



Enhancing MRI

Pioneering research could revolutionise MRI in hospitals

Super-fast DNA testing

Speeding up medical diagnosis and crime scene investigation

Materials at the nanoscale

Smaller, faster, smarter devices

Innovative antibiotic design

Penetrating bacterial membranes

In this issue

Welcome to *Chemistry New Boundaries*, the University of Southampton's chemistry research magazine. In this issue, you will discover how research in Chemistry is addressing some of the most challenging issues facing society through multidisciplinary collaborations.

The research carried out in Chemistry ranges from the search for new inorganic materials for the production of essential chemical feedstocks in sustainable processes, to molecular diagnostics and therapeutics where new ways to treat human diseases are explored.

Pioneering research that could revolutionise MRI in hospitals and lead to the early detection of cancerous cells is described on page 4. You can also read about new super-fast DNA tests, with applications for both medical diagnosis and crime scene investigation research by a collaborative team from Chemistry and Medicine, on page 10.

Along with innovative projects and forward-thinking researchers, today's research needs cutting-edge techniques to confirm results and at Southampton we are world-leaders in X-ray crystallography. Home to the National Crystallography Service, Chemistry has the most powerful and sophisticated lab-based crystallography instrument in the world. Find out more on page 14.

As well as new diagnostic tools and high-tech techniques, research here is looking at how nanotechnology can help develop faster computers, smarter sensors and more energy-efficient mobile phones. Find out how on page 16.

Southampton is also a fantastic place for young researchers with opportunities for up-and-coming talent to forge careers. Find out more from one of Chemistry's early career researchers on page 20.

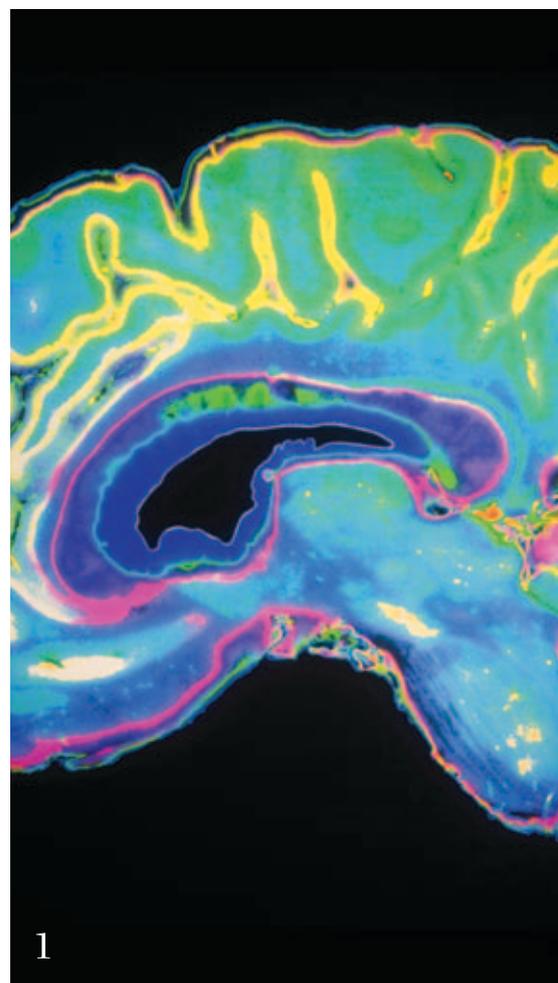
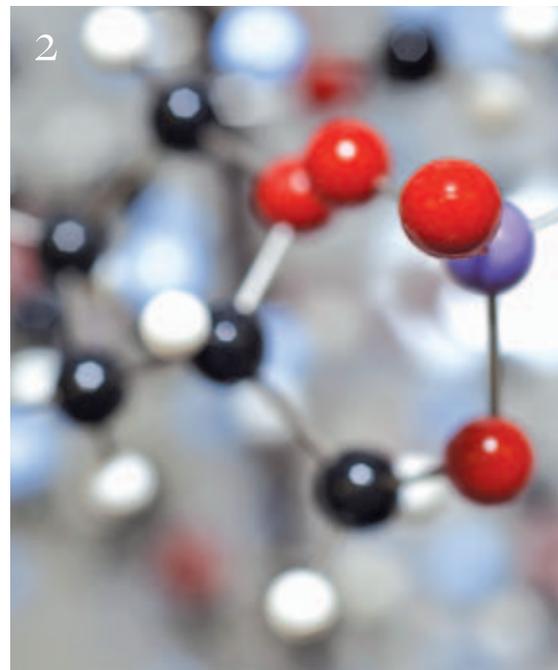
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1 Enhancing MRI

Pioneering research could revolutionise MRI in hospitals.
Page 4

2 Super-fast DNA testing

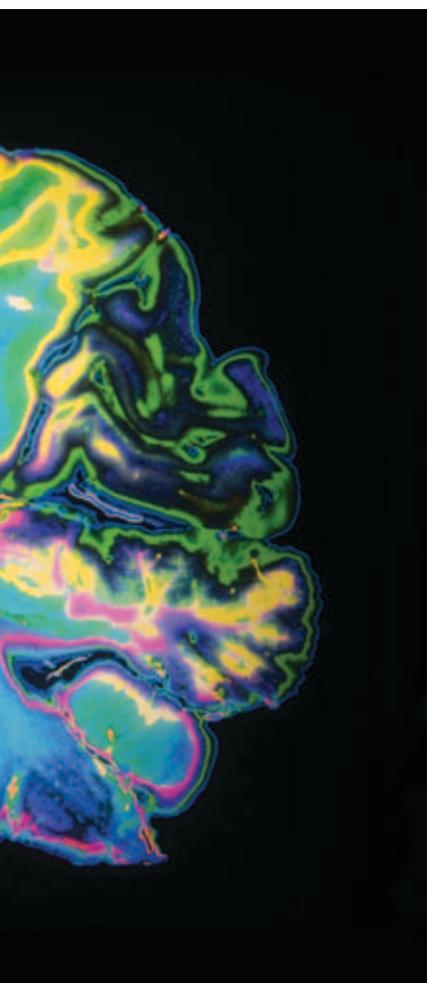
Groundbreaking research that could lead to faster medical diagnosis and crime scene investigation.
Page 10

