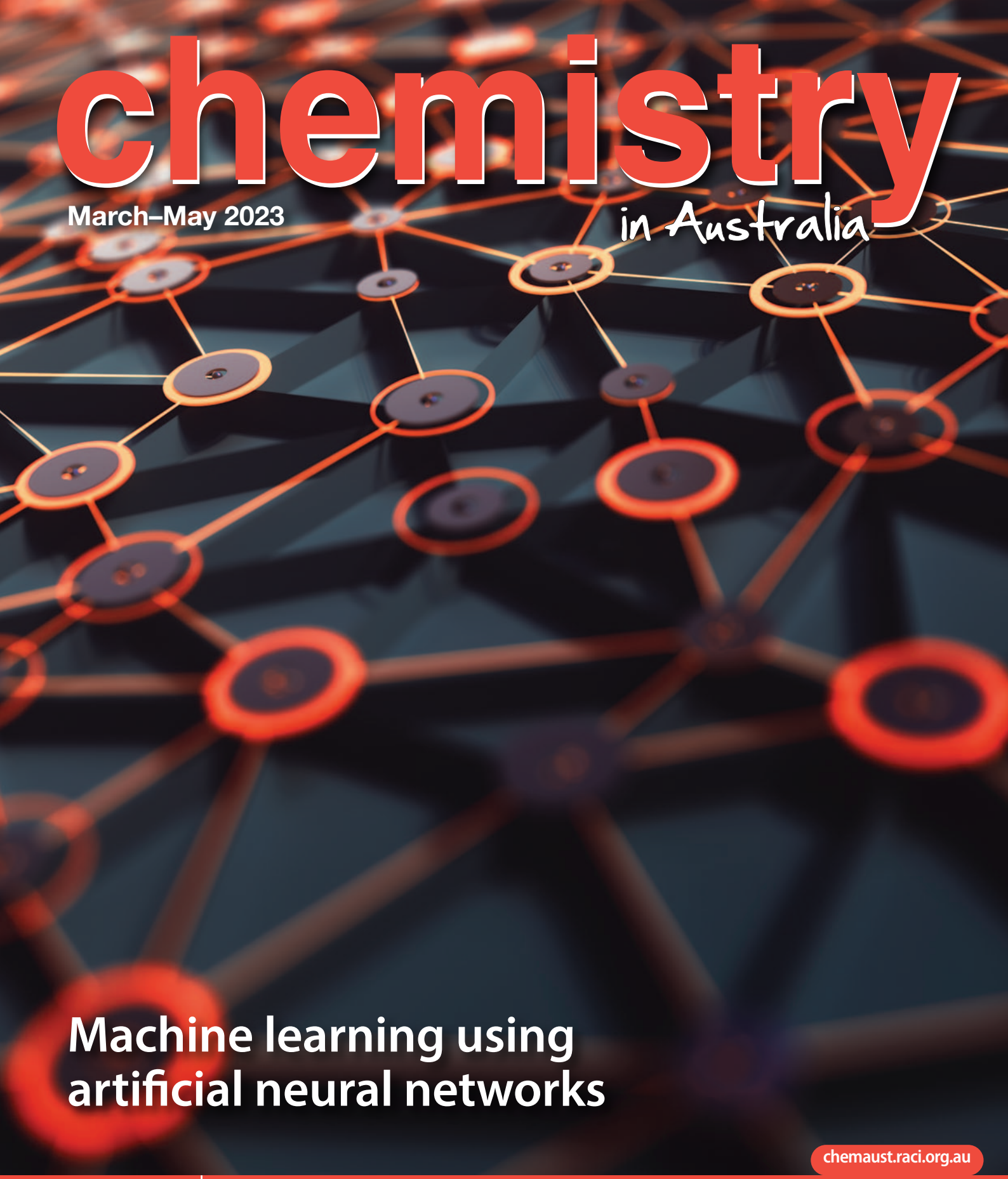
chemistry in Australia

March–May 2023



Machine learning using artificial neural networks

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- Reverse osmosis and Australia's water security
- A remedy for fragmentation in our chemical organisations
- A decade of RACI Careers and Mentoring

chemistry in Australia

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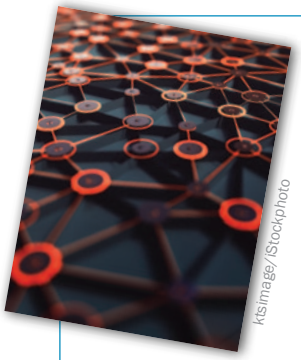

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Machine learning: a shortcut in fluorescent polymer selection

The first commercial LED lights came out in the 1960s, but it wasn't until the colour could be fully tuned, nearly 40 years later, that their full utility was realised. Recent work aims to do the same thing for fluorescent polymers and other novel materials, but in a fraction of the time, using machine learning.

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LSD – ageing of a 'problem child'

On 19 April this year, Bicycle Day (not to be confused with UN World Bicycle Day on 3 June) marks 80 years since an unusual bicycle ride made by Swiss chemist Albert Hofmann after his first intentional dose of lysergic acid diethylamide (LSD).

Five years before that ride, while continuing work begun by biochemist Arthur Stoll (a senior colleague at Sandoz Laboratories) on isolating ergot alkaloids, Hofmann accidentally absorbed a lysergic acid derivative through his skin. What followed, wrote Hofmann in *LSD: my problem child* (bit.ly/3XFAeCJ) were a couple of hours of 'fantastic pictures, extraordinary shapes with intense, kaleidoscopic play of colors'.

Ergot is the common name for fungi of the genus *Claviceps*, which attack cereal crops such as rye. The medicinal properties of ergot extracts have been exploited for centuries, and Hofmann was investigating the pharmaceutical potential of ergot alkaloids using one of their key constituents, lysergic acid, as a starting point.

Archives of Hofmann's research are now housed at the Institute for the History of Medicine in Bern, and the project 'From Ergo to LSD' (2015–2019), funded by the Swiss National Science Foundation, aimed to address some important gaps in the drug's story.

Bern University associate researcher Beat Bächi, author of *LSD in the country: production and collective action of psychotropic substances* (Konstanz University Press, 2020), described the background to the project (bit.ly/40Az8u5):

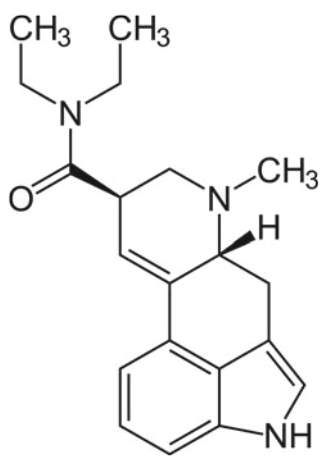
> *What is completely lacking so far [in the story of LSD] is a history of the production of the starting material for LSD production, namely ergot. The selection, breeding and cultivation of appropriate types of grain as well as the vaccination, production and harvesting of the ergot show the complexity of producing a psychotropic substance in the field, so to speak. Only numerous negotiation processes between industrial research, science and agriculture made LSD and other products based on ergot possible.*

Producing LSD from ergot was just one of many complexities in this story. In the 1960s, widespread misuse of LSD and other psychedelics prompted strong government interventions, and the early 1970s saw previously burgeoning psychedelics research virtually cease.

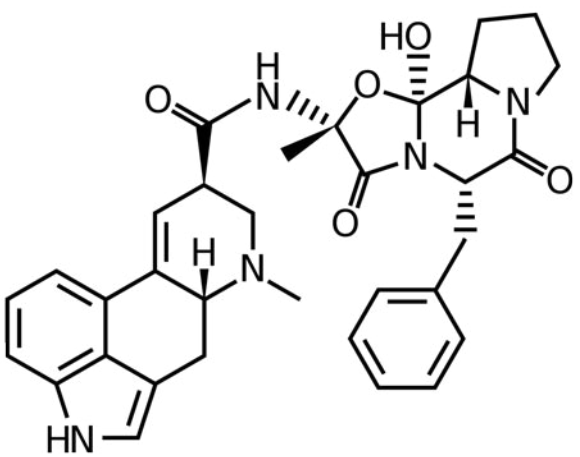
In a recent article in *Psychological Medicine*, Wayne Hall, Emeritus Professor at the National Centre for Youth Substance Use Research and Queensland Alliance for Environmental Health Sciences, reported that 'The demise of psychedelic drug research was not solely due to the "War on Drugs". It was hastened by tighter regulation of pharmaceutical research, the failure of controlled clinical trials to live up to the claims of psychedelic advocates, and the pharmaceutical industry's lack of interest in funding clinical trials' (bit.ly/3wwAgkw).

Although Hofmann's unintentional LSD dose in the lab produced pleasant effects, his intoxicated bicycle ride in April 1943 was the beginning of a bad trip in every sense – Hofmann's experience, described in his book, featured 'wicked creatures' and he felt 'demonically possessed'. After Hofmann's arrival at home, a kindly neighbour appeared as a 'malevolent, insidious witch with a colored mask'.

Although Hofmann's unintentional LSD dose in the lab produced pleasant effects, his intoxicated bicycle ride in April 1943 was the beginning of a bad trip in every sense ...



Lysergic acid diethylamide (LSD-25), Hofmann's 25th lysergic acid derivative. NEUROtiker, Public domain, via Wikimedia Commons



Ergotamine, an alkaloid first extracted by Arthur Stoll. Benrr101, Public domain, via Wikimedia Commons

In his foreword to *LSD: my problem child*, Hofmann remarked on both the potential help and harm of this psychedelic:

> *I share the belief of many of my contemporaries that the spiritual crisis pervading all spheres of Western industrial society can be remedied only by a change in our world view. We shall have to shift from the materialistic, dualistic belief that people and their environment are separate, toward a new consciousness of an all-encompassing reality …*
>
> *… LSD finds such an application in medicine, by helping patients in psychoanalysis and psychotherapy to perceive their problems in their true significance.*
>
> *Deliberate provocation of mystical experience, particularly by LSD and related hallucinogens, in contrast to spontaneous visionary experiences, entails dangers that must not be underestimated.*

In the year before Hofmann's death in 2008 at the age of 102, Swiss physician for psychiatry and psychotherapy Peter Gasser commenced psychotherapeutic experiments on patients with life-limiting diseases such as cancer, with the approval of Swiss medical authorities and a positive reception by Hofmann. After more than three decades, studies into the therapeutic uses of LSD were again underway.

In Australia, current clinical trials are investigating the use of a range of psychedelic substances as part of treatment for depression, opioid addiction and late-stage cancer, among others. On 3 February, the Therapeutic Goods Administration announced that 'from 1 July this year, medicines containing the psychedelic substances psilocybin and MDMA (3,4-methylenedioxy-methamphetamine) can be prescribed by specifically authorised psychiatrists for the treatment of certain mental health conditions' (bit.ly/3Rw4wWr). This follows applications and public submissions calling for these to be rescheduled in the context of medical use (from prohibited substances to controlled drugs) in the Poisons Standard.

Sally Woollett
(editor@raci.org.au)

Readings and reflections

As usual, the December 2022 – February 2023 issue was full of interesting and readable articles. *Chemistry in Australia* is one of the great assets and benefits of RACI membership, but it is a pity that it is now only four times a year. Following are some comments on several articles that I related to.

Firstly, I was saddened to read about the demise of John Lane. I also started work at the CSIRO Division of Physical Chemistry in Fishermens Bend in 1965, albeit as a junior technical assistant, where a favourite past-time was watching construction of the West Gate Bridge. I remember John as a quiet and gentle but approachable scientist, in contrast to Bill Mansfield who was more outgoing but also easy to talk with. Bill told us that the problem with the film to prevent evaporation of lakes and dams was that wind caused waves to break up the film coating.

Secondly, re Ian Rae's article 'Poisoned underpants?', I also suffered as a child with a sensitivity to woollen underwear, with skin rashes etc. However, my mother also discovered that a contributing factor was the washing powders available in Australia in the 1950s; some were very harsh and added to my sufferings. Today's washing detergents are much gentler and better formulated, often developed for sensitive skins, with many thanks to the development team with Peter Strasser of Albright & Wilson. Peter and I worked together in the 1970s on trying to get a 'freshly laundered aroma' impregnated into newly washed clothes.

Thirdly, re the International Day of People with Disability, I have spent the last six years volunteering with young adults with a disability who are training to gain employment, mainly hospitality. Although the article was interesting, I consider that some examples of the people with disabilities who are actually working in STEM-related occupations would have enhanced it.

Lastly, my thanks to Geoff Scollary for his many years of wine articles. I have not always agreed with his jottings, particularly regarding the large number of food additives and processing aids permitted in a beverage that is regarded as 'natural', but I was grateful for the opportunity to learn more about the intricate details of the science and art of winemaking. I spent many years servicing the wine area and related products areas with flavours and food additives, but usually wine makers are reluctant to reveal their secrets; not so Geoff.

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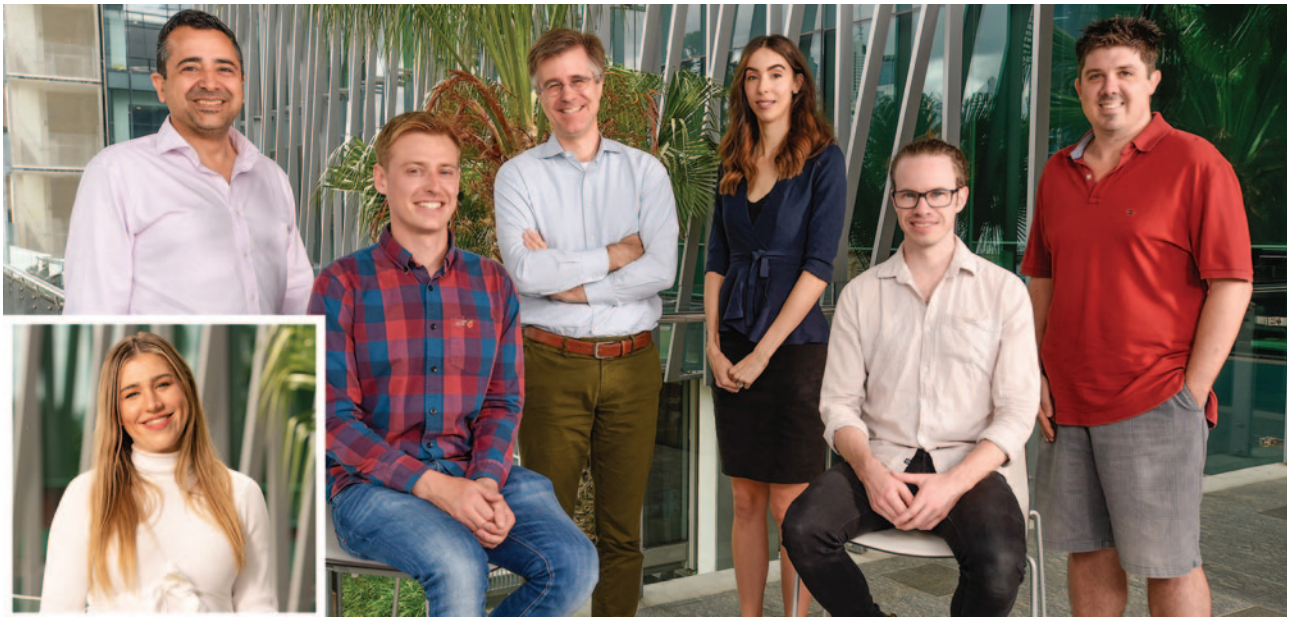
Tackling plastic pollution with law and chemical coding



Dr Hope Johnson (inset). From left: Professor Afshin Akhtar-Khavari, Dr Joshua Holloway, Distinguished Professor Christopher Barner-Kowollik, Annastasia Bousgas, Lewis Chambers and Associate Professor James Blinco.

An innovative proposal to tackle the global plastic pollution crisis with a combination of DNA-like encoding of plastics and international law has been put forward by a transdisciplinary team of Queensland University of Technology researchers.

Plastic pollution has been identified as an environmental problem similar in scope and complexity to global challenges such as climate change.

The team, from chemistry and law, have published their approach in *Polymer Chemistry* (doi.org/10.1039/D2PY01180H).

The researchers are Dr Hope Johnson, Dr Lewis Chambers, Dr Joshua Holloway, Annastasia Bousgas, Professor Afshin Akhtar-Khavari, Associate Professor James Blinco, and ARC Laureate Fellow Professor Christopher Barner-Kowollik, and they are part of QUT's Centre for Materials Science and Centre for a Waste Free World.

Barner-Kowollik said one of the biggest challenges was tracing the polluting plastic back to the source, which resolves the anonymity of plastic waste.

'If a technology existed that allowed us to give unique "DNA" to each batch of plastic that was produced, plastic waste could be traced back to the producer, given the information stored in the "DNA" could be simply read-out.'

Barner-Kowollik said that several emerging advances in polymer chemistry could play a part in identifying plastic.

One solution could be chemically labelling batches of plastic production using sequence-defined polymers, that could be decoded in a way similar to DNA, although at this point reading information from sequence-defined polymers is challenging. However, new and simple technologies for reading information from such sequence-defined polymers embedded into plastics are emerging.

If polymer science can develop the means of uniquely identifying plastics and tracing each piece back to its producer, there still remains the issue of enforcing responsibility – which is where the legal researchers around Johnson come in.

'One of the first challenges with an international problem such as this is the obvious one of jurisdiction, and also where in the regulatory process we can best intervene to create sustainable change', Akhtar-Khavari said.

'A considerable challenge is the implementation in international frameworks so that malicious actors cannot identify loopholes

'A careful and coordinated international approach is of the essence, yet establishing it will require initial careful research into the underpinning international governance principles and subsequent coordinated approaches for implementation.'

The researchers describe their paper as a 'discussion starter', not only on the plausibility of using sequence-defined polymers for coding and reading 'DNA' embedded in plastics and the associated governance challenges, but also for a broader conversation.

