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May 2018

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- Surface coatings from concept to commercial reality
- The p -value: a misunderstood research concept

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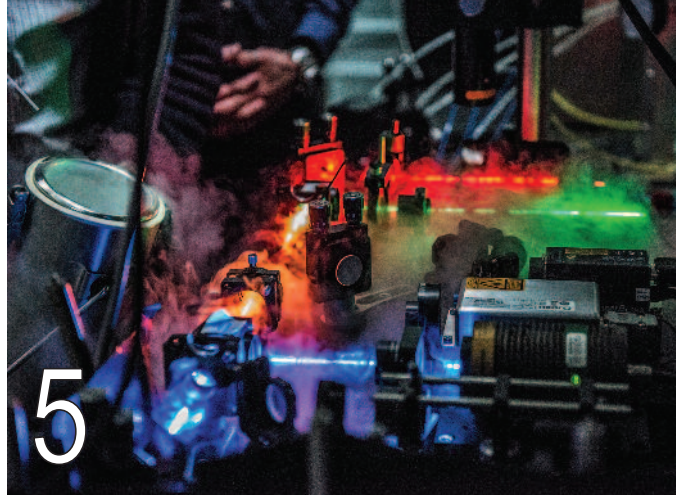
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chemistry

in Australia

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cover story

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From the President

By the time you read this, the second annual March for Science will have been held in Townsville in mid-April. I plan to march again this year as I hope do other chemists and scientists to ensure we continue to have a voice in the community and in politics. Last year, the March for Science was held essentially worldwide in attempts to have scientists of all disciplines recognised for what they do and to ensure science is funded to levels required. Let's hope it builds into a bigger and better event at all sites to keep science at the forefront of politicians' minds.

During a recent research trip to Japan, I visited Nagoya to meet Professor Hisashi Yamamoto, President of the Chemical Society of Japan. Before visiting, I mentioned I would like to talk to him about diminishing membership in our Institute and the possibility of a kindred agreement between the two societies. He felt the latter was something that he would need to discuss further with his Board members, and we will re-address this in March, when I attend the Chemical Society of Japan's 140th birthday celebrations at their 98th annual conference. Along with presidents of many other chemical societies, I have been invited to attend and speak at their international function as part of this celebration.

Professor Yamamoto provided me with some ideas on what the Chemical Society of Japan was doing to stem the lowering of membership. These ideas included:

- offering school students membership and a monthly newsletter. For a little extra, students get access to the monthly magazine. This brings in 200 new members every year
- giving a year's free membership to high-profile international speakers at conferences
- making a video of high-profile conference speakers available to members upon request (presumably those who could not attend the conference).

The next president of the Chemical Society of Japan will be Professor Maki Kawai (Okazaki University), who will be their

first female president. The society currently has 28 000 members and plan to build a new headquarters in Tokyo, a 20-storey building, and use the lower seven floors, while renting out the upper 13 for income. The society has 40 people working in their office.

These are ideas I will be working on with the Board of the RACI (except perhaps for the building of a sky-scraper!). If members have any other innovative ideas, please feel free to contact me.

In a similar vein, I will be travelling to France in July to attend the ICOMC conference in Florence (I am on the international advisory board after chairing the last meeting in July 2016 in Melbourne). Immediately prior to this meeting, the French Chemical Society will be holding a small symposium and part of that will be a signing of a kindred agreement between the two societies.

Hopefully, members will see these two agreements as beneficial.



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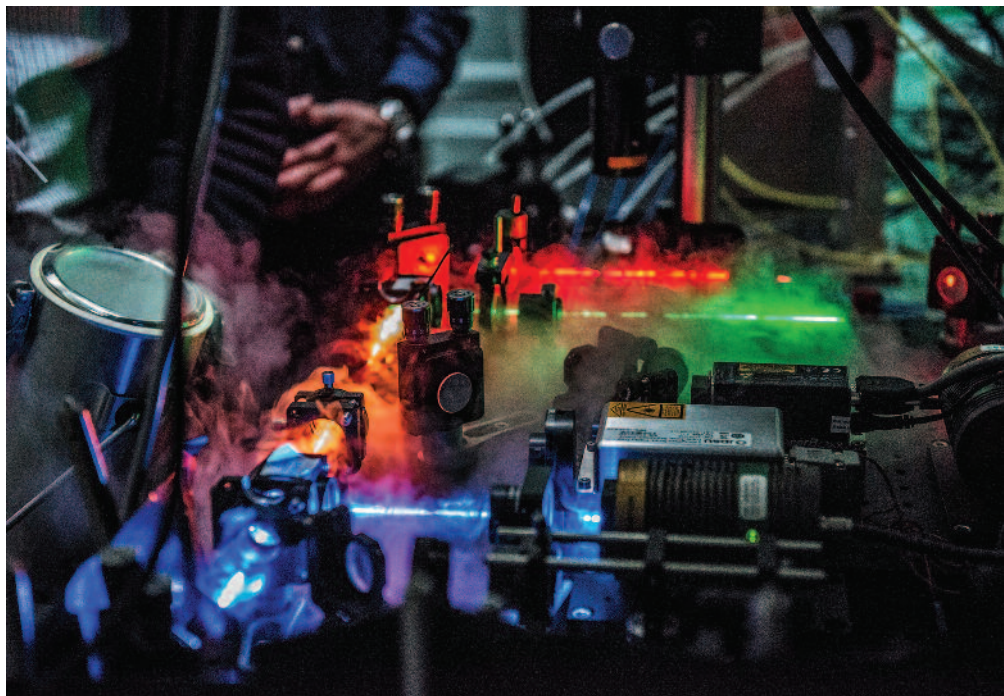


New interaction mechanism of proteins discovered

Proteins are among the most important biomolecules and are the key mediators of molecular communication between and within cells. For two proteins to be able to bind, specific regions of their three-dimensional structure have to exactly match one another – like a key that fits into a lock. The structure of proteins is extremely important for their functioning and for triggering the required response in cells. Now researchers at the University of Zurich, together with colleagues from Denmark and the US, have discovered that unstructured proteins can also have ultra-high-affinity interactions.

One of these proteins is histone H1, which as a component of chromatin is responsible for DNA packaging. Its binding partner, prothymosin α , acts as a kind of shuttle that deposits and removes the histone from the DNA. This process determines whether or not genes in specific parts of the DNA can be read. Both proteins are involved in several regulatory processes in the body, such as cell division and proliferation, and therefore also play a role when it comes to a number of diseases, e.g. cancer. Ben Schuler, professor at the Department of Biochemistry at the University of Zurich and head of the research project published in *Nature* (doi: 10.1038/nature25762), explains: 'The interesting thing about these proteins is that they're completely unstructured – like boiled noodles in water'. How such disordered proteins should be able to interact according to the key-lock principle had puzzled the team of researchers.

What is remarkable is that the two proteins bind to one another much more strongly than the average protein partners. The research team used single-molecule fluorescence and NMR spectroscopy to determine the arrangement of the proteins. Observed in isolation, they show extended



Single molecule fluorescence spectroscopy. Christoph Schumacher, dunkelweiss

unstructured protein chains. The chains become more compact as soon as both binding partners come together and form a complex. The strong interaction is caused by the strong electrostatic attraction, since histone H1 is highly positively charged while prothymosin α is highly negatively charged. Even more surprising was the discovery that the protein complex was also fully unstructured, as several analyses confirmed.

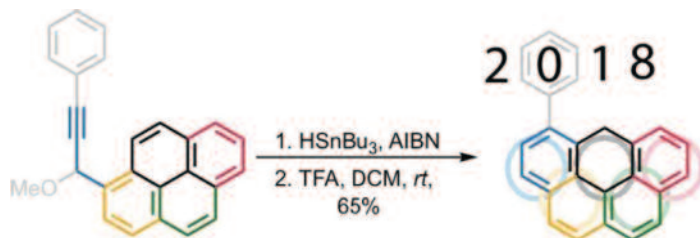
To investigate the shape of the protein complex, the researchers labelled both proteins with fluorescent probes, which they then added to selected sites on the proteins. Together with computer simulations, this molecular map yielded the following results: histone 1 interacts with prothymosin α preferably in its central region, which is the region with the highest charge density. Moreover, it emerged that the complex is highly dynamic: the proteins' position in the

complex changes extremely quickly – in a matter of approximately 100 nanoseconds.

The interaction behaviour is likely to be fairly common. Living beings have many proteins that contain highly charged sequences and may be able to form such protein complexes. There are hundreds of such proteins in the human body alone. 'It's likely that the interaction between disordered highly charged proteins is a basic mechanism for how cells function and organise themselves', concludes Schuler. According to the biophysicist, textbooks will need to be revised to account for this new way of binding. The discovery is also relevant for developing new therapies, since unstructured proteins are largely unresponsive to traditional drugs, which bind to specific structures on the protein surface.

University of Zurich

‘Olympic ring’ molecule in time for winter games



In the FSU team's technique, an additional hexagonal ring of carbon atoms is fused to the zigzag edge of an existing carbon-rich molecule. Igor Alabugin

As the world's premier winter athletes were preparing to take to the slopes, rinks and tracks for the 2018 Olympic Winter Games, Florida State University researchers were hard at work making a gold-medal discovery of their own.

Far away from the snowcapped peaks of PyeongChang, scientists from FSU's Department of Chemistry and Biochemistry unlocked a novel strategy for synthesising a highly versatile molecule called olympicene – a compound of carbon and hydrogen atoms named for its familiar shape.

'An olympicene is a molecule consisting of five rings that resemble the shape of the famous Olympic rings', said Cottrell Family Professor of Chemistry and Biochemistry Igor Alabugin. 'This new process for synthesising these molecules offers a unique tool for the preparation of structurally precise carbon-rich nanostructures.'

The team's findings were published in *Angewandte Chemie* (doi: 10.1002/ange.201712783).

Olympicenes are like the decathletes of nanoscale molecules. Their range of

potential applications includes sophisticated sensors, information and energy storage, solar cells and high-tech LEDs.

The first olympicene molecule was unveiled by British chemists in anticipation of the 2012 London Olympics. Until now, synthesising these unique structures was only possible through an arduous and intensive seven-step process based largely on chemistry dating back to the 1960s.

In the FSU team's new technique, an additional hexagonal ring of carbon atoms is fused to the zigzag edge of an existing carbon-rich molecule in two quick steps. Think plodding cross-country skier versus agile speed skater.

'Our success in developing this strategy allowed us to accomplish a two-step synthesis that is much shorter than the previously reported route, even though both methods used the same starting material', Alabugin said.

It is olympicene's relationship to graphene – a two-dimensional, single-layer lattice of carbon atoms – that may hold the most promise for these

recognisably shaped molecules. Graphene is a world-beating material with truly Olympian properties: it is an efficient conductor of electricity and heat, it is almost completely transparent and, at 200 times stronger than steel, it is the mightiest material ever tested.

Soon after olympicenes were successfully synthesised, researchers recognised the important connection they shared with graphene. Now, with their new strategy for accelerated olympicene synthesis, Alabugin and his team may have revealed a way to better facilitate the production of what some have dubbed a 'miracle material'.

'Our approach will allow chemists to synthesise a variety of olympicenes that can serve as stepping stones for the preparation of precisely shaped and functionalised graphene substructures', Alabugin said.

In honour of this year's Olympic Games, the team christened the product of their innovative synthesis strategy 'Ph-olympicene' – the 'P' reflecting both the phenyl group crucial to the synthesis of the molecule and a subtle nod to the host city PyeongChang.

Alabugin said he considers the timing of his team's discovery a rare, lucky moment of scientific serendipity.

'The exact timeline for designing, discovering and then having your findings peer reviewed is never certain', he said. 'Publishing this new synthesis of olympicene just in time for the Winter Olympics is indeed a fortunate coincidence.'

Florida State University

It is olympicene's relationship to graphene ... that may hold the most promise for these recognisably shaped molecules.

Problems with herbicide-resistant weeds become crystal clear

Herbicide-resistant weeds are threatening food security, but University of Queensland researchers are one step closer to a solution after a new discovery.

A UQ School of Chemistry and Molecular Biosciences study led by Associate Professor Luke Guddat uncovered how penoxsulam, the active ingredient in the world's largest-selling rice herbicide, works.

'Penoxsulam controls weeds such as key grass, broadleaf and sedge, and has become a focus of research due to an increased number of weeds that have developed resistance to herbicides', Guddat said.

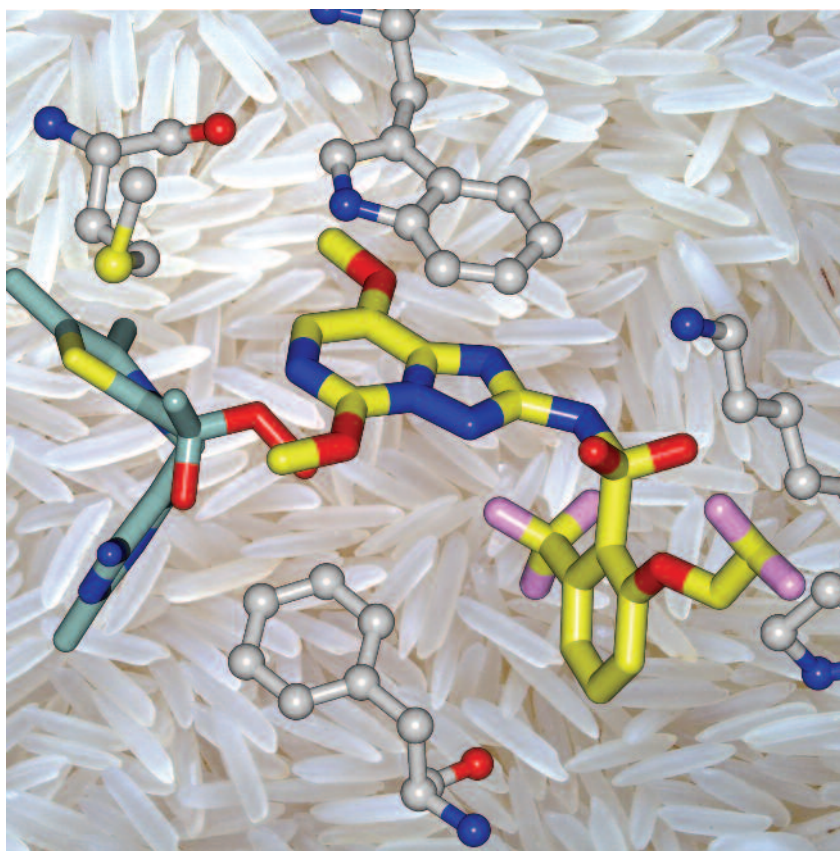
'Understanding how it works will assist in managing herbicide resistance not only for rice growers but also for wheat, turf and wine producers globally.

'These compounds have been shown to have extremely low levels of toxicity to the environment.'

The researchers hope the discovery will contribute to the design of the next generation of safe and commercially effective herbicides to counter the growing number of weeds becoming resistant.

Herbicide-resistant weeds result in lost income for the world's crop producers despite the \$30 billion they spend globally on herbicides each year, threatening food security.

The research conducted by Dr Thierry Lonhienne and PhD student Mario Garcia used crystallographic studies, which show



Penoxsulam, in yellow, binds to the surface of the enzyme (acetohydroxyacid synthase). Penoxsulam is a leading herbicide for crop protection, especially for rice (background) and wheat. Courtesy the research team

the precise structure of molecules at incredibly high resolutions, enabling them to capture the molecular mechanisms of the herbicide in action.

Guddat said the team discovered that penoxsulam combined with an enzyme in the weed and prevented it from carrying out its normal function – to produce amino acids.

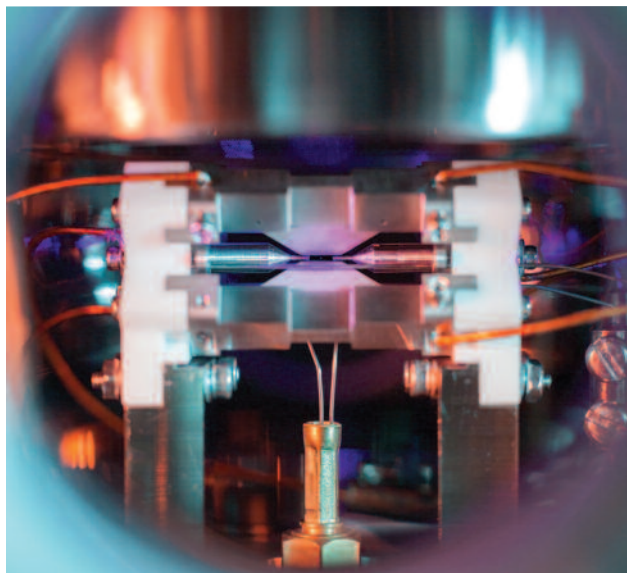
'Luckily, humans and other animals don't have that enzyme so penoxsulam compounds are relatively safe at the concentrations used in field applications.'

The study is published in *PNAS* (doi: 10.1073/pnas.1714392115).

University of Queensland

... penoxsulam combined with an enzyme in the weed and prevented it from carrying out its normal function – to produce amino acids.

Single trapped atom captures science photography competition's top prize



Single Atom in an Ion Trap. David Nadlinger – University of Oxford

An image of a single positively charged strontium atom, held near motionless by electric fields, has won the overall prize in a UK science photography competition, organised by the Engineering and Physical Sciences Research Council.

Single Atom in an Ion Trap, by David Nadlinger, from the University of Oxford, shows the atom held by the fields emanating from the metal electrodes surrounding it. The distance between the small needle tips is about two millimetres.

When illuminated by a laser of the right blue-violet colour, the atom absorbs and re-emits light particles sufficiently quickly for an ordinary camera to capture it in a long exposure photograph. The winning picture was taken through a window of the ultra-high vacuum chamber that houses the ion trap.