3 Materials at the nanoscale

Smaller, faster, smarter devices.
Page 16

4 Innovative antibiotic design

Penetrating bacterial membranes to prevent the spread of disease.
Page 20



More highlights

One-stop shop for crystallography

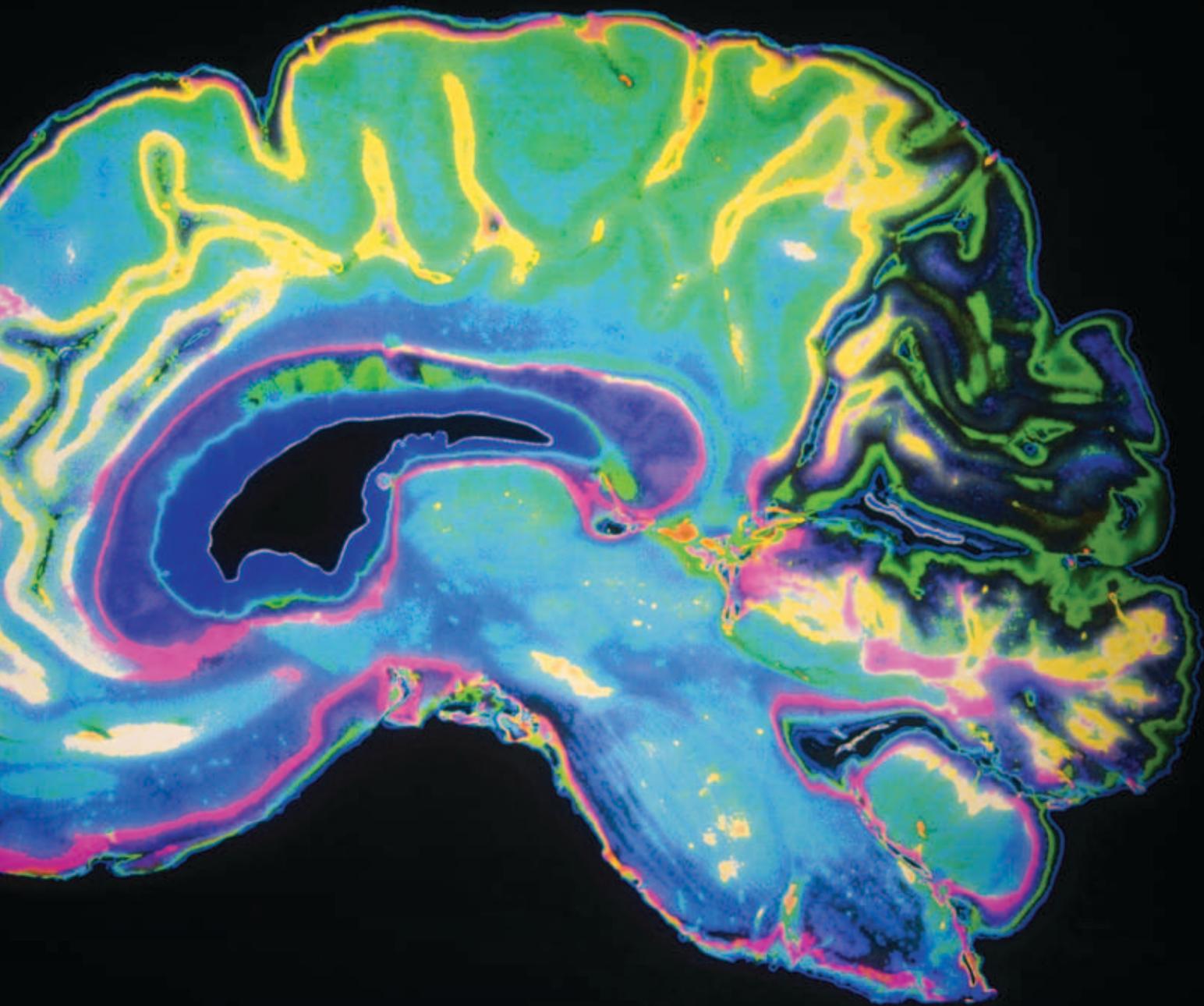
Cutting-edge techniques to support world-leading research.
Page 14

Restoring sight

Treatments for eye disease explored.
Page 22

Knowledge and innovation

Southampton spin-outs successfully exploit research ideas.
Page 25



“This technique could pave the way to many different opportunities in MRI that are currently not possible and ultimately, it can benefit us all.”

Richard Brown,
Professor of Organic Chemistry

Enhancing MRI

New research from the University of Southampton could lead to enhanced MRI scans, producing brighter and more precise images, and potentially enabling doctors to detect cancerous cells early, before they cause health problems.

“This method could allow us to detect oxygen levels in cells. When oxygen levels are depleted, this can mean that cells are metabolising more quickly, which can suggest that the cells are cancerous.”

Malcolm Levitt,
Professor of Magnetic Resonance





MRI scans showing arteries and veins in the body could be brighter and more detailed in the future

Professor Malcolm Levitt from Southampton has been awarded a grant from the European Research Council of €2.8m to support research into enhanced nuclear magnetic resonance (NMR). Along with collaborators Professor Richard Brown and Dr Giuseppe Pileio from the University and Dr Lynda Brown, a Royal Society Dorothy Hodgkin Fellow, Malcolm hopes the research will lead to a range of clinical applications, including the early detection of cancer.

NMR is the physical principle underlying MRI scanning, which is used routinely to detect abnormalities such as tumours. NMR was discovered in the 1950s and is a technique where the nuclei of atoms, many of which are magnetic, interact with magnetic fields. The technique can be used to probe the molecular structures and properties of materials. Images of how the nuclei are distributed can then be created, which is the basis for MRI.

Strengthening signals

NMR signals are inherently very weak. However, methods have been developed recently which lead to substances exhibiting a phenomenon called hyperpolarisation, which gives rise to NMR signals that can be more than 100,000 times stronger than normal. The problem is that this incredible enhancement only lasts a short amount of time – up to one minute in optimum conditions.

Research at Southampton has previously demonstrated the existence of quantum states that have extremely long lifetimes relative to the norm of several seconds – up to half an hour in the case of the common substance nitrous oxide. The new research grant has been awarded for a project that involves a combination of the hyperpolarisation effect with the long-lived

quantum states developed at Southampton. The combination could give the best of both worlds – enormously enhanced NMR signals, which last long enough to perform an MRI scan.

Malcolm says: “This could have benefits for MRI scanning. If you have strong signals, you can detect smaller amounts of substance that are less concentrated. For example, some substances naturally occur in a cell as part of the metabolism process, but occur in greater amounts in cancerous cells. Through this method, we should be able to detect when these substances are present and cells are potentially cancerous, earlier than ever before.”

Isotope labelling

Richard and Lynda are working on the design and synthesis of molecules that are labelled with stable isotopes such as carbon-13 with the objective of supporting these very long-lived quantum states.

Carbon-13 is an isotope of carbon that can be used in NMR because it is magnetically active, but its natural abundance is only 1.1 per cent, explains Richard. “Common MRI markers enriched with carbon-13 still do not have long enough lifetimes so that their potential for MRI cannot be fully exploited,” adds Giuseppe.

One group of compounds showing promise are synthetic carbon-13 labelled molecules that are derived from a natural product found in the human diet. “We are mainly looking at the synthesis of the molecules – that is the priority – but we are also still thinking about whether the molecules are soluble in water and compatible with human tissue,” says Lynda. “We don’t know the toxicology of the molecules yet; they would need to be tested, but we are keeping it in mind to make sure we stay on the right path,” she adds. ▶



A new NMR machine will be able to perform small-scale MRI experiments to test new concepts

“What we are really excited about is the prospect of seeing the first in vivo images using the technique.”