'Research is done with focus, but sometimes there needs to be a broader lens', Barner-Kowollik said.

'There is a critical need for the social and natural sciences to work more closely together in the future, breaking currently still prevailing siloed structures.'

The combined approach, of polymer science and international law, is looking at the single outcome of enforcing responsibility on polluters.

The paper says that identifying the people responsible for the plastic pollution could lead to a phasing out of plastics.

Queensland University of Technology

Speeding up sugar's conversion to fuel

Researchers have found a way to more efficiently convert sugarcane into a building block of aviation fuel and other products. By zeroing in on a specific enzyme, a University of Queensland team working in collaboration with the Technical University of Munich has sped up the slowest step in processing sugar into isobutanol.

Professor Gary Schenk said isobutanol from a renewable resource could be used to make fuels, plastics, rubbers and food additives.

'Our research into this particular enzyme means we can accelerate the production rate and yield of isobutanol from sugarcane, ultimately enabling biomanufacturers to make diverse products at scale sustainably and efficiently', Schenk said.

'Usually during a biomanufacturing process, cells such as yeasts are used as a production platform, but in our research only a small number of a sugar acid-specific dehydratase enzyme was used.

'Having sugar-converting enzymes operate outside a cellular environment meant we could bypass many of the pitfalls of the more traditional cell-based biomanufacturing methods.

'This has led to much higher yields of isobutanol with fewer unwanted side products.'

Cell-based production of isobutanol from sugar creates about 25 grams per litre of liquid cell culture but in this study, the cell-free method produced at least 10 times that amount.

'The cell-free method gives biomanufacturers more control and results in much higher yields, meaning a higher return on their investment and a more sustainably produced product – it's a win-win', Schenk said.

'One limitation in creating bulk products like aviation fuel with a cell-free process has been the availability of enough enzymes, but developments in enzyme engineering and production mean large-scale production is now achievable.

'We're only at the dawn of what is a very exciting age in this space.'

Rufino Uribe

Professor Damian Hine from the university's Queensland Alliance for Agriculture and Food Alliance said the research proved the enormous potential of cell-free biomanufacturing.

'While there have been commercial limitations to producing the enzymes, we now have enough evidence to show that large-scale manufacturing using the cell-free enzymes process is commercially viable and should play a major role in future biomanufacturing', he said.

This research is published in *Chemistry – a European Journal* (doi.org/10.1002/chem.202203140).

University of Queensland

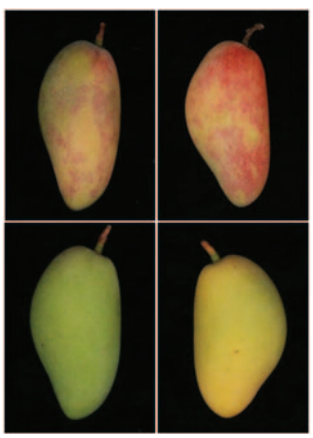
Blue light means sweeter mangoes

Researchers report in the *Journal of Agricultural and Food Chemistry* (doi.org/10.1021/acs.jafc.2c07137) that mangoes can become redder, sweeter and more ripe when exposed to blue light over several days.

Plants rely on sunlight to carry out photosynthesis and ripen their fruits. Studies have shown that exposure to light can affect the appearance of some fruits' peels and can increase the amount of sugar and pigments in fruits such as tomatoes, which contain chlorophyll throughout their flesh. However, other fruits such as mangoes only contain this pigment in their thick peels, which could change how light affects the flesh. Plus, sunlight contains many colours, so different wavelengths could have different effects.

Yuanwen Teng and colleagues wanted to investigate how blue light affects the quality and ripeness of mangoes. They placed a group of mangoes in blue light and another group in darkness for nine days. They found that mangoes in blue light contained far more anthocyanins in their peels, making them redder than those left in the dark. The flesh of these mangoes was also softer, sweeter and more yellow, and had more sucrose and carotenoids than the other group.

In further tests, the team found that light-responsive genes involved in the photosynthesis pathway, as well as key genes involved in producing sucrose, anthocyanin and carotenoids, were upregulated under blue light. This meant that the mangoes could directly perceive this light and trigger an internal genetic signalling pathway, say the researchers. The effect was more pronounced in the peel than in the flesh, indicating that the blue light did not penetrate much past the skin. The researchers say that this work could help explain on the complex relationship behind coloured light and the internal quality of fruit.



Mangoes exposed to blue light over several days were redder and sweeter (top) than those placed in the dark (bottom).

Adapted from the *Journal of Agricultural and Food Chemistry*, doi.org/10.1021/acs.jafc.2c07137

American Chemical Society

Long-life electrode material for solid-state batteries

Scientists have developed a positive electrode material that doesn't diminish after repeated charging cycles, for the manufacture of durable solid-state batteries.

Electric cars are widely regarded as our best bet to replace conventional cars with a more environmentally friendly alternative. However, electric cars and other electric vehicles will most likely run on lithium-ion batteries, which currently don't deliver the necessary performance and durability at a reasonable price.

Solid-state batteries (SSBs), however, have gained much traction over the past few years among researchers looking for alternatives. While conventional lithium-ion batteries contain a liquid electrolyte in which lithium ions flow during the charge/discharge process, SSBs are made entirely from solid materials. Besides a massive improvement in operational safety – since these batteries won't spill toxic liquids when punctured – SSBs can be charged much more quickly.

But until now, a problem has limited their durability. When lithium ions are inserted into or extracted from the electrodes of the battery, the crystalline structure of the material changes, making the electrode expand or shrink. These repeated changes in volume damage the interface between the electrodes and the solid electrolyte and cause irreversible alterations in the crystal chemistry of the electrodes.

A team of scientists led by Professor Naoaki Yabuuchi of Yokohama National University, Japan, investigated a new type of positive electrode material with unprecedented stability in SSBs. Their work, which was published in *Nature Materials* (doi.org/10.1038/s41563-022-01421-z), was co-authored by Associate Professor Neeraj Sharma from the University of New South Wales and Dr Takuhiro Miyuki from LIBTEC, Japan.

The material was $Li_8/7Ti_2/7V_4/7O_2$, a binary system composed of optimised portions of lithium titanate (Li_2TiO_3) and lithium vanadium dioxide ($LiVO_2$). When ball-milled down to an appropriate particle size in the order of nanometres, this material offers high capacity thanks to its large quantity of lithium ions that can be reversibly inserted and extracted during the charge/discharge process.

Unlike other positive electrode materials, $Li_8/7Ti_2/7V_4/7O_2$ has nearly the same volume when fully charged and fully discharged. The researchers concluded that this property is the result of a fine balance between two independent phenomena that occur when lithium ions are inserted or extracted from the crystal.

Although the removal of lithium ions, or 'delithiation', causes an increase in free volume in the crystal, which makes it shrink, some vanadium ions migrate from their original position to the spaces left behind by the lithium ions, acquiring a higher oxidation state in the process. This causes a repulsive interaction with oxygen, which in turn produces an expansion of the crystal lattice.

'When shrinkage and expansion are well balanced, dimensional stability is retained while the battery is charged or discharged, i.e. during cycling', Yabuuchi said.

'We anticipate that a truly dimensionally invariable material – one that retains its volume upon electrochemical cycling – could be developed by further optimising the chemical composition of the electrolyte.'

The research team tested this new positive electrode material in an all-solid-state cell by combining it with an appropriate solid electrolyte and a negative electrode. This cell exhibited a remarkable capacity of 300 mA h g^{-1} with no degradation over 400 charge/discharge cycles.

By further refining dimensionally invariant electrode materials, it may soon be possible to manufacture batteries that are good enough for electric vehicles in terms of price, safety, capacity, charging speed, and lifespan.

'The development of long-life and high-performance solid-state batteries would solve some of the problems of electric vehicles', Yabuuchi said. 'For instance, it may be possible to fully charge an electric vehicle in as little as five minutes.'

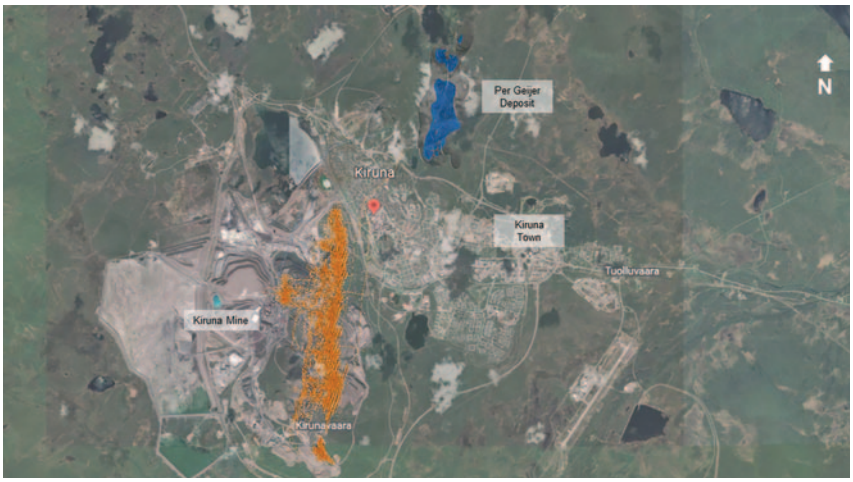
University of New South Wales

Europe's largest deposit of rare earth found in Sweden

Swedish company LKAB has identified significant deposits of rare earth elements at the Per Geijer deposit near Kiruna in far north Sweden. Mineral resources of rare earth metals exceeding one million tonnes of rare earth oxides, the largest known deposit of this kind in Europe, have been reported.

No rare earth elements are currently mined in Europe, and demand is expected to increase dramatically as a result of electrification, which will lead to a global undersupply, and this at a time of increasing geopolitical tensions. According to the European Commission's assessment, the demand for rare earth elements for electric cars and wind turbines, among others, is expected to increase more than fivefold by 2030.

LKAB has already started to prepare a drift in Kiruna's nearby LKAB iron ore mine towards the new deposit in order to investigate it at depth and in detail.



More extensive studies show an increase from 400 million tonnes of mineral resources with high iron content to over 500 million tonnes, and that the Per Geijer deposit contains up to seven times the grade of phosphorus as the orebodies that LKAB mines in Kiruna today. Phosphorus is one of three nutrients in mineral fertilisers necessary for food production and is on the EU's list of critical minerals. The rare earth elements in Per Geijer occur together with phosphorus in the mineral apatite, in what is mainly an iron ore deposit and which may therefore be by-products.

LKAB

Magnetic method to clean PFAS-contaminated water

Researchers at the University of Queensland have pioneered a simple, fast and effective technique to remove perfluoroalkyl and polyfluoroalkyl substances (PFAS) from water.

Using a magnet and a reusable absorption aid that they developed, polymer chemist Dr Cheng Zhang and PhD candidate Xiao Tan at the Australian Institute for Bioengineering and Nanotechnology have cleared 95% of PFAS from contaminated water in under a minute.

'Removing PFAS chemicals from contaminated waters is urgently needed to safeguard public and environmental health', Zhang said.

'But existing methods require machinery like pumps, take a lot of time and need their own power source.

'Our method shows it is possible to remove more of these chemicals in a way that is faster, cheaper, cleaner, and very simple.

'Because our process does not need electricity, it can be used in remote and off-grid communities.'

PFAS substances are synthetic compounds used in industry and consumer products since the 1950s, but they persist in the environment, potentially leading to human health problems.

The PFAS removal technique developed by Zhang and Tan involves treating contaminated water with a new solution, called a magnetic fluorinated polymer sorbent.

PhD candidate Xiao Tan holds a magnet attracting PFAS particles to the side of a vial of contaminated water, watched by Dr Cheng Zhang.

'This solution that we developed coats the PFAS particles and then we can use a magnet to attract, isolate and remove them', Zhang said.

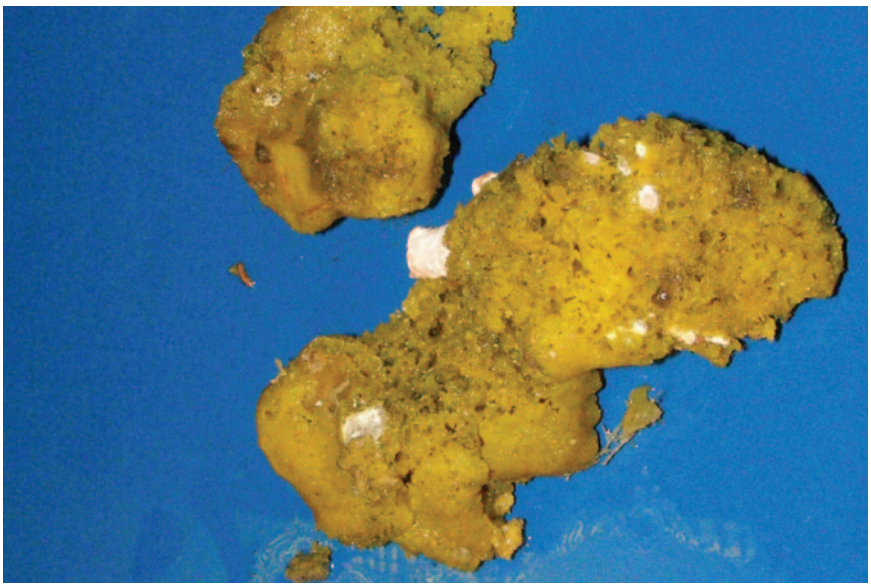
'The solution itself can be reused up to 10 times.

'Our team will now scale up the testing and we hope to have a commercially available product ready in the next three years.'

The study has been published in *Angewandte Chemie* (doi.org/10.1002/anie.202213071).

University of Queensland

Ocean-based molecule could fight Parkinson's



Lissodendoryx florida (PIBOC 047-283).
Photo by spongiologist Vladimir B. Krasokhin. Provided by Sophia Kolesnikova, G.B. Elyakov Pacific Institute of Bioorganic Chemistry

... lissodendoric acid A, appears to counteract other molecules that can damage DNA, RNA and proteins and even destroy whole cells.

Organic chemists at the University of California, Los Angeles have created the first synthetic version of a molecule recently discovered in a sea sponge that may have therapeutic benefits for Parkinson's disease and similar disorders. This molecule, lissodendoric acid A, appears to counteract other molecules that can damage DNA, RNA and proteins and even destroy whole cells. The findings are published in *Science* (doi.org/10.1126/science.ade0032).

And in an interesting twist, the research team used an unusual, long-neglected compound called a cyclic allene to control a crucial step in the chain of chemical reactions needed to produce a usable version of the molecule in the lab – an advance they say could prove advantageous in developing other complex molecules for pharmaceutical research.

'The vast majority of medicines today are made by synthetic organic chemistry, and one of our roles in academia is to establish new chemical reactions that could be used to quickly develop medicines and molecules with intricate chemical structures that benefit the world', said Neil Garg, UCLA's Kenneth N. Trueblood Professor of Chemistry and Biochemistry and corresponding author of the study.

A key factor complicating the development of these synthetic organic molecules, Garg said, is called chirality, or 'handedness'. Many molecules – including lissodendoric acid A – can exist in two distinct forms that are chemically identical but are 3D mirror images of each other, like a right and left hand. Each version is known as an enantiomer.

When used in pharmaceuticals, one enantiomer of a molecule may have beneficial therapeutic effects while the other may do nothing at all – or even prove dangerous. Unfortunately, creating organic molecules in the laboratory often yields a mixture of both enantiomers, and chemically removing or reversing the unwanted enantiomers adds difficulties, costs and delays to the process.

To address this challenge and quickly and efficiently produce only the enantiomer of lissodendoric acid A that is found almost exclusively in nature, Garg and his team employed cyclic allenes as an intermediate in their 12-step reaction process. First discovered in the 1960s, these highly reactive compounds had never before been used to make molecules of such complexity.

'Cyclic allenes', Garg said, 'have largely been forgotten since their discovery more than half a century ago. This is because they have unique chemical structures and only exist for a fraction of a second when they are generated.'

The team discovered that they could harness the compounds' unique qualities to generate one particular chiral version of cyclic allenes, which in turn led to chemical reactions that ultimately produced the desired enantiomer of the lissodendoric acid A molecule almost exclusively.

While the ability to synthetically produce an analogue of lissodendoric acid A is the first step in testing whether the molecule may possess suitable qualities for future therapeutics, the method for synthesising the molecule is something that could immediately benefit other scientists involved in pharmaceutical research, the chemists said.

Holly Ober, University of California

Recyclable mobile phone batteries a step closer with rust-busting invention

Mobile phone batteries with a lifetime up to three times longer than today's technology could be a reality thanks to an innovation led by engineers at RMIT University.

Rather than disposing of batteries after two or three years, we could have recyclable batteries that last for up to nine years, by using high-frequency sound waves to remove rust that inhibits battery performance, the team says.

Only 10% of used handheld batteries, including for mobile phones, are collected for recycling in Australia, which is low by international standards. The remaining 90% of batteries go to landfill or are disposed of incorrectly, which causes considerable damage to the environment.

The high cost of recycling lithium and other materials from batteries is a major barrier to these items being reused, but the team's innovation could help to address this challenge.

The team is working with a nanomaterial called MXene, a class of materials they say promises to be an exciting alternative to lithium for batteries in the future.