Laser-cooled atomic ions provide a pristine platform for exploring and harnessing the unique properties of quantum physics. They can serve as extremely accurate clocks and sensors or as building blocks for future quantum computers, which could tackle problems that stymie even today's largest supercomputers.

The image came first in the Equipment & Facilities category, as well as winning overall against many other stunning pictures, featuring research in action.

Nadlinger explained how the photograph came about: 'The idea of being able to see a single atom with the naked eye had struck me as a wonderfully direct and visceral bridge between the minuscule quantum world and our macroscopic reality. A back-of-the-envelope calculation showed the numbers to be on my side, and when I set off to the lab with camera and tripods one quiet Sunday afternoon, I was rewarded with this particular picture of a small, pale blue dot.'

Engineering and Physical Science Research Council (UK)

American Chemical Society releases 2018 advocacy agenda

The American Chemical Society (ACS) has released its 2018 advocacy agenda. The Society's highest priorities fall into four broad categories.

Support US innovation: ACS seeks public policies to ensure that federal investment in scientific research is predictable and sustained. A strong innovation ecosystem requires support and maintenance at all levels, including federal scientific investment and incentivising US corporate research and development, to guarantee long-term competitiveness.

Invest in US science education to empower students to be future innovators who can compete in the global economy: ACS advocates enhanced support for quality teacher training and creating opportunities for traditionally under-represented students to pursue graduate degrees in science, technology, engineering and mathematics (STEM) fields. The Society encourages policymakers to work toward bipartisan solutions to improve access to a multitude of STEM career pathways through new and innovative methods of workforce training and career preparation. The Society supports state efforts to strengthen STEM teacher training programs, invest in infrastructure improvements and prioritise rigorous hands-on science components in schools across the country.

Ensure scientific integrity and the role of science in the public policy arena: The government both supports the scientific enterprise and relies on scientific information to fulfil its obligations to serve the public. To ensure that accurate, reliable scientific information is available to all stakeholders, scientists must be able to contribute to the development and dissemination of scientific information without fear of reprisal for their work. ACS seeks public policies that sustain the role of expert peer review in evaluating scientific opportunities, protect scientists from political interference in the scientific process, and help government bodies obtain and integrate scientific assessments into policy development and implementation.

Advance science that benefits society: Some science-intensive issues rise to a level of particular importance due to their impact on human and environmental well-being. As a scientific society and leader on science policy issues, ACS advocates for solutions to complex issues on which it can offer specific expertise. Given the threat posed by climate change and the central role chemistry must play in addressing it, ACS seeks public policies that mitigate the impact of climate change and forestall its worst effects, enhance the ability to produce energy economically and efficiently and promote sustainability as a core component of the chemical enterprise.

American Chemical Society

Hidden details revealed in Picasso Blue Period painting

An international partnership of the Northwestern University/Art Institute of Chicago Center for Scientific Studies in the Arts (NU-ACCESS), the Art Gallery of Ontario (AGO) and the National Gallery of Art, Washington, has used multiple modes of light to uncover details hidden beneath the visible surface of Pablo Picasso's painting *La Miséreuse Accroupie* (The Crouching Woman), a major work from the artist's Blue Period.

The 1902 oil painting, owned by the AGO in Toronto, Canada, depicts a crouching and cloaked woman, painted in white, blues, greys and greens.

With knowledge of an underlying landscape revealed long ago by X-ray radiography, researchers used non-invasive portable imaging techniques, including infrared reflectance hyperspectral imaging and X-ray fluorescence imaging, to detail buried images connected to other works by Picasso as well as the presence of a landscape likely by another Barcelona painter underneath *La Miséreuse Accroupie*.

The researchers used non-invasive methods they adapted to the study of paintings. One finding was that Picasso painted over another painter's work after rotating it 90° to the right, using some of the landscape forms in his own final composition of *La Miséreuse Accroupie*. Picasso incorporated the lines of the cliff edges into the woman's back, for example.

AGO's conservation department had observed distinct textures and contrasting underlying colour that peaked through the crack lines and did not match the visible composition. X-ray radiography was the first non-invasive tool used to uncover hidden information in the painting; it revealed a horizontal landscape by a different unknown Barcelona painter under the visible surface.

John Delaney, senior imaging scientist at the National Gallery of Art, then studied the painting with infrared

reflectance hyperspectral imaging, which records underlying images depending on their relative transparency of the paint layers. He found that Picasso had made a major compositional change. The artist initially painted an arm and a disc under the surface of the painting. They were covered by her cloak in the final work. Delaney's imaging method provides improved visibility of earlier compositional painted elements.

For a more detailed understanding of the repositioned arm, NU-ACCESS scientists investigated the painting by using an X-ray fluorescence (XRF) scanner.

This system produces greyscale images showing the distribution of elements associated with various pigments of the painting. The scientists were able to analyse 70% of the painting in 24 hours. Together with micro-samples extracted from strategic locations, the XRF results, along with further images generated by Delaney from the hyperspectral reflectance, reveal the steps of creation taken by Picasso.

The iron- and chromium-based pigments of the surface layer correlated with the painting's current structure and its palette of mostly blues (painted with the iron-based Prussian blue and with ultramarine, Picasso's Blue Period blue of choice) and yellow-greens (painted with chromium-based yellows). The elemental maps of cadmium- and lead-based pigments, however, revealed the presence of the woman's right arm and hand beneath the visible surface.

The imaging techniques have allowed Kenneth Brummel, the AGO's assistant curator of modern art, to better understand Picasso's style, influences and process.

'When we saw the rendering of the lead elemental map, it became clear to me that the arm hidden under the visible surface of *La Miséreuse Accroupie* is the same as the proper right arm of a crouching woman in a Picasso watercolour recently sold at auction',



Pablo Picasso. *La Miséreuse Accroupie*, 1902. Oil on canvas, 101.3 × 66 cm (39 7/8 × 26 in.). Art Gallery of Ontario. Anonymous gift, 1963. © Picasso Estate

Brummel said. The watercolour is titled *Femme Assise* (1902).

Images generated by Delaney – by selecting different bandwidths in the near infrared – confirmed the relationship between *La Miséreuse Accroupie* and the watercolour.

'After seeing the lead map from the XRF scanning, we were able to make a map of pigment lead white, which, when overlaid with the false colour infrared, gives a more complete image of an upstretched arm, sleeve, disc and fingers', Delaney said.

'We now are able to develop a chronology within the painting structure to tell a story about the artist's developing style and possible influences', said Sandra Webster-Cook, AGO's senior conservator of paintings.

Northwestern University

Digital technologies in chemical plant operations fuelling further investments

Digital adoption is increasing in chemical companies' plants as more firms recognise the technologies' financial and operational value, according to Accenture's new Digital Technology in Chemical Plant Operations survey. Yet, digital technologies are still in the early stages of deployment on the plant floor.

The survey of 360 chemical executives from 12 countries revealed 80% of respondents are investing more, or significantly more, in digital technologies for their plant environments, and 85% expect overall digital investment to increase in the next three years. Moreover, 92% of chemical executives are satisfied with the benefits received from their digital investments, with effective plant management the top cited benefit, followed by improved product quality.

An overwhelming number of respondents (95%) are also seeing the tangible financial value of using digital in their operations. Just under one-third (31%) saw an operating profit improvement in production/manufacturing operations of 10–20%, with an additional 20% seeing gains of 20–40%. This is supported by Accenture's recent research that showed that combining technologies such as augmented reality/virtual reality, autonomous vehicles, big data analytics and digital twin to increase operational efficiency could realise initial savings of more than US\$90 000 per chemical company employee.

Although many chemical companies have started pilot programs across their operations, full deployment of digital technologies remains limited. Even for technologies where executives see more widespread adoption, including cloud, robotics, artificial intelligence, mobility/wearables and cybersecurity, less than one-third of respondents cited using each technology broadly.

When it comes to pilot programs, analytics is the technology in which chemical companies are investing most often, cited by 43% of respondents. Just under half (46%) listed analytics in their top three digital investment areas over the next three years, as it provides a way to drive more value from the large amounts of generated data.

'In the chemical industry, there is a growing understanding of the potential for the digital reinvention of industry – or Industry X.0 – where businesses use advanced digital technologies to transform their core operations, worker and customer experiences and business models', said Tracey Countryman, managing director and lead for Industry X.0, Accenture Resources. 'By harnessing this reinvention, chemical companies can release value trapped in the enterprise not only by realising efficiencies through smart connected assets, but also through new digitally enabled sources of revenue.'

Meanwhile, chemical firms' plant operations are becoming increasingly connected, leaving them open to the growing threat of cyberattacks. In the past 12 months, 73% of respondents had more than 30 attempted breaches of their plant operations, 54% suggested more than 30 attacks were successful, and 50% indicated it took days, weeks or even months to detect them.



Yet, faced with this challenge, chemical companies' abilities to identify, handle and respond to the threats are severely lacking. Currently, only 42% can manage the financial risk due to a cybersecurity event targeting their plant operations, or minimise the disruption. Even less (39%) can identify the cause of a breach, and only 33% are able to monitor for breaches.

The repercussions of successful cyberattacks could be considerable. 'Commercial consequences' was cited as the top cybersecurity risk to plant operations by 16% of respondents. This encompasses production loss and breach of customer supply contracts, which demonstrates that successful cyberattacks could have a serious impact on profits. Environment, health and safety (15%) and operational reliability (14%) risks were ranked second and third, respectively. The former suggests cyberattacks on plant operations could present a threat to the security and health of employees and the wider public.

'Chemical companies must invest urgently to bolster cybersecurity resilience and response capabilities for their industrial operations', said Robert Boyce, managing director and cybersecurity lead, Chemicals & Natural Resources, Accenture. 'As chemical plants typically have legacy operational technology systems, the technology across sites is not standardised and there are gaps in their security controls, leaving them exposed. Agile and adaptive capabilities are needed that can effectively react to and intervene with cyber threats to protect industrial operations.'

Accenture conducted an online survey of 360 C-level and top international management executives and functional leaders in the chemical industry. The survey focused on chemical companies with a total annual revenue ranging from US\$500 million to more than US\$20 billion that are currently leveraging digital technology in their core operations.

Accenture



Phosphorus pollution dangerously high in global fresh water

Human-driven phosphorus pollution is reaching dangerously high levels in freshwater basins around the world, according to a study looking at agricultural activity. The researchers estimated the global amount of phosphorus entering freshwater bodies between 2002 and 2010 from human activity as 1.47 teragrams. China contributed 30% of the phosphorus, followed by India (8%) and the US (7%). Less-populated regions like Australia have smaller phosphorus use but less fresh water to accommodate pollution, the authors say.

The study is published in *Water Resources Research* (doi: 10.1002/2017WR020448).

Phosphorus is a common component of mineral and manure fertilisers because it boosts crop yields. However, a large portion of phosphorus applied as fertiliser is not taken up by plants, and either builds up in the soil or washes into rivers, lakes and coastal seas, according to the study's authors.

The study also assessed whether human activity had surpassed the Earth's ability to dilute and assimilate excess levels of phosphorus in freshwater

bodies. The authors found phosphorus load exceeded the assimilation capacity of freshwater bodies in 38% of Earth's land surface, an area housing 90% of the global human population.

Phosphorus pollution leads to eutrophication, which causes algal blooms, which can lead to the mortality of fish and plants due to lack of oxygen and light.

The authors gathered data on how much fertiliser is applied per crop in each country, and estimated domestic and industrial phosphorus production by looking at protein consumption per capita per country.

The largest contribution to the global phosphorus load came from domestic sewage (54%), agriculture (38%) and industry (8%). The phosphorus load from agriculture grew by 27% over the study period, from 525 gigagrams in 2002 to 666 gigagrams in 2010.

The study also estimated the water pollution level of Earth's major river basins by comparing the amount of fresh water needed to dilute the excess phosphorus to an allowable concentration compared to the basin's actual river run-off. If a freshwater basin

An algal bloom caused by eutrophication.
Wikicommons/F. Iamiot/CC BY-SA 2.5

has a water pollution level above one, water quality standards are being violated and the basin is receiving more phosphorus pollution than it can assimilate.

The results show freshwater basins with a water pollution level above one cover 38% of Earth's land surface, excluding Antarctica. These basins often pertain to densely populated areas or regions with intensive agriculture, according to the authors.

The most severely polluted freshwater areas include the Aral drainage basin, the Huang-He (Yellow) river in China, the Indus and Ganges rivers in India and the Danube river in Europe.

Less-populated regions such as Australia and northern Africa also suffer from high water pollution levels, according to the study. These regions have smaller phosphorus loads than areas such as China and Europe, but they have much less water available to accommodate their excess phosphorus.

University of Nebraska and National University of Singapore

Uranium potential in bulk chemical production

Uranium can perform reactions that previously no one thought possible, which could transform the way industry makes bulk chemicals, polymers and the precursors to new drugs and plastics.

Writing in *Nature Communications* (doi: 10.1038/s41467-017-01363-0), the chemists from the University of Manchester, UK, have determined that uranium can perform reactions that used to be the preserve of transition metals such as rhodium and palladium. And because uranium sits between different types of reactivity of lanthanides and transition metals, it might be able to combine the best of both to give new ways of producing materials and chemicals.

This discovery is also profiled in a new video ([youtube.com/watch?v=3m3CbQct0pM](https://www.youtube.com/watch?v=3m3CbQct0pM)) produced by the School of Chemistry.

The latest discovery means that industry might now be in a position to develop new compounds that can't be made in any other way.

What's more, uranium is one of the elements we know the least about and while it is associated with nuclear weapons and nuclear power, the new discovery suggests other uses.

Professor Steve Liddle, author of the paper, said: 'This discovery will lead to some monumental developments that could change the way we live. Development work like this really could pave the way for new medicines and also the creation of truly biodegradable hard plastic.'

'It is comparable to the discovery of liquid crystal displays, which happened 20 years before everyone sat up and realised that they could be used in modern computer displays and TVs.'

University of Manchester

Next-generation semiconductors

A team of scientists at Technische Universität Dresden, Germany, have used the SuperMUC supercomputer at the Leibniz Supercomputing Centre to refine its method for studying organic semiconductors. The team uses semiconductor doping to introduce impurities into a material to give it specific semiconducting properties. The results are published in *Nature Materials* (doi: 10.1038/s41563-018-0030-8).

'New kinds of semiconductors, organic semiconductors, are starting to get used in new device concepts', said team leader Dr Frank Ortmann. 'Some of these are already on the market, but some are still limited by their inefficiency. We are researching doping mechanisms to understand these semiconductors' limitations and respective efficiencies.'

Small changes in material make-up can lead to big changes in a material's characteristics. Conversely, the underlying forces are generally weak and short-range, so researchers have to accurately compute atomic and molecular interactions as well as the densities of electrons and how they are transferred among molecules.

Introducing specific atoms or molecules to a material can change its conducting properties on a hyperlocal level. This allows a transistor made from doped material to serve a variety of roles in electronics, including routing currents to perform operations based on complex circuits or amplifying current to help produce sound in a guitar amplifier or radio.

The team used density functional theory to efficiently predict the variety of complex atomic interactions.

'Electrical conductivity can come from many dopants and is a property that emerges on a much larger length scale than just interatomic forces', Ortmann said. 'Simulating this process needs more sophisticated transport models, which can only be implemented on high-performance computing architectures.'

To test its computational approach, the team simulated materials that already had good experimental datasets as well as industrial applications. The researchers first focused on C₆₀ (buckminsterfullerene). In addition, the researchers simulated zinc phthalocyanine, another molecule used in photovoltaics, but with a flat shape and a metallic atom (zinc).

As its dopant the team first used the well-studied molecule 2-Cyc-DMBI (2-cyclohexyldimethylbenzimidazole). 2-Cyc-DMBI is considered an n-dopant, meaning that it can provide its surplus electrons to the semiconductor to increase its conductivity. N-Dopants are relatively rare, as few molecules are 'willing' to give away an electron. In most cases, molecules that do so become unstable and degrade during chemical reactions, which in this context can lead to an electronic device failure. 2-Cyc-DMBI dopants are the exception because they can be sufficiently weakly attractive for electrons – allowing them to move over long distances – while also remaining stable after donating them.

The team got good agreement between its simulations and experimental observations of the same molecule-dopant interactions. This indicates that they can rely on simulation to guide predictions as they relate to the doping process of semiconductors. They are now working on more complex molecules and dopants by using the same methods.

Gauss Centre for Supercomputing

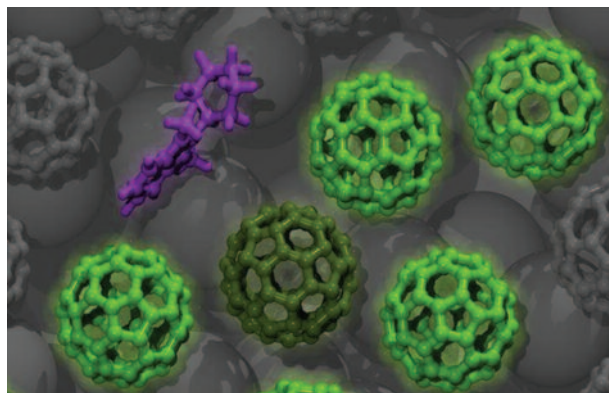


Illustration of a doped organic semiconductor based on fullerene C₆₀ molecules (green). The benzimidazole dopant (purple) donates an electron to the C₆₀ molecules in its surrounding (dark green). These electrons can then propagate through the semiconductor material (light green). S. Hutsch/F. Ortmann, TU Dresden

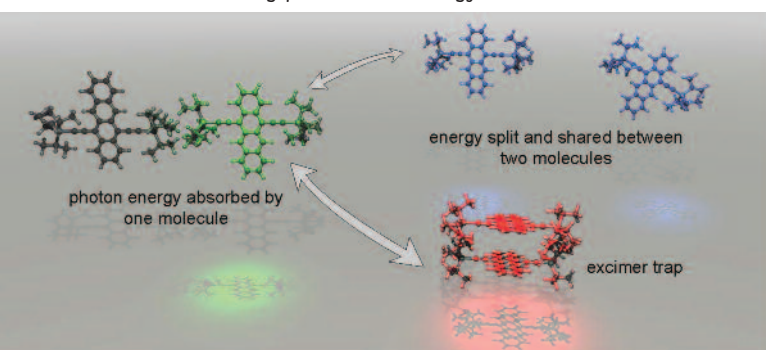
Pathway opens to minimise waste in solar energy capture

Researchers at the ARC Centre of Excellence in Exciton Science have made an important discovery with significant implications for the future of solar cell material design that could help push solar efficiency beyond 30%.