Richard Brown,
Professor of Organic Chemistry

Richard explains that another option would be to investigate metabolites as potential molecules to label. However, a lot of pre-existing work in the area of imaging focuses on metabolites. Their advantage is that they are not toxic as they are involved in metabolic pathways in the body, but the drawback has been that they can only be kept in an excited state for a matter of seconds, so it is impossible to track them to specific organs in the body.

Through this project Southampton researchers will be pushing the boundaries of what is known about molecules in hyperpolarised states and explore them in more detail. While they are in a hyperpolarised state for long periods of time, the team can manipulate the molecules to explore their unique properties, bind them to proteins with the aim of delivering them to certain organs in the body, or tag them to other proteins so they can follow their movements.

Meeting milestones

“At present we have got two classes of molecules that can support these hyperpolarised states,” says Richard. “Already the lifetimes we are achieving are very interesting and way beyond what is in existence for carbon-13 magnetisation. As we get information back from the NMR experiments using these molecules, we can then refine the design,” he adds.

The team’s collaborators at GE Healthcare in Copenhagen are currently carrying out in vitro studies on the first set of molecules that Richard and his team have developed. “So it is actually moving really fast – the project is progressing really well because we have two groups here that can work closely and quickly together. The close cooperation between the synthesis and NMR groups, where the molecules containing stable isotopes are made and then assessed for their suitability for progression, or refinement of

the molecular design, is really what counts,” Richard says. “We have met some of the major milestones already,” he adds.

New equipment

In addition to funding the research, the grant will allow for two new pieces of equipment to be installed at Southampton. One will be a polariser, which will be designed and constructed at the University and will generate substances exhibiting the hyperpolarisation phenomenon. The second piece of equipment will be a NMR spectrometer equipped to perform small-scale MRI experiments, to test out the new concepts in preparation for performing experiments on a clinical MRI scanner.

Malcolm explains that one of the possibilities in applying this research to MRI scanning is that the images will have better resolution and be brighter. This could be important when imaging small structures like coronary arteries. “Additionally, this method could allow us to detect oxygen levels in cells. When oxygen levels are depleted, this can mean that cells are metabolising more quickly, which can suggest that the cells are cancerous.”

Aiding existing therapies

From talking to medical experts, Malcolm has discovered that what the medical community really want is to image oxygen levels in cells to detect cancerous cells early. Doctors could then treat the affected area with radiotherapy at a very early stage and have a better rate of success. The enhanced-NMR technique could also be used in conjunction with radiotherapy to monitor the progress of cancer. “At present, the only way to tell if radiotherapy is working is to wait and see if the tumour grows again or regresses,” he says. “What you need is a marker the day after the radiotherapy treatment to tell you if it has worked. By looking at oxygen levels in the tissue we might be able to do that.”

The team hopes that this research, which will run over the next four years, will lead to the development of new tools for clinicians to detect all sorts of metabolic or anatomical

abnormalities in the body. “This technique could pave the way to many different opportunities in MRI that are currently not possible and ultimately it can benefit all of us,” says Richard.

Malcolm says that although the project is still at an early stage, the first results are promising. “The potential impact on medicine is quite large,” he says. Applying the fundamentals of this enhanced NMR technique to MRI could lead to better quality images of all the body’s internal organs.

The key to the versatility of the technique is to develop molecules that can stay in the hyperpolarised state for much longer amounts of time – as long as 30 minutes. This would allow the molecules to be used for many different applications. “What is exciting for the field of imaging is that if the lifetime issue can be overcome, it will really open the door again to major advances,” says Lynda. “Such a long lifetime will give access to remote organs – this is not possible with current techniques – or allow images with enhanced contrast by allowing the agent to accumulate over a longer period. It could also be possible to tag the hyperpolarised long-lived agent onto a molecular vehicle to deliver it to the desired target – either a cell, tissue or organ,” adds Giuseppe.

The technology is basically static at the moment and there is a limit to the organs we can image, explains Richard. “What we are really excited about is the prospect of seeing the first in vivo images using the technique,” he says.

For more information, visit www.southampton.ac.uk/chemistry

Super-fast DNA testing

Southampton researchers are developing an innovative technique for DNA testing that is paving the way to point-of-care tests for medical conditions and faster crime scene analysis.



The ability to diagnose disease and identify people from the DNA sequence of their genome has revolutionised medicine and forensic science. However, the time-consuming nature of this type of test causes problems when the results are needed quickly. Southampton researchers are leading the way in developing super-fast DNA tests.

In partnership with international analytical science company LGC, Southampton researchers have developed a new way of fluorescently labelling DNA with special probes, known as HyBeacons. “HyBeacons are like little balls of loosely screwed up string that uncoil easily and find their targets,” says project leader Tom Brown, Professor of Chemical Biology. The HyBeacons light up when they attach to a specific target sequence of DNA. Their advantage over existing systems is their very simple structure, which makes them more predictable: they bind faster to their targets and always work. “In theory you could diagnose any infectious

or genetic disease by using HyBeacons on the DNA sequence of bacteria, viruses or people,” says Tom.

Towards faster diagnosis

Tom’s team is currently developing a fast test for chlamydia, a common sexually transmitted infection (STI) that is becoming a big problem, particularly in the western world. Chlamydia can usually be treated with antibiotics – but only a quarter of women and half of men with the condition show any symptoms, so most people are unaware that they have the infection and so continue to spread it. If left untreated, chlamydia can lead to long-term painful infections in women that result in infertility. Ectopic pregnancy is a life-threatening condition that has also been linked to prior chlamydial infection.

Despite these serious complications, many patients who have tested positive for chlamydia don’t return for their results. “Previous studies have shown that up to 40 per cent of people diagnosed with chlamydia

did not return for treatment,” says Ian Clarke, Professor of Molecular Microbiology at Southampton. “This obviously increases the risk of passing on this infection, so it would be far better for diagnosis and treatment to occur at the same visit to a clinic.”

To address this issue, Southampton researchers led by Ian, in partnership with LGC and Optigene – a company that manufactures systems for analysing DNA – are designing a chlamydia test that aims to produce results within 15 minutes. Having secured £480,000 of funding from the Engineering and Physical Sciences Research Council (EPSRC) and the UK’s Technology Strategy Board, they are developing the new test using HyBeacons to detect the presence of the *Chlamydia* bacterium in urine samples. In the future doctors could use this type of test to diagnose several different bacterial infections from one sample, which would be particularly useful for diagnosing STIs, as they often occur at the same time. ▶



“Previous studies have shown that up to 40 per cent of people diagnosed with chlamydia did not return for treatment, so it would be far better for diagnosis and treatment to occur at the same visit to a clinic.”