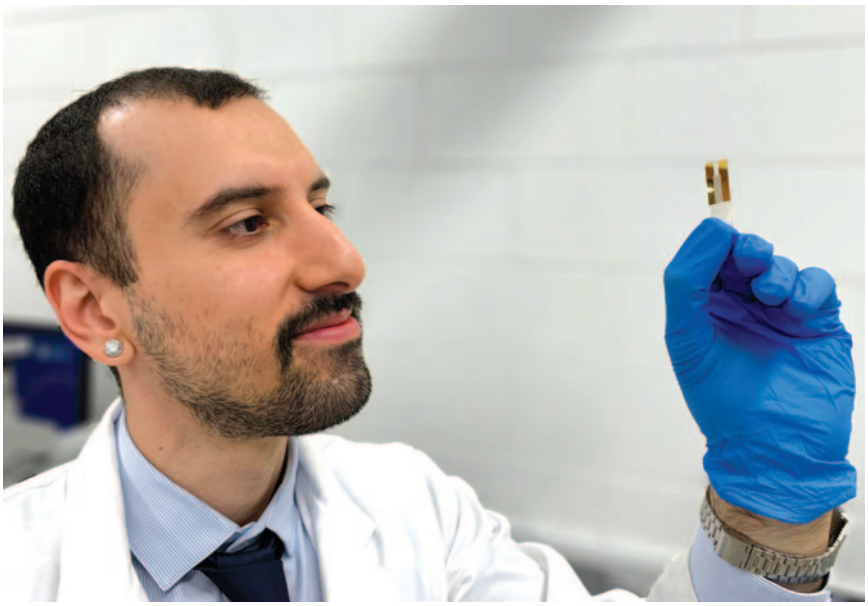
Leslie Yeo, Distinguished Professor of Chemical Engineering and lead senior researcher, said MXene was similar to graphene with high electrical conductivity.

'Unlike graphene, MXenes are highly tailorable and open up a whole range of possible technological applications in the future', said Yeo.

The big challenge with using MXene was that it rusted easily, thereby inhibiting electrical conductivity and rendering it unusable, he said.

'To overcome this challenge, we discovered that sound waves at a certain frequency remove rust from MXene, restoring it to close to its original state.'

The team's innovation could one day help to revitalise MXene batteries every few years, extending their lifetime up to three times, he said.



Mr Hossein Alijani with the new rust-busting device. RMIT University

'The ability to prolong the shelf life of MXene is critical to ensuring its potential to be used for commercially viable electronic parts', Yeo said.

Co-lead author Mr Hossein Alijani, a PhD candidate, said the greatest challenge with using MXene was the rust that forms on its surface in a humid environment or when suspended in watery solutions.

'Surface oxide, which is rust, is difficult to remove especially on this material, which is much, much thinner than a human hair', said Alijani.

'Current methods used to reduce oxidation rely on the chemical coating of the material, which limits the use of the MXene in its native form.

'In this work, we show that exposing an oxidised MXene film to high-frequency vibrations for just a minute removes the rust on the film. This simple procedure allows its electrical and electrochemical performance to be recovered.'

The team says their work to remove rust from MXene opens the door for the nanomaterial to be used in a wide range of applications in energy storage, sensors, wireless transmission and environmental remediation.

Associate Professor Amgad Rezk, one of the lead senior researchers, said the ability to quickly restore oxidised materials to an almost pristine state represented a gamechanger in terms of the circular economy.

'Materials used in electronics, including batteries, generally suffer deterioration after two or three years of use due to rust forming', said Rezk.

'With our method, we can potentially extend the lifetime of battery components by up to three times.'

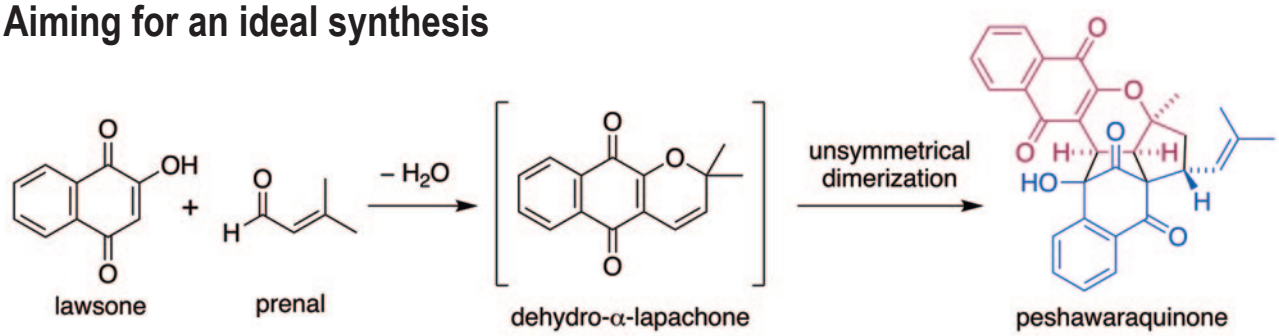
While the innovation is promising, the team needs to work with industry to integrate its acoustics device into existing manufacturing systems and processes.

The team is also exploring the use of their invention to remove oxide layers from other materials for applications in sensing and renewable energy.

The research is published in *Nature Communications* (doi.org/10.1038/s41467-022-34699-3).

RMIT University

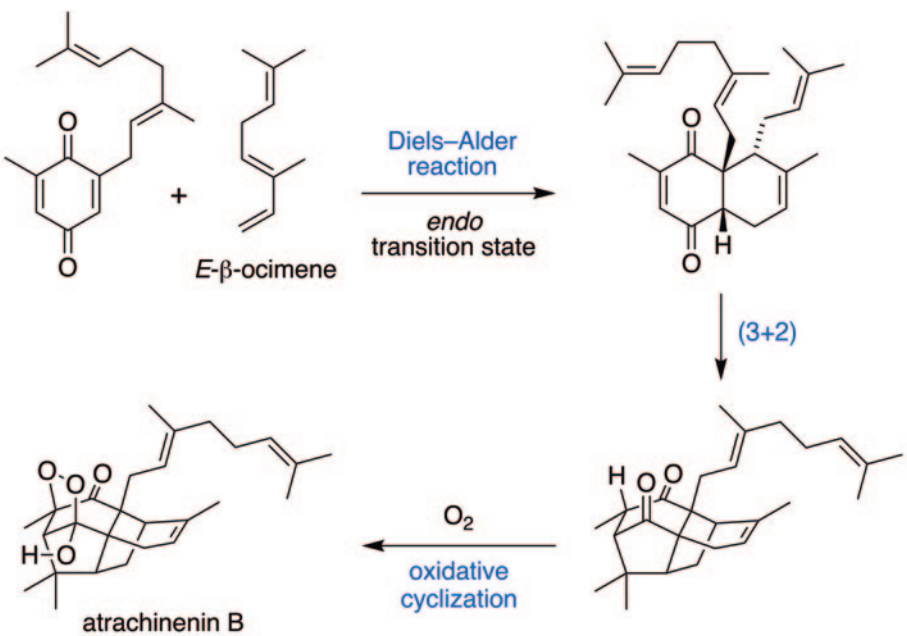
Aiming for an ideal synthesis



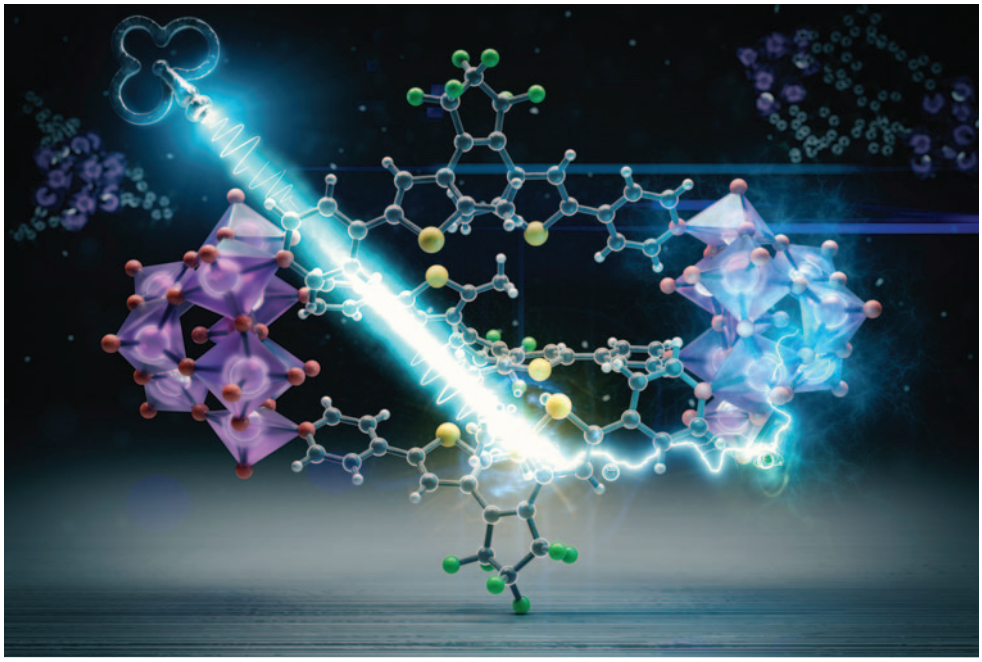
An important concept in organic chemistry is that of an ideal synthesis. According to Wender, 'ideal syntheses are those in which the target molecule is assembled from readily available starting materials in one simple, safe, economical, and efficient operation'. With this goal in mind, researchers at the University of Adelaide and the University of Edinburgh recently speculated that a complex natural product, peshawaraquinone, could be synthesised in one step from lawsone and prenal (Vieira de Castro T., Huang D.M., Sumby C.J., Lawrence A.L., George J.H. *Chem. Sci*. 2023, **14**, 950–4). In a forward sense, these readily available starting materials would combine to form dehydro-α-lapachone, a natural product that was co-isolated with peshawaraquinone from the heartwood of the flowering tree *Fernandoa adenophyllum* at the University of Peshawar, Pakistan. An unsymmetrical dimerisation of dehydro-α-lapachone then gives peshawaraquinone via a spectacular sequence of electrocyclic reactions and cycloadditions that are based on the proposed biosynthetic pathway. Although low yielding, this one-step, biomimetic synthesis meets several requirements of Wender's 'ideal synthesis'. Furthermore, the four-component cascade reaction generates six bonds and six stereocentres in one step, enabled by the conversion of six trigonal planar carbon atoms in the reactants to six tetrahedral centres in the product.

Reflecting on a racemic natural product

Stereochemically complex natural products are almost always found as single enantiomers, with each stereocentre constructed under exquisite enzymatic control. Racemic natural products with multiple stereocentres are far less common as they must be formed via stereoselective but non-enzymatic chemical reactions. Their existence must therefore be explained by highly predisposed biosynthetic pathways, which can be investigated in a biomimetic total synthesis. For example, atrachinenin B is a structurally intricate but racemic meroterpenoid natural product recently isolated from the rhizomes of *Atractylodes chinesis*, a plant widely used in traditional Chinese medicine. Researchers at the University of Adelaide have completed a concise total synthesis of this natural product using three key stereoselective reactions (French S.A., Sumby C.J., Huang D.M., George J.H. *J. Am. Chem. Soc.* 2022, **144**, 22 844–9). First, an intermolecular Diels–Alder reaction between *E*-β-ocimene and a naturally occurring quinone preferentially forms an *endo* adduct, which then undergoes an intramolecular (3+2) cycloaddition. Finally, a simple aerobic oxidation completes the cage-like pentacyclic ring system of racemic atrachinenin B, with seven contiguous stereocentres and a peroxyhemiacetal bridge.



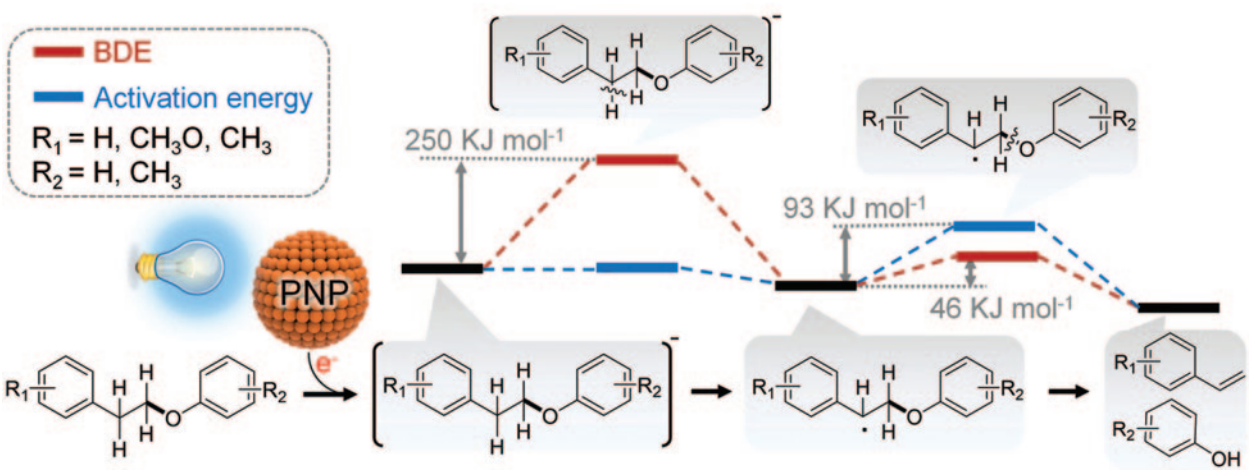
Photoresponsive molecular capsule



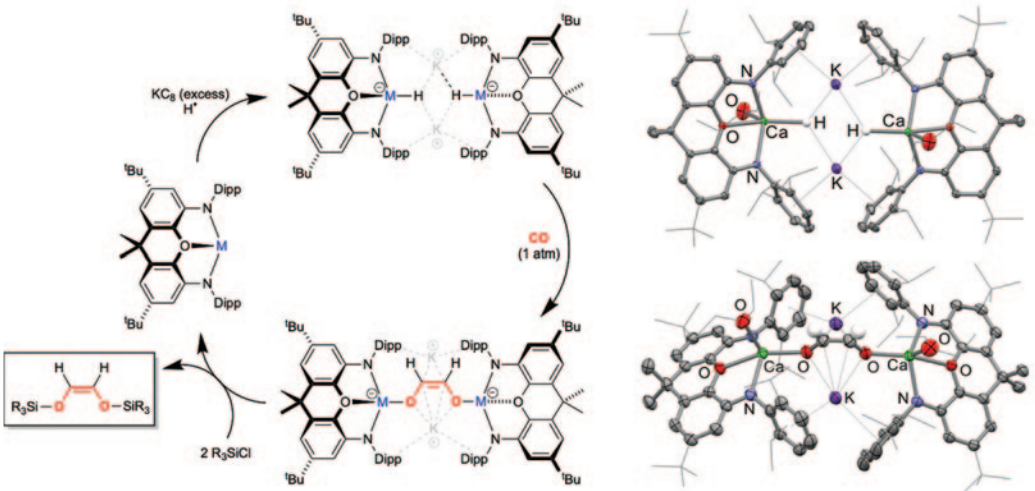
A collaboration led by the Monash University and involving the University of Melbourne, University of Lille and University of Strasbourg has led to the discovery of a self-assembled photoresponsive molecular capsule with intriguing photophysical properties (Choudhari M., Xu J.J., McKay A.I., Guerrin C., Forsyth C., Ma H.Z., Goerigk L., O'Hair R.A.J., Bonnefont A., Ruhlmann L., Aloise S., Ritchie C. *Chem. Sci.* 2022, **13**, 13 732–40). The study used $[PMo_9O_{31}(py)_3]^{3-}$ $\{PMo_9\}$ as an inorganic polyanionic ligand to direct the coordination of three organic diarylethene (DAE) photoswitches at specific sites on the molecular metal oxide's surface. As the DAEs were constrained to exist in photo-active conformations, photochromism was observed on illumination by an appropriate light source. Solution-state transient absorption spectroscopy, spectro-electrochemistry, NMR spectroscopy and DFT calculations were used to interrogate the photochemical process, revealing sequential ring closure of the DAEs, as well as a latent photoinduced electron transfer from the DAE to the polyanion following electrocyclisation. Ongoing research includes further elaborate syntheses and studies of self-assembled polyoxometalate–diarylethene compounds to generate more advanced photoresponsive materials.

Plasmon-catalysed selective C–H activation

The selective activation of robust C(sp^3)–H bonds is of great interest in organic synthesis. However, high reaction temperatures or powerful catalysts are required to activate these bonds, adversely affecting product selectivity. Recently, researchers from the Queensland University of Technology, collaborating with researchers from Hunan University, Shanxi Normal University and the Chinese Academy of Sciences, found that light-generated hot electrons from visible light-illuminated plasmonic nanoparticles (PNPs) can significantly lower the bond dissociation energy of the C(sp^3)$_\alpha$–H bond of an alkyl aryl ether. Moreover, the precise scission of the C(sp^3)$_\alpha$–H bond enables the cleavage of the alkyl ether C_α–O bond under mild conditions, yielding aromatic compounds with unsaturated, substituted groups in excellent yields (Han P., Mao X., Jin Y., Sarina S., Jia J., Waclawik E.R., Du A., Bottle S.E., Zhao J.-C., Zhu H.Y. *Angew. Chem. Int. Ed.* 2023, **62**, e202215201). Thermal catalysis and other photocatalytic systems do not produce these products. Furthermore, the C(sp^3)$_\alpha$–H bond scission does not promote cleavage of the C_α–O bonds of other ethers, even though the C_α–O bonds have a lower bond dissociation energy than the C_α–O bond. The plasmon-driven selective activation of the C(sp^3)–H bond provides a new synthesis approach under mild conditions.