The team, led by Professor Timothy Schmidt at the University of New South Wales, has been looking at ways to capture the energy of visible light that is currently wasted because of the limitations of silicon, which can only access approximately 25% of the solar spectrum. To illustrate, silicon on its own can only use about half the energy of green light, which is the peak of the solar spectrum in terms of energy availability.

One of the ways to reduce this waste is by designing materials that can be coated on top of silicon to capture some of the energy of light that silicon cannot. By incorporating singlet exciton fission, a process that generates two excitons from a single photon, it is hoped that silicon solar cell efficiencies can be boosted beyond 30%.

The work, published in *Nature Chemistry* (doi: 10.1038/nchem.2926), examines the role of a short-lived (about eight billionths of a second), excited molecular complex called an excimer in singlet exciton fission and overturns previous thinking by demonstrating that these singlet fission materials must avoid excimer formation to reach full potential in enhancing photovoltaic energy conversion.



Photon energy splitting is done directly by two molecules, not via an excimer state.

Schmidt explained, 'As we look to find ways to bring down the cost of solar energy harvesting, we should be designing materials that avoid excimer formation.'

Their result suggests that what had previously been considered as an intermediate in the fission process may in fact be a source of loss. With this understanding Schmidt et al. propose an important new direction in our search for materials that enable higher efficiency solar cells,' said Professor Marc Baldo, member of the Centre's International Scientific Advisory Committee and Director of the Center of Excitonics at MIT, Massachusetts, USA.

ARC Centre of Excellence in Exciton Science

New Eclipse peptide synthesiser

Eclipse™ is a smart new peptide synthesiser providing the peptide chemist and user, for the first time, software that analyses any sequence no matter how difficult and provides a protocol. Eclipse™ presents the user with a synthesis strategy in an easy to interpret graphical display. Our exclusive Smart Synthesis software is based on an algorithm compiled from AAPPTec's 35 years of experience synthesising difficult peptides.

The Eclipse™ is the research scale peptide synthesiser used by novices and experts alike.

The Eclipse™ Smart Synthesis software will automatically generate and carry out the synthesis protocol without additional input. Experienced peptide researchers can create custom protocols, including double and single couplings, longer or shorter reaction times or variable temperatures. They can change the number of washes

or even utilise different coupling chemistry for each amino acid. While the instrument is running, one can change the protocol without interruption or set up the next synthesis.

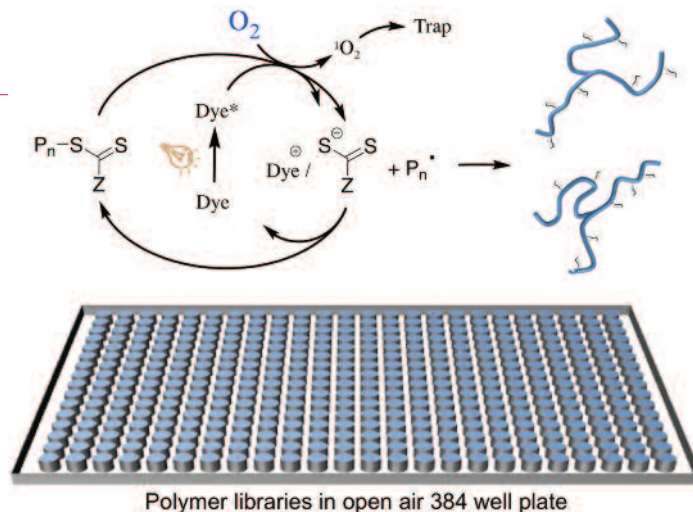
The Eclipse™ was developed to automatically provide synthesis protocol and efficient peptide synthesis without additional user input. The Eclipse™ Smart Synthesis software evaluates the peptide sequence and generates a graphical report of the expected difficulty of each amino acid. It predicts when double coupling would be required, thus improving synthesis efficiency. The algorithm also predicts when and where to modify the chemistry either by double coupling, substituting pseudo proline dipeptides, Dmb protected dipeptides or amino acid, double coupling and extended de-protection etc. Thus, these modifications improve synthesis efficiency and increase the quality of crude peptide by reducing the side products. The algorithm also suggests that the use of different chemistries shows a great increase in yield and superior crude peptide.

For further information, email info@scientex.com.au or visit www.scientex.com.au.



Radical polymerisation in air

Two decades ago, controlled radical polymerisation (CRP) techniques revolutionised the ability to make well-defined polymers with complex architectures. Unfortunately, the sensitivity of CRP techniques to oxygen makes the high-throughput synthesis of structurally diverse polymers challenging, particularly when working at low volumes and high dilutions. This limits the ability to probe the relationship between a polymer's structure and its biological properties. Now the Boyer and Chapman groups at the University of New South Wales, in collaboration with researchers at Rutgers University, USA, have developed an oxygen-tolerant photoinduced electron transfer reversible addition–fragmentation chain-transfer (PET-RAFT) polymerisation that is unaffected by the presence of air (Gormley A.J., Yeow J., Ng G., Conway Ó., Boyer C., Chapman R., *Angew. Chem. Int. Ed.* 2018, **57**, 1557–62). The system enables high-throughput synthesis of bioactive polymers with excellent control and high conversions at low volumes

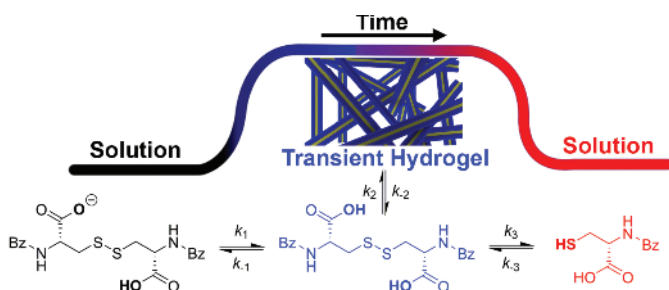


Polymer libraries in open air 384 well plate

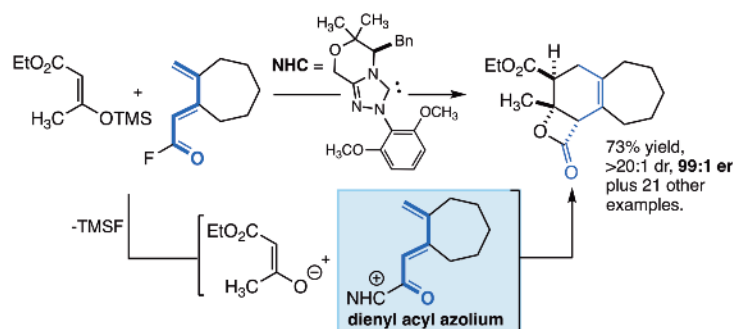
(40 μL) and monomer concentrations (0.5 M). This method was used to build polymer libraries and to investigate the effect of glycopolymer architecture on their binding affinity to lectin proteins. It is expected that a similar approach could be used to investigate structure–activity relationships for a wide range of polymer–protein interactions and to improve the design of bioactive macromolecules.

Transient programmable self-assembly

Tubulin and many other self-assembled structures in nature are transient non-equilibrium structures that use some of the free energy provided to form them to perform mechanical work. The synthesis of such a bioinspired transient system based on small molecules has recently been achieved with the development of a transient supramolecular gel by the Thordarson group at the University of New South Wales (Wojciechowski J.P., Martin A.D., Thordarson P. *J. Am. Chem. Soc.* 2018, **140**, 2869–74). The new transient hydrogel system uses orthogonal methods for activation and deactivation, namely the competition between the gelation of the oxidised cystine form of the *N,N'*-dibenzoyl-L-cystine (DBC) gelator and its reduction to the soluble cysteine by a chemical reducing agent, tri(2-carboxyethyl)phosphine (TCEP). Detailed kinetic analysis of the system allowed the researchers to program the lifetime of the gels with good accuracy down to 15 minutes. Furthermore, the team could generate multiple transient hydrogel cycles (sol↔gel oscillations) simply by periodically adding more of the DBC gelator to a TCEP 'bath'. The general concept of this work is applicable not only to redox-active systems but to systems responsive to other stimuli, which should aid the design of next-generation spatiotemporal hydrogel materials.



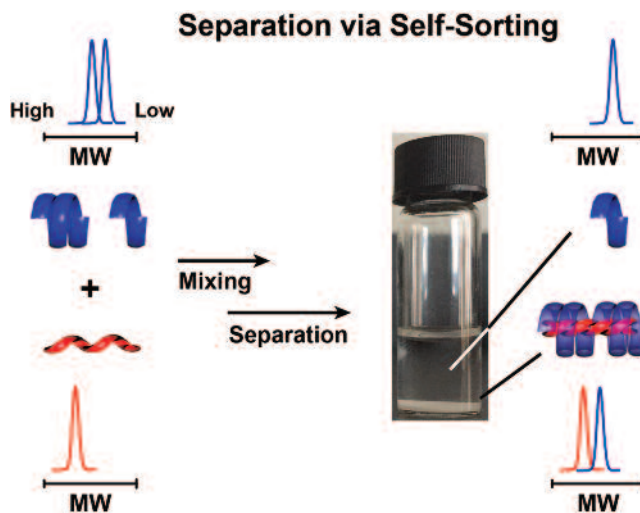
Diene to do a (4 + 2)



Central to many *N*-heterocyclic carbene-catalysed transformations is the α,β-unsaturated acyl azolium. In contrast, the dienylyl acyl azolium has received little attention, with only one reaction reporting its involvement to date. Recently, studies by Rachel Gillard, Jared Fernando and David Lupton at Monash University have led to the discovery of the first enantioselective reaction using the dienylyl acyl azolium as a key intermediate (Gillard R.M., Fernando J.E.M., Lupton D.W. *Angew. Chem. Int. Ed.* <https://doi.org/10.1002/anie.201712604>). The reaction exploits readily accessible acyl fluorides and trimethylsilyl enol ethers to give rise to densely functionalised β-lactone products. In most cases, excellent diastereo- and enantio-selectivity was observed (most >20:1 d.r., most >97:3 e.r.). In addition, the tetracyclic products are reminiscent of natural products yonanolide and scabrolide. Thus, the reaction can potentially be exploited in target synthesis.

Triple-helix self-sorting separations

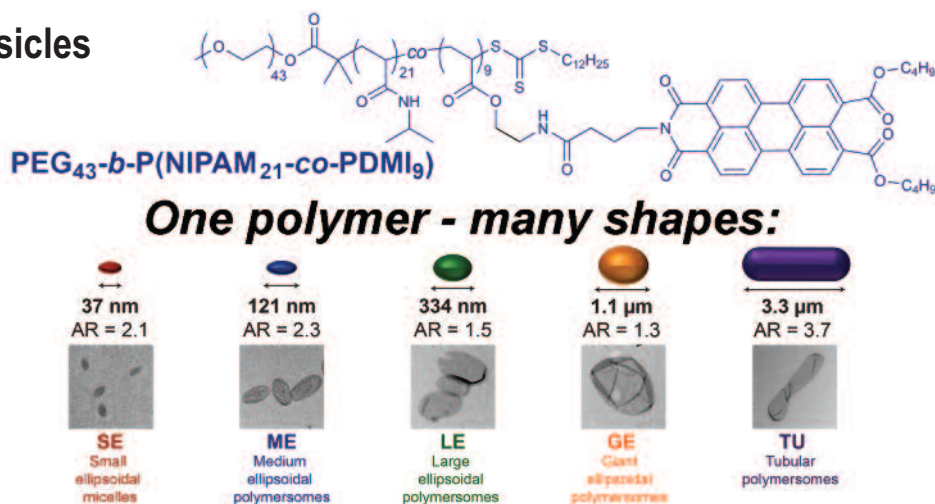
The triplex-helix conformation formed by self-assembly of complementary stereoregular poly(methyl methacrylate) strands is a striking synthetic analogue of the double-helix structure of DNA. The groups of Greg Qiao at the University of Melbourne and Craig Hawker at the University of California, Santa Barbara, USA, have recently shed new light on the synthetic helical stereocomplexes formed from oligomeric methyl methacrylate (OMMA) (Ren J.M., Lawrence J., Knight A.S., Abdilla A., Zerdan R.B., Levi A.E., Oschmann B., Gutekunst W.R., Lee S.-H., Li Y., McGrath A.J., Bates C.M., Qiao G.G., Hawker C.J. *J. Am. Chem. Soc.* 2018, **140**, 1945–51). The precise synthesis and isolation of near-discrete stereoregular oligomers allowed the researchers to empirically determine the minimum chain length required for triple-helix formation. Remarkably, they also observed competitive binding between complementary OMMA of different chain lengths – a ‘self-sorting’ phenomenon that proved effective for separating polymer mixtures through stereocomplex formation. This finding further strengthens the analogy with DNA, for which self-sorting is prevalent between



different strand lengths and sequences, yielding more thermodynamically stable supramolecular helices. The specificity of the interactions observed in this work holds promise for the development of novel bio-inspired nanotechnologies with increased versatility and functionality.

Tuneable non-spherical vesicles

Very little in nature is perfectly spherical. Most biological structures, such as cells, bacteria and viruses, come in a variety of shapes, including tubes, rods, squashed spheres, or ellipsoids. But it has proven difficult for scientists to synthesise particles that are not perfectly round. A collaboration between the Thordarson and Stenzel groups at the University of New South Wales has led to a breakthrough in the ability to make non-spherical polymersomes – artificial vesicles – with tuneable and predictable structures (Wong C.K., Mason A.F., Stenzel M.H., Thordarson P. *Nat. Commun.* 2017, **8**, 1240). In a break from previous work in this field, the team achieved this significant advance using a single block-copolymer, poly(ethylene glycol)-*b*-poly(*N*-isopropylacrylamide-*co*-perylene diester monoimide) (PEG₄₃-*b*-P(NIPAM₂₁-*co*-PDMI₉)) and by

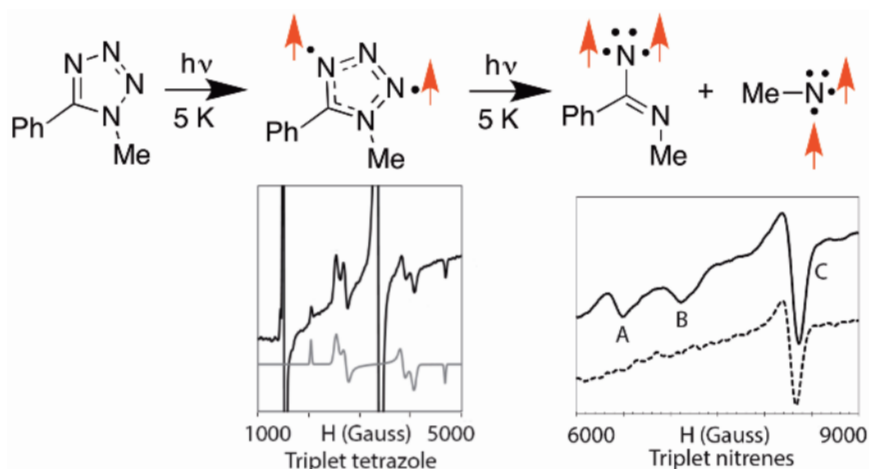


simply varying the polymer concentration when triggering self-assembly in going from an organic solvent to water. This approach takes advantage of the dual directional and hydrophobic nature of aromatic (π - π) interactions between the perylene units on the polymer side-chains, allowing the size and shape of

the structures formed to be programmed and fine-tuned. This elegant solution to making non-spherical structures has potential implications for the development of nanoparticles for medical applications and complex ‘lifelike’ structures for use in systems chemistry.

Glimpsing reactive intermediates

Nitrenes (R–N) are important reactive intermediates in numerous chemical transformations. Imidoynitrenes R–C(=NR′)–N have been postulated frequently as intermediates in syntheses of benzimidazoles and carbodiimides, but direct evidence for their existence has been lacking. Now, Curt Wentrup of the University of Queensland and Manabu Abe of Hiroshima University, Japan, have generated and observed the first imidoynitrene, PhC(=NMe)–N in its triplet ground state, by photolysis of 5-phenyl-1-methyltetrazole at 5 K and have investigated it by electron spin resonance (ESR) spectroscopy (Abe M., Bégué D., Santos-Silva H., Dargelos A., Wentrup C. *Angew. Chem. Int. Ed.* 2018, **57**, 3212–16). Previous attempts to observe such nitrenes had failed because the singlet states undergo rearrangement to carbodiimides or cyclisation to 1*H*-diazirines with very low activation



barriers, thus escaping detection. In contrast, photolysis of tetrazoles at 5 K immediately generates their triplet excited states, which could be observed directly by ESR spectroscopy in this work. Further photolysis at 5 K caused loss of N₂ with formation of the imidoynitrene directly in its triplet state. Alternative

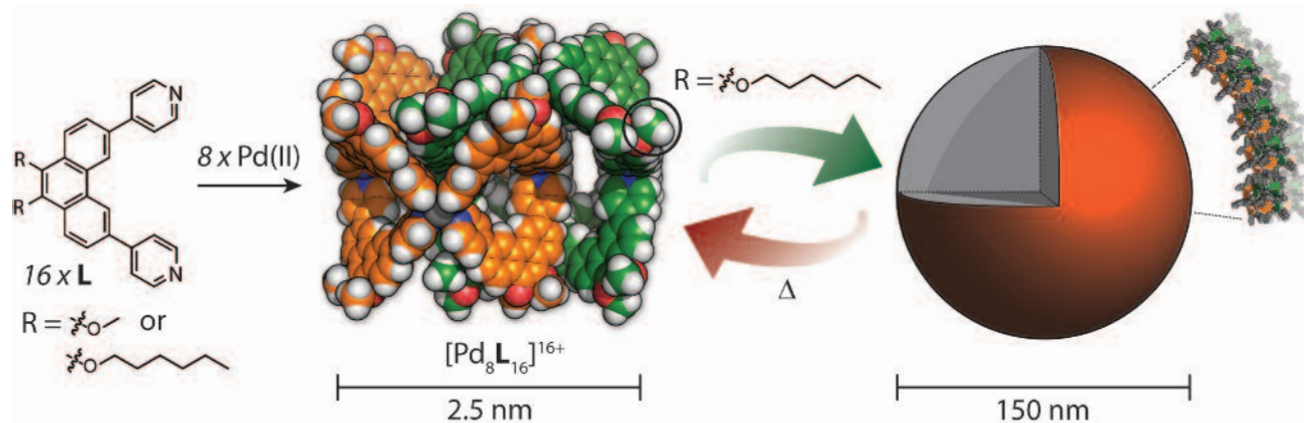
fragmentation of the tetrazole yielded benzonitrile and triplet methylnitrene, Me–N. The potential energy surface including all the reactive intermediates was evaluated computationally by Didier Bégué and co-workers at the Université de Pau et des Pays de l'Adour, France.