Ian Clarke,
Professor of Molecular Microbiology

Personalised medicine

HyBeacons could also be valuable for accurately prescribing medicines. Many people who are susceptible to deep vein thrombosis (DVT) take warfarin to prevent their blood from clotting. The dosage of this drug needs to be tailored for each person; however, HyBeacons could make this process easier in the future. Using HyBeacons, doctors could use a person’s individual genetic make-up as part of the calculation and work out the dosage much more easily. HyBeacons could also have a role for testing a patient’s susceptibility to the side-effects of certain medicines, such as statins, the cholesterol-lowering drugs that are taken by around seven million people in England alone. Side effects of statins can be anything from cramp to kidney failure. If statins became available over the counter, a 15-minute test that tells people whether they are likely to get any side effects would be crucial to helping them make an informed choice.

The University’s Nucleic Acid Research Group, led by Tom, made a groundbreaking advance in personalised medicine in the 1990s. In collaboration with AstraZeneca, they invented a novel real-time polymerase chain reaction (PCR) method, which copies a DNA sequence millions of times for rapid analysis. The method, known as Scorpion Technology, helps researchers identify mutations in a person’s genome. “Scorpion Primers enable treatment to be tailored to the genetic nature of the disease to ensure that the correct therapy is given,” says Tom.

“If you can understand which drugs are going to work for which people, you can avoid unnecessary expense and stress, and if there is more than one possible drug, you can give them the right one. This could have a huge impact – prolonging life and saving money.”

Rapid crime scene analysis

We all have our own unique genetic ‘barcode,’ which is what forensic scientists use to identify people from traces left at a crime scene by comparing DNA samples with, for example, the UK’s National DNA Database. However, finding a ‘match’ from a DNA sample is a lengthy process and suspects often need to be released from custody before the results are ready. Now Southampton scientists and LGC are developing an ultra-rapid portable test that could be carried out by non-experts.

As a species we share more than 99 per cent of our DNA; some of the differences between us lie in the length of the DNA sequence between certain sections of our genome known as short tandem repeats (STRs). To create a genetic profile, forensic scientists take a sample of hair or saliva, extract the DNA and make multiple copies of the STRs at 11 key points in the human genome. To measure the length between the STRs, forensic scientists currently need to run the DNA strands through a polymer gel at a high voltage, which takes about a day and needs specialist equipment and expertise. HyBeacons could be the key to much faster tests. In the same way as for diagnostic tests, they bind to the DNA taken from a crime scene, producing a fluorescent glow. When the mixture is



“In theory you could diagnose any infectious or genetic disease by using HyBeacons on the DNA sequence of bacteria, viruses or people.”

Tom Brown,
Professor of Chemical Biology

Multi-coloured HyBeacons can be used in human diagnostic and forensic applications

heated gradually, it stops glowing at a certain temperature, proportional to the length of the DNA strands. This so-called ‘melting temperature’ shows the type of STRs present and the exact length of the DNA strands between them, which can be compared to the DNA database in order to identify a suspect.

“This is particularly valuable if you want to very quickly determine if someone was present or absent at the scene of a crime,” says Tom. “If you have someone in a custody suite and you can only keep them for a certain length of time, you need a fast test to enable you to retain them for longer. If you combine this with the portable equipment, you can do this at the scene of the crime,” he explains.

This research is now in the commercial arena: LGC are hoping to commercialise the technique and they are working with ATDBio, a company based at the University of Southampton and co-founded by Tom, to make the probes. There are also several of our PhD students further developing HyBeacons at the University, funded by ATDBio.

The applications of HyBeacons don’t stop there; they could be used for a whole host of other areas, including paternity testing, making sure rare parrots have been bred legally in captivity rather than illegally imported from the wild, testing sheep for the prion disease, scrapie and also for foot and mouth disease. “A portable test for scrapie and foot and mouth could become important at any time,” says Tom. “HyBeacons make it possible to test for these out in the field rather than taking samples back to the lab,

which minimises the risk of spreading the infection,” he adds.

Building on strong foundations

Southampton’s Nucleic Acid Research Group has an impressive history of innovation, multidisciplinary working and enterprise. Tom founded the company Oswel Research Products, which synthesises chemically modified molecules such as DNA, and co-founded two spin-out companies, ATDBio and PrimerDesign. In 2008, in collaboration with PrimerDesign, Tom’s team produced the first H1N1 swine flu test kit, which was used in Mexico at the early stages of infection. The team has recently developed a novel technique for linking DNA strands together using chemical methods. Still in its early stages, this could eventually have implications in molecular biology and biotechnology. The team’s future plans include developing small molecules that interact with nucleic acids to switch off disease-causing genes – a big challenge because the human body is extremely adept at finding ways of adjusting to change.

“One of the great things for me about doing research at Southampton is that we have such fantastic facilities,” says Tom. “We have great students and a lot of collaborations across the University. With the development of the new Institute for Life Sciences, we are looking forward to being able to collaborate more and more across the disciplines.”

For more information, visit www.southampton.ac.uk/chemistry



One-stop shop for crystallography

Today's research needs cutting-edge techniques to confirm results. At Southampton we are pioneering X-ray crystallography that supports and develops research across all the sciences. Dr Simon Coles, Director of the Southampton Diffraction Centre (SDC), explains how our facilities can help you unambiguously confirm the most challenging chemical structures.

Q *What is crystallography?*

Crystallography involves the scattering of beams of X-rays when they are passed through crystals. Researchers can then analyse the scattered rays using computer software to determine the structure of chemicals for a wide range of applications. By confirming the structures of materials that can store greenhouse gases, for example, crystallography can help combat climate change. It can also help save lives by identifying the composition of potential new drugs, as well as enzymes and proteins.

Q *Why is crystallography important?*

It is the most unambiguous way to identify a chemical structure, providing the chemical is in its solid form. It provides extremely accurate structural information that can then be related to the properties of the material. It is not possible to get that level of accuracy with any other technique and so you get the definitive answer.

Q *Can you explain the aim of the SDC?*

The SDC provides a one-stop shop for everything single-crystal based. It has several functions such as providing a University-wide service to solve crystal structures of small molecules such as pharmaceuticals, through to large macromolecules such as proteins. It provides a commercial service for industry, carries out research to push the boundaries of the field and provides researchers from across the UK with the National Crystallography Service (NCS), which incorporates state-of-the-art laboratory equipment and expertise.

Q *What services does the NCS provide?*

The NCS provides two types of service to those eligible to apply to the Engineering and Physical Sciences Research Council (EPSRC) for funding. The first service is to solve crystal structures for researchers when they don't have the sufficient instrumentation available locally to do it themselves. The second service is a more in-depth, complete analysis of the chemical structure of their compound, as well as help publishing the work.

Q *How did Southampton become the home of the NCS?*

The University of Southampton won the bid to keep the NCS here in 2010, because of a University-wide effort to obtain the contract. We were one of six institutions tendering for the contract, but due to the University's support and the expertise we have here, we were able to secure the Centre.