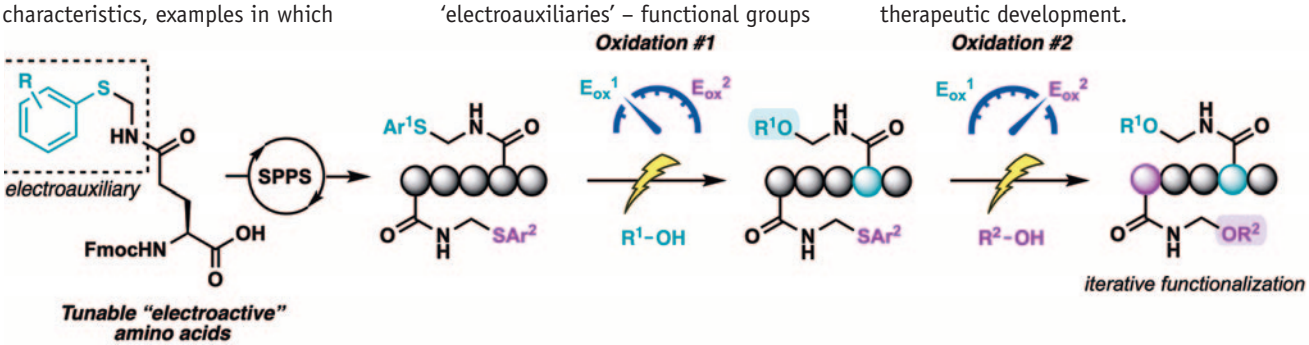
Transforming CO into fine chemicals



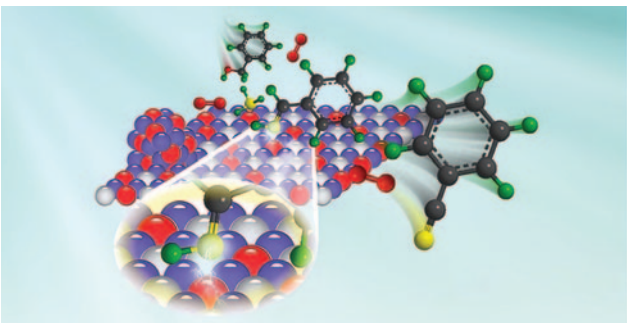
Combustion is an effective way to take complex mixtures of organic molecules and oxidise them into simple C_1 products (CO and CO_2). However, reversing this reaction (i.e. transforming C_1 starting materials into useful organic molecules), is a considerable fundamental challenge, but one that could lead to significant environmental benefits. An international team led by Jamie Hicks at the Australian National University has reported that using a novel series of earth-abundant, anionic group 2 hydride reagents, CO can be selectively transformed into a range of useful organic molecules (McMullen J.S., Huo R., Vasko P., Edwards A.J., Hicks J. *Angew. Chem. Int. Ed.* 2023, **62**, e202215218). The team is currently investigating whether this chemistry can be used to synthesise sustainable chemical feedstocks as potential replacements for some of our currently used crude oil-derived feedstocks.

Dialling in the potential for tuneable electrochemical peptide modifications

The use of electricity to drive chemical reactions is an appealing approach to green and sustainable synthesis. In addition, electrochemistry provides powerful opportunities for the precise control of chemical reactivity by enabling practitioners to 'dial in' the potential or current at which a reaction is performed. For highly functionalised molecules, this tunability provides unprecedented opportunities for targeted chemical modifications. Despite these appealing characteristics, examples in which electrochemistry is applied to the tuneable modification of peptides are scarce. A recent collaboration between the Connal and Malins labs at the ANU Research School of Chemistry, led by PhD student Dhanya Karipal Padinjare Veedu, has produced a method for the tuneable, iterative electrochemical modification of peptides (Veedu D.K.P., Connal L.A., Malins L.R. *Angew. Chem. Int. Ed.* 2023, **62**, e202215470). The technique uses designer amino acids adorned with 'electroauxiliaries' – functional groups predisposed to electrochemical oxidation – which are electronically programmed to oxidise at different electrochemical potentials. The incorporation of these amino acids into peptides enables selective, iterative modifications, affording valuable modified peptides and unlocking a new level of orthogonality in peptide synthesis. The strategy has promising applications for the preparation of peptide libraries, including for therapeutic development.



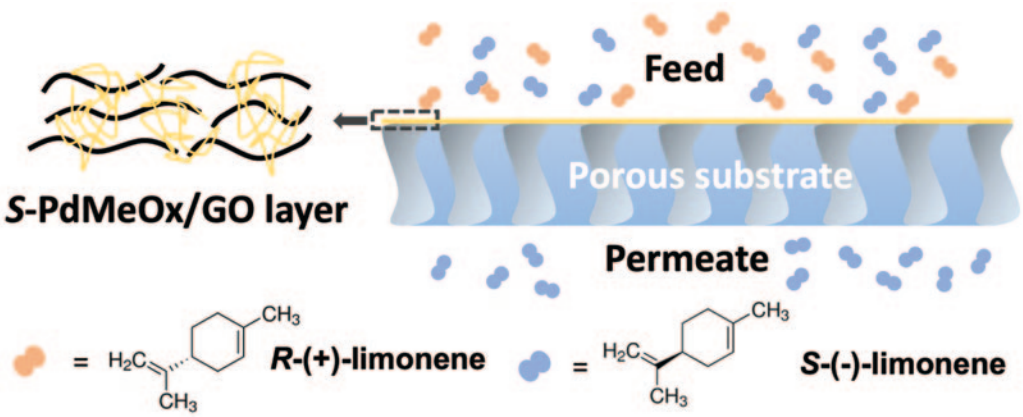
Economical photocatalysts for high nitrile yields from aerobic alcohol ammoxidation



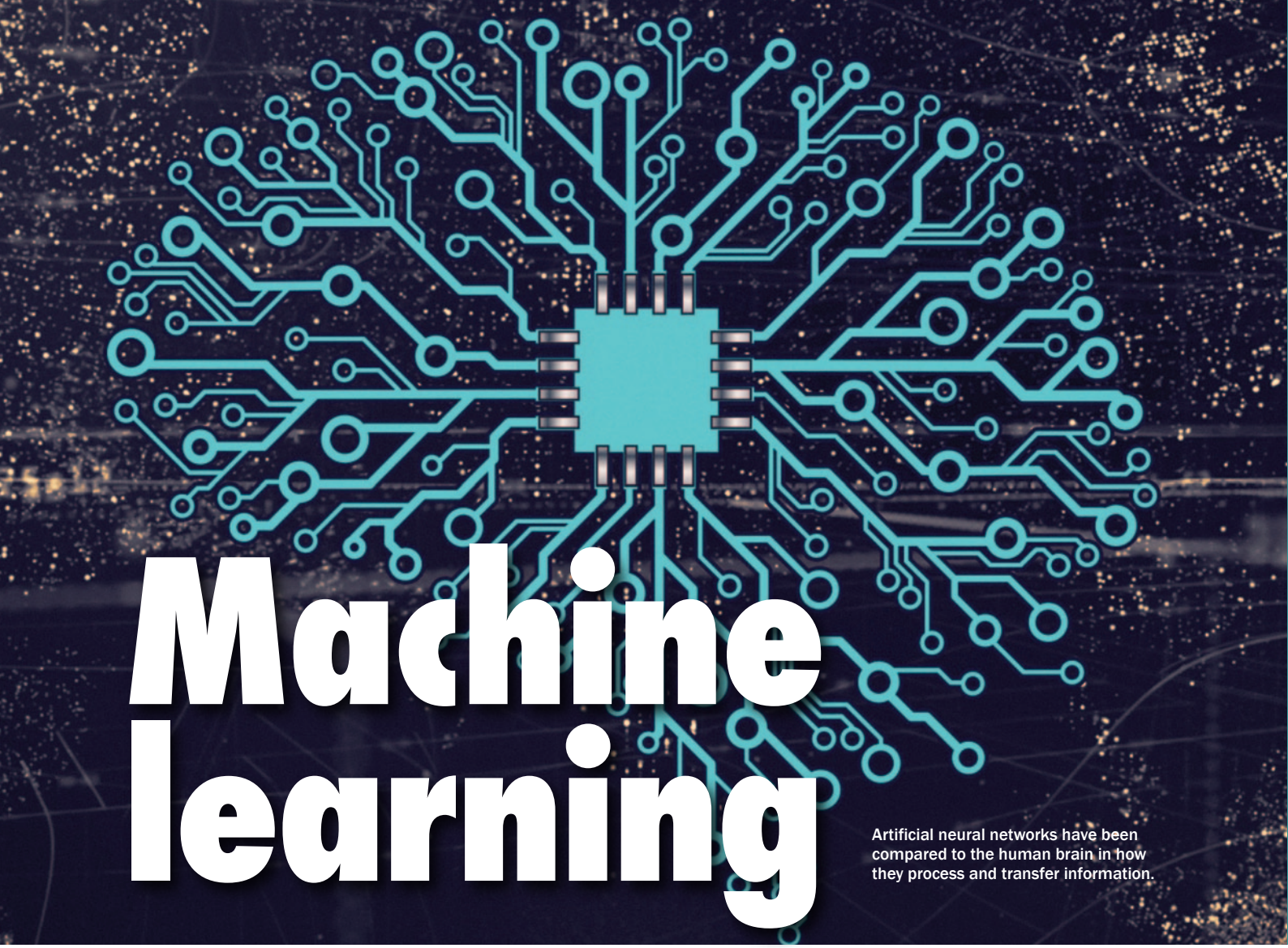
Nitriles are important intermediates in organic synthesis, and catalytic ammoxidation of alcohols into nitriles is an essential route to their production. But most thermal-catalytic systems require high reaction temperatures and high-pressure oxygen, which can produce a range of undesirable by-products. Now, researchers from the Queensland University of Technology and South-Central Minzu University (China) have developed robust and economical photocatalysts consisting of Fe(III)-modified titanium dioxide (TiO_2) for room-temperature ammoxidation using O_2 at atmospheric pressure as a benign oxidant, ammonia as the nitrogen source, and ammonium bromide as an additive (Xian C., He J., He Y., Nie J., Yuan Z., Sun J., Martens W.N., Qin J., Zhu H.Y., Zhang Z.H. *J. Am. Chem. Soc.* 2022, **144**, 23 321–31). Various (hetero)aromatic nitriles were synthesised at high yields, and aliphatic alcohols could be transformed into corresponding nitriles. The modification of TiO_2 with Fe(III) facilitates the formation of $^{\bullet}O_2^-$ radicals and increases the adsorption of ammonia and amino intermediates on the catalyst, accelerating ammoxidation to yield nitriles. The Br^- anions consume the photogenerated holes and $OH^{\bullet}$ radicals, which are strong oxidants, preventing over-oxidation and improving nitrile selectivity. The synergy of the catalyst modification and bromide additive opens new avenues for fine chemical synthesis.

Efficient POx-based chiral separation membranes

Membrane-assisted chiral separations enable continuous harvesting of enantiomers and have potential applications in the food and pharmaceutical industries. But challenges remain in the scalable fabrication of membranes with both high enantioselectivity and enantiomer flux. Poly(2-oxazoline)s (POx) are a class of synthetic polymers whose physiochemical properties can be tuned via the introduction of functional groups in the 2-position of their monomers. Due to their ease of synthesis and structural and chemical diversity, POx are good candidates for making efficient chiral separation membranes. A team led by Huanting Wang and Kristian Kempe groups at Monash University has recently used *S*-poly(2,4-dimethyl-2-oxazoline) (*S*-PdMeOx) macromonomers to make an efficient enantioselective membrane scaffolded by graphene oxide (GO) nanosheets (Wang F., Pizzi D., Lu Y., He K., Thurecht K.J., Hill M.R., Marriott P.J., Banaszak Holl M.M., Kempe K., Wang H. *Angew Chem. Int. Ed.* 2023, **63**, e202212139). The *S*-PdMeOx/GO membrane was prepared by a simple solution-based casting method and used for the separation of a racemic limonene mixture. The membrane showed a 98.3 ± 1.7% enantiomeric excess of *S*-(–)-limonene over *R*-(+)-limonene and a flux of 0.32 mmol m^{-2} h^{-1}. This work establishes a new route to the preparation of efficient enantioselective membranes using synthetic homochiral polymers.



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.*, *Chem. Sci.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.



Machine learning

Artificial neural networks have been compared to the human brain in how they process and transfer information.

A shortcut in fluorescent polymer selection

The first commercial LED lights came out in the 1960s, but it wasn't until the colour could be fully tuned, nearly 40 years later, that their full utility was realised. Recent work aims to do the same thing for fluorescent polymers and other novel materials, but in a fraction of the time, using machine learning.

BY **NASTARAN MEFTAHI, DAVE WINKLER, SALVY RUSSO** AND **ANDREW J. CHRISTOFFERSON**

Machine learning is a hot topic, but like so many hot topics there is hype and confusion about what it is, and what it can (and can't) do. Machine learning, which is a subset of artificial intelligence, can help experimental researchers achieve results they could not otherwise obtain quickly and easily. Machine learning models are trained on (ideally) thousands of data points to 'learn' the complex relationships between the data points and properties of interest, and are sometimes described as not being easily interpretable by humans (the so-called 'black box'), although this is changing.

Deep learning is a subset of machine learning. Although this powerful technique is gaining popularity, deep learning is not always the best tool for the job. Like any research project in chemistry, the optimal machine learning technique depends on what you're trying to achieve, and what information is available to you.

A library of polymer systems

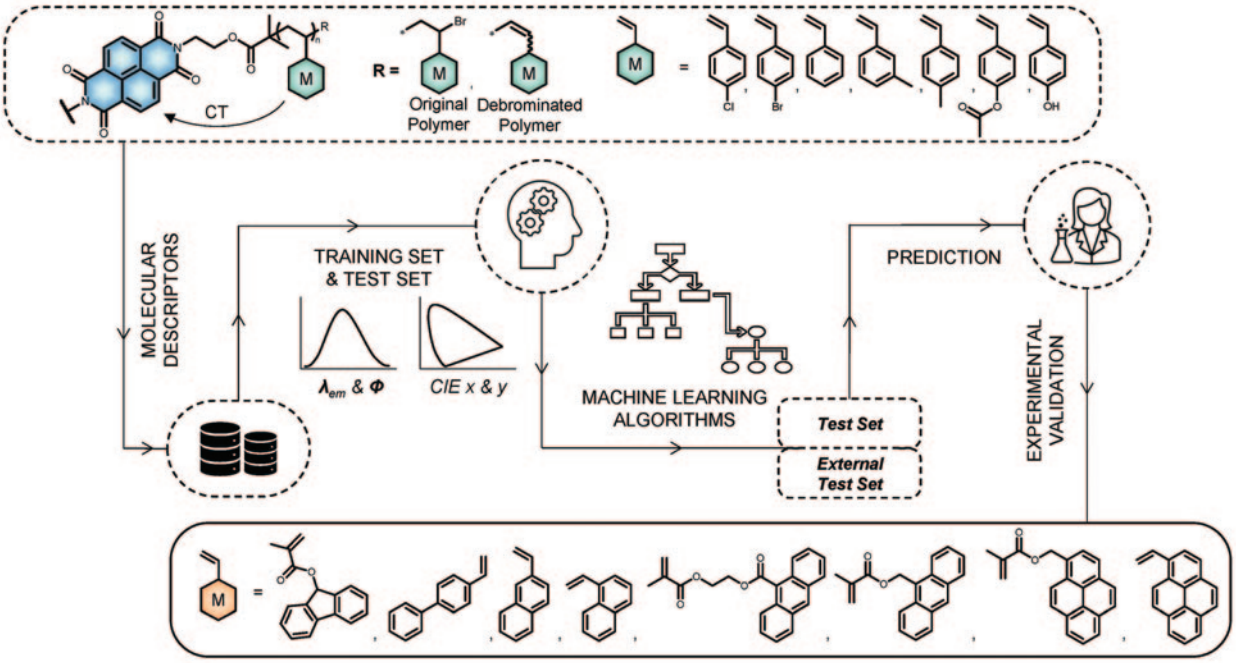
In our efforts to achieve full-colour tuneability in fluorescent polymers, our experimental collaborators developed a library of 71 polymer systems where the number and chemical composition of the electron donor monomers were varied, but the electron-accepting core remained constant. For each system, properties such as colour and intensity were measured. Simply by trial and error, our colleagues were able to produce a variety of colours, but the goal was to be able to quickly produce polymers of any desired colour. This is where machine learning was invaluable. Machine learning models trained on the chemical composition and number of monomers in the polymer can predict the colour of the resultant polymer. Because machine learning can only make models out of numerical data, the colour of each system was described using CIE 1931 chromaticity coordinates, where the observed colour is translated into Cartesian x and y numerical values.

Choosing a machine learning model

The next step was to decide what type of machine learning model to use. Machine learning can be further broken down into linear and non-linear methods (although it's a bit more nuanced than that). One of the most straightforward linear methods is multiple linear regression, where the equation $y = mx + b$ is repeated for multiple x variables x_1, x_2, x_3 and so on (also known as descriptors or features), and the algorithm solves for the constants b, m_1, m_2, m_3 and so on. Once the model is optimised, the m values can tell you how strongly each descriptor contributes to the final property, and whether the effect of each descriptor is positive or negative. This ability to interpret the model and understand the contribution from each descriptor is one of the main advantages of multiple linear regression. One of the main disadvantages is that it only works when the relationship between the descriptors and the property of interest is linear.

Artificial neural networks are some of the most popular non-linear machine learning methods. They have been compared to the human brain in how they process and transfer information. In contrast to deep learning (multiple hidden layers containing large numbers of neurons that require very large training sets), shallow neural networks (a single hidden layer with few neurons) are able to generate robust models with a relatively small number of data points. The main limitation of these models is not so much their modelling accuracy but their small domains of applicability. In other words, they are not as good at predicting properties of things that are substantially different from the data set that was used to train the model. While artificial neural networks have the advantage of being able to determine non-linear relationships between descriptors and the property of interest, the contribution of each descriptor is a local rather than global property for non-linear models. This means that the magnitude and direction (positive or negative) of the contribution depends on where on the complex, multidimensional response surface the importance is assessed, and this is not easily obtained from the model. Simply put, artificial neural networks are good at predicting properties based on descriptors, but it is difficult to interpret how they achieved this prediction (the black box).