Hierarchical aggregates from interlocked molecules

Traditionally, research on interlocked molecules has focused on exploring the dynamic properties that are introduced by their mechanical bond. From a structural viewpoint, however, their densely packed architecture is also an interesting feature that offers a unique platform to examine functionalisation and supramolecular aggregation. Recently, a team led by Witold Bloch at the University of Adelaide and Guido Clever at TU Dortmund, Germany, reported the synthesis of a novel

24-component catenane that spontaneously self-assembles into large vesicle-like aggregates (Bloch W.M., Holstein J.J., Dittrich B., Hiller W., Clever G.H. *Angew. Chem. Int. Ed.* 2018, <https://doi.org/10.1002/anie.201800490>). The Pd₈L₁₆ [2]catenane is composed of two interlocking Pd₄L₈ barrel-shaped containers, whose assembly is facilitated by the presence of nitrate counter-ions. When functionalised with hexyloxy chains, the interlocked molecule can

spontaneously self-assemble into a colloid of vesicle-like aggregates measuring 150 nm in diameter. The hierarchical aggregation is facilitated by the dense hydrophobic interactions between catenane molecules and can be completely reversed by applying a heat stimulus. This research delivers new knowledge on interlocked structures and opens up the possibility of using their hierarchical aggregates as molecular delivery and release vessels.



Compiled by David Huang MRACI CChem (david.huang@adelaide.edu.au). This section showcases the very best research carried out primarily in Australia. RACI members whose recent work has been published in high impact journals (e.g. *Nature*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.

Project Deal, or collective bargaining?

In between bouts of procrastinating over ARC Discovery Grant writing, we read about the German initiative known as Projekt Deal (www.projekt-deal.de/about-deal), in *Chemistry World* (2018, vol. 15(2), p. 12) the Royal Society of Chemistry's excellent magazine.

It tells the story of a consortium of German universities and research institutes that have cancelled their subscriptions to Elsevier journals. The push has come from Germany's National academy of Sciences, the Fraunhofer Society and the German Research Foundation who all want publicly funded German research to be open access in that country. The article suggests that paying costs only at the time of publication would substantially lower the subscription fees to the institutions. Intriguingly, German researchers are resigning from editorships and journal advisory boards to protest the move. Dare we say it, it would seem that collective action is bearing fruit because Elsevier has declined to act by restricting access to their collections.

The consortium wants a Publish and Read model where all articles from the participating institutions would be open access on being published (the Publish component) and then all the participants allowed perpetual electronic access to the publisher's collections (the Read component). Elsevier would then get an appropriate price determined by a formula that takes into account articles published and the cost of processing the articles, paid annually. And any German academic institution can participate. The publisher responded: 'paying for German-authored articles to be open access doesn't cover the cost for access to papers from the rest of the world' (bit.ly/2FB0AjB).

It appears that coalitions of like-minded institutions in the Netherlands, Finland and Austria and the UK are trying to achieve similar consideration in their own countries. According to a media report (bit.ly/2vho7P1), SpringerNature and Wiley are much more amenable to the idea. The same report puts the

collective cost to the world's libraries at some \$11.9 billion in subscriptions. Sounds like academic publishing is a very lucrative business as a large proportion of libraries' budgets go to these three publishers.

Academic publishing for profit is a lucrative business! It's worth noting that researchers do the research, write the paper and then sign the rights over to the publisher for no financial recompense. When you throw in that the majority of this research is paid for by the public purse, then it seems a farce. A fit plot line for an upcoming episode of *Yes, Vice Chancellor!* While we appreciate that costs are incurred by the publisher, there are reports of large profit margins (bit.ly/2vho7P1). Also, don't forget all the free reviewing work that we put in; one wonders whether if we charged for this, it might become financially more sustainable to do research. It's clear that a journal's worth is judged by the quality of work published in it as determined by the peer review process.

Conversations among colleagues over the years have revolved around only using society publishers, but this often is rebutted by reference to performance assessment exercises that require us to publish in high-impact journals. If journals are accessible to all, then the quality and impact of the work will be the only determinant of citations.

The question is can we the workers in universities and libraries adopt Project Fair Go and tackle the publishers who are making obscene profits from the fruits of our labour and public funds. A question to be resolved at the coalface is how would it work at individual universities; would they use their library budgets to pay for the open access or street it back to the researcher? Is our market big enough to influence Wiley, Elsevier and SpringerNature? Why don't we give it a go and find out?

George Koutsantonis FRACI CChem and John D. Wade FRACI CChem Co-Editors-in-Chief, *Australian Journal of Chemistry*

Our 2018 media kit is now available at chemaust.raci.org.au.

For further information, contact Mary Pappa:
mary.pappa@raci.org.au,
(03) 9328 2033



Bog bodies

Still here in the hereafter

Bog bodies such as Tollund Man provide a fascinating insight into biochemical action below the ground.

BY **DAVE SAMMUT** AND
CHANTELLE CRAIG



On 13 May 1983, the partially preserved head of a woman was discovered buried in peat at Lindow Moss, near Wilmslow in Cheshire, England. Police suspected a local man, Peter Reyn-Bardt, whose wife had gone missing two decades before. 'It has been so long, I thought I would never be found out', confessed Reyn-Bardt under questioning. He explained how he had murdered his wife, dismembered her body and buried the pieces near the peat bog.

Before the case could go to trial, carbon dating of the remains showed that the skull was around 17 centuries old. Reyn-Bardt tried to revoke his confession, but was convicted and sentenced to life imprisonment.

Lindow Woman and other 'bog bodies', as they have come to be known, are surprisingly common. Under just the right set of natural conditions, human remains can be exceptionally well preserved for extraordinarily long periods of time.

When bog water beats bacteria

Records of bog bodies go back as far as the 17th century, with a body discovered at Shalkholz Fen in Holstein, Germany. Bog bodies are most commonly found in northwestern Europe – Denmark, the Netherlands, Ireland, Great Britain and northern Germany. The oldest specimen recorded, Koelbjerg Man (Syddanmark, Denmark), has been dated to around 8000 BCE, during the Mesolithic period. The oldest fleshed body is that of Cashel Man (County Laois, Ireland), dating to around 2000 BCE during the Bronze Age.

The best-preserved specimens are found in colder bogs, particularly those closer to salt water. Until the 19th century, they were mostly reburied in Christian burials, but as science developed so did the study of this remarkable phenomenon. We now know that to be preserved, a body at the time of death must be in a bog when the water temperature is less than 4°C, and ideally in a sphagnum bog that has an average annual temperature of less than 10°C.

At these temperatures, oxidation conditions and pH, the immediate bacterial action causing putrefaction is retarded, giving time for the bog waters to infiltrate the body.

Bog waters are very rich in humic acids and very low in mineral content. Sphagnum mosses, particularly *Sphagnum chamaedaphne*, have negatively charged cell surfaces. They tend to take in cations, replacing them with acid, to reach pH levels as low as 3.3–4.5. Sugary substances released by dying moss cells then tan the tissues to form a type of leather. The skin turns brown, and the hair red.

The highly porous sphagnum cells absorb a lot of water, up to 90% of their mass, and with the accumulation of dead cell matter they quickly form substantially anaerobic environments, even within 30–50 millimetres of the exposed surface. Provided that the rate of evaporation is less than the rainfall (so that the bog stays wet), then these



Bogs of sphagnum moss have ideal conditions for the preservation of bodies. Wikimol/CC-BY-SA-3.0

bogs can form the ideal conditions for the preservation of tissue over long periods of time.

Something rotten in the state of Denmark

Perhaps the most famous and best-studied bog body, Tollund Man (see opposite and cover images), was found in 1950 on Denmark's Jutland Peninsula. He died some time in the fourth century BCE, yet his face could almost be that of a man asleep, still with a three-day growth of stubble on his chin.

Tollund Man was found wearing a belt but no clothes. That's either an odd fashion choice, or an indication that the clothes themselves rotted away over the ages. This is common to the bog bodies catalogued, with most of them found either naked or wearing only head gear.

Teams of scientists and doctors have examined the remains of Tollund Man, taking approximately 16 000 CT-scan images, plus X-rays, IR and UV images and endoscopic investigation.

The structures in his head – brain, tongue, larynx – are remarkably intact because specific efforts have been made by scientists to further preserve them.

The key task in preserving the tissues was to replace the bog water initially occupying space in the cells. To achieve this, the head was placed in ethanol, then toluol, then liquid paraffin at 83°C. Bees' wax, with similar properties to paraffin, is known to be non-perishable, with Viking-era samples having been preserved this way for more than 1000 years underground.

The best-preserved specimens are found in colder bogs, particularly those closer to salt water.

Without similar efforts at preservation, the remainder of Tollund Man's body deteriorated rapidly after exposure to air. Now entirely dry, it is little more than a skeleton.

Tollund Man's hair has been examined by Professor Karin Margarita Frei of the National Museum of Denmark, together with that of Haraldskjaer Woman (fifth century BCE, found in 1835 near Jutland,

Denmark) and Huldremose Woman (second century BCE, found in 1879 near Huldremose, Denmark). Using studies of trace strontium-86 and -87, Frei was able to prove that both of the women had travelled substantial distances over their last few years of life.

Results for Tollund Man were inconclusive. With only 2–3 centimetres of hair, as compared to around

50 centimetres for the two women, there was much less history to work with. Because of the slow rate at which hair grows, Frei was able to use it as a record of the environmental strontium at the time of growth. Comparing the isotope levels and ratios to known geographical and time-based data gives meaningful information about a person's movements during the 2–3 years before death.

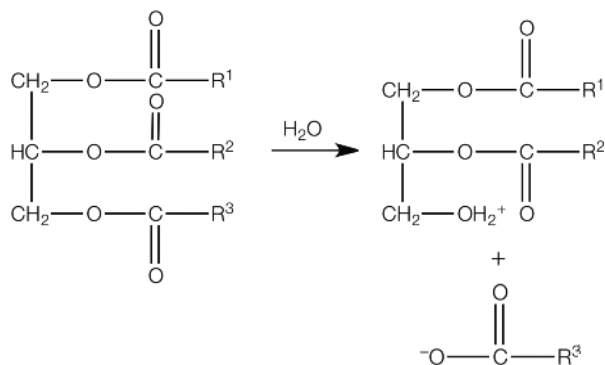
The messy stuff

When I was asked to write an article about human decomposition chemistry, I was a little concerned about the depths of my ignorance in biochemistry. But then I thought 'Surely I can dig something up'. As it turns out, the chemistry of human decomposition is complex, messy and super-gross.

The human body is composed of approximately 64% water, 20% protein, 10% fat, 1% carbohydrate and 5% minerals. Once the blood stops flowing, oxygenation of the tissues ceases, and cell reaction products – particularly CO_2 and H_2O – start to accumulate. These combine to form carbonic acid, which in combination with existing digestive enzymes spontaneously starts to degrade the complex macromolecules (particularly proteins and lipids) via a process called autolysis.

In combination with autolysis, the body rapidly passes through the first four stages of death (pallor mortis, algor mortis, rigor mortis and livor mortis) to putrefaction, which is a highly complex decomposition of the body's proteins (proteolysis), and eventual breakdown of the connective tissues.

Proteins in the gastrointestinal tract are the first to break down, then proteins in other organs – the pancreas, brain, liver and kidneys – then muscle proteins, then hard proteins such as collagen and keratin. This is why hair is often found on corpses, even after long periods. The breakdown products are proteoses, peptones, polypeptides and amino acids, and the



Shortly after death, neutral lipids are hydrolysed by enzymes known as lipases.

further breakdown of those amino acids gives the characteristic amines putrescine (tetramethylenediamine) and cadaverine (1,5-pentanediamine), together with hydrogen sulfide, ammonia and methane, all of which are classically associated with the strong odours of decomposition.

As a demonstration of the complexity of the multiple reactions, the Australian Facility for Taphonomic Experimental Research (AFTER) identified 452 volatile organic compounds released from a range of human and animal remains over a six-month period. Of these, human and pig decomposition products were the most similar across species.

Lipids, mainly associated with adipose tissue (fat cells), are particularly rich in triglycerides. These are hydrolysed by lipases (enzymes), liberating the fatty acids from their glycerol backbone. Under anaerobic conditions, the fatty acids undergo hydrogenation, transforming the unsaturated bonds to saturated. However, under highly anaerobic conditions, further oxidation of the fatty acids to aldehydes and ketones is retarded.

Both autolysis and putrefaction are substantially aided by bacteria, many of which are already present when the body is living. However, the environmental conditions where the bog body is placed combine to preserve the remains. At or below 4°C , both enzymic and bacterial processes are essentially stopped. The water in which the body is submerged, and the generally anaerobic conditions both prevent exposure of the tissues and associated oxidation. And the high levels of humic acids further retard the putrefaction reactions. Ultimately, the sphagnum bog environment provides the ideal conditions of low temperature, low oxygen and high acid for the natural preservation of the tissues.

However, those same conditions typically also result in the demineralisation of the remains, and it is common to find bog bodies missing bones and teeth. Put simply, the mineral (calcium hydroxyapatite and osteocalcium phosphate) portion of the bones is leached out, leaving the organic (collagen and other proteins). This process was very well demonstrated by Dr Rob Morrison in an experiment for RACI's '100 Reactions for RACI 100' project in 2017.

Violent ends

Frei's work adds a new dimension to the ongoing conjecture regarding cause of death. Overwhelmingly, bog bodies show evidence of violence. Tollund Man, for example, had been strangled, with the rope still around his neck when he was discovered. Many bodies show much more horrific wounds. Lindow Man's injuries (dating to around the time of the Roman invasion, found in 1984 in Cheshire, England) included blows to the top and back of his head, a possible garrotte, stab wound to the neck and broken neck, which finally killed him.

The two dominant theories are that the bodies represent either human sacrifice or the execution of criminals. Both have their origin in contemporaneous Roman accounts of their encounters with Northern European peoples. Frei's studies found that the clothing (unusually) found with both women was of high quality, imported, probably dyed and expensive. 'You sacrifice something that is meaningful and has a lot of value. So maybe people who [had] travelled had a lot of value', Frei told National Geographic at the Euroscience Open Forum in Copenhagen in 2014.

Frei went on to suggest that, rather than the sacrifice of slaves (as might be expected of human sacrifice, and as occurred in Viking culture), these apparent sacrifices were 'fine ladies', and that the travel in their final years might even have been associated with the ritual.

At the Copenhagen forum, other hypotheses were presented, including the idea that the two women died of natural causes, and may have been buried in the bog because as 'geographical outsiders' the locals did not know their funerary customs. Simply, there is no real way of knowing for sure the beliefs and practices of cultures from 2000 years ago that left no written records.

However, the question of whether the bog bodies might have actually represented a funerary custom does



Tollund Man was discovered in a bog close to Bjældskovdal, about 10 kilometres west of Silkeborg, in Denmark. The Silkeborg Museum houses Tollund Man's remains.

Museum Silkeborg

point to an interesting new trend. In the modern era, the traditional Western burial customs are being slowly displaced, mostly by cremation, but also by a range of exotic alternatives. People can now choose to have their ashes formed into artificial diamonds, be mixed with concrete to be made into artificial reefs, be pressed into a playable vinyl record or even launched into space. Bodies can be preserved with plastic and displayed, or donated

for study at one of the 'body farms' such as AFTER (see box).

Perhaps being preserved as a bog body might just enter that pantheon of options. It fits the rock'n'roll philosophy: 'Live hard, die young, and leave a good-looking corpse'.

Dave Sammut FRACI CChem and **Chantelle Craig** are the principals of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries.

Fighting *creepy*



with *crawly*

The Australian sheep industry is crippled by drug-resistant parasitic worms, but the unique chemistries in spider venoms are showing promise as a new class of drenching agent.

BY **SAMANTHA NIXON**

It's a sight all too common for Australian farmers. A ewe collapses while being driven into the yard, her lamb circling anxiously by her side. The farmer carefully checks around her eyes and gums. They're pale, almost white instead of a healthy, rosy pink. This sheep is anaemic, her blood being drained from the inside by thousands of parasitic worms.

Eaten alive: the barber's pole worm

The barber's pole worm (*Haemonchus contortus*) is one of the most virulent parasitic worms of sheep. It lives in the abomasum – the fourth stomach – where it feeds on sheep blood. The name comes from the worm's blood-filled intestines, which twist around white ovaries along the length of its

body, giving it a barber's pole-like appearance with red and white stripes.