Q *Why is the SDC cutting-edge?*

What makes SDC and therefore the NCS cutting-edge is that we have the most powerful lab-based single crystal X-ray diffractometer in the world here. We also not only have the expertise here to use it, but we have the expertise here to design and develop it. There isn't another instrument like it in the world and we worked very closely with the manufacturers to build it. What we mean by the most powerful in the world is that it produces the most intense beam of X-rays of any lab-based machine. It's about five times more powerful than anything else out there.

Q *Is having the most powerful diffractometer important?*

Having the most powerful lab-based instrument in the world is important because it means we can push the boundaries of the technique to look at weaker and smaller crystals. This means that on demand we can tackle the most difficult problems researchers can throw at us. For example, there are members of staff at Southampton that have reinvigorated their research after using the SDC. After gaining very accurate structural information from samples of tiny crystals that in the past were just thought to be powders, they have been able to take their research in a different direction.

Q *What is the NCS's biggest challenge?*

It is an enormous challenge to stay cutting-edge, and that is why we have developed an academic strategy around the National Service. We need to keep developing the machines and software we have. The contract will be up in the next five years so we still need to show we are developing the field through our research.

Q *Does the SDC offer any other services?*

The SDC as a whole is very open to approaches for collaborative work. We also actively go out and seek collaborations, both academic and on a more industrial level. Once we have a partnership in place, we can play a major part in grant applications and the research that results. We offer commercial services, from just solving crystal structures to long-term crystallography projects that are carried out by members of our team. An example of a current commercial partner is Argenta.

Q *How do you help train the next generation of crystallographers?*

Because we are a cutting-edge facility and a service, we have the opportunity to train people to a higher level. So we run training events and a number of different training exercises, from work shadowing to placements. We also run workshops with manufacturers of the crystallography software in order to further train researchers who are already experts in the technique, solve complex reoccurring problems and overcome limitations with the system.

For more information, visit www.southampton.ac.uk/sdc

Materials at the nanoscale

Scientists have secured £5m of funding for research into nanotechnology that could result in faster computers, smarter sensors and more energy-efficient mobile phones.

High-tech materials underpin a wide range of photonic and electronic devices, including recording and medical equipment. By depositing these materials onto surfaces in specific structures and patterns manufacturers can build the components for the gadgets we use every day. Computer chips and data storage devices are produced using material deposition techniques, but in order to keep up with consumer demand for faster computers and larger data storage devices, smaller and more complex structures are needed.

Smaller, faster, smarter devices

Now, a collaboration of research teams led by the University of Southampton and funded by the Engineering and Physical Sciences Research Council (EPSRC), aims to develop the technique of supercritical fluid electrodeposition to make and enhance materials at the smallest scale possible.

“The drive is always to make technological devices faster, smaller and smarter,” says project leader Professor Phil Bartlett, from Southampton. “And smaller and faster often match up in these terms because the speed at which a component works is usually based on how close together the individual bits are in order to send signals backwards and forwards,” he adds.

Phil explains that electrochemistry has been used for many years as a way to coat objects such as cutlery and jewellery with other metals. By using an electric current, you can control the thickness of the plating, or stop it and switch to another material so that you can deposit different layers on the same surface. The problem with using the technique for really small nanoscale devices – a human hair

is 70µm across, which is 70,000 nanometres (nm) – is that liquids are unable to penetrate the tiny pores on the surfaces due to surface tension and therefore the quality of the coating is compromised.

Collaborative effort

“Electrodeposition of materials into pores with diameters smaller than a few tens of atoms is very difficult, if not impossible, from liquids,” says Phil. “But using supercritical fluids – halfway between a liquid and a gas – means we could potentially fill pores of less than two nanometres. Supercritical fluids can completely fill a space, like gas, but have the properties of a liquid that can be altered by temperature or pressure. Their extreme penetrating powers will enable electrodeposition to apply to structures far smaller than anything achieved to date.”

The five-year programme brings together researchers from the universities of Southampton, Nottingham and Warwick with expertise in electrochemistry, supercritical fluid science, synthetic chemistry and materials physics. Professor Gill Reid, from Southampton, leads the synthesis team whose primary role in the project is to prepare new, tailored molecular reagents and electrolytes – charged salt species that carry electrical charge – that will aid the deposition of nanostructured materials via the supercritical fluid electrodeposition route.

“We have two strands to our part of the work; one is making the electrolytes and the other is making the metal reagents that supply the elements we wish to deposit,” says Gill. “The properties that we need for the supercritical fluid electrodeposition means we have to develop bespoke reagents.

It’s all about solubility of the reagents and clean deposition, so we work closely with the electrochemists in Phil’s team and the supercritical fluid team in Nottingham,” she adds.

Carrying out the electrodeposition using a supercritical fluid as a solvent brings its own challenges, explains Phil. As supercritical fluids behave like gases, the reactions have to be carried out at high temperatures and pressures in order to dissolve the reagents in the fluid and contain all the reactants in the same place. “Typically the conditions we are using at the moment are something in the region of 80–90°C and up to 300bar of pressure. So this has to be done in a closed vessel with thick steel walls,” says Phil. “The advantage of this is that when we insert our structure that we want to deposit onto, into the vessel, the pressurised fluid with the metal reagent dissolved inside fills all the holes in the structure. The size of the holes we want to deposit into are a couple of nanometres across, but they may also be 100nm in length, so we will end up with deposited nanowires,” he adds.

Right equipment

Southampton physicist Dr David Smith explains that one of the aspects of the project his team is looking at is the design of the reactors so that higher temperatures and pressures can be investigated. “We could be talking about reactions with temperatures of 300°C and 1000bar of pressure and for that you need the right equipment. We produce the vessels that are used at the moment that withstand 300bar of pressure; these can be opened simply by unscrewing a nut. But we will need to go to a whole new ▶



“The drive is always to make technological devices faster, smaller and smarter.”

Phil Bartlett,
Professor of Electrochemistry

The team deposits materials onto different electrode surfaces and then analyses the quality of the resulting layers



Reaction vessels for the electrodeposition experiments need to be able to withstand high temperatures and pressures

“This is a distinctive team with complementary and unique skills and expertise.”

David Smith, Doctor of Physics

level of technology to support the elevated temperatures and pressures needed for subsequent tests,” he says.

So far Phil’s electrochemistry team has been able to deposit metals such as silver and copper using the supercritical electrodeposition technique. This is a good result because they are the kind of contact materials that are used in electronic devices, explains Phil. In addition, they have also managed to deposit metals such as nickel, cobalt and iron, which are used in magnetic and data storage devices. “We are moving on to depositing elements such as germanium, which is a semiconductor. This signifies a major step forward as another semiconductor silicon, forms the basis of the electronics that we use every day,” he says.

The success of the nanofabrication technique is firmly embedded in the collaborative nature of the project, explains Gill. “None of us could do the project alone. We need all four elements of synthesis, electrochemistry, supercritical fluid properties and characterisation of the resulting structures in order to achieve success,” she says. “And from a synthesis perspective we are discovering new families of molecules with new properties.”