Fluorescent polymers with full-colour tuneable solid-state emission enabled by machine learning. Reprinted from Ye et al., *Chem* 2023, vol. 9, pp. 1–24, with permission from Elsevier



The machine learning modelling process that was used to predict the colour of polymers as a function of type and number of monomers.
Reprinted from Ye et al., *Chem* 2023, vol. 9, pp. 1–24, with permission from Elsevier

Both linear and non-linear machine learning methods require descriptors. Descriptors are mathematical entities that encode chemical and physical properties of materials. There are literally thousands of possible descriptors for each molecule or material, and most are not particularly informative. Unless the set of descriptors is reduced to those containing the most relevant information, models will be overfitted and degraded by the presence of uninformative descriptors (noise). A very efficient way to select the best subset of relevant descriptors that avoids the possibility of chance correlation between descriptors is the use of sparse feature selection methods that set less relevant descriptors identically to zero, improving model predictivity and interpretability.

Predicting promising polymers

In our models of photoluminescent properties of fluorescent polymers, our aim was to use molecular descriptors that are both efficient and chemically interpretable to describe the emission wavelength, quantum yield and CIE *x y* coordinates that define the colour, to provide guidance for the synthesis of new polymers of interest. We deliberately avoided using descriptors based on experimentally determined properties or derived from computationally expensive quantum chemical calculations, because they are unsuitable for predicting properties of materials not yet synthesised, or are very resource demanding. Instead, we chose the smallest number of simple descriptors that could produce a reliable model and were easily determined without synthesis or computationally expensive calculations, such as number of monomers in the polymer, type of monomer based on percentage of carbon or halogen atoms, and nature of the terminating group of the polymer.

We used both multiple linear regression and artificial neural networks to create our models and, in both cases, divided the experimental data set of 71 polymers into a training set of 57 and a test set of 14 polymers. It is standard practice in machine learning to divide the data set this way and use about 80% for the training set and 20% for the test set, in order to ensure that the model is not overfitted to the training set and can still predict the properties of materials it wasn't trained on. While artificial neural networks produced slightly better models, multiple linear regression models allowed us to interpret how the characteristics of the polymers, as given by the descriptors, affected each property of interest.

Based on the outcomes from machine learning, our experimental collaborators synthesised and characterised new polymers from an additional eight monomers not previously used, and we used this data as an external test set to further validate our models. The properties of seven out of eight were predicted well. The eighth monomer had a significantly different structure from the monomers used in the model training sets, which emphasises that when the data set is small, machine learning

often cannot be used to predict the properties of materials that are substantially different from those in the data set. The solution, of course, is that the new materials can then be added to the data set and used to develop new and better models (called active learning).

In general, to identify functional polymers with targeted performance, it is very time consuming and expensive to synthesise and characterise a large library of polymers one by one, considering all possible combinations of monomers, chain lengths, end group functionalisation, and so on. Using machine learning techniques, experimental scientists can greatly save time and resources by avoiding the experimental screening process and only synthesising the polymers predicted by machine learning to be promising. When there is a need to select polymer structures from a large pool of candidates, the machine learning models would play a pivotal role in reducing the working load for time-consuming and expensive synthesis.

Still, there are some considerations for experimental researchers to keep in mind if they are interested in using machine learning to optimise their research. For those not familiar with machine learning, it is important to emphasise that the property of interest is the output, not the input, of the model. If, for example, we wanted to produce a polymer that is green, the machine learning model can't necessarily tell us what to synthesise. Instead, we can input thousands of possible combinations of monomers, chain lengths, and end group functionalisations as descriptors, and the models will predict in a matter of seconds which of those are most likely to be green. In the case of multiple linear regression, the interpretability of the model allows us to narrow down the choice of possible combinations most likely to be green.

Using machine learning techniques, experimental scientists can greatly save time and resources by avoiding the experimental screening process and only synthesising the polymers predicted by machine learning to be promising.

Another important consideration is that machine learning doesn't always work. This could be because of the data set, particularly if the data set is compiled from the work of different experimental groups, or simply because there is no clear relationship between the descriptors chosen and the property of interest. In both cases, the solution can be the same: use a larger data set produced by a single group and, if possible, try different descriptors.

Machine learning and the Sustainable Development Goals

Our world is rapidly changing, and in materials discovery and development we can't afford to wait 40 years between the initial innovation and full commercial utilisation. In the future, machine learning will be essential to achieve the Sustainable Development Goals outlined by the United Nations, particularly affordable and clean energy, industry, innovation and infrastructure, and climate action.

In collaboration with experimental colleagues across Australia and beyond, we have already developed machine learning models for organic and inorganic solar cells that have improved their efficiency and provided non-intuitive guidelines for further optimisation, and we are currently working on developing and optimising carbon capture technologies for commercial use. In addition to materials composition, machine learning can provide models and predict other variables such as temperature, duration and cost/efficiency ratios that will factor into the commercial implementation of the materials and systems. Machine learning is undoubtedly becoming an essential component of materials discovery, design and implementation, and has enabled us to achieve outcomes more quickly and efficiently than ever possible previously.

Dr Nastaran Meftahi, **Professor Salvy Russo** and **Dr Andrew J. Christofferson** are at the ARC Centre of Excellence in Exciton Science, RMIT University. **Professor Dave Winkler** FRACI CChem (Honorary) is at the La Trobe Institute for Molecular Science, La Trobe University.

Congratulations to the 2022 RACI National Awards recipients.

Leadership in the chemical sciences

Leighton Memorial Medal

Recognises eminent services to chemistry in Australia in the broadest sense. Commemorates the distinguished career of A.E. Leighton

Professor George Koutsantonis, University of Western Australia

A member for nearly 40 years, I am proud to have advocated for the internationalisation of chemistry in Australia, working to create opportunities to build national and international networks and profiles. My support of the *Australian Journal of Chemistry* has given me immense pride and I believe the journal has a prominent role in the Australian chemical community, reflective of its rich history, and deserving of continuing support from all. In science, I am very grateful for the efforts of my students and collaborators, who collectively have made it possible to make inroads into modern challenges in multidisciplinary areas, including catalysis, materials science and molecular electronics.

Margaret Sheil Leadership Award

Recognises an outstanding female leader working in the chemical sciences

Professor Colette Boskovic, University of Melbourne

Colette's research interests lie in the fields of molecular magnetism, rare earth chemistry, redox-active ligands, inelastic neutron scattering and switchable molecular materials. She sits on several conference International Advisory Boards. She is co-Chair of the forthcoming 2030 International Conference on Coordination Chemistry (ICCC), which will be held in Brisbane. Colette is strongly committed to increasing the participation of women in chemistry and served as a guest co-editor of the 'Women in Chemistry II' special issue of the *Australian Journal of Chemistry*. She is also the University of Melbourne's representative on the Australian Institute of Nuclear Science & Engineering Council.

Colette is Chair of the Inorganic Chemistry Division and Divisional Archivist. She has been active in the Victorian Branch's Inorganic Chemistry Group over many years.

Fensham Medal for Outstanding Contribution to Chemical Education

Recognises outstanding contributions to the teaching of chemistry and science in general over an extended period; the Fensham Medal is the most senior award for education in RACI

Associate Professor Daniel Southam, Curtin University

I strive to adapt the traditional ways of teaching chemistry by structuring learning in new ways that support cognitive and affective development of learners. In my experience, I have discovered that encouraging students to be active learners and reflect on their learning processes while working in teams leads to qualitatively better learning and enables emotional satisfaction with this process.

Citations Award

There are a considerable number of chemists – members of RACI – who make substantial contributions to chemistry, and, especially to the progress of the profession over a period of many years.

Bruce Graham

I'm proud of my cadet training in analysis and my education in chemistry at Sydney Technical College and the University of New South Wales. The focus on thoroughness, precision and logic was a good basis for a lifetime in applied science. In industry, I worked with chemicals, food and pharmaceuticals; in government with poisons, medicines, medical devices, public health and manufacturing regulation. One of my last tasks was, as a consultant, to screen imported chemicals for compliance with multiple regulations, using chemistry learnt in 1950. I joined RACI as a student member and became heavily involved with three Groups, two as a founder and one that had an important educational focus. I was surprised and delighted for my contributions to be recognised.

Dr Eveline Baker, scientific consultant
Eveline has been principal scientist in an environmental engineering and scientific practice for more than 20 years. She has held a range of senior positions in private, federal and state public sectors, such as International and National Accreditation bodies. She has conceived, developed and presented courses and lectures at diverse venues, including several Australian universities, industry and government-focused adult education. Of particular importance is the specialist material produced and presented to meet international standards in analytical method validation for the purpose of laboratory accreditation.

Her research has covered rare earths and enzyme models, as well as therapeutic substances. She has significant experience in post-tertiary, tertiary, post-secondary education, management and staff training. To augment her scientific career, she accepted secondments to management and human resources positions.

Dr Nathan Kilah, University of Tasmania
I am a passionate advocate for RACI and the promotion of chemistry in the community. I have undertaken many activities, including RACI-branded public chemistry shows and science outreach activities in schools and in the community. I have written articles in magazines and online, and been interviewed for TV and radio. I also mentor and supervise students and volunteers in the promotion of chemistry. The outreach activities I've undertaken would be impossible without their collaboration, and my hope is that these experiences will broaden the diversity of voices and perspectives of chemistry engagement.

Professor Debra Bernhardt, University of Queensland
I strive to use theoretical and computational approaches to advance the fundamental understanding of the behaviour of matter at the atomic or molecular level. I enjoy finding mathematical relationships to describe physical and chemical phenomena and applying computational methods to study a wide range of problems, particularly transport in nanoscale systems, non-equilibrium flow, design of materials, energy storage and conversion. Working with wonderful collaborators, colleagues, group members and students has made my academic journey particularly rewarding. I greatly value being part of the chemistry community in Australia and was honoured to chair the RACI National Congress in 2022.

Distinguished Fellowship

Recognises highly distinguished contributions to the profession in academia, government or industry and RACI

Professor John Carver, Australian National University
I have had a somewhat peripatetic career at universities in Australia (Wollongong, Adelaide, Australian National University) and England (Oxford). My research has investigated peptide and protein structure, function and interactions, mainly addressing the mechanisms of protein aggregation in relation to diseases, particularly cataract, Alzheimer's and Parkinson's. The role of molecular chaperones in inhibiting protein aggregation has been a major focus. Most of the credit for this work must go to the many students, postdoctoral fellows and national and international collaborators with whom I have worked.

In the latter part of my career, I was heavily involved in administration as head of three schools at the University of Adelaide and ANU. Throughout my career, I received excellent support and mentorship from colleagues, for which I am very grateful. As a result, I have made many friends along the way.

Applied Research Award

Given to a member of RACI who has contributed significantly towards the development of, or innovation through, applied research, or in industrial fields

Professor Paul Burn, University of Queensland
We have developed sensitive and selective sensing materials for explosives, chemical warfare agents and narcotics, and detector platforms. Along the way, the team has debunked myths in the field that have held back innovation. One aspect of the technology is now in market, which is exciting for us all, and I believe a key reason for the award.

Weickhardt Medal for Distinguished Contribution to Economic Advancement

For significant contributions towards the economic advancement of the Australian economy through work in the chemistry area

Professor David Lewis, Flinders University
Some of the most satisfying moments in my professional career have been seeing my inventions on the shelf and speaking to people who use them. Through my industrial and academic career, I have been fortunate to work with a range of exceptional colleagues to conceive, manufacture and commercialise a range of products. Most recently, we have launched a patented engineered hardwood made from sustainably sourced plantation timber and leveraged the chemistry of the materials and process to create something unique through a start-up called 3RT. This award is a wonderful opportunity to highlight the contribution of chemistry to the world around us through the commercial outcomes from research, and I am thrilled to be a recipient.

Achievements in research and innovation

(See p. 21 for the winner of the Applied Research Award, and p. 23 for winners of the Cornforth and the Rennie Memorial Medals.)

H.G. Smith Memorial Award

Recognises contribution to the development of some branch of chemical science

Professor Christopher Barner-Kowollik, Queensland University of Technology
Our research is focused on the in-depth understanding of photochemical reactions and their application to macromolecular chemistry, in particular advanced light-reactive soft matter inks for 3D printing. Specifically, we have shown in detailed studies over the last decade that – surprisingly – the absorbance spectra of photoreactive molecules are no reliable predictor of photochemical reactivity. We illustrate this discrepancy via so-called 'action spectra', where the reactivity of photochemically reactive molecules is probed wavelength by wavelength with a tuneable laser system, exposing the reaction to identical numbers of photons at each wavelength. Our action spectra thus allow us to determine the optimum wavelength for a given photochemical reaction. These findings have wide-ranging implications for designing materials that rely on photochemical curing applications – from dental materials, to surface coating systems in the automotive and aerospace industries, and 3D printing systems.

Excellence in the education sector

(See p. 20 for the winner of the Fensham Medal for Outstanding Contribution to Chemical Education.)

RACI Chemistry Educator of the Year Award

Designed to encourage developing teachers, and is open to tutors, lecturers and senior lecturers (academic levels A, B and C) teaching in undergraduate or postgraduate university courses

Dr Stephen George-Williams, University of Sydney
While there are many components that make an effective teacher, I believe that the main two are adaptability and being evidence based. Not all students are alike, but teaching using research-supported methods (or trying new things and generating new data!) provides a much more solid foundation than simply following one's instincts. Our understanding of effective teaching and learning experiences is constantly evolving, so having an awareness of as many as possible to draw upon when working with a diverse range of students is key to successful student learning outcomes.

Women in chemistry

(See p. 20 for the winner of the Margaret Sheil Leadership Award.)

Rita Cornforth Lectureship

Offered to an outstanding female early-career chemist for an opportunity to gain broader recognition of their career achievements to date

Dr Annie Colebatch, Australian National University
Annie completed her BSc(Hons) and PhD in organometallic chemistry at the Australian National University. She then moved to the UK to undertake postdoctoral research and returned to ANU in 2019. Her research interests span inorganic chemistry, synthesis, catalysis, supramolecular chemistry and electrochemistry. In particular, she is looking at the way multiple chemical entities can 'cooperate' to achieve a particular chemical outcome and designing systems capable of utilising these effects. Her team is developing bimetallic complexes and investigating the interplay of two metals on the chemical reactivity as well as physical properties such as electrochemical and photochemical properties. A key focus of the group's work is ligand design to support such systems where multiple metal centres can bind and interact.

Annie is a proactive supporter of women in chemistry as well as diversity more broadly.

Chemistry students and early career chemists

(See p. 22 for the winner of the Rita Cornforth Lectureship.)

Cornforth Medal

The medal, bearing the words 'For a Thesis on Chemical Research', is designed to give recognition of outstanding achievement in chemistry and to promote chemical communication.

Dr Harshal Patel, University of Adelaide
I am honoured to be awarded a prize in memory of John Cornforth's achievements and acknowledge the significant contributions of Rita Cornforth to that success. Thank you, Thomas Fallon for those PhD years, where we established new synthetic methods towards two fascinating molecular groups – the exotic, shape-shifting molecule bullvalene and the endiandric acid family of natural products. Co-workers and collaborators have my gratitude. Time for me to go on vacation.

Rennie Memorial Medal

Recognises excellence in research in chemical science

Dr Lara Malins, Australian National University
My lab focuses on the development of efficient methods for the synthesis and modification of biologically relevant small molecules, peptides and proteins. We are particularly interested in the use of electrochemistry, photochemistry and molecular strain as driving forces for new modes of chemical reactivity. It is an honour to receive this award on behalf of the incredibly talented and motivated team of students and postdoctoral fellows who make all the work underway in my lab possible.

Masson Memorial Scholarship Prize

Established as a memorial to the late Sir David Orme Masson, founder of RACI, and open to RACI members who are eligible to proceed for a year's study of Chemistry at BSc Honours level

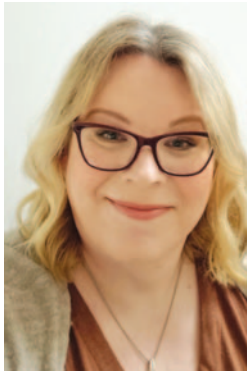
Eve Poland, University of Tasmania
I have contributed to several projects within organometallics and catalysis throughout summer research projects and my honours year at the University of Tasmania. Winning the Masson Memorial award has been a great encouragement for me for the work I've put in over the past five years and has given me confidence to continue this trajectory.

New awards

A suite of new awards was added in 2022 to ensure all demographic groups are addressed by our awards portfolio.

Welcome Award

Established to honour and welcome a chemist who is new to Australia



Professor Tanja Junkers, Monash University
Since arriving in Australia, with my team, I have worked at Monash University at changing the way we do synthesis. We have developed many tools in laboratory continuous-flow chemistry, and have shown that flow chemistry is a perfect tool for producing highly precise polymers. Further, we dived into machine learning and artificial intelligence, working on data-driven polymer synthesis. While still in its infancy, it is clear that machine learning will change the way all chemists are doing things. We are glad to contribute with our work to the proud Australian chemistry sector, and look forward to the years ahead.

Ochre Award

Established for First Nations Australians, in recognition of a passion for Chemistry

William Frazer, Inside Policy
I am a proud Wiradjuri man who grew up on Bundjulung country in Casino in northern New South Wales. I have a BSc and an LLB from Macquarie University on Dharug country.

Since year 8, I have been involved with the National Indigenous Science Education Program. I learnt about bush medicines, climate and ecological practices known by Indigenous people for thousands of years in a university context. This culminated in my capstone unit where I was able to adapt methods for chemistry experiments on native plants testing for properties such as starch and pH for use at Macquarie University's Bush University in Arnhem Land. Seeing the blend of Western and Aboriginal science can move us towards reconciliation as a whole if done right.