These worms are only three centimetres long, but they have numbers on their side. As many as 10 000 of these writhing worms can infest a sheep, draining it of up to 10% of its blood each day. This makes the sheep anaemic, weak and malnourished, reduces its ability to produce wool and meat, and can be rapidly fatal.

Drug resistance in Australia's sheep industry

Gastrointestinal roundworms, like the barber's pole worm, cost the Australian sheep industry more than \$400 million each year in treatments and lost productivity. Farmers usually treat these worms by 'drenching' them with an oral dose of a de-worming drug.

However, we only have four main classes of drugs available, and the worms have become widely resistant to all of them. As many as 90% of Australian sheep properties now have drug-resistant worms, with multi-drug resistance becoming increasingly common. For the sake of the sheep and the sustainability of the Australian sheep industry, we desperately need to find new treatments.

How spiders can help save sheep

Surprisingly, it may be spiders that hold the key to sheep survival. The unique and complex chemistries in spider venoms have formed the basis of my research for the past three years at the University of Queensland's Institute for Molecular Bioscience and CSIRO Agriculture and Food, where I

investigate venoms as potential sources of new antiparasitic drugs. Venoms have evolved over millions of years to become fine-tuned cocktails of bioactive molecules. They are fast-acting, potent and selective, which makes them excellent drug candidates. Spider venoms have already been shown to be useful insecticides and promising treatments for chronic pain, stroke and epilepsy.

There are about 47 000 species of spiders, all possessing complex venoms made of inorganic salts, small organic molecules, neurotoxins, peptides and larger proteins. Some spiders produce venoms containing more than 1000 unique peptides, leading to a conservative estimate of more than 10 million unique peptides in spider venoms. It is these exciting qualities that make spider venoms such a vast and untapped resource for drug discovery.

Spider milking 101

To study venom you need to collect it from the spider. As an arachnophobe, this is the part that I find most challenging, and frankly a little terrifying. It begins by shepherding a large tarantula out of its container and onto the lab bench. We usually work with tarantulas because their large size makes them relatively easier to handle and results in larger venom yields. Then, with fast hands (and a slightly faster heartbeat), we carefully pick the spider up by its fused head and thorax, and position it over a tube

covered in a tough plastic wrap. Using tweezers, we then gently coax the tarantula's fangs to puncture the plastic covering over the small collection tube. A small electric shock (enough to stimulate the venom glands but not hurt the spider) is applied to the muscles over the venom gland, which squeezes out a few tiny drops of precious venom.

Using small amounts of this venom, we can then investigate the antiparasitic properties of the extracted venom by testing it against the early life stages of the barber's pole worm.

Stopping the infection cycle

Female barber's pole worms in the stomach of a sheep can lay thousands of eggs every day. These eggs are expelled in the sheep's faeces onto the pasture, where they grow up to the infectious third larval stage. They then crawl up blades of grass to be eaten by sheep, so that the cycle of infection continues.

To experiment on the worms I therefore have to dig through sheep manure to find the eggs. I hand-filter the sheep poo and use centrifugation to separate the eggs from the debris, before finally bleaching the eggs to remove bacteria and viruses.

Once the eggs are collected, they are hatched in a dish and the larvae grown in venom solution. I observe their development, looking for signs of paralysis or behavioural abnormalities that might signify antiparasitic activity.

Venoms have evolved over millions of years to become fine-tuned cocktails of bioactive molecules. They are fast-acting, potent and selective, which makes them excellent drug candidates.

After a week, I count how many worms have survived to develop to the infectious third larval stage. If we can inhibit or prevent this development, it indicates that the venoms are antiparasitic.

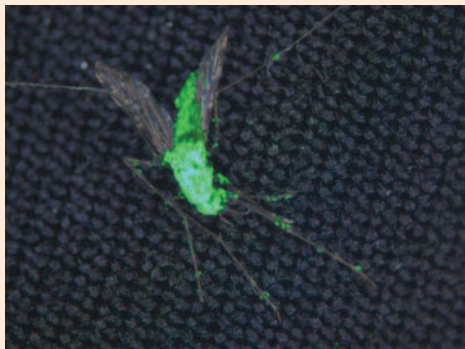
Once an active venom is identified, we use chromatography to fractionate the venom according to the chemical properties and sizes of its components. Using this technique, I can then test and retest the venom fractions against the parasites until the individual molecules responsible for the antiparasitic activity are isolated.

Then I study the masses and structures of the active compounds. I also investigate how the venom is working, because identifying new

Barber's pole worm is a roundworm that grows up to 30 millimetres long and sucks blood from the lining of the sheep's stomach, causing anaemia. Symptoms include swelling under the jaw (bottle jaw), weight loss and reduced wool growth and tensile strength. In lactating ewes, milk production can decline. More severe infections can prove fatal. Female worms have a red and white striped appearance, from which the common name 'barber's pole' worm is derived. Barber's pole worms are the highest egg producers of all sheep worms. Females can lay up to 10 000 eggs per day. CSIRO



Genetically engineered fungi could help fight malaria



This composite image shows a dead female *Anopheles gambiae* *Metarhizium pingshaense*, which has been engineered to produce spider and scorpion toxins. The fungus is also engineered to express a green fluorescent protein for easy identification of the toxin-producing fungal structures.

Brian Lovett

Malaria kills nearly half a million people every year, according to the World Health Organization (WHO). In some of the hardest-hit areas in sub-Saharan Africa, the mosquitoes that carry the malaria parasite have become resistant to traditional chemical insecticides, complicating efforts to fight the disease.

A study from the University of Maryland (USA), Burkina Faso, China and the University of Queensland's Institute for Molecular Bioscience suggests that a mosquito-killing fungus genetically engineered to produce spider and scorpion toxins could serve as a highly effective biological control mechanism to fight malaria-carrying mosquitoes. The fungus is specific to mosquitoes and does not pose a risk to humans. Further, the study results suggest that the fungus is also safe for honey bees and other insects. The study was published in *Scientific Reports* (doi: 10.1038/s41598-017-03399-0).

'In this paper, we report that our most potent fungal strains, engineered to express multiple toxins, are able to kill mosquitoes with a single spore', said Brian Lovett, a graduate student in the University of Maryland Department of Entomology and a co-author of the paper. 'We also report that our transgenic fungi stop mosquitoes from blood feeding. Together, this means that our fungal

strains are capable of preventing transmission of disease by more than 90% of mosquitoes after just five days.'

The researchers used the fungus *Metarhizium pingshaense*, which is a natural killer of mosquitoes. The fungus was originally isolated from a mosquito and previous evidence suggests that the fungus is specific to disease-carrying mosquito species, including *Anopheles gambiae* and *Aedes aegypti*. When spores of the fungus come into contact with a mosquito's body, the spores germinate and penetrate the insect's exoskeleton, eventually killing the insect host from the inside out.

On its own, however, the fungus requires fairly high doses of spores and a large amount of time to have lethal effects. To boost the fungus's deadly power, the researchers engineered the fungus with several genes that express neurotoxins from spider and scorpion venom – both alone and in combination with other toxins. The toxins act by blocking the calcium, potassium and/or sodium channels required for the transmission of nerve impulses.

The researchers then tested the engineered fungal strains on wild-caught, insecticide-resistant mosquitoes in Burkina Faso. Each engineered strain killed mosquitoes more quickly and efficiently than the unaltered fungus. But the most effective strain used a combination of two toxins, one derived from the North African desert scorpion *Androctonus australis* and another derived from the Australian Blue Mountains funnel-web spider *Hadronyche versuta*. The scorpion toxin blocks sodium channels, while the spider toxin blocks both potassium and calcium channels.

... the most effective strain used a combination of two toxins ...

Both of these toxins have already been approved by the US Environmental Protection Agency for insecticidal use.

'The WHO has identified insecticide resistance as the major threat to effective mosquito control, which is relevant not only to malaria but to a number of mosquito-borne diseases such as dengue, yellow fever, viral encephalitis and filariasis', said Raymond St Leger, a distinguished university professor in the University of Maryland Department of Entomology and senior author of the study. 'Unlike chemical insecticides that target only sodium channels, many spider and scorpion toxins hit the nervous system's calcium and potassium ion channels, so insects have no pre-existing resistance.'

When Lovett, St Leger and their colleagues inserted the toxin genes into the *Metarhizium* fungus, they included an additional failsafe: a highly specific promoter sequence, or genetic 'switch', which ensures that the toxin genes can only be activated in the blood of insects. As a result, the fungus will not release the toxin into the environment.

To further ensure the safety of non-target insect species, the researchers also tested the engineered fungal strains on honey bees. Working in Burkina Faso, the team deliberately infected local bees by both passive methods (exposing the bees to spore-coated fabric) and direct methods (spraying the bees with spores suspended in liquid). After two weeks, no bees had died as a result of the toxin-boosted fungus.

'The toxins we're using are potent, but totally specific to insects. They are only expressed by the fungus when in an insect. Additionally, the fungus does nothing at all to bees and other beneficial species', St Leger said. 'So we have several different layers of biosecurity at work.'

Encouraged by the results of the current study, the researchers plan to expand their on-the-ground testing regimen in Burkina Faso.

University of Maryland

... we are looking to produce these venom molecules in the lab, using genetically engineered bacteria or synthetic chemistry.



Spiders have evolved unique and complex venoms over millions of years. These venoms are fast-acting, potent and selective, which are important criteria for drug development. Tarantulas like this whistling tarantula (*Selenotholus foelschi*) are useful specimens because they produce larger amounts of venom for study. Researchers at the University of Queensland and CSIRO Agriculture and Food are investigating whether these venoms can be used to fight blood-sucking parasitic worms. UQ Institute for Molecular Bioscience

drug targets is highly useful for long-term research to continue fighting drug resistance.

A safe targeted solution inspired by nature

Once we understand the nature of the active molecule, we can begin optimising it, making structural modifications and seeing how this affects selectivity, stability and potency – all essential qualities for an effective and targeted drug. We then need to investigate whether these molecules have any side effects and make sure that they are safe to give to sheep. Fortunately, most spiders are relatively harmless to mammals – less than 1% of all spider species are actually dangerous to humans – so these molecules are likely to be safe to use as drugs.

It is essential that we identify the active components from the venom. It would not be possible to get enough venom from spiders to be useful for the 70 million sheep in Australia. Instead, we are looking to produce these venom molecules in the lab, using genetically engineered bacteria or synthetic chemistry. It is vital that these molecules can be produced

cost-effectively at scale to ensure these treatments are accessible to Australian farmers.

We have found that spider venoms contain molecules that can stop the worms in their tracks. These venom molecules show no cross-resistance to the drug-resistant strains of barber's pole worms, providing hope that we can overcome Australia's serious problem of widespread multidrug resistance.

From farm animals to suburban pets: the global impact of parasitic worms

The problem of parasitic worms, however, is not limited to Australia. The barber's pole worm is found around the world, posing serious threats to sheep and goat production in many regions.

Our beloved pets aren't safe, either. Heartworm, hookworms and roundworms cause serious infections in cats and dogs, requiring regular drug treatment. Mass drug treatment is also the mainstay for many major human parasitic worms as well. Worms such as *Brugia malayi*, *B. timori* and *Wuchereria bancrofti* cause the tropical disease lymphatic filariasis.

This causes serious disability in 40 million people worldwide, as the worms infest the lymphatic system and cause large and painful swellings. With 1.1 billion people at risk of this disease and needing regular treatment, this presents a major burden for public health.

At the University of Queensland and CSIRO, we are working with an international team of researchers to investigate whether spider venom molecules can be applied more broadly against such parasitic worms. Already, one particular tarantula venom molecule is a highly promising drug candidate, showing no signs of toxicity in animal models but strong activity against a major human parasitic worm.

So next time you encounter a tarantula – and yes, we do have Australian tarantulas – take a moment to say thanks. It may just save our Australian sheep industry from these devastating parasitic worms.

Samantha Nixon is a Westpac Future Leaders Scholar and University of Queensland Global Change Scholar, studying her PhD at the University of Queensland's Institute for Molecular Bioscience and CSIRO Agriculture and Food. Reproduced from *Australasian Science* (austscience.com).

The *art* of invention

An attorney's perspective



Mike Zammit uses a surface coatings example to illustrate the process of developing an invention, from concept to

How does one go about inventing something? Why are some people serial inventors, whereas others find it difficult to invent, or their discoveries are not considered 'worthy' of patent protection? Is it a certain way of thinking that leads some people to develop valuable IP (intellectual property)? Perhaps it is simply an understanding of what constitutes an invention and the commercial value of that solution.

In addressing these questions, the first point to clarify is what constitutes an 'invention' and an 'innovation'. Generally, an innovation results from developing a new idea and putting it into practice. In other words, innovations are concerned with the commercialisation of new ideas, usually involving the process of interaction and exchange of feedback

during the various stages of the product development process. In contrast, an invention may not be directly associated with commercialisation, and is considered as the generation of a new idea or knowledge, which aims to solve a specific technical problem. As not all inventions are commercialised, not all inventions result in innovations. Indeed, a great number of new ideas are conceived, but most die a lonely death, never seeing the light of commercial success.

Through my work as a patent attorney, I have contributed to my client's innovations to varying degrees. Most often I am involved in exploring the scope of the invention and working to define the broadest form of that invention in a patent application. However, more and more I am being asked to work with clients to

brainstorm ideas to real-world problems, and to sit in on R&D meetings to discuss the results of the research, and to assist in setting the direction of future investigations in the context of what IP might be protectable.

A client's preliminary concept

A client of mine recently identified a particular opportunity in the marketplace – he had identified a specific technical problem, the solution to which could result in a profitable business venture. At that time, no experiments had been undertaken to attempt to solve that problem, although my client had a preliminary concept in mind that involved the use of a specific surface coating. A brainstorming meeting was held with a coatings manufacturer (a specialist in the coatings field, and who was contracted to conduct the R&D) and their attorney to jointly brainstorm the research from a technical perspective, and to consider what IP might be protectable at each stage of that research, and what commercial issues could arise.

During the initial meeting, the question arose as to whether it was possible to seek patent protection for the concept itself. From a patenting perspective, it can be difficult to obtain protection of a concept per se without sufficient examples demonstrating how that concept may be implemented in practice. This means that some experimentation is usually required, although this can vary with different fields of technology.

Trialling solutions

During that preliminary discussion, a number of potential solutions were considered. While there was some 'gut feel' regarding which of the solutions might be best, it was decided that the contractor should trial a number of surface coating types to assess their performance in solving the problem at hand. If they all happened to work, then, from a patenting perspective, it

might be possible to pursue broad method claims, along the lines of: 'A method comprising applying a surface coating to ... [insert outcome here]'. If it were possible to obtain such broad protection, this would effectively equate to protection of the concept itself, and would be quite valuable IP.

One critical question, however, was whether anyone had used that same method in the past, or something similar. To find out, a search of the 'prior art' would be required. If no relevant prior art could be found, then there may be an opportunity to file for patent protection of the method just described. However, if the concept was already disclosed in the prior art, further research would be required to devise a solution that performs better than these prior art solutions.

In this situation, a few commercial issues become relevant. In particular, from a commercial perspective, these prior art solutions would stand as competing technologies to my client's eventual product, and could therefore impact on the viability of the proposed business venture. These prior art solutions may also result in issues of patent infringement that we need to deal with. Additionally, assuming that a better solution could be invented, it would need to have advantages over and above the prior art solutions for it

... it may be difficult to secure patent protection for using a known compound, having known properties, being used in a known way, in a known surface coating, to achieve what is arguably a predictable outcome.

to have any chance of being adopted commercially. For instance, it would need to be significantly cheaper and/or provide significantly better performance.

Assuming that none of the proposed coatings worked to solve the problem (or if all the proposed coatings worked), clearly some further R&D would be required to develop 'improved' coatings.

Trialling 'improved' solutions

One option considered during this next phase of the R&D was to trial additives known in this field of art that might be inherently suited to assist in solving the identified problem. Some additives are well known for their ability to confer certain benefits due to their inherent chemistry or properties. Trials could be undertaken with these modified coatings and potentially some (or all) of them may deliver a reasonable outcome.

From a patenting perspective, there are issues with this approach. In particular, it may be difficult to secure patent protection for using a known compound, having known properties, being used in a known way, in a known surface coating, to achieve what is arguably a predictable outcome. In this case, there is a high likelihood of running into serious 'obviousness' rejections when prosecuting the patent application before a patent office, making the prospects for patentability low – although from a commercial/marketing perspective, it still may be appropriate to file for protection. This of course assumes that there is no 'new working interrelationship' with the base coating composition into which the additives are added, i.e. no synergy. If some unexpected synergy can be identified, the prospects for securing patent protection become significantly better.

Again, assuming that none of these 'improved' coatings solved the problem sufficiently (or if all them solved the problem), clearly further R&D would be required.



How to invent a solution to a problem

The question is then how to go about developing a new surface coating that solves the problem at hand. This is difficult to answer. Some guidance can be found in the famous quote from Isaac Asimov:

The most exciting phrase to hear in science, the one that heralds new discoveries, is not 'Eureka!' but 'That's funny ...'

This suggests that innovations emerge from noticing something out of the ordinary, or from a departure from what is otherwise expected. From a patent perspective, a departure from what is otherwise expected strongly suggests an 'inventive step', but from a practical perspective the question is really where the researcher should be directing their efforts (while at the same time keeping an eye out for that elusive departure from the ordinary).

From the perspective of a patent attorney working with inventors on a daily basis, and drafting and prosecuting many dozens of patents here and abroad over the last 15 years, I can offer several suggestions. Some avenues to consider might be:

- 'new' additives not already known for being inherently suitable for

addressing the problem

- a system or group of additives that might synergistically solve the problem
- some additives that might be found to serve multiple functions.