“This is a distinctive team with complementary and unique skills and expertise,” agrees David. “Discovering new properties of materials is what makes the project exciting,” he adds. He explains that if the team can deposit inside 1.5nm pores, the coating could have an entirely new crystalline structure compared to the bulk material. Scientists have known for a while that the surface of a material is not necessarily the same as the bulk, because the atoms can rearrange on the surface. This can lead to topological insulators where electrons and therefore an electric current can move along the surface, but not through the rest of the bulk material; it remains an insulator. “If we deposit nanowires of 3nm in diameter or lower into pores on a structure, the whole nanowire could exhibit properties dominated by the surface,” says David.

Potential for commercialisation

Looking to the future, the team is hoping to investigate whether layers of materials that are just one atom thick can be deposited. They also hope to investigate electrodeposition at higher temperatures and pressures. “When you go to higher temperatures, the atoms and molecules are more mobile and you tend to get better quality materials deposited,” says Phil. “However, the problem with increasing the temperature is that you have to increase the pressure – if you just increase the temperature, the supercritical fluid will become less dense, will expand and then your metal reagent will not dissolve, so the electrochemistry will not work.”

Phil and his collaborators can demonstrate that their technique really works to deposit good quality materials on nanoscale structures, but their aim is to make some exemplar devices in well-defined pores on a chip array that really shows the benefit of the technique and pushes the boundaries of nanotechnology. Deposition of silicon into nanometre-sized pores on structures would prove that the technique could be used widely in the electronics industry.

Phil believes that the supercritical electrodeposition technique could have real potential for commercialisation in the silicon industry. “In a silicon microfabrication plant electrodeposition is used to make the interconnects between components on chips. Supercritical fluids are also used for cleaning chips before they are inserted into the microfabrication system. So from an engineering perspective, both these technologies are already used and they could be brought together in one process,” he says.

The technology might not win on cost, but the driver here is to develop something unique that will allow manufacturers to gain faster components and higher amounts of data storage than any other competitors in the business, Phil explains.

For more information, visit www.southampton.ac.uk/chemistry

Innovative antibiotic design

Dr Syma Khalid joined the University of Southampton in 2007. She explains that the support and advice that was available here helped her to form a pioneering research team that uses biomolecular computing to design potential antibiotics that could be truly life-saving.

Q *What does your research involve?*

My research is in biomolecular computing. Most of the work we do is based around biological membranes.

The general theme in my group is to build computer models that find the best ways for drug molecules to penetrate bacterial membranes. This is important because if you want to design new antibiotics that are going to kill bacteria and stop them causing infections, the drugs need to be able to get past the protective cell membrane to be effective.

Q *How did you get interested in this topic?*

I was always interested in computers in a geeky kind of way, and I was always better at theoretical chemistry than practical chemistry. I didn't really enjoy synthesis and I wasn't very good at it, so it was the ideal solution. I was always good at calculations and physical chemistry and through that I got into a computational project and I have never turned back.

Q *What is the impact on society of your research?*

My research is theoretical chemistry, but there are certain things that you can do in a computational model that you just can't do using an experimental method. For example, you can look down at individual atoms in the model and see what they are actually doing, whereas experimentally this is very difficult. The potential implication from our models is that, through rational design, novel antibiotics will be more effective than current ones. In terms of the practical development of new antibiotic drugs, potentially a lot less money should be wasted, as we will be able to predict which molecules have a greater chance of being

successful as therapeutic agents. If we can provide guidelines for people making these drugs, then the discovery process should speed up.

Q *Will your research have an impact on personalised medicine?*

Yes, we also work with a company called Oxford Nanopore Technologies that is trying to develop a DNA sequencing device to meet the \$1,000 genome challenge. Many biotech companies all over the world are racing to be the first to sequence the entire human genome for \$1,000. This would mean anyone could pay \$1,000 to find out the kind of diseases they might be susceptible to in the future. This would take personalised medicine into a new realm and our simulations are playing a big role in aiding the design of the device that Oxford Nanopore Technologies is developing.

Q *Is multidisciplinary collaboration important in your research?*

Yes, definitely, collaboration is vital in modern research. The nature of academic research is that we are all becoming more and more specialised. We strive for excellence in our own field, for which we have to focus on specific research questions. But that's certainly not the full picture; we need other researchers who are equally good at their own specialist area to build up the whole story, so collaborations are essential to good research.

Q *With technology leaping forward, do you think it is easier to collaborate than it used to be?*

I think so; the internet has made a massive difference. You can just fire off an email that someone can read at their leisure, rather than

trying to catch them on the phone. And also things like collaborative initiatives have been really helpful.

Q *Why did you choose to work at Southampton?*

My previous position was at the University of Oxford and at the time I decided to move to Southampton I still had two years of funding, so I wasn't at the stage that I needed a job. Research facilities here are excellent and my colleagues are also really supportive. Another benefit of Southampton is that it is home to *Iridis 3* – the most powerful university-owned supercomputer anywhere in the UK. And as my work is computational chemistry, that's a fantastic selling point.

Q *How would you rate Southampton for early career researchers?*

I would rate Southampton as excellent for early career researchers. I have been helped with funding for studentships, have been assigned a mentor and been given help and advice on grant applications. My mentor and other senior members of staff from Chemistry are always available for help and advice. In particular there is always the chance to have grant applications read through by someone more senior than me before submission.

Q *What would you say your biggest achievement has been here?*

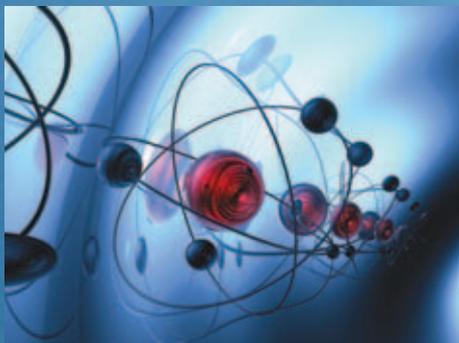
I would have to say that building up a good research group in difficult economic times has been my biggest achievement to date. I have eight researchers working for me now and many collaborative projects to get my teeth into.

For more information, visit www.southampton.ac.uk/chemistry

Syma Khalid's research in biomolecular chemistry could lead to the practical development of new antibiotics



In brief



Dial-a-molecule

A major constraint to progress in many areas of science is the time it takes to make molecules. It has an impact on technological progress and ultimately commercialisation of products. With this in mind chemists at Southampton are leading the EPSRC funded 'Dial a molecule' Grand Challenge, based on a vision that in 20 to 40 years, scientists will be able to deliver any desired molecule within a timeframe useful to the end user through safe, economically viable and sustainable processes.

Currently, many researchers in academia and industry use simple molecules in their research because they can be easily obtained. However, these are rarely the best, explains Professor Richard Whitby, the project lead. "It should be as easy to get the right molecule as picking up the telephone and asking someone to send it the next day," he says.