Currently, I work for Inside Policy – a social research and evaluation company that aims to make government programs and policies work better for Aboriginal people. My goals are to continue to work in community engagement and knowledge sharing, including science communication. I know the impact this can have on young people and would love to see the belief and mentoring that I received in science continue to inspire the next generation of Indigenous chemists.

Centenary of Federation Teaching Award in Chemistry

For the recognition and reward of outstanding excellence in the teaching of chemistry in Australia at both primary and secondary school levels

From left: Amanda Tauber, Stephanie Schweiker and Stephan Levonis

The Bond University team led by Dr Stephanie Schweiker, Bond University
The Bond chemistry team comprises Dr Stephanie Schweiker, Dr Stephan Levonis and Dr Amanda Tauber, who are from Bond University on the Gold Coast. They created The Virtual Scientist – a website that gives school and university students access to virtual lab experiments, combining 360-degree tours with embedded interactive videos, which students can navigate in their own time. The high level of interactivity, gamification and step-by-step instruction provides a unique and genuine lab-teaching environment, with added accessibility of digital resources.

The Virtual Scientist has averaged approximately 2000 views per month since its launch in late 2021, and has benefitted many students around the world.

Catalyst Award

Established to recognise an early career chemist – for outstanding innovation in applied chemistry in the workplace

Dr Rachel Pepper, Queensland University of Technology
My work focuses on developing new materials for energy and water applications. I work in a team that excels in industry-partnered research. These partnerships have really driven the translation of our research beyond the lab, most notably in the development of an agile process to produce high-purity alumina, which is used in lithium-ion batteries. I am honoured to have been acknowledged by RACI through this award, which recognises the important role that chemistry has in solving big problems related to sustainability and the environment, and highlights the benefits of working with industry to create innovative solutions.

Vicki Gardiner Advocacy Award

Established to recognise outstanding leadership in the areas of promotion of chemistry, outreach, mentorship and inspiration and the provision of a more equitable workplace

William Li, ANSTO
Since 2018, I have actively promoted RACI and careers in chemistry through the New South Wales Early Career Chemists Group, New South Wales Branch Committee and Careers Development, helping many around Australia with their career search while also getting people to appreciate the great diversity of the industries that chemists work in and to recognise that chemistry is inclusive of everyone regardless of, for example, cultural background, seniority or gender. I wholeheartedly thank RACI as the inaugural recipient of this award and will continue to do this advocacy work within RACI and elsewhere.

IUPAC's emerging technologies: call for proposals

The search is underway for the the 2023 top 10 emerging technologies.

This call for proposals is open to the global science community as well as to the general public.

To make a nomination, search 'emerging technologies 2023' at iupac.org.

Have your say by 31 March.

ACES Early Career Travel Bursary

Established to support an early career chemist to present a paper at a national conference

Dr Yu Heng Lau, University of Sydney
Yu Heng is a senior lecturer and Westpac Research Fellow. Yu Heng completed a PhD in organic chemistry at the University of Cambridge, then moved to Harvard Medical School as a Sir Henry Wellcome Postdoctoral Fellow in bioengineering. In mid-2017, he was recruited back to Sydney as a lecturer and DECRA fellow, where he has established a research program that spans the fields of medicinal chemistry and synthetic biology.

Yu Heng is recognised for developing new chemical methods for peptide cyclisation to target oncogenic protein–protein interactions. He has also established genome-scale engineering methods for the reprogramming of synthetic microorganisms, and protein engineering methods for manipulating in vivo self-assembly. Currently, the two main research themes in his lab are: developing cancer therapeutic leads for protein complexes that dysregulate genome stability at telomeres, and engineering protein cages as synthetic organelles for controlling biocatalysis.

RACI National Awards 2023

Through our national awards program we recognise and promote the contributions and achievements of our members.

Nominations for this year's National Awards are invited from 1 April.

See the outside back cover for further details.

Jelina Preethi/iStockphoto

A decade of making a difference

It gladdens my heart every time someone says, 'RACI Careers made a difference to my life'. After all, that's why our volunteers contribute so much.

The wonderful news is that we hear these words often. 2023 is the tenth year that the RACI Careers and Mentoring programs have been running. Over the years, we have directly mentored nearly 300 early career scientists. They have gone off to have wonderful careers in an amazingly diverse range of fields. And many of our former mentees have returned as mentors, sharing their experiences to continue the cycle of opportunity.

Take Tiffany Reeves. Tiffany attended one of our Intensive Careers Workshops for active jobseekers a few years ago, and quickly became an active participant in RACI Careers mentoring, events and networking. More than just training, we pair these workshops with facilitated networking to help our participants with targeted approaches to find key opportunities in their preferred field. Based on her success, Tiffany has been building a fabulous career as an analytical R&D team leader in a clinical stage ophthalmology company. She is a successful mentor for our program, and she has taken a leadership role alongside other former mentees Travis Hochwallner (Technical Officer, Australian Racing Forensic Laboratory) and Emma Xu (Business Development Associate, Monash University) in a committee to design and organise RACI Careers' schedule of engaging events.

Tiffany, Travis, Emma and a committee of volunteers in RACI Careers Events and Webinars are organising a flagship event to celebrate the tenth anniversary of our careers work. We will be hosting a National Online Careers Fair on 31 March 2023, bringing more than 40 employers together with more than 400 students and early career scientists across Australia, in the cities and regions. It will be a half day of active professional networking and key careers talks, and we invite every one of our RACI members to get involved (bit.ly/3xlTJF0).

This is just one of the activities in 2023 that has me so excited about the growing good that we can achieve. We are setting up a calendar of more than 30 events in 2023 alone: workshops, webinars, networking events and more, delivered both face to face and online, so that we can achieve access for our full membership in both the main cities and regionally.

William Li (ANSTO) and his colleagues are working on a series of new workshops, collaborating with outside parties to develop truly engaging new educational opportunities, starting with a workshop on postdoc opportunities. Yvonne Mah (BASF, Victorian Branch Past President and former RACI Board member) is leading a project to better engage both with our RACI Groups, Sections, Divisions and Branches and with related societies such as AIP, SETAC, STA and AIFST. Michael Hides (iNova Pharmaceuticals) and colleagues are leading a marketing and sponsorship initiative to grow our reach.

Another team of volunteers is working on a revolutionary Careers Map project, via which we aim to give guidance to students and early career chemists on the amazing range of career pathways and opportunities available to them. Once ready, this will be an incredible resource to help students and early career scientists find inspiration and guidance to better target their career ambitions.

In 2022, I personally piloted a project that is dear to my heart: Job Advocacy. The aim is to reverse the recruitment

paradigm, and to help find great jobs for RACI members from backgrounds that are overlooked by employers, particularly intersectional groups. For example, in our 2022 pilot a group of us (notably including Jovana Sobat of CS Executive Group) volunteered our time to assist a member who had come to Australia from Egypt. A qualified and experienced pharmaceutical analytical chemist, she had been in Australia for 11 months without being able to find any form of employment. By working with her to give her some training and assistance, and particularly by using our professional networks to help her find the right contacts and opportunities, we were able to help this member find a high-quality professional position in her field within just one month!

Following up with her after a couple of months, she was delighted to report: 'The lab is a very busy and rich lab and even after this time there is still a lot to learn; what is worth mentioning is that the team is amazing, and my trainer is a highly knowledgeable person that I learn a lot from'.

The point of our job advocacy is that there is a great job for everyone, even if their background doesn't always attract as much attention from potential employers: culturally and linguistically diverse (CALD), lower socioeconomic background (LSEB), living with a disability, Indigenous, returning to the workforce after a career break, lack of experience, and intersectional groups facing more than one challenge. Notwithstanding their great skills and attitude, and regardless that they would make fabulous long-term employees if they're just given a chance, such people can struggle to find work. And no matter how resilient they may be, months of unemployment can destroy the most robust confidence. But some simple intervention, and the use of networks to bypass the impersonal approach of resumés, can make a transformative difference to these lives. Frankly, I get a little bit emotional just thinking about the difference that a small contribution of time and energy can make.

Amazingly, the challenge for our work is not in achieving the outcomes. With so much goodwill, so many mentors, volunteers and supporters contributing their time, their energy and their professional networks, we achieve spectacular results: roughly 90% of our student mentees graduate from uni with a job waiting for them (or, if they've waited to only look once they complete their studies, then within one month of starting their search). In 2021, 100% of our mentees reported that 'RACI Careers training helped me in my job search' and that 'RACI Careers helped me build my network'. Over more than 50 activities in 2021, our wider careers outreach reached more than 2100 people!

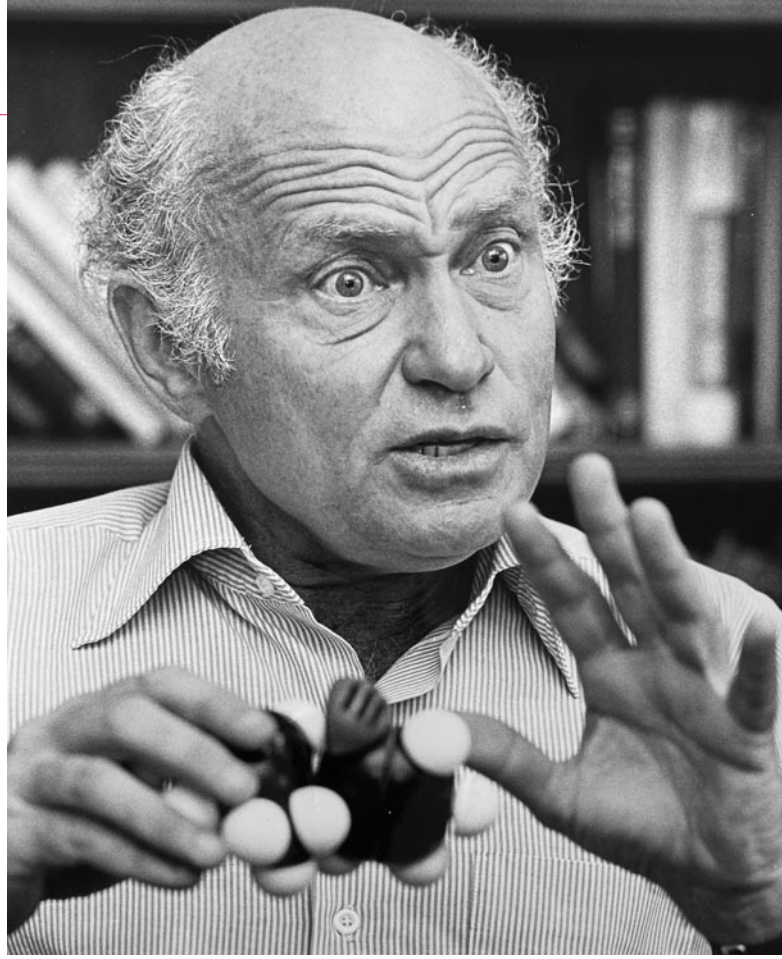
Instead, the challenge for our work is primarily in getting the word out: making sure that students and academics are aware of the breadth of free activities and resources that we offer; getting engagement with our events in an era of 'Zoom fatigue'; and recruiting mentors to offer time one on one, or just to be available for networking purposes.

I'd like to enthuse and engage every single member who is reading this magazine. Spread the word. Talk to your employer about sponsoring the program (please). Get involved. As a person, as a committee member of a Group, or Branch, or Division, reach out to us here at mentoring@raci.org.au. We're eager to hear from you.

Dave Sammut FRACI CChem

Vale Sev Sternhell (1930–2022)

Influential organic chemist



Sev Sternhell DSc AO FAA FRACI CChem was a prominent figure in Australian organic chemistry, academia and public life for more than 40 years. He held the Chair of Organic Chemistry at the University of Sydney from 1977 until his retirement in 1998. Sev was very influential, not only directly through his science, but indirectly through the graduate students that he inspired and mentored, and the thousands of undergraduates he taught over the years.

Severyn Marcel ('Sever', 'Sev') Sternhell was born into a Jewish family on 30 May 1930 in Lwow, Poland (now Lviv, Ukraine). Sev's experiences during World War II in Nazi-occupied Europe were horrific, and he escaped the Holocaust on several occasions by the narrowest of margins. Sev and his family spent time in the Bergen-Belsen concentration camp in Germany, from which they escaped, eventually settling in Australia in 1947. Sev was just 16 years old.

Sev obtained his Leaving Certificate in 1947 at Newington College, Stanmore, and in 1948 he enrolled in Science at the University of Sydney, where he majored in Organic Chemistry. He graduated with First Class Honours in 1951 under the supervision of Dr Francis Lions, and then undertook an MSc supervised by Professor Arthur Birch in 1952.

Sev worked briefly in industry and in 1955, he took up a position in CSIRO (Division of Coal Research) at North Ryde. While at CSIRO, he was awarded a scholarship to undertake a PhD with D.H.R. Barton (later Sir Derek Barton, and 1969 Nobel Laureate) at Imperial College, London. His PhD was on the structure of limonin – one of the natural oils in citrus fruit. At Imperial College, he developed the unusual conversion of hydrazones into vinyl iodides and geminal diiodides – a reaction now known as the Barton–Sternhell reaction.

Sev was also introduced to NMR spectroscopy at Imperial College. NMR was just emerging as a powerful tool for determining the structure of organic compounds and NMR would become one of Sev's major research areas for the rest of his career.

Sev was appointed as senior lecturer in organic chemistry at the University of Sydney in 1964. He rose through the academic ranks and, in 1977, he was appointed to the Chair of Organic Chemistry and Head of Department following the sudden death of Professor Ern Ritchie. Sev served as Head of the School of Chemistry at the University of Sydney on two occasions.

Sev is probably best known for his research into the use of NMR as a tool to unravel the structures of organic compounds. His seminal monograph (with Lloyd Jackman) *Applications of nuclear magnetic resonance spectroscopy in organic chemistry*, published in 1969, became a 'bible' to generations of organic chemists.

Sev was elected as Fellow of the Australian Academy of Science in 1992. In 2001, he was awarded the Centenary Medal for his service to Australian society and science in organic chemistry. He was awarded the Order of Australia in 2019 for services to chemistry and to higher education. Sev was unbelievably proud of this recognition.

Besides his science, Sev had a passion for the great outdoors, and he walked, climbed and abseiled through most of the canyons, valleys and peaks in the greater Blue Mountains. Sev's true obsession was with the Himalayan high peaks and mountain passes in Nepal. He returned to Nepal some 14 times – mostly on trekking trips he organised himself – with different groups of people. He nearly died at least twice in the harsh blizzard conditions on the high passes in Nepal and he credited his survival to his Sherpa guide Bir Bahadur Sarki Tamang with whom he struck a lifelong friendship.

Sev was a very down-to-earth, pragmatic man of keen intelligence, persistence and dogged determination. Sev always identified himself among the 'sincere chemists' – he kept a mental list of those he considered 'sincere chemists' – those with a deep understanding of the discipline who literally lived, breathed and deeply understood chemistry. Sev leaves an incredible legacy – the students and researchers who can be identified as part of the 'Sternhell academic family tree' occupy positions in academia, in government, in industry etc. throughout Australia and all over the world.

Sev is survived by his wife (of 59 years) Alice (who's also a Holocaust survivor), sons James and Roger, and his eight grandchildren Elizabeth, Robert, Leanne, Samson, Lucy, Molly, Leo and Eddie. His son Peter, sadly, predeceased him in 2015.

Les Field AM FAA FRACI CChem FRSN

Earthshot: how to save our planet

Butfield C., Hughes J., John Murray, 2021, hardback, ISBN 9781529388626, paperback, ISBN 9781529388633, ebook, ISBN 9781529388657, 338 pp., $26–35

Earthshot is both the title of this book and an international foundation aimed at saving our planet from the scourges we have inflicted on it (and ourselves). The name draws inspiration from Moonshot, where President John F. Kennedy announced in 1961 a plan to land a man on the Moon within ten years. As we know, this project was spectacularly successful and brought with it many useful discoveries and spin-offs.

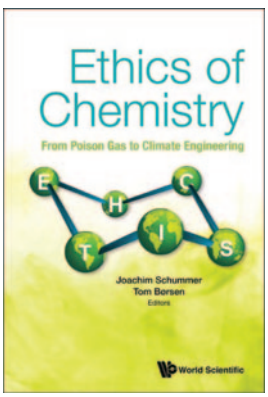
The Earthshot Foundation, which draws its support from international philanthropy, asserts we have ten years to achieve five targets if we are to save our planet, and attempts to draw together people from all walks of life to achieve this. The goals are simple, universal and yet complex to achieve: namely, to protect and restore nature; to clean our air; to revive our oceans; to build a waste-free world; and to fix our climate. Each year until 2030, Earthshot Prizes (in 2021 these were each £1 million) will be awarded in each of these five Earthshot Goals by a committee chaired by HRH Prince William.

So, what of the book? It begins with an erudite and inspirational introduction by HRH Prince William, guaranteed to mollify even the most ardent Australian republican. Subsequently, the book is organised into three sections: a critique of these five major problems facing the planet and why the next decade will be crucial for their amelioration; a discussion on their extent and impact, including how those problems could be tackled; and ways in which we could individually and collectively make a beneficial difference. The writing and the message are both quite clear. Surely, there cannot be many people who would not agree that the challenges outlined in this book are absolutely real and their solutions urgently critical for our very survival on Earth. There is no Planet B; either we fix these problems (largely of our own making) or they will surely fix us. I am not generally convinced that throwing large prizes about leads very far on environmental issues (but that could change in the blink of an eye if I were a winner!) We all have a pretty good grasp of the problems. What we lack is both strongly committed yet subtle leadership to implement, what may seem to many, draconian policies. If you want to know what I mean by 'subtle', think 'nudge'. You could do worse than listen to Toby Park at www.youtube.com/watch?v=cVQ3-1ITsBg in this regard. To put it simply, we can all suffer a bit now so subsequent generations may thrive, or we can continue on our present trajectory and leave our legacy of a much nastier planet. In summary, for me, the book gives a message of hope, but also despair.