Experimentally, one could compile a generous list of additives, compounds or materials from a variety of fields to trial, and then embark on a comprehensive research program to search for a new combination of features that solve the problem, or especially some combination that provides a surprising or unforeseen outcome, i.e. the elusive 'that's funny' moment. Alternatively, or additionally, new relevant technology might be available that could be explored. Of course, another line of research would be to undertake deeper investigations into the actual cause of the problem at hand, since knowing the chemistry and physics at play can often reveal unforeseen mechanisms that, when addressed in a new way, can be suitable subject matter for patent protection. The commercial drivers for the new invention will often dictate the resources that are allocated to this part of the process.

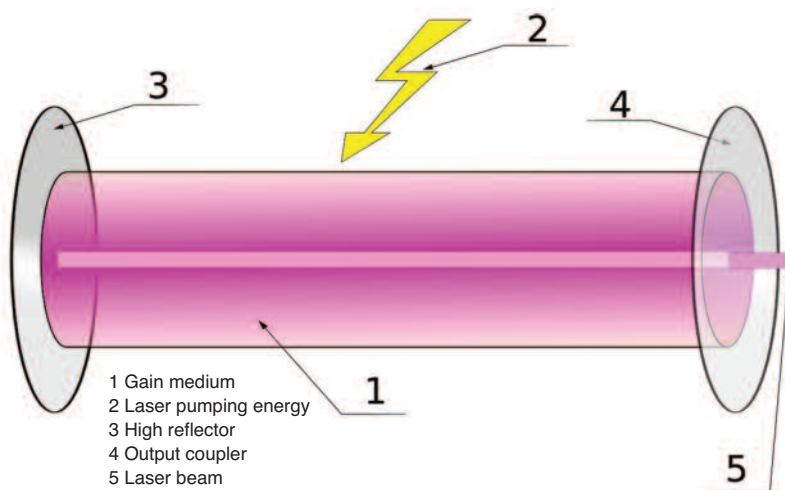
In terms of attitudes, I find that many inventors challenge conventional wisdom, especially when that

conventional thinking is a road block to achieving a superior outcome. Also, the inventors who I meet often can think in a counterintuitive way.

Thinking ahead, and turning to the considerations of what IP might be protectable, assuming that a new solution to the problem was developed, it may be possible to obtain method claims along the lines of: 'A method comprising applying a surface coating comprising features X, Y, Z [i.e. defining the specifics of the new coating] to ... [insert outcome here]'. It may also be possible to obtain patent claims directed to the improved coating composition itself. These patent claims would be valuable IP to the proposed business venture.

IP considerations at every stage of research

It should be clear from the details of this example that, at every stage of the research, the prospects for IP protection were considered. It is also important to consider the commercial realities at each stage of the research. For example, if the proposed solution is unrealistically expensive, there is little chance that it will be commercialised, which may affect the decision on whether to file for IP protection. Also, if the new coating is



The basic components of a laser, shown here, and the first use of the acronym, were detailed in the late 1950s in a notebook of American physicist Gordon Gould, who is widely credited with the laser's invention. Gould spent more than 30 years trying to obtain patents from the US Patent and Trademark Office. Tatoute/CC-BY-SA 2.5

... many inventors challenge conventional wisdom, especially when that conventional thinking is a road block to achieving a superior outcome.

better than a prior art coating, but is not significantly better, this may affect the decision on whether to commercialise the new coating and seek IP protection of it. There may also be competitor IP to consider.

This example is but one course that might be followed during a program of R&D, and there are, no doubt, other ways to invent a new solution to a specific technical problem. Also, new 'solutions' are developed in laboratories around the world each day without an associated 'problem' in mind. An example of this is Arthur Schawlow, who co-invented the laser and who was granted a patent in 1960. He and his colleagues had not

considered any applications of their invention during their R&D, and it was left to others to devise ways of exploiting this invention in a commercial product. Schawlow has commented:

We thought it might have some communications and scientific uses, but we had no application in mind. If we had, it might have hampered us and not worked out as well. (Bell Labs, 1998)

From coatings to other chemistry

Innovation often starts with a deep understanding of what problems need to be addressed in the marketplace, and progresses to devising new technical solutions to those problems,

all the while keeping an eye on the commercial realities of those solutions, and the prospects for IP protection.

The specific example of a surface coating has been used in this article, but this could be replaced with another technical solution. What is more important is the methodology that was followed. This general methodology might serve as a template for your own research activities.

Mike Zammit MRACI CChem completed a PhD in polymer chemistry at the University of New South Wales before working in industry for five years. Mike then trained to become a patent attorney and is currently a senior associate at Shelston IP. The content of this article is general in nature, and must not be relied on in lieu of advice from a qualified professional in respect of your particular circumstances.



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Andrey Kiselev/Adobe

Centenary fellows

RACI's centenary ends on 30 June, and as part of this special year the RACI Board, Branches and Divisions are suggesting names for consideration for fellowship status. Congratulations to the following people on becoming Centenary fellows during the centenary year so far.

The first group of Centenary fellows was announced on pp. 26–28 of the April issue.



Professor Phil Andrews
Monash University



Professor Evan Bieske
University of Melbourne



Professor James De Voss
University of Queensland



Professor Bart Follink
Monash University



Professor Maria Forsyth
Deakin University



Dr Anita Hill
Future Industries CSIRO



Professor Steven Langford
Swinburne University of
Technology



Ms Regina Menz
O'Connor Catholic College,
Armidale



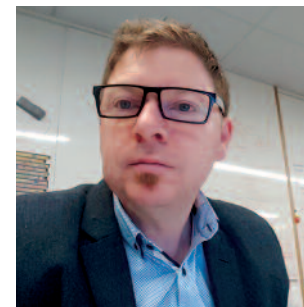
Rev Dr Tim Nicholson
University of Queensland



Professor Martina Stenzel
University of New South Wales



Dr Matt Sykes
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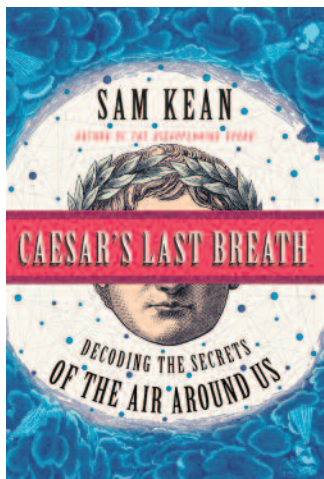
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Caesar's last breath: decoding the secrets of the air around us

Kean S., Little, Brown and Company, Hachette Book Group, 2017, hardcover, ISBN 9780316381642, 373 pp., \$US21.66 (Amazon)

For all people with an interest in science, Sam Kean, the bestselling science writer of *The tale of the dueling neurosurgeons* (on brain function) and *The disappearing spoon* (on the discovery of the elements), has now added a most entertaining and educational book about

the air we breathe. Inevitably, it covers the composition of Earth's atmosphere, but in Kean's typical fashion it also offers historical facts on chemical discoveries and intriguing anecdotes about significant discoverers.

Kean outlines the evolution of Earth's gaseous atmosphere over 4.5 billion years, and this provides a perspective on other possible 'life' in the universe. He also describes the contribution of each gas in our atmosphere and how much we statistically inhale; for example, for nitrogen, 78% of the air (780 000 parts per million), you inhale nine sextillion molecules every time you breathe. Why *Caesar's last breath*? Well, the air we breathe has circulated around the planet for several thousand years and it may be that we breathe molecules used by Caesar on that fateful 'Ides of March' some 2000 years ago.

Kean provides stories of several natural disasters that have contributed to the composition of our gaseous atmosphere, notably volcanic eruptions ...

Kean provides stories of several natural disasters that have contributed to the composition of our gaseous atmosphere, notably volcanic eruptions, and he deftly uses Mount St Helens as a recent example. He weaves in several, not so natural disasters too, such as the 'The Fallout of Fallout', the flip side to how the atmosphere has shaped human beings.

This diversion is about US nuclear weapons tests at Bikini Atoll (July 1946). Kean examines the massive expenditure and some weird outcomes. For example, of 5000 rats, 204 goats and 200 pigs planted on board a substantial fleet of decommissioned naval vessels, one pig (#311) miraculously survived. This animal was used to reassure the public about the

safety of nuclear weapons, and accelerate the nuclear weapons testing program – 200 more tests over the next two decades. Consider what other 'nuclear' nations have subsequently contributed (and continue to contribute) to our 'valued' atmosphere. However, my real concern is the loss of life of individual scientists working on relatively open laboratory experiments to 'start' (controlled) nuclear chain reactions with small plutonium spheres using tungsten-carbide, and later beryllium as neutron reflectors. Accidents happened – the control spheres were dropped, setting off mini nuclear bombs and obituaries for Harry Daghlian, Louis Slotin and Alvin Graves.

Kean draws on the technologies employing atmospheric gases. From nitrogen fixation in the Haber process that 'transformed the very air we breathe into bread', to the harnessing of water and steam power revolutionising transport, industry and power generation; and the Bessemer process (1856) employing controlled blasts of air (oxygen) applied to molten cast iron to reduce its carbon content to produce at least four types of steel today (with a little magnesium alloying thrown in).

As chemists, we all know about the above discoveries, but Kean weaves in more personal revelations. For example, the German industrial chemists Fritz Haber and Carl Bosch (the latter the mastermind of the Haber production process) were hailed as national heroes for their discoveries and won Nobel Prizes, but both were later condemned as international war criminals. In a similar vein on energy using explosives, 'the movement of gases at high speed', Kean notes that Alfred Nobel provided great benefits in the construction industry and mining, but when his products were employed as weapons of war, he was portrayed as 'The Merchant of Death'. However, his final eulogy came from establishing, from his amassed fortune, the distinguished Nobel Prizes, which have all but 'exploded' his earlier reputation. Finally, structural steel became the material of choice following the tragic collapse of the brittle cast-iron Tay Bridge in Scotland in 1879, and the loss of 150 train passengers.

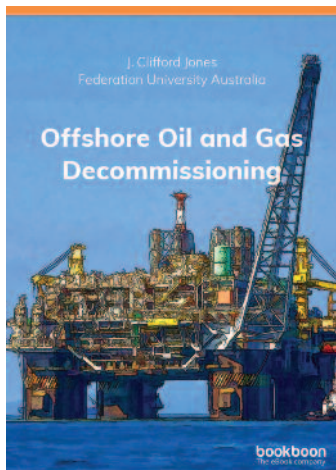
Similarly, most chemists learn about the discovery of oxygen (e.g. shining a beam of sunlight onto mercuric oxide powder), but few realise that Joseph Priestley spilled the beans in an enthusiastic presentation he gave at the French Academy of Sciences about a 'gas' he had discovered. A guest at Priestley's presentation, Antoine-Laurent Lavoisier, had performed similar experiments but failed to isolate any gas. He repeated the experiments following Priestley's disclosure and named the emergent gas 'oxygen'. Plagiarism or co-discovery? Priestley's fixation with the theory of phlogiston was not helpful. The 'Priestley Riot' (Birmingham, 1791) saw him literally burned out of his primary profession (preacher) due to his outspoken views on contentious religious issues, and his strong support of the French Revolution. By 1794, he had moved to teach chemistry at the University of Pennsylvania (founded by his old friend Benjamin Franklin). The 'royalist' Lavoisier met a grislier end under the blade of a Jacobian guillotine in 1794.

Kean's discussion on the atmosphere and 'weather', especially its control and prediction following 'cloud seeding' by Langmuir culminates in a conclusion that the number of variables concerning Earth's weather system are just too great to make the two objectives viable, even when chaos theory is considered. A critical debate about 'climate change', or humans' over-utilisation of limited fossil fuel resources is lacking. Kean does touch on the impact of CFCs, but this appears rather as an introduction to an intriguing story of 'the' Albert Einstein, as co-inventor (1930) of an absorption refrigerator having no moving parts and requiring only a small heat source to operate.

The book also offers some coverage of the most important theoretical foundations of gases, of developments in anaesthesia and its associated 'drug' culture (of that time); and as light relief, there is a story of the French entertainer of the 1890s, Le Pétomane.

Like Sam Kean's earlier books, this one is difficult to put down until you have completely read it. It is so refreshing and offers great incentives, especially to youngsters, to recognise the joys of scientific discovery, as well as a few of the real horrors.

Alan J. Jones FRACI CChem



Offshore oil and gas decommissioning

Jones J.C., bookboon.com, e-book, ISBN 9788740319224, 313 pp., free

Concern for the environment and the on-going impact of redundant industrial facilities started to become an issue in the 1960s. Prior to this period, facilities were often left 'to rot' in their own time, which has been a boon for industrial archaeologists, especially when facilities were abandoned in remote locations. Since the 1960s, the principal driver has

been to ensure rehabilitation of the site to the state that existed prior to construction of the facility. Where this proves difficult, including where costs are prohibitive, alternative remedies are sought. A good example is old gas-works sites that frequently contain a high level of contamination and are often remediated as playgrounds or similar amenities.

Prior to the new enlightenment, companies and government agencies were under no obligation to remediate industrial facilities when they reached the end of their useful life. Nowadays, industrial companies, miners, and oil and gas companies carry a significant contingent liability in their accounts to pay for remediation. However, as the on-going issue of the Townsville nickel refinery shows, a positive outcome is not always achieved in practice.

Another aspect of this approach is that any contingent liability for remediation has to be factored into new developments. For Australian mining businesses, for instance, this means new ventures must generate sufficient cash during the operational phase to pay for end-of-life remediation.

Offshore oil and gas decommissioning comprehensively tells the story and the methods used for decommissioning offshore oil and gas facilities, the offshore nature of which can be particularly problematic in rehabilitating to pristine conditions.

The book details and compares a variety of decommissioning methods with case studies taken principally from the Gulf of Mexico and the North Sea, where offshore oil and gas facilities expanded rapidly from the 1960s and many of the early operations have now been abandoned and decommissioned. Removal of all types of facilities, from underwater units (well-heads, umbilicals, pipelines and the like) to above-water structures is comprehensively described and referenced to company and government documents via interactive hyperlinks.

Prior to the new enlightenment, companies and government agencies were under no obligation to remediate industrial facilities when they reached the end of their useful life.

The first chapter of the book gives an overview of the history of the offshore oil and gas industry and decommissioning approaches since 1890s' California. This is followed by seven chapters covering cutting techniques, lifting vessels (including their use in offshore wind farm decommissioning), well-head removal, the use of jack-up rigs and other vessels used. Chapter 7 covers miscellaneous issues such as the use of suction dredgers for underwater spoil removal, pipeline removal and the conversion of rigs into artificial reefs. The next chapter discusses the scrapping of floating structures such as floating, production, storage and off-take (FPSO) vessels.

Chapter 9 is devoted to North Sea decommissioning and a discussion on International Maritime Organisation guidelines for structures toppled and similar. A chapter on other places where offshore oil and gas fields have been developed makes it evident that most activity occurs in the developed western world, primarily the North Sea and Gulf of Mexico. Other places with longstanding offshore oil operations, such as the Caspian Sea, have not seen any decommissioning, and oil facilities in Lake Maracaibo in Venezuela are allowed to degrade and pollute the environment.

As well as decommissioning, mothballing of offshore facilities is explained with the extensive use of corrosion

inhibitors and cleaning agents. Mothballing allows re-commencement of oil/gas production in times of high oil price – so called ‘late-life operations’.

Many offshore structures are brought to shore for final break-up and disposal. This optimises the quantity of steel that can be recycled. A chapter details some of the specialist yards and converted shipyards that do this. However, this can also generate large amounts of more intractable waste such as paint ash, which requires subsequent disposal. As well as steel content, on-shore breaking up of structures allows recycling of other components such as copper and fluorescent tubes (containing mercury); for example, there were 3500 tubes on the Brent Delta platform. The 2015 decommissioning of the Stybarrow FPSO vessel and similar facilities off north-west Australia are also discussed.

Chapters 9 and 10 report costs of decommissioning and the trade-offs in terms of costs and achieving a sufficiently low level of risk. The decommissioning costs based on removal of unit quantities of structural steel are estimated. A discussion of estimates for the carbon footprint of decommissioning of various North Sea facilities is also included.

Chapter 18 provides details of various regulatory standards and discussion of when a structure can be left in situ and converted to an alternative use, completely removed or toppled and converted into a reef; also covered is the removal of artificial islands constructed during the early days of the Californian oil boom of the 1920s. Each facility requires its own decommissioning plan and risks are discussed and the logistics train required is outlined.

A chapter covers Gulf of Mexico hurricane damage. Decommissioning of damaged platforms involves a greater degree of risk and can cost more than three times the cost of removal of an undamaged rig. Case studies are presented to illustrate the salient points.

Decommissioning of offshore oil and gas facilities has hardly begun in areas outside the Gulf of Mexico and the North Sea. In the not too distant future, when decommissioning begins in earnest (for example, in the Bass Strait and Otway basins or the many other offshore locations in South East Asia), there will be considerable interest in the subjects covered by this book. This interest will range from regulators concerned with the application of the best approaches and the standards to be applied, to companies wishing to become involved with various aspects of the process from structure removal to recycling of parts of the facilities.

One minor criticism is that the topic is a field extensively covered by the Society of Petroleum Engineers in its journals and conference proceedings, yet that is not discussed here. However, the book does contain a wealth of information and references from web sources, especially government reports, which adequately covers the field.

Duncan Seddon FRACI CChem

RACI National Awards 2018 Call for nominations

Nominations are called for the following awards. You can apply for some of these awards yourself; others require nomination. **All national awards except the Post Graduate Student Travel Bursary (closing date 15 May) close on 15 June.**

- Applied Research Award
- C.S. Piper Award
- Citations
- Cornforth Medal
- Distinguished Contribution to Economic Advancement – Weickhardt Medal
- Distinguished Fellowship
- Fensham Medal for Outstanding Contribution to Chemical Education
- H.G. Smith Memorial Award
- Leighton Memorial Medal
- Margaret Sheil Lectureship Award
- Masson Memorial Medal
- MRACI Post Graduate Student Travel Bursary
- RACI Chemistry Educator of the Year Award
- Rennie Memorial Medal
- Rita Cornforth Lectureship

See www.raci.org.au/events-awards/awards or email awards@raci.org.au for more information about the requirements for nominations for each award.