The aim is to meet the challenge of being able to programme the synthesis of any chemical efficiently and effectively, using a combination of innovative chemistry and new technology. Many disciplines outside of chemistry have key roles to play, for example informatics, computer science, mathematics, biology and engineering.

Through collaborating with a range of academic disciplines and end-users in industry, the resulting network will encourage creativity and adventure in the development of synthesis technology.



Ultrasonic water

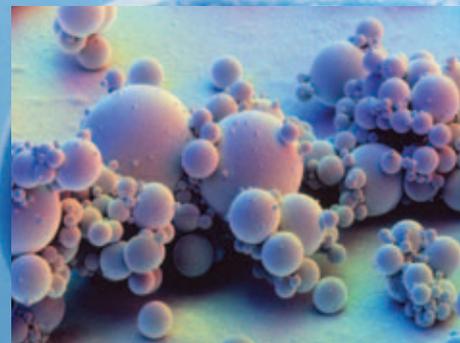
A team from Southampton has developed a revolutionary ultrasonic attachment for taps, which massively enhances the ability of water to clean.

Currently, industry uses excessive water, power and additives for cleaning and many industrial processes also generate large quantities of contaminated run-off. Purifying run-off is costly – each cubic metre of water used for cleaning in the nuclear industry can cost around £10,000 to treat.

Dr Peter Birkin from Chemistry and collaborator Professor Tim Leighton from the Institute of Sound and Vibration Research (ISVR) have developed a device that works with cold water, minimal additives and consumes as much electrical power as a light bulb.

The new nozzle generates both bubbles and ultrasound waves. Both travel down the water stream to the dirty surface and there the bubbles are driven into oscillation; under these conditions they seek and enter crevices and structured surfaces to remove dirt efficiently.

In recognition of their invention, Peter and Tim were awarded the Royal Society Brian Mercer Award for Innovation 2011. "The Brian Mercer award represents a significant milestone for the development of this technology and its possible exploitation," says Peter.



Restoring sight

Age-related macular degeneration (AMD) is one of the leading causes of vision loss in the western world and researchers at Southampton are looking to polymer chemistry for a cure.

AMD targets photoreceptor cells in the retina at the back of the eye and impairs the function of the fragile membrane underneath the retina – the Bruch's membrane – leading to loss of central vision. Dr Martin Gossel and colleagues, in partnership with charity Gift of Sight – established by Andrew Lotery, Professor of Ophthalmology at the University – are now investigating ways to deliver stem cells to the retina as well as ways to replace damaged parts of the Bruch's membrane with a synthetic version, to reverse AMD damage.

The team has synthesised biocompatible microspheres from a blend of poly(L-lactide) and poly(DL-lactide-co-glycolide) that stem cells can be attached to. The aim is to then inject the microspheres under the retina at the damaged site. They are also developing fibrous biopolymer networks based on polymethyl methacrylate that could replace the damaged parts of the Bruch's membrane, so that it can function again.

"We are coming at the problem from two angles – repairing damaged retina cells and regenerating the Bruch's membrane," says Martin. "The next step is to move into animal models to check biocompatibility."



Antibiotic attack

With the increase in antibiotic-resistant bacteria and the continued interest in biological weapons, there is an urgent need for new and effective antibiotics. Now, chemists at Southampton, in collaboration with the Defence Science and Technology Laboratory (Dstl), are looking at ways to switch off the ability of bacteria to cause disease.

Bacterial cells have receptors on their surfaces that monitor their surroundings.

These signals can tell the bacteria that they are in a mammalian host and need to produce suitable virulence factors and modulate their metabolism appropriately for survival. A team led by Dr Peter Roach from Southampton and Dr Petra Oyston from Dstl are looking at switching off the formation of guanosine pentaphosphate (pppGpp), one particular signalling molecule in this process.

Proteins are chains of amino acids linked together by the ribosomal machinery,

explains Peter. When bacterial cells run out of nutrients, the ribosome stops working which stimulates the formation of pppGpp. "So if we can switch off this process, the bacteria wouldn't be able to produce the proteins they need to survive and cause disease, and would just die," says Peter.

"The kind of antibiotics we hope to develop could be used to counter multi-resistant bacteria in both civilian and military settings," he adds.

In brief

Sustainable manufacturing

Southampton scientists are working together with industrial partners to make nylon – a polymer used traditionally in the clothing and carpet industries – in a more green and sustainable way. Using a solid that can catalyse the two individual steps of the process, the team can reduce the amount of byproducts, harmful waste products and the cost involved.

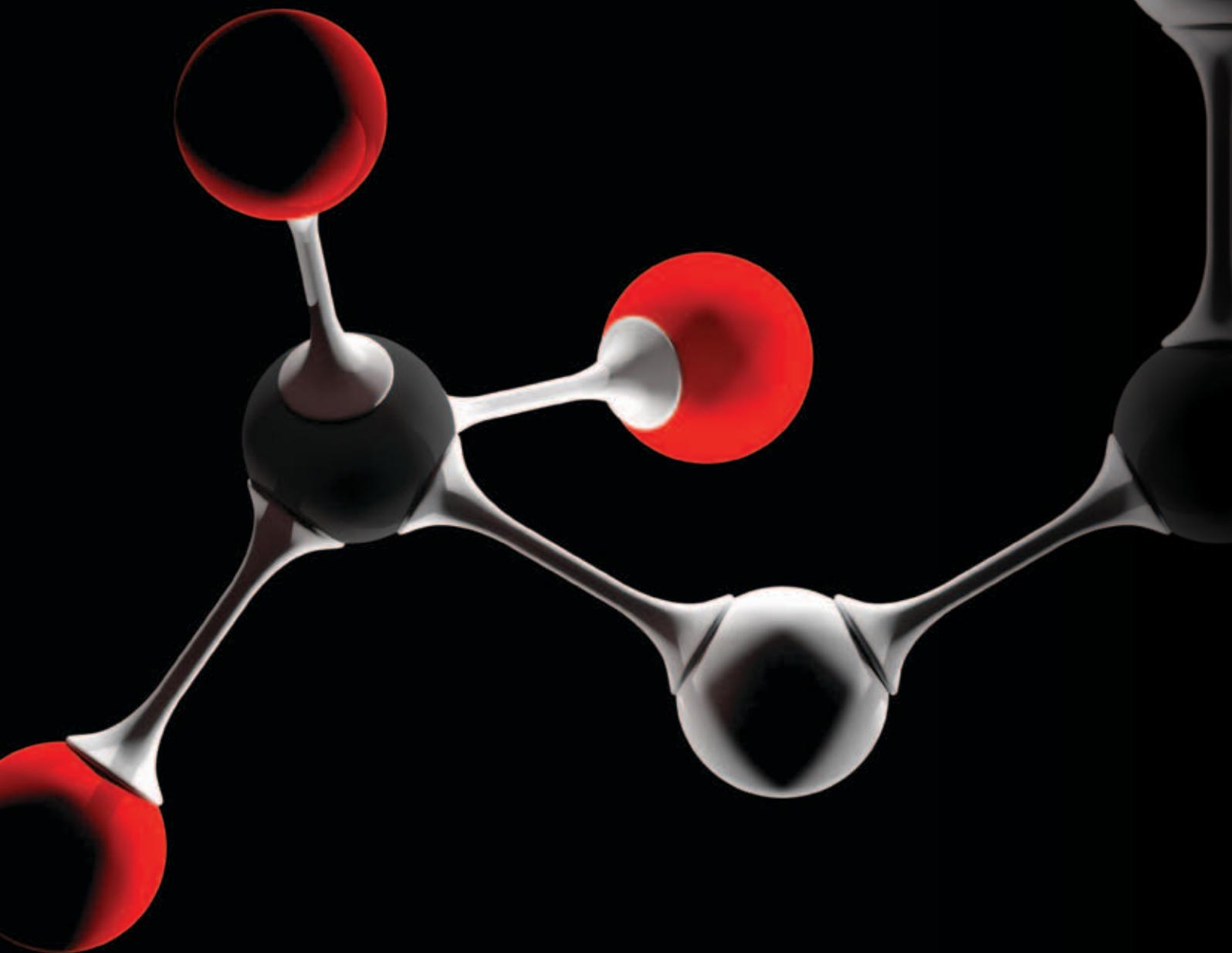
Nylon can be made using a two-step process that converts the ketone, cyclohexanone,