Authors Butfield and Hughes are co-founders of Studio Silverback, with extensive experience in film making, including production of WWF's *Our planet* project (Butfield) and Sir David Attenborough's *A life on our planet* (Hughes). The book is well written, is 'friendly' in its language, targets a general audience seeking an understanding of planetary environmental issues and is very moderately priced. What's not to like?

R.J. Casey FRACI CChem

Ethics of chemistry: from poison gas to climate engineering



Schummer J., Borsen T. (Eds), World Scientific Publishing Co., 2021, paperback, ISBN 9789811249488, 560 pp., $120–195 (incl. delivery), hardback, ISBN 9789811233531, $302–570 (incl. delivery)

Ethics of chemistry: from poison gas to climate engineering is a mind-shattering and ground-breaking book. There is little published on the ethics of chemistry available in readily accessible book form. It is probable most individual chemists operate without very much influence from ethical issues (How often do you see OHS issues discussed in the revelation of new molecules or new syntheses?), while many companies from time to time wrestle with conflicts around ethics versus their balance sheets. (Think Bhopal; think thalidomide.) What ethical message did the Nobel Prize Committee send to the world when it awarded the 1918 Chemistry award to the inventor of chemical warfare (Fritz Haber)? What are the ethical responsibilities of defence scientists who develop materials such as napalm, later used contrary to the rules of *jus bellum*, in the Vietnam War (known in Vietnam as 'The American War')? My point is that chemistry is certainly not lacking in ethical dilemmas and the so-called 'Nuremberg Defence' remains as spurious now as it was then.

This book is complex: it is a scholarly work, at times quite depressing reading because it is concerned largely with failure, but enormously enlightening in guiding the reader through the ethical consequences of chemical actions. Over the last century or so, chemistry has come in for a generous share of bad press.

Ethics of chemistry: from poison gas to climate engineering is a serious and successful attempt to develop an ethically balanced view of chemistry. It does this via a series of very interesting case studies from which ethical issues may be drawn. These range from the gas warfare of World War I, to the development of weapons of war, to the Bhopal disaster, to the development of thalidomide, to the use of Agent Orange and DDT, through to issues associated with the use of bisphenol-A and PVC and more. Each chapter describes the problem and its consequences and then offers well-rounded commentary on the

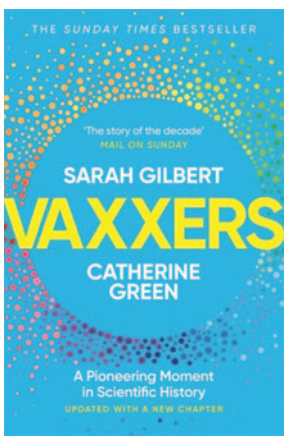
ethical issues it presents. There are 18 contributing authors cited ranging from scientists to philosophers to lawyers. All appear well qualified and suited to the task.

The issue and treatment of whistle blowing is undervalued in the book. It takes considerable bravery, maybe even foolhardiness, to blow the whistle on unethical corporate or individual behaviour. It usually results in 'shooting the messenger': a manifestly unsatisfactory outcome.

You will note the enormous price ranges for this book (sourced from Booko) and recall an earlier enjoinment where I advocated 'shopping around'. My copy (paperback) cost $97 (including delivery) in February 2022, so maybe I should add 'buy early'! Erudition does not come cheap.

This book would make a wonderful text for a university unit on chemical ethics. Every chemist ought to read it and reflect on its messages. Who knows, it might just make the world a bit better place. I commend it most highly.

R.J. Casey FRACI CChem



Vaxxers: a pioneering moment in scientific history

Gilbert S., Green C., Hodder and Stoughton, 2021, hardback, ISBN 9781529369854, $50, paperback, ISBN 978152969878, 352 pp., $25

Vaxxers, co-written by Professor Sarah Gilbert and Dr Catherine Green, both from Oxford University and pioneers in development of the AstraZeneca vaccine against COVID-19 (now known as SARS-CoV-2), is a really interesting and very readable book. Basically, Sarah Gilbert, whose team developed the vaccine from their generic vaccine platform, and Catherine Green, whose team worked up the vaccine to a point where there was adequate supply of injectable formulation to engage in human trials, present in alternate chapters the development of the vaccine. This is all very clearly explained and absolutely accessible for general readers. The book hangs together superbly.

The big question is surely why would one want to read this book? We have endured lockdowns, curtailment of travel, very limited access to social and cultural pursuits, and loss of loved ones in conditions preventing adequate mourning, just to name a few, as a result of the waves of COVID pandemic. My own hometown, Melbourne, has morphed from 'world's most liveable city' to 'world's most locked-down city'. Our political masters morph back and forth between bouts of inspiration (aspects of JobKeeper) and ineptitude (the handling of hotel quarantine). Since Chinese authorities informed the World Health Organization of the virus on 31 December 2019, this virus has killed at least 5.4 million people and we are still counting. In short, we have all had quite enough of COVID, thank you very much.

There are numerous reasons this book is interesting and worth reading. First, it may expand your knowledge about how vaccines work and the processes of developing vaccines. What I also particularly liked was the way the book lets us into the lives of the authors. No doubt, the authors are very clever and accomplished people, but they are also human beings, with much the same faults and foibles as the rest of us. Just like Australian academics, they are perpetually chasing research funding, fighting their way through the abundance of university oversight committees, lying awake worrying about progress or, just occasionally, having a 'bright idea', trying to get the balance right between work and family relations. This, for me, was the real highlight of the book. Science is not done exclusively by stern-faced bespectacled men in long white coats, frequently worshipped for their great sagacity (but occasionally far less admirable at a personal level). Rather, it is done by clever people of all genders, shapes, sizes and colours, with all the imperfections inherent in the human condition.

But there is also a far bigger reason to read this book. The very rapid roll-out of vaccines shortly after the emergence of COVID-19 and the millions of lives saved by these vaccines is an enormous resounding triumph for biomedical science. In so many ways, we have all derived enormous benefit and comfort from the highly skilled scientists whose role has been watching for the ebb and flow of viruses about the globe, anticipating and rapidly identifying emergent pandemics, and expeditiously getting ameliorating vaccines out of the laboratory and into use.

So, how was the AstraZeneca vaccine developed and scaled up so quickly? Because the Oxford group was working on a 'vaccine platform' approach: build a broad vaccine platform, which can then be rapidly modified to act against whatever particular virus emerges. This strategy paid off handsomely. As at August 2021, more than a billion doses had been manufactured and the vaccine had various forms of approval in 121 nations (*New Scientist*, 14 August 2021, page 8).

Undoubtedly, this approach succeeded in saving very many lives. The AstraZeneca vaccine came under attack because of public association with very rare instances of blood clotting (vaccine-induced thrombotic thrombocytopenia, VITT) and the consequent public fears this engendered. To be fair, all medical interventions have both benefits and costs. The Oxford/AstraZeneca vaccine has delivered enormous benefits globally and at extremely minimal risk to human health.

Buy the book and read it! You will greatly enjoy it and learn a lot on the journey.

R.J. Casey FRACI CChem

Space debris and elevated atmospheric CO_2

iStockphoto/dottedhippo

Over the past 60 years, we have sent into Earth orbit 15 000 satellites, rocket stages and other objects. According to the European Space Authority (ESA), there are 130 million pieces of human-generated debris smaller than one centimetre and 32 000 larger items of space junk, all travelling at great speed. These small fragments have resulted from satellite–satellite and satellite–debris collisions over the past six decades. There are now about 9600 satellites in orbit with 6800 of these being defunct. That number of orbiting satellites is increasing massively, with the recent ongoing addition of so-called 'mega-constellations' of satellites by private corporations such as SpaceX and Amazon. These mega-constellations offer the great benefit of connectivity for poorer countries and communities that otherwise would not have access to the internet infrastructure. They also extend the future possibility of involvement in the huge space-sector economic growth for such disadvantaged populations. An unusual example of such a benefit is the provision of SpaceX internet services by Elon Musk companies to Ukraine while it is resisting the invasion by Russia.

These great benefits come with an increasing risk as the overfull orbit with its associated collisions behaves like a grinder of satellites. With the expectation that there will be up to 12 000 SpaceX satellites in the future, the risk is that at some point any new satellites added to orbit will be destroyed or damaged by increasing numbers of debris collisions. This would mean that access to the many strategic advantages of the global internet to humanity could be extinguished, including GPS navigation, weather, climate change monitoring, security, science and entertainment. This risk has been given the name the Kessler syndrome.

The key to avoiding such a disaster is to develop approaches to remove dead satellites. However, while a series of possible removal strategies have been conceptualised by space agencies, no single item of space debris has yet been intentionally removed from orbit. ESA has a project with a timeline of 2025 that involves a chaser satellite attaching itself firmly via a harpoon to a large rocket-stage debris target. Robotic arms will be used to secure the target to the chaser and any damage fragments retained by a net. The chaser plus target is then programmed to carry both as a unified unit into Earth's atmosphere to safely burn up. The company Airbus is involved in developing harpoon capture and removal technologies. Other removal technologies involve lasers in orbit or a laser on a land base. Small debris items can be ablated by laser and the directional pressure of ablation vapour propels the small item either into the atmosphere or into deep space.

The materials commonly used in satellites include approved light metals, polymers and carbon composites. During the disintegration of a dead satellite re-entering the atmosphere, the properties of these materials are important in minimising the quantity and nature of debris reaching Earth's surface. The recent case of a large Chinese rocket stage falling uncontrollably to Earth has caused international safety concerns among space agencies and media because of the possibility of it landing in a populated zone. Uncertainties about the materials used in the rocket stage have added to these international concerns.

At least one NASA-approved polymer has a chlorofluorocarbon mer unit. This material is related to the chlorofluorocarbon monomer refrigerants that were implicated decades ago in the catalytic chain-decomposition of the ozone shield by photolytically generated chlorine atoms. Atmospheric burn-up of such a polymer associated with satellite re-entry could in principle release such catalytic chlorine atoms. At this stage, the extent to which this specialty polymer is used in space devices is not clear.

A concerning aspect of a connection between re-entry science and elevated carbon dioxide levels of the atmosphere from increasing human use of fossil fuels has been reported. Elevated atmospheric carbon dioxide levels increase the density of the lower atmosphere but decrease the density of the upper atmosphere, where the satellite burn-up mainly begins. This loss of upper atmosphere density has been measured at a surprising 20%. Further, the research group exploring this effect claims that the decrease in density could be much greater if carbon emissions continue to grow. The result would be that the ability of Earth's upper atmosphere to capture dead satellites would be sharply reduced. This in turn would mean that this natural pathway of dead satellites moving out of orbit would be substantially reduced and so the number of dead satellites remaining in orbit much longer would progressively increase with time. Instead of an average satellite remaining in orbit for 15 years, it could continue to remain in orbit for several decades. The overall effect would cause the barrier to the addition of new critical satellites to arrive much sooner than previously projected.

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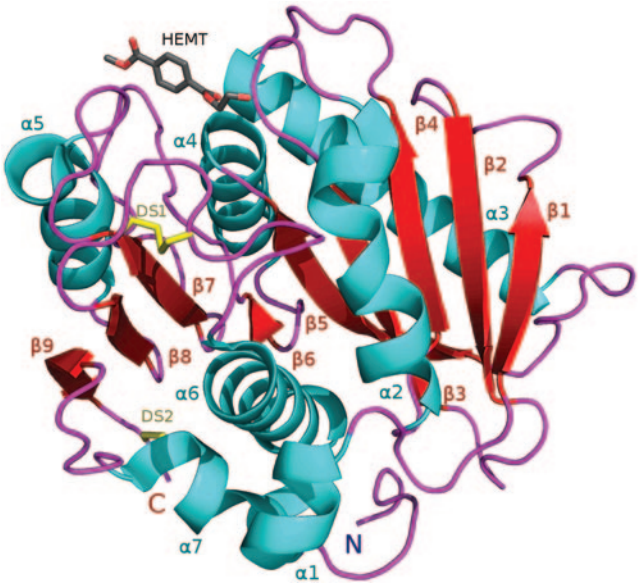
How science fiction predicted recent high-tech developments in chemistry

Real-world technology is often foretold by science fiction. In 1927, characters in the film *Metropolis* made video calls to each other. Star Trek creator Gene Roddenberry hung flat-screen colour monitors on the walls of the *Enterprise* decades before we did the same in our living rooms.

The most obvious examples of technology in science fiction tend to focus on artificial intelligence, communication and transport. But futuristic chemistry is embraced by sci-fi writers too. For example, a central feature of Aldous Huxley's 1932 novel *Brave New World* is a chemical antidepressant.

In recent years we've seen incredible leaps in chemical technologies – to the point where, as a chemist, I'm frequently reminded of some of my favourite fiction while reading about the latest big developments.



1.3 Å crystal structure of a PETase R103G/S131A mutant enzyme in complex with HEMT from *Ideonella sakaiensis* strain 201-F6. PDBID 5XH3. Keministi

A plastic world

While environmental issues are a common thread in science fiction, not many deal with the blight of plastics. An exception is the 1972 novel *Mutant 59: the plastic eaters*. This story, featuring a bacteria that digests plastic, would have seemed far-fetched a few years ago. After all, plastics have only been around for 80 years or so, which hardly seems long enough for nature to evolve a mechanism to eat them.

Yet plastics are carbon-based compounds, in many ways similar to natural polymers such as collagen (in animals), cellulose (in plants) and bee waxes. Over eons, bacteria and fungi have evolved many biochemical tools to scavenge the carbon from every dead organism.

CSA-Archive/iStockphoto

So maybe it shouldn't have been a surprise when, in 2016, scientists sifting through a recycling plant in Kyoto, Japan, discovered a bacteria literally feeding on plastic bottles. Since then, several other research groups have isolated the digestive enzymes involved and engineered them to be more efficient. The hope is we can use these modified natural systems to clean up our plastic mess.

The most recent attempts to do so have a distinctly futuristic feel. A group in Austin, Texas, fed the digestive enzymes' structure into a neural network. This artificial intelligence predicted the best parts of the enzyme to tweak to increase its efficiency. With the AI's advice, the group produced an enzyme that completely degraded a plastic punnet in just a couple of days.

Chemical engineers are already developing large-scale recycling plants using bacteria. The bacteria in *Mutant 59* was also engineered in a lab – but let's hope the parallel stops there. In the novel, the bacteria escapes and causes devastation as it rips through our world, rotting the plastic infrastructure that holds society together.

Dishing up science fiction

From William Gibson's *Neuromancer* to the *Expanse* series, vat-grown meat is a common trope of science fiction. Characters are rarely content with the results, frequently complaining about how synthetic meat is a poor substitute for the real thing.

With the AI's advice, the group produced an enzyme that completely degraded a plastic punnet in just a couple of days.

Many fake meats already line our supermarket shelves, but most are formed from plant-based ingredients blended to mimic the taste and texture of flesh. As a vegetarian, I actually quite enjoy them. But they are easily distinguishable from the real meat of my memories.

Growing meat in a vat is a different affair. It is more like brewing, but using animal cells instead of yeast. The process needs people with a good understanding of cell biology, nutritional chemistry and chemical engineering to work.

The process begins by growing a dense broth of cells. The mix of nutrients within the vat is changed, triggering the cells to differentiate into tissue types – muscle, connective tissue, fat cells. Finally, the cells coalesce into something resembling a pulp of meat, which is harvested and processed into your nuggets, burgers and such like. The advantage, of course, is that you get something with the texture, taste and nutritional content of meat, but without the slaughter.

Back in 2013, the first edible burger made this way cost $300 000. Nine years later, costs have plummeted and investors have poured in billions of dollars. The industry is poised to start selling its products, and is just waiting for the regulatory frameworks to be put in place. Singapore led the way in approving cultured meat in 2021, the US Food and Drug Administration recently gave its seal of approval, and UK and EU regulators are not far behind.

A word of caution

However, sometimes aspirations of real-world science struggle to progress from their fictional inspiration. In 2003, Elizabeth Holmes, aged only 19, founded Theranos. Ten years later, the company was worth $10 billion.

Holmes raised the funds with her promise to deliver a revolutionary technology that could deliver cheap, rapid diagnostics from just a drop of blood. The idea seemed closer to the medical scanners in Star Trek sickbays than anything in reality. And it turned out the promises made by Holmes were criminally over-inflated, earning her an 11-year prison sentence for fraud.

The Theranos story may have set back investors' confidence in plausible applications for the lab-on-a-chip technologies that Holmes championed. But we are actually quite familiar with them already, in the form of COVID lateral flow tests. An even more extraordinary, real example reminded me of the almost-instant DNA sequencing depicted in the 1997 film *Gattaca*.

Early in 2022 at Stanford University, a small group of researchers sequenced an entire human genome in just over five minutes. Contrast that to the 13 years it took to sequence the first human genome, published in 2003. This could help speed up rare disease diagnosis from years to hours.

These astounding leaps forward in diagnostics, recycling and food are just a few areas of chemistry that were once considered science fiction. Many others – such as high-density batteries allowing quicker and fewer charges, atmospheric cleaning technology to remove CO_2 from the air, and 3D 'printed' personalised medication – are also under development. Let's just hope the dystopias so often depicted in science fiction don't emerge alongside the technologies they describe.

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The role of reverse osmosis in securing Australia's water supply

The availability of clean water for drinking and other uses has been a hot-button issue in Australia for at least two decades. The Millennium Drought, which ravaged Australia between 1996 and 2010, made water supply front-page news across the country and led to the construction of Australia's first large-scale municipal desalination plant, in Perth, followed by similar plants on the Gold Coast and in Sydney, Melbourne and Adelaide. At the same time, Brisbane was constructing the largest recycled water scheme in Australia, consisting of three advanced water treatment plants that together can produce 180 megalitres of purified recycled water per day.