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Lab-made hormone may reveal secret lives of plants

By developing a synthetic version of the plant hormone auxin and an engineered receptor to recognise it, Howard Hughes Medical Institute (HHMI) Investigator Keiko Torii and colleagues are poised to uncover plants' inner workings.

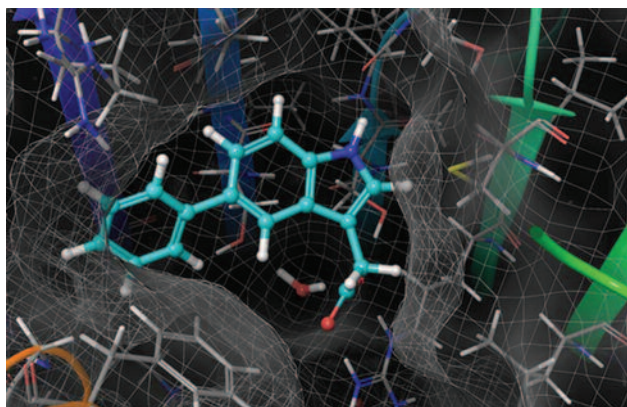
The new work, described in *Nature Chemical Biology* (doi: 10.1038/nchembio.2555) is 'a transformative tool to understand plant growth and development', says Torii, a plant biologist at the University of Washington (USA). That understanding may have big agricultural implications, raising the possibility, for instance, of a new way to ripen strawberries and tomatoes.

To plants, the hormone auxin is king. Among many other jobs, auxin helps sunflowers track sunlight, roots grow downwards and fruits ripen. This wide range of jobs, as well as the fact that every cell in a plant can both produce and detect auxin, makes it tricky to tease apart the hormone's various roles. 'It's been a huge mystery as to how such a simple molecule can do so many different things', Torii says.

She and her colleagues set out to create a new way to study plants' responses to auxin by designing a lab-made version of the hormone that can be precisely controlled. Working with synthetic chemists in Japan, the researchers added a little bump to auxin's structure – hydrocarbon rings that auxin doesn't normally contain. The researchers then tweaked plants' auxin receptor, a protein that sits on the outside of plant cells and detects auxin. This time, the researchers removed a bulky amino acid from the receptor, creating a perfect-sized hole that cradles the lab-made auxin. That simple switch, called a 'bump and hole' strategy, 'is really elegant, actually', Torii says.

Next, the researchers tested whether this matched set – the synthetic auxin and the synthetic receptor – could do the same jobs as the cells' natural auxin-receptor pair. The intricately designed system worked beautifully, experiments on roots showed.

Normally, roots exposed to auxin stop growing down, and instead grow sideways by activating stem cells that break out



A synthetic version of auxin and its protein receptor (light blue) nestle together, creating a matched set that behaves just like the natural one. Keiko Torii / University of Washington/HHMI and Shinya Hagihara/Nagoya University



of the main root. Torii compares the process, called lateral root development, to aliens bursting through stomachs. After detecting synthetic auxin, *Arabidopsis* plants genetically engineered to produce the synthetic auxin receptor behaved just like normal – growing the same sideways baubles of root branches.

What's more, roots that didn't have the synthetic auxin receptor were essentially 'blind' to synthetic auxin, proof that the artificial hormone is detected by only the artificial receptor. Torii and her colleagues call this switch to synthetic auxin 'chemical hijacking' – a well-controlled takeover that will now allow researchers to tease apart the tangled web of auxin's jobs in plants.

With their system up and running, the researchers tested a long-standing question in plant biology. Scientists knew that germinating seedlings use auxin to grow quickly. But the identity of the exact receptor that allows this process to happen wasn't settled.

The scientific community had a suspect in mind. Torii's team produced a plant that lacked an auxin receptor called TIR1, and instead possessed a synthetic version. When exposed to artificial auxin, these seedlings began to grow rapidly, behaving exactly as if they had the normal receptor. The results suggest that seed elongation does indeed happen through the TIR1 receptor.

Other fundamental scientific questions can be addressed with this system, Torii says, such as auxin's role in corn ripening and in opening the stomata, the structures that let plants breathe.

One day, synthetic auxin might even find a place in agriculture. Auxin is currently sprayed on fruits to hasten ripening. But in high concentrations, the hormone can act as a plant-killing herbicide. Fruits engineered to carry the synthetic receptor could be ripened with the synthetic auxin hormone, Torii says, eliminating the need to spray auxin indiscriminately. But, she cautions, much more testing needs to be done before a synthetic hormone system can be used for growing food.

Howard Hughes Medical Institute

p -values – abused but not abandoned

One afternoon in the south of England circa 1919, the biologist Ronald Fisher poured a cup of tea and handed it to his colleague Miss Muriel Bristol. She declined, saying that she preferred the taste of tea when the milk had been poured before the tea, and not the other way around.

She insisted that she could taste the difference, prompting a third person, William Roach, to suggest a blind tasting. Afterwards, Roach enthusiastically declared that Bristol could, in fact, tell the difference.

He may not have been entirely objective (he later married Bristol), and the details surrounding Bristol's achievement are, unfortunately, undocumented. But the episode with the tea had a long-lasting impact on science.

It prompted Ronald Fisher, a gifted mathematician, to develop the basic principles for statistical analyses – principles that are still used widely by scientists today.

Science based on tea

The tea experiment was the starting point of a famous examination in Fisher's book, *The design of experiments*.

He pictured a scenario where there are eight cups. In four of them, the milk was poured first, in the last four the tea was poured first. The eight cups are presented to Bristol in random order. Now the question is: if she correctly points out the four cups in which the milk has been poured first, can we then conclude that she is actually able to identify the order in which the drinks were mixed?

Fisher reasoned that if Bristol could not taste the difference, but merely guessed (the null hypothesis), then he could calculate the probability that she would correctly identify the four cups in the experiment by chance.

The result is 1/70 or about 1.5%. Since this probability is small, we can reject the null hypothesis that Bristol was simply guessing, and recognise Bristol's impressive tea tasting skills.

The 1.5% is called the p -value or probability value. Simply put, the p -value generally reflects the probability of achieving the observed test result if the null hypothesis is true.

An integrated part of quantitative research

The p -value is interesting because its calculation is probably the most used, most misunderstood and most criticised procedure in modern experimental research, and has big financial, societal and human consequences.

Here is a more scientific sounding scenario.

A research team measures the ability of a new drug to lower blood pressure in a group of people with hypertension. At the

same time, they measure the effect of a known drug in a control group. If the new drug works better than the old drug in the experiment, can we then be certain that this applies to the patient population in general?

The null hypothesis is conservative and predicts that the two drugs work equally well. Due to random variation, you could still observe differences between the drugs. But if the probability for this – the p -value – is low, then we can reject the null hypothesis and conclude that the new drug works best (i.e. we disregard the possibility that the old drug is best).

The p -value is interesting because its calculation is probably the most used, most misunderstood and most criticised procedure in modern experimental research, and has big financial, societal and human consequences.

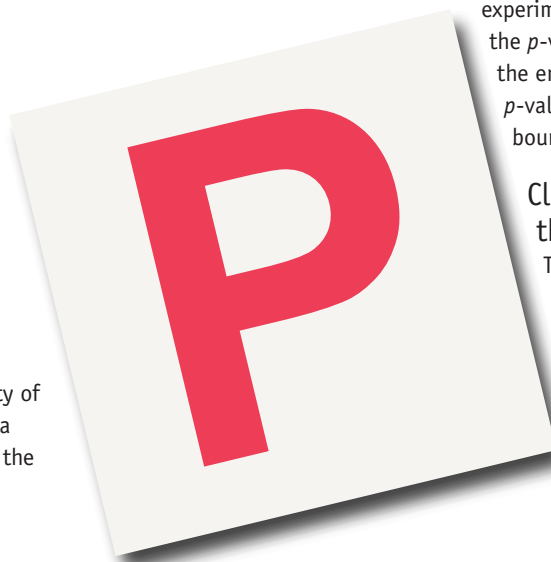
But a high p -value would suggest that the observed difference could easily have occurred by chance and that the two drugs are in fact equally good. In that situation, you would accept the null hypothesis that the effect is the same for both drugs.

But how small should the p -value be before we reject the null hypothesis?

Of course, there is not a fixed boundary. Fisher drew the line at 1/20 (five per cent). This convention is still widely used, for example in medical science. The result of an experiment is considered 'significant' when the p -value is less than five per cent, and the entire procedure of calculating the p -value and checking that it crosses this boundary is called a 'significance test'.

Classic misinterpretation of the p -value

The p -value is commonly misinterpreted. Fisher's hypothetical-deductive approach is straightforward, but there are countless examples where even the researchers themselves get it wrong.



<u>P-VALUE</u>	<u>INTERPRETATION</u>
0.001	HIGHLY SIGNIFICANT
0.01	
0.02	
0.03	
0.04	SIGNIFICANT
0.049	
0.050	OH CRAP. REDO CALCULATIONS.
0.051	ON THE EDGE OF SIGNIFICANCE
0.06	
0.07	HIGHLY SUGGESTIVE, SIGNIFICANT AT THE $P < 0.10$ LEVEL
0.08	
0.09	
0.099	HEY, LOOK AT THIS INTERESTING SUBGROUP ANALYSIS
≥ 0.1	

xkcd.com/CC BY-NC 2.5

If you find a stronger effect of the new drug with a p -value of four per cent, many people might subtract 4 from 100 and conclude, 'The experiment showed a whopping 96% probability that the new drug works best'.

But the probability does not directly relate to the assumption that the new drug is best. It concerns the observation (the difference in effect during the test) under the assumption that the effect of the two drugs is actually the same.

One statistician compared it with confusing the two questions: 'Is the Pope a Catholic?' and 'Is a Catholic the Pope?' The answer to the first question is 'yes', whereas the answer to the second question is 'unlikely'.

The correct conclusion is: 'If the new and old drug worked equally well, the probability of randomly observing the effect recorded during the experiment (or an even bigger difference) would be four per cent'.

The p -value must also be analysed

A common point of criticism is that scientists are overly reliant on the p -value compared to the many other quantitative measures that are available to summarise experimental results.

The size of the observed effect is especially important. Does the new drug work only slightly better or much better? Even though a very low p -value strongly implies that the new drug is

better, the difference in effect can easily be too small to have any practical importance.

Besides, a p -value less than five per cent is not a complete guarantee of a difference in effect. As long as the p -value is not extremely low, the result could still have occurred randomly even though there is no real difference (the p -value is the size of that risk by definition).

You can, on the other hand, risk reporting a p -value higher than five per cent, thereby maintaining the null hypothesis that both drugs work the same – even though there actually is a difference. This could occur if the experiment is not sensitive enough because there are too few test subjects – in technical terms, the experiment lacks power.

Overlooking a more efficient new drug is of course unfortunate, but it is also unfortunate to falsely conclude that the new drug does not have worse side effects than the old, based on an insignificant p -value.

The official authorities that approve the introduction of new drugs are expected to be aware of these errors. But it is important to note that the risk of making them is an inevitable problem, which follows from the core principles of significance tests.

p -value hacking

Many scientists think that the conventional significance level of five per cent has gained an unreasonable level of importance. Numerous researchers have first committed to using the five per cent criterion, only to calculate a higher p -value later – for example, eight per cent.

This can lead to despair as it forces them in principle to maintain the null hypothesis. In the example above, the conclusion would be that the new drug is no better than the old one. This can be a great disappointment when much time and money has been invested in the hope of a difference. Often, a 'non-significant' p -value (above five per cent) is considered an uninteresting outcome that is unlikely to be published.

In this situation, some scientists argue that eight per cent is not so far from five per cent, and use phrases such as 'nearly significant' or 'in reality significant'. A humorous list of more than 500 examples of similarly creative expressions have been compiled by Matthew Hankins from the University of Southampton.

Another common reaction is to recalculate the p -value using different statistical models, hoping to get below the five per cent – a dubious practice known as p -hacking. Others resort to filtering their data to achieve the desired level of significance.

These issues have implications for another well-known problem in the world of science: the lack of publication of negative results, even though they can be very informative. We will delve into this further in part 2.

Ole Kjørulff is at the Neuropharm and Genetics Lab, University of Copenhagen, Denmark. First published at sciencenordic.com.

Targeting loose language about science

Usually, my 'Science for Fun' piece is an experiment for people to try, or an explanation of a science topic. This time, I am taking a look at some examples of loose language in science – some harmless and some less so. As a science communicator, accurate language is something that I take extremely seriously, and I see a lot of use of inaccurate language in all forms of media.

Recently a *Chemistry in Australia* reader pointed out to the editor some examples of inaccurate science they have observed. These are the subject of my column.

I have a prescription medication that boldly states 'Do not take potassium without medical advice'. I wouldn't take potassium even if it was prescribed by my doctor!

This misinformation is technically incorrect, but unlikely to be dangerous. The reader was referring to the element potassium (atomic symbol K), a *very* reactive metal. If you put metallic potassium in water, it will react violently. Depending on the size of the piece of metal, it may fizz, catch fire or explode. In schools and universities, small amounts of potassium (or similar metals such as sodium) are put into water to demonstrate their high levels of reactivity. A video showing the reactivity of these metals with water can be seen at bit.ly/2BSz5kf.

Potassium in elemental form is not going to be part of a medication. However, potassium in the form of ions (K^+) is an important part of some medicines, and indeed a crucial component of the human body.

This distinction between forms of chemicals is extremely important, and sometimes deliberately manipulated to provide misleading information. A classic example of this is the issue of mercury as a preservative in vaccines. Yes, mercury is a very toxic heavy metal. Yes, some vaccines contained mercury. However, the mercury was only present in small amounts – way below established safety thresholds, and in a chemical form (called thimerosal) that allowed rapid excretion from the body. The evidence in this case still shows that exposure to mercury from vaccines was safe, but public perception and fear resulted in removal of all mercury from vaccines. See a fact sheet about thimerosal at bit.ly/2CJiPyX.

In our local media there have been ads for 'chemical-free food'. Can food be 'chemical free'?

I know for sure that our reader knows the correct answer to this. By definition, literally everything is chemicals. The intention with the term 'chemical free' is to market something as being perhaps organic, natural, healthy, clean, safe etc., but unfortunately this use of language can result in an unnecessary and dangerous phobia of 'chemicals'.

Now don't get me wrong, I'm not suggesting that minimising or avoiding *toxic* or *harmful* chemicals is a bad thing – far from it! It is the use of language that I disagree with. Perhaps people conveniently forget that some of the most dangerous chemicals known – including components of snake venom, botox and cigarette smoke – are 'organic' and 'natural'. In addition, as with the example of mercury, the toxicity of all chemicals is dependent upon the dose. Even water is toxic if you consume enough of it (bit.ly/1XfYcio).

Our previous Prime Minister reportedly said that 'carbon dioxide is a weightless gas'.

The political debate around climate change, and the carbon tax is full of loosely used language such as this. Carbon dioxide is not weightless, and is indeed a more dense gas than the air around us. Even by a less scientific definition, 'weightless' refers to something 'lacking apparent gravitational pull'. A simple experiment, where one balloon is filled with air, and another is filled with carbon dioxide, provides evidence that this gas is in no way weightless. Drop both balloons at the same time and the carbon dioxide balloon will fall to the floor due to gravity much more quickly than the air balloon. Again, this may not be critical misinformation, but is further evidence of the loose language used in discussions of scientific issues.

It seems to me that one of the major problems in science journalism in Australia is the decline of specialised science journalists in the mainstream media. This, among other reasons, has contributed to an increase in the careless or inaccurate language. I won't address these ideas in detail here, as they were succinctly covered last year by Professor Joan Leach, Director of the Centre for the Public Awareness of Science at ANU, in an article in *The Conversation* entitled 'Science journalism is in Australia's interest, but needs support to thrive' (bit.ly/2GMcrtg). Professor Leach discusses the importance of accurate scientific reporting, and reasons for the decline of specialised science journalists. She points out that, thankfully, 'as the number of science correspondents has fallen, the science sector has rushed in to fill the online void with blogs and social media sites'.

In answer to the reader's question, my opinion is that yes, we should be doing all we can to assist in the accurate portrayal of science in the mainstream media. How exactly to do this though, I honestly don't know. Ultimately, this is of critical importance, as more accurate reporting allows the public to make more informed decisions when it comes to things such as voting for our government, who creates and enforces policy.



Jeremy Just MRACI is a Hobart-based PhD candidate in organic chemistry and a passionate science communicator, specialising in chemistry shows and demonstrations.

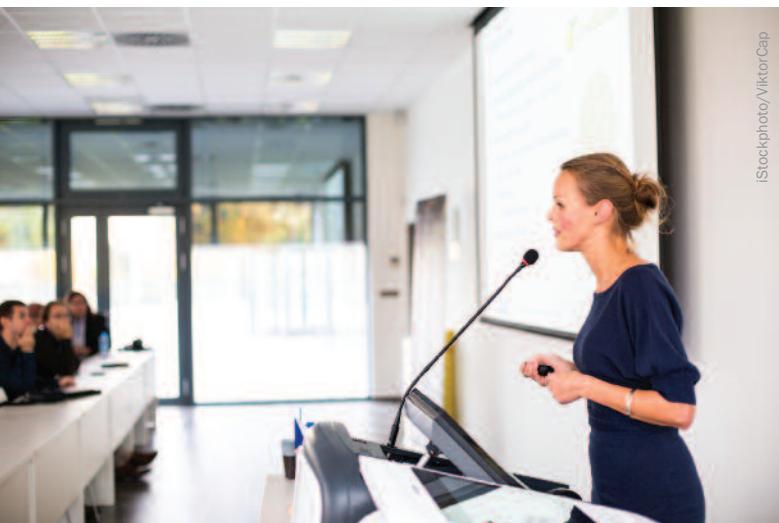
New research shows explaining things to ‘normal’ people can help scientists be better at their jobs

In times when fake news and alternative facts circulate in society, spreading scientifically based findings is more important than ever. This makes science communication one of academia’s most vital tasks. But despite the pivotal role scientific communication plays in society, communicating with the general public is not always prioritised among researchers.

