard but not too hard, don’t be afraid to ask for help, and take good advice at key stages. And enjoy yourself! You’ll be amazed at what can be achieved and how much fun it will be.

Has the status of women in chemistry changed during your career?
I sometimes get depressed at the lack of female role models in science generally, not just in chemistry. But on the other hand, there have been huge efforts made in the last few years in this area and some of it is beginning to pay off – for example, in the diversity of women award-winners in science prizes, and in the representation of women on panels and in chemistry departments at universities. There is work still to be done.

What gets you out of bed in the morning?
When you have a job like the one that I have, you really want to get out of bed in the morning, because working with students and staff in universities is fantastically and enduringly interesting. Working in science has opened up opportunities to me that I could not have dreamed of when I was at school.

What would you have done if you hadn’t been a chemist?
I’m actually not very good at anything else. I always rather fancied being one of the backing singers in a famous band, but I can’t sing!
School of Chemistry
Open Days 2019

Friday 14 June
Saturday 15 June
Saturday 7 September

bristol.ac.uk/opendays