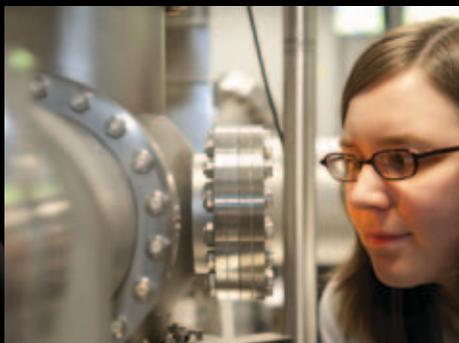
to caprolactam – the precursor to nylon. Corrosive reagents such as nitric and sulfuric acids are used generating large amounts of byproducts such as ammonium sulfate, causing environmental concerns and cost implications.

Now Dr Robert Raja and his team have developed a catalyst composed of aluminium and phosphorus bridging blocks, with either cobalt or manganese incorporated to catalyse both steps. These metal centres

catalyse the first step of the process producing water as the only byproduct. The surrounding framework architecture initiates the second step simultaneously resulting in caprolactam formation.

“We can catalyse stage one and two separately with two solid catalysts; but this can also be engineered in a one-pot synthesis with a synergistic catalytic approach,” says Robert. “Not only is it more sustainable, but cost effective too.”





Knowledge and innovation

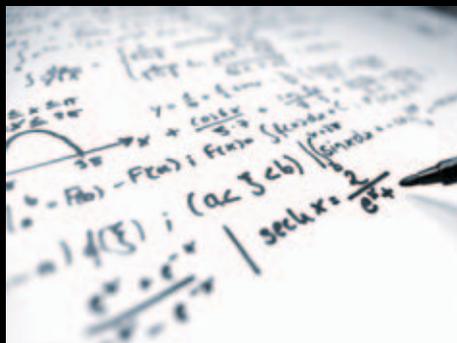
Strong links with business and industry encourage enterprise and innovation in research and Chemistry has a fantastic record of successful exploitation of research ideas into spin-out companies.

The range of companies spun-out from Chemistry showcases the variety of cutting-edge research being carried out here. Spin-out company Nanotecture seeks to exploit the properties of new materials for nanofabrication, while ATDBio pushes the boundaries of diagnostic DNA research.

Another notable spin-out is Karus Therapeutics, co-founded by chemists and researchers based in Medicine, for Cancer Research UK. This company investigates the biological properties of a series of novel compounds that have particular interest as potential treatments for a number of different cancers.

Materials-focused company Ilika, started by Professor Brian Hayden, forms new alloys that have interesting catalytic, electronic and magnetic properties. Many products Ilika has developed impact on broad and diverse markets, including the energy sector, for example, developing lithium ion batteries for use in electric and hybrid vehicles.

"Ilika provides direct evidence of the value of basic scientific research at universities, and the company's formation is a testament to the University's ability to help academics make best use of the intellectual property arising from their research," says Brian.



Transforming calculations for chemists

Innovative software could hold the key to major breakthroughs in the discovery of new drugs, energy sources or agents to tackle pollution. Chemists at Southampton are leading the way in developing these computer-based aids.

The principles for a theory needed to simulate molecular reactions were established in the 1920s, and when computers were invented, these paper-based theories became programs. However, the new science of quantum chemistry became more relevant with the arrival of supercomputers which can carry out trillions of calculations every second.

Dr Chris Skylaris has been developing new computational methods that enable chemists to simulate complex, lengthy and expensive molecular experiments at an atomic level. He has led the development of the ONETEP program which is already used extensively by academics worldwide and is marketed to industries through Accelrys.

Calculating the potential results when molecules react at an atomic level is an enormous task requiring huge computing power, but ONETEP achieves satisfactory results using IT facilities available at most universities. "Scientists need to have a way of predicting what molecules will do in reactions before testing them in the laboratory, to find out if they could be used for drugs or other purposes. They can then weed out unsuccessful candidates at an early stage," Chris says.



Radiolabelling metal complexes

Radiolabelled molecules are used to detect organ abnormalities or damage in patients, allowing early diagnosis and treatment of diseases such as cancer. Now, researchers at Southampton are developing new radiolabelling agents to make the process more effective.

The favoured radioisotope is fluorine-18, with its short half-life of 110 minutes. Once bound to a target molecule it can be injected into the body, delivered to the particular organ, imaged by positron emission tomography (PET), and then will decay safely. However, traditional methods to make fluorine-18 labelled molecules often involve lengthy, multi-step processes, limiting their clinical application.

Professors Gill Reid and Bill Levason, in collaboration with GE Healthcare, are taking a different approach to fluorine-18 radiolabelling using coordination chemistry. Using metal-fluorides bound to macrocyclic molecules, they hope to produce stable fluorine-18 labelled compounds that can be attached to a peptide and delivered to the target organ in a clinical setting.

"We are looking to use metal fragments that allow us to introduce the radio-label efficiently and rapidly, at room temperature, at the last stage of the synthesis," says Gill. "The idea is that in future this stage will be performed in the clinic, just before the imaging agent is administered to the patient," she adds.

For more information on these stories, visit www.southampton.ac.uk/chemistry

Journal papers published from January 2011 – February 2012

Southampton's chemistry academics have contributed to over 200 papers in leading scientific journals in the past year; here are just a few. For more research papers, please view individual staff profiles online.

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