This is in part because although scientists tend to be great at doing the research and discovering results, they are not always so great at then communicating these findings to a wider audience. Writing about research for people outside academia requires a wider perspective on science matters, and a completely different writing style. And many scientists may simply not know how to communicate their research to wider society. The low importance placed on this in the past, and the limited (if any) training students get in science education also isn’t helping.

This is short sighted, particularly as my recent study found, encouraging science students to write about their work for a non-academic audience helped them to discover and discuss different ideas within their thesis. And this in turn helped them to realise the importance and societal impact of their work.

... the students found it easier to deal with different perspectives and levels of abstraction in their scientific thesis after first having written a popular text on their degree project.



Science for dummies

The research showed that across their writing, the students successively added different aspects to their texts, to make it more relevant to a general audience. The students also changed the ways they discussed subject matter – from a specific, detailed level, to a more general, holistic interpretation. This meant that an overall wider societal perspective emerged along with the students’ writing process.

These findings are similar to an earlier study that looked at science students’ experiences of writing a popular science article on their degree project – at bachelor or masters level. Many of these students described how writing for non-academics helped them to create a ‘bigger picture’ of the subject and see what relevance their research project could have in a larger context.

Some of the students especially emphasised the popular writing helped them to clarify the aim of their project. Others pointed out how the writing made them reflect on their own knowledge and realise how much they had actually learned during their studies.

Lasting impact

In the recent study (<https://doi.org/10.1080/21548455.2017.1371355>), students also said they found that writing for a non-academic audience actually helped with their scientific writing. In particular, the students found it easier to deal with different perspectives and levels of abstraction in their scientific thesis after first having written a popular text on their degree project.

It is not hard to see how communication with different audiences can help scientists find connections to other disciplines and see the societal relevance of their own research. And in this way, training future scientists to communicate with different audiences could help to facilitate research and development across disciplinary borders.

It could also help to increase people’s knowledge and interest in science, thereby giving a higher likelihood of informed political decisions in society.

What all this shows is the huge potential science communication could have on learning, research and democracy. But to make use of this power, scientists need to be able to ‘zoom out’ and connect their research to the world outside. It also needs to be held up as one example of how new knowledge can be spread. Because ultimately it is by recognising and rewarding these efforts that new and original research could develop – as well as increasing the likelihood of scientific learning and literacy across society.

Susanne Pelger is a senior lecturer in science education, Lund University, Sweden. First published at theconversation.com.

Sterile filtration of wine

In the April issue (p. 40), I introduced wine filtration as a controversial issue, controversial because many regard filtration as introducing an industrial step in the process of making wine with minimal interference. James Halliday, writing in the *Australian Wine Companion*, comments that ‘sterile filtration is the most controversial form of what is a controversial subject at best [filtration generally], although the controversy is seldom created by winemakers; it is more frequently due to wine writers who have no practical knowledge of the subject’ (bit.ly/2FWEJlx).

Fighting words from Halliday perhaps. However, given the number of industry articles that address issues such as why and how, I am not sure that it is just wine writers who have an issue with filtration, especially sterile filtration. In essence, there are two stability issues that require filtration – physical stability and microbiological stability – the latter requiring sterile filtration. Matt Holdstock, an oenologist at the Australian Wine Research Institute, has published a succinct note on sterile filtration on the Wine Australia website (bit.ly/2tkqMef). Matt comments on the need for winemakers to know the wine composition when deciding when or if to filter. For example, residual sugar (glucose, fructose) and malic acid are classic food sources for yeasts and bacteria, thereby underlying the need for sterile filtration.

Among all the controversy regarding filtration, perhaps Matt Holdstock’s words are appropriate: ‘A well performed filtration of the appropriate grade will not have a negative effect on wine quality’.

The relationship between sterile filtration and winemaking practice raises a terminology issue. Many winemakers will pass their wine through a 0.45 μm filter and claim that it is a sterile filtration. There are some difficulties with this simple strategy. First, it is essential that the filter used has an ‘absolute’ pore size; that is, it is capable of removing 90–99% (manufacturer-dependent criterion) of particles at or above the stated pore size. Filters with a ‘nominal’ pore size of 0.45 μm may only retain 60% or more of particulate material at or above this pore size.

The second difficulty is that some bacteria in wine are smaller than 0.45 μm and so wine filtered through 0.45 μm

cannot be said to be truly sterile. Greg Howell MRACI CChem from Vintessential has described the terminology dilemma rather succinctly (bit.ly/2oQDnAA). Yeasts are generally between 5 and 10 μm , so relatively easy to remove by filtration. Bacteria are much smaller, with size or diameter depending on the shape. Spherical cocci, such as *Oenococcus oeni* and *Pediococcus*, have diameters between 0.5 and 3 μm , whereas the rod-shaped bacilli, such as in *Lactobacillus*, range from 0.2 to 2 μm . *Acetobacter*, the acetic acid producing organism, tends to be 0.6–0.8 μm .

Thus, there seems to be a need for a 0.2 μm standard to ensure that filtration produces a sterile product. I am not aware that this is used in routine winery processing and Greg Howell notes (bit.ly/2oQDnAA) that ‘many, if not most, winemakers have a great concern’ about filtration at this size, the argument being ‘that such fine filtration will most likely remove much of the positive attributes from the wine’.

With 13–15% alcohol wines that have low residual sugar, low pH, have been through malo-lactic fermentation and have a good sulfur dioxide regime, the chances of microbial spoilage without filtering are generally low. However, lower alcohol sweet wines with poor sulfur dioxide management are severely at risk of spoilage unless they are filtered before bottling.

Ensuring sterility in the bottled wine does involve more than good filtration. Even with the most careful filtration procedure, microbial contamination can still occur in the final step in preparing the wine for market, the bottling process. Bottling lines are notorious for harbouring yeasts and bacteria and even the occasional mould. Dr Tina Tran and colleagues from the AWRI have discussed the packing process in detail (see bit.ly/2ItTcGk). Good quality assurance practice is necessary to ensure cleanliness before passing the ‘sterile filtered’ wine through the line to the bottle. Hot water above 80°C is reasonably effective in sterilising the lines, as is steam containing caustic cleaning agents, provided all traces of caustic are removed before commencing bottling. Checking places where wine may be trapped, such as joins, seals and O-rings is always helpful to ensure that old wine has been removed prior to the next bottling run. Water used in the sterilisation process needs to be clean as well. Simple filtration of the water is usually sufficient. While microbial contamination can be checked by plating samples from the bottling wine onto a suitable growth medium and monitoring the growth of colonies, this is a slow process and not an overly useful routine quality check. None-the-less, good QA is far better than having the wine returned as ‘spoilt’ with consequent loss of customer satisfaction.



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‘Tort’ Jamieson

David Collins and I wrote the biographical memoir of Professor John Swan (1924–2015) for the Australian Academy of Science and it was published in *Historical Records of Australian Science*, 2017, vol. 28(1), pp. 58–65. Most chemists never see this journal, so if you are interested in this commemoration of the life and work of one of Australia’s leading chemists, let us know and we will provide an electronic copy.

Like many successful people, John mentioned that his career choice had been influenced by a teacher, in this case his chemistry teacher at Scotch College, Melbourne, one William Rotherham Jamieson (1871–1953), who taught at Scotch for 40 years before retiring in 1948. Jamieson had studied at the University College of Aberystwyth and University College Bristol before graduating BSc from the University of London in 1892 with honours in mathematics and physics. Migrating soon after, he taught at Queen’s School in North Adelaide and then at Roseworthy Agricultural College before coming to Scotch in 1908.

Swan recalled that Jamieson was always called – but not necessarily to his face – ‘Tort’, probably a reference to one of his tools of trade, the retort. A history of the school suggests that Jamieson’s profile, featuring a large nose and prominent Adam’s apple, reminded students of that glassware.

In 1917 Jamieson’s book *Australasian text book of chemistry. Part 1* was published locally. In his preface, Jamieson wrote that it was the first part of a complete course of chemistry for schools, covering a ‘two-year’s course for boys (and girls, too, for that matter) from the age of 14 to that of 16’. Atomic theory was not included, but deferred for inclusion in part 2, because Jamieson felt that it was impossible for a boy to grasp it adequately until he had mastered the material in part 1. When I got a copy out of the library, it seemed strangely familiar, and I realised that I had a copy of it, a copy so battered that the title page had been lost and so I was unaware of the author’s name.

Jamieson thanked his wife for reading the proof-sheets and making helpful suggestions, so I wondered if she might have been educated in chemistry, too. She also contributing the drawings (there were lots), and he wrote that ‘it was only after I had commenced to write this book that I realized her assistance in this direction to be indispensable for its satisfactory completion’.

In 1926, Jamieson published a different kind of book entitled *Elementary physical science*, in which he began his preface with ‘There is a strong body of opinion holding that the science courses of secondary schools are unduly specialized, and that breadth of culture is sacrificed to an intensive treatment that is out of place in the earlier stages, at least, of a boy’s education’. A.C.D. Rivett, Professor of Chemistry at the University of Melbourne, had read the text in proof and he provided an introduction in which he expressed broad

agreement with Jamieson’s views. Jamieson thanks a number of people from industry for helping with the text and illustrations, but perhaps most significantly credits ‘most of all’ a former pupil of his, C.W. Ross, who assisted with the compilation of the text to the extent that ‘whatever merit the book possesses is due in large measure to him’. Ross graduated in medicine and made his career in the Australian Army Medical Corps.

Jamieson wrote several other school chemistry texts, starting in the 1920s with several versions of junior and senior courses and culminating in 1941 with *Revision chemistry for schools*. It was quite short and contained no equations or diagrams. It concentrated on the language of chemistry and Jamieson wrote that it was intended ‘to help students integrate their work, as so many of them fail to see the wood for the trees’.

When he retired in 1948, Jamieson’s students composed a tribute for him that found its way into the school history. Probably sung to an unidentified tune, it contains hints of the lecture room (where Tort was known for his Latin aphorisms) and the laboratory:

In the dry way, in the wet way,
Testing for an unknown salt,
A priori, fortiori
In the customary way.

Chorus:

Test for chloride, test for nitrate, Test for sulphate, arsenate,
‘Tisn’t sulphide or hydroxide –
Would it not make one irate!

Sublimation, condensation
Avogadro, Berthollet,
Saturation, titration
Dalton and Lavoisier

Chorus

Oxidation, levigation
Is it arsenic or lime?
Perspiration, resignation,
Try again another time!

At the 1907 Congress of the Australasian Association for the Advancement of Science, held in Adelaide, Jamieson gave a talk about educational methods in the teaching of mathematics and science. Rosemary Polya’s comment, in her 1986 review of science textbooks, noted that the advanced ideas he expressed in Adelaide were like those of modern educationalists. However, she described his chemistry textbooks as ‘virtually recipe books’ but did acknowledge that he had always stressed the need for teaching because the textbook alone was not sufficient.



Ian D. Rae FRACI CChem (idrae@unimelb.edu.au) is a veteran columnist, having begun his Letters in 1984. When he is not compiling columns, he writes on the history of chemistry and provides advice on chemical hazards and pollution.

events

ALTA 2018 – Nickel-Cobalt-Copper, Uranium-REE & Gold-PM Conference & Exhibition

19–26 May 2018, Perth, WA
altamet.com.au/conferences/alta-2018

AOCR-5 – 5th Asian & Ocean Regional Congress on Radiation Protection

20–23 May 2018, Melbourne, Vic
aocrp-5.org

Units 3 & 4 Chemistry Extended Practical Investigation Made Easier

30 May 2018, Monash University, Vic
ivvy.com.au/event/VCG774

22nd Annual Green Chemistry & Engineering Conference

18–20 June 2018, Portland, Oregon, USA
gcande.org

Macro 18 – World Polymer Congress

1–5 July 2018, Cairns, Qld
macro18.org

ICCE2018 – International Conference on Chemical Education

10 July 2018, University of Sydney, NSW
ivvy.com.au/event/CED681

ICCE 2018 – 9th International Conference on Chemistry and Chemical Engineering

11–18 July 2018, University of Liverpool, Liverpool, UK
icce.org

ICABC 2018 – 5th International Conference on Advances in Biology and Chemistry

6–8 August 2018, National Taipei University of Technology, Chemical Engineering & Biotechnology, Taipei, Taiwan
icabc.org

8th IUPAC International Conference on Green Chemistry

9–14 September 2018, Bangkok, Thailand
greeniupac2018.com

8th International Conference on Environmental Chemistry and Engineering

20–22 September 2018, Berlin, Germany
environmentalchemistry.conferenceseries.com

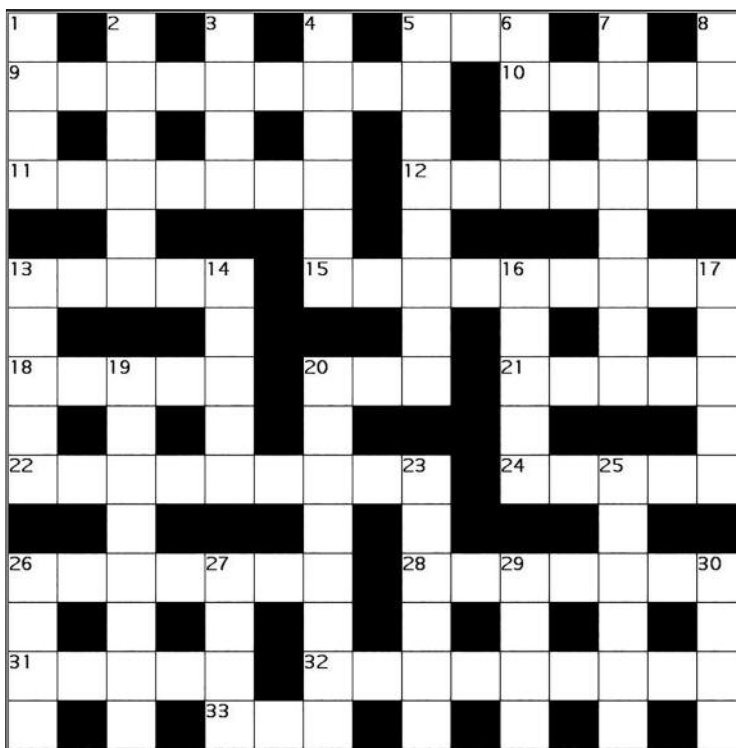
CBEE 2018 – 10th International Conference on Chemical, Biological and Environmental Engineering

27–29 September 2018, Hotel Berlin, Berlin, Germany
icbee.org

Organic 18 – 24th RACI Organic Chemistry Conference
2–6 December 2018, University of Western Australia, WA
ivvy.com.au/event/OGD780

RACI events are shown in blue.

cryptic chemistry



Across

- 5** Reference conditions for $\text{Na}_5\text{P}_3\text{O}_{10}$. (1.1.1.)
9 Mathematician re bullion grab. (9)
10 Two acyl groups bound to nitrogen initially in massive international development exercise. (5)
11 Streets broken up by scientists. (7)
12 Nucleobase held back during the nine days. (7)
13 Entertains crowds. (5)
15 Soap humor fails without long-range order. (9)
18 Activates ionic inclusion over unwanted disturbance. (5)
20 Made from the last three 11 Across with little residue. (3)
21 Associate with first legitimate $\text{H}_2\text{C}=\text{CH}-\text{CH}_2-$. (5)
22 Elements 89 to 103 feign inside change. (9)
24 Gives 1 + 16. (5)
26 Recipe for my upload alternate. (7)
28 Flame crime wave which is short-lived. (7)
31 Mount graduated system. (5)
32 Held carbon on detain order. (9)
33 Egg masses loudly to make a side by side arrangement. (3)

Down

- 1** A wager to encourage criminal behaviour. (4)
2 Combs ridges. (6)
3 Pointed head makes 6 + 1. (4)
4 Ionised state as lamp breaks. (6)
5 Sulfur ions all lead to examples of $\text{R}_3\text{Si}-\text{OH}$. (8)
6 π -polyethylene duct? (4)
7 $\text{RC}(\text{NR}')-$ bonded to a nitrogen ion dimly burning. (1-7)
8 Two element code. (4)
13 Bird with sodium dye. (5)
14 Two elements and another put back patina. (5)
16 An element for every pleasing person. (5)
17 Good person came back on two elements compounds. (5)
19 Four elements within. (8)
20 Happiness of 14 Down. (8)
23 13 Down drops hydrogen for silicon pigment. (6)
25 Putting tag on selection. (6)
26 Quick time pursuing two elements. (4)
27 Consumer of three elements. (4)
29 Scorch three elements. (4)
30 Bars poles. (4)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University. Solution available online at Other resources.



Invitation to ANCQ 2018

The RACI invites all students to participate in the ANCQ 2018, being held in Australia on Thursday 2 August 2018.

The quiz has been in operation since 1982, growing from humble beginnings into an international event spread over 21 countries, seven languages, 1400 schools and more than 100 000 students.

The ANCQ is a unique chemical education activity.

It provides a major focus for secondary school students on the relevance of chemistry in an exciting and stimulating way. It is not a nationwide assessment of chemistry knowledge, but rather a promotion of chemistry that allows teachers and students to gauge their level of teaching and learning.

The quiz comprises 30 multiple-choice questions and takes one hour to complete. It is available both in hard copy and online.



**Registrations close:
Friday 8 June 2018**

Entry cost: \$6 per student

Website: www.ancq.com

For further information,
including quiz dates for other
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