The technology that makes all this possible is reverse osmosis. Modern reverse osmosis technology consists of semipermeable membrane sheets spiral-wound around a central tube that collects and transports the desalinated water. To separate salt water or brackish water into a purified stream and a concentrated stream, sufficient pressure must be applied, both to overcome the osmotic pressure of the feed water and to push the water through the cylindrical membrane element. For seawater, pressures of about 6000 kilopascals are typical, while for water recycling, where the salt concentration in the feed is much lower, pressures are 1000–1500 kilopascals. While this gives desalination in particular a reputation for being an energy-intensive technology, when considered at a household level, the energy usage required to provide desalinated water to a family of four is comparable to the energy used to power a family-sized refrigerator. Many water authorities also choose to power their desalination plants with renewable energy.

Reverse osmosis technology for drinking water production originated in the mid-20th century and provided an alternative to thermal desalination (distillation), which was already in use in the Middle East at that time. Since its inception, reverse osmosis has spread around the world, becoming the dominant desalination technology in Australia, the US, Mediterranean Europe and North Africa. The Middle East has also embraced the technology alongside the continuing use of thermal techniques, which remain in play due to the availability of cheap thermal energy in that region.

Reverse osmosis technology is now well understood, but it is not without its challenges. A large desalination plant houses tens of thousands of individual membrane elements collectively worth tens of millions of dollars. If poorly managed, contamination with hydrocarbons or uncontrolled introduction of oxidising agents such as chlorine can cause millions of dollars' worth of damage, while biological fouling can lead to significant increases in energy usage.

Reverse osmosis also produces a concentrated waste stream called brine that needs disposal. For seawater desalination plants, this brine is typically discharged back into the ocean through diffusers, which are designed to ensure that the salinity of the surrounding ocean returns to background levels quickly, minimising the impact to the receiving environment. For inland reverse osmosis plants without the advantage of an ocean disposal pathway, waste disposal is not so straightforward, and can involve complex treatment processes such as brine concentrators and crystallisers for a zero liquid discharge solution. Beneficial reuse of desalination wastes is often discussed in the industry but is yet to become common because of a combination of technical and economic considerations.

It is clear to all who work in the water industry that reverse osmosis technology will be a key part of our national water infrastructure in the future. Sixteen years since the first major desalination plant in Australia was officially opened in 2007, new or expanded desalination plants are now on the cards in five states with the combined potential to add hundreds of millions of litres of water per day to the nation's supply.

In addition to this expansion in desalination, water recycling is still a viable option for drinking water augmentation that has by no means been discarded by planners. The Western Corridor Recycled Water Scheme in Queensland has to date been used only for industrial customers, but it was designed to meet the strict regulatory requirements for use as drinking water. The purified recycled water it produces is able to be discharged into Wivenhoe Dam, from which point it could be traditionally treated as a part of Brisbane's drinking water supply. In New South Wales, Sydney Water is currently building a purified recycled water demonstration plant and visitor centre at Quakers Hill in the Sydney's north-west. The plant is for education purposes only and the water produced will not be added to the city's drinking water supply, but the technology used is robust and able to meet the strict requirements for drinking water use.

Although some Australians may still feel reluctant to drink purified recycled water, there are parts of the world where this is a well-established reality with a proven track record of safety and reliability. In Orange County, California, purified recycled water has been used since the mid-1970s to replenish the groundwater basin from which the region draws its drinking water. Closer to home, Singapore's NEWater recycling scheme purifies water through membrane filtration (including reverse osmosis) and ultraviolet disinfection before discharging it to

... at a household level, the energy usage required to provide desalinated water to a family of four is comparable to the energy used to power a family-sized refrigerator.

A worker inspects the reverse osmosis room at the Gold Coast Desalination Plant, where approximately 2100 pressure vessels collectively contain almost 17 000 reverse osmosis elements.

reservoirs where it mixes with rainwater before being further treated and added to the city's water supply. NEWater will celebrate its 20th anniversary of operation this year.

Water recycling plants typically use a combination of technologies, but reverse osmosis is usually a core element due to its ability to remove pathogens, salts and other contaminants from a wastewater matrix. Reverse osmosis technology was designed to remove salts from seawater, and as a consequence has a pore size of about 1 nanometre or less. Common pathogens (bacteria, viruses and protozoa) are at least one, and often many, orders of magnitude larger, which makes reverse osmosis a highly effective physical barrier to disease-causing microorganisms. The percentage removal of chemical contaminants by reverse osmosis is lower, but still substantial, with factors such as the size, charge and hydrophobicity of the molecule influencing how readily it is removed by reverse osmosis membranes. If reverse osmosis alone is insufficient to reduce chemical contaminants to the required level, it is often accompanied by other technologies that use oxidation, adsorption or other mechanisms to further reduce trace chemicals.

On Australia's east coast, rainfall patterns in recent decades have oscillated between famine and feast. A severe drought between 2017 and 2019 was followed by the arrival of a La Niña weather pattern in 2020 that has brought floods to Australia's eastern states with alarming frequency in the years since. Desalination and water recycling are primarily considered to be drought mitigation measures, but recent floods have again brought them to the fore in ways that might surprise some. Flooding has affected the quality of water catchments by bringing silt, ash and organic matter into rivers and dams. This degraded raw water quality has been challenging for conventional water treatment plants in many regions. Desalination plants, because of both their technology and their feed water source, are less affected by these challenges and have been used to take the pressure off stretched traditional treatment plants.

Desalination is being considered as part of a strategy to manage flood risks in some cities. Supplementing water supplies with desalination may allow planners to operate dams at lower levels, giving communities additional flood protection through the freeboard created between the operational water level and the height of the dam.

Taken together, the benefits of reverse osmosis make it a highly valuable technology in any strategy for a reliable, climate-resilient water supply for the future.

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Natural products and drug-like chemical space

To quote Douglas Adams (*The hitchhiker's guide to the galaxy*): 'Space is big. Really big. You just won't believe how vastly hugely mind-boggling big it is'. If space is big, then chemical space, the virtual (meta) space populated by every conceivable chemical structure, is even bigger. One metaphor that tries to convey this bigness goes something like '… to make a milligram of each of even a small subset of molecules that occupy drug-like chemical space would consume the entire mass of the known universe', where 'drug-like chemical space' refers to a hypothetical set of chemicals that have the potential to inspire all past, present and future drugs.

Irrespective of the merit of the underlying arithmetic, the metaphor successfully speaks to the vastness of chemical space and introduces the concept that drug-like molecules might be concentrated in a smaller and perhaps more manageable region known as 'drug-like chemical space' – if only we knew what this space really was. Unfortunately, defining drug-like chemical space is no simple task, as known drugs belong to a bewildering array of chemical classes, and no one really knows what space is occupied by yet-to-be-discovered drugs! Assuming we accept that drug-like chemicals can be assembled into a common space, this begs the following questions. Can we really differentiate what chemicals fall within and without? Can we exploit this knowledge to better guide the discovery of new drugs?

As noted above, setting boundaries for drug-like chemical space is problematic. The sheer number of molecular permutations makes it impossible to synthesise and experimentally test every conceivable chemical for efficacy against every conceivable disease or medical indication by every conceivable assay, before flagging them as drug-like or not. Consider, for example, the 51 amino acid peptide insulin. To synthesise all possible stereoisomers would involve making more than 2×10^{15} compounds, which is >10 000 000-fold more than all the compounds currently known to science (i.e. listed in *Chemical Abstracts*), requiring any boundaries to be predictive not experimental. What follows is an account of two philosophies for predicting the occupancy of drug-like chemical space, one based on in silico rules that favours synthetics, and the other based on evolution that favours natural products.


hanohiki/iStockphoto

Briefly, the in silico approach draws on a subset of known drugs to identify, calculate and define the acceptable range for each of an array of predictive characteristics (i.e. molecular weight, polar surface area, partition coefficient, and the number of H donors, acceptors, rotatable bonds and atoms etc.), thereby establishing quantifiable rules that define drug-like chemical space.

While the in silico approach can readily detect rule violations, and thereby catalogue and populate said space, it suffers from some significant limitations. For example, by assuming that a limited set of known drugs uniquely defines all of drug-like chemical space, the in silico approach excludes any drugs that possess molecular characteristics that fall outside these pre-defined parameters. This is much like a mining geologist confronted by a near-exhausted ore body restricting all future exploration to locations within the boundary of the current mining lease. Even if the lease is big, and is inclusive of related ore bodies, such self-limiting boundaries are inherently counter-productive – especially if you own a coal lease and are exploring for gold!

Another shortcoming of the in silico approach is that the known drugs used to derive its rules exclude natural products and natural product inspired drugs. To put this in perspective, natural product drugs include nearly all known antibacterials (vancomycin, rifampicin, daptomycin) as well as antifungals (echinocandins, nystatin), antiparasitics (avermectins), antimalarials (artemisinin), anticancer agents (taxanes), insecticides (spinosins), antilipidemics (statins), immunosuppressives (cyclosporin, rapamycin, tacrolimus) and many, many more! This exclusion was rationalised on the basis that the structural complexity of natural products made it near impossible to arrive at a simple and universal set of in silico rules that defined drug-like chemical space. Returning to our humble geologist, this exclusion is akin to deciding not to explore a vast mineral-rich region with a complex geology simply because it's easier to search the gaps between coal seams where the geology is better understood and highly predictable. Again, such a path may be valid for opening up a new coal seam but is clearly unhelpful if the objective is to discover new lithium or copper deposits.

Simple rules may be attractive, but they need to be fit for

purpose. The exclusion of natural products would not be such a problem if it was more generally acknowledged and factored into decision making. Sadly, this has not always been the case. For example, one of the early applications of the in silico approach was to validate the purported drug discovery potential of combinatory chemistry (combichem) libraries, massive collections of structurally simple, achiral synthetic small molecules that were seen by some as a more accessible and exploitable alternative to natural products. Caught up in the predictive surety of a new paradigm, some employed in silico rule violations to downplay the drug-like potential of natural products. While not the only factor at play, such misguided absolutism fuelled a trend that saw the pharma industry turn away from natural products late last century, to seek inspiration elsewhere. Some 20–30 years on, and confronted by near empty drug discovery pipelines, and pharma are still in search of inspiration (see www.science.org/content/blog-post/combichem-into-drugs-many). Notwithstanding a bumpy start, a more nuanced appreciation of the in silico approach might see it repositioned from gatekeeper to drug-like chemical space to that of a tool to optimise and develop drug leads derived from a wider diversity of chemical space inclusive of natural products. This prompts the question, what is the relationship between natural products, drugs and drug-like chemical space?

At its simplest, natural products chemical space can be defined as that region of chemical space occupied by natural products. For a definition of natural products, I refer you to my earlier column 'Natural products – mainstream but not always natural' (September–November 2022, pp. 36–7). While history provides numerous examples of successful, indeed game-changing, natural-product-inspired pharmaceuticals and agrochemicals, it's worthwhile pausing for a moment to consider why. As life on Earth evolved from simple to more complex forms, survival of the fittest went hand in hand with genetically acquired traits that enhanced survival. Natural products featured prominently among these traits and included chemicals that improved intra- and inter-species and even inter-kingdom defence and communication (i.e. anti-infectives to protect against infection, as well as pigments to hide from, and bitter-tasting, painful or poisonous chemicals to defend against predators, as well as sex, trail, alarm and other pheromones). They could also enhance predatory prowess (i.e. venoms to better hunt and rapidly immobilise prey).

Natural products are unique in co-evolving with life on Earth to be biocompatible (i.e. produced by and of value to life), often operating with exquisite selectivity and potency, binding to and changing the biochemical behaviour of chiral macromolecules and assemblages (i.e. proteins, DNA, RNA, carbohydrates, extra and intracellular membranes, biochemical pathways, tissues and organs). Current natural products are far from a random assortment of complex molecular structures; rather they have co-evolved and diversified with all the species of life on Earth, benefitting from billions of years of genetic mutation and natural selection, a near-infinite investment unconstrained by ethics, time or resources, that shamelessly exploited the emergence and extinction of trillions of individuals and countless species. Given this pedigree, it's hardly surprising that natural products would feature prominently in drug-like chemical space.

Natural products were, are and always will be key players in drug-like chemical space, inspiring the development of urgently needed future drugs.

Recent years have seen dramatic advances in the technologies and methodologies of natural products science, and in our understanding of the genetic machinery responsible for their biosynthesis, their molecular targets and mechanisms of action, and our ability to detect, isolate and identify, as well as evaluate, optimise and repurpose their chemical and biological properties. That said, drug-like chemical space is no more uniquely defined by natural products than by in silico rules. Natural selection does not optimise natural products for oral bioavailability, shelf life, ease and cost of manufacture, for example. In many cases, natural products provide valuable drug leads, but it's medicinal chemistry that reaches beyond natural products chemical space to develop and deliver practical drugs to the market.

So where does this leave drug-like chemical space? Early last century in a pre in silico era, the drug discovery pendulum swung heavily in favour of natural products, which delivered the revolution in health care that is the foundation of modern medicine (think penicillin). Late last century, and driven by many factors including the 'commercial' need to be different to attract investment, the drug discovery pendulum over-corrected in favour of an in silico philosophy. Like many things in life, balance is the key. Perhaps the true value of drug-like chemical space lies more in its acceptance as a concept that embraces both natural and synthetic chemicals, rather than an absolutist and strict adherence to rules and rule violations. Natural products were, are and always will be key players in drug-like chemical space, inspiring the development of urgently needed future drugs.

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Australian chemical organisations: a remedy for fragmentation

More than 1100 RACI members and friends attended last year's very successful Congress in Brisbane. As expected, by far the majority of presentations and posters had a strong academic focus. The few non-academic presentations included sessions run by the HS&E and Industrial Chemistry Divisions and presentations by the Medicinal Chemistry and Analytical and Environment Divisions. Other than these and some CSIRO lunchtime presentations, the Congress had little appeal to the 3000 or so RACI members who are not academics, not to mention the many non-member chemists in Australia.

The authors of *Chemistry for a better life: the decadal plan for Australian chemistry 2016–25* (bit.ly/3ku98zN) appeared to avoid involving other chemical-based societies and organisations in their deliberations. This was a pity and a weakness because thousands of people with chemistry qualifications, experience and backgrounds were unintentionally excluded from contributing to this important work.

A few years ago, RACI played a significant role in establishing the Federation of Asian Chemical Societies. It was also active when Commonwealth Chemistry, the Federation of Chemical Science Societies in Commonwealth countries, was established. Maybe it is now time to play another significant role and take the initiative to set up what we might call the Federation of Australian Academic and Applied Chemical Societies (FAAACS).

Science & Technology Australia (formerly known as Federation of Australian Scientific and Technological Societies, FASTS) is the umbrella organisation for all science and technology societies in Australia, representing the interests of more than 90 000 scientists and technologists. The proposed FAAACS would be the equivalent for chemists, focusing on the interests of chemists, chemical engineers and chemical technologists working in academia, teaching and industry.

Establishing links

We need to recognise that many chemists, particularly those working in industry, no longer belong to RACI because of perceived lack of relevance. In a letter to *Chemistry in Australia* (May 2008), Albright & Wilson (Australia) Senior Manager John O'Donnell described his membership of the Australian Society of Cosmetic Chemists as 'being open to scientists involved in the industry at large' rather than 'based on a scientific discipline'. Unfortunately, the impression gained by many chemists working in industry is that RACI appears aloof and uninterested in who they are or what they do. This may not really be true, but the impression is still around and needs to be rectified. If industrial chemists won't join RACI, RACI needs to collaborate and work with the organisations they do join.

If RACI truly wants to be the voice of chemistry in Australia, I believe it should find ways of establishing links with all relevant organisations. Just as RACI took the initiative to establish the Federation of Asian Chemical Societies, I think it is now time for it to advocate for the 90% of qualified chemists in this country who are not currently RACI members, not just the 10% who are.

How might this be implemented? How about regular

We need to recognise that many chemists, particularly those working in industry, no longer belong to RACI because of perceived lack of relevance.

meetings with all groups involved in chemistry-related research, development, manufacture, importing, selling or using chemicals, including representatives from the organisations listed below, with RACI taking a lead role in spearheading this initiative? Most of the organisations have their own annual meetings, often quite large affairs. Maybe a way could be found for future RACI Congresses to be combined with these other annual meetings. There should also be regular forums of all the chemical societies, institutes and organisations to address common problems.

Scope of the opportunity

Many scientific societies, institutes and organisations in Australia cater for the interests of chemists in specific industries. These include organisations such as Surface Coatings Association Australia, the Australian Society of Cosmetic Chemists, the Australasian Plastics and Rubber Institute, the Australian Institute of Food Science and Technology, the Society of Dyers and Colourists of Australia and New Zealand, the Australian Institute of Occupational Hygienists, and the Australian Institute of Energy. The total number of members of all of these organisations with chemistry qualifications would run into several thousand. Then there are the Institution of Chemical Engineers, the Royal Society of Chemistry, the Society of Chemical Industry, and the American Chemical Society, nearly all of which have strong contingents of Australian members, only some of whom are also members of RACI. I am sure there are more societies, but these are enough to be going on with!

We could also add the industry associations covering chemical companies employing chemists in production, research and development, marketing and general management, such as Chemistry Australia (formerly the Plastics and Chemicals Institute of Australia, PACIA), ACCORD (hygiene, cosmetic and specialty products) and Fertilizer Australia. It is likely that the number of employees of member companies of these Associations with chemistry qualifications would probably also run into the thousands.

And what about teachers? A very rough estimate suggests that there may be 14 000–15 000 science teachers in Australia, a significant number of whom are chemists (although unfortunately not all chemistry teachers have chemistry qualifications). The Science Teachers Association has branches in every state, but a key association specifically for chemistry teachers is the Chemistry Education Association based in Victoria. They have a broad membership, but not many chemistry teachers are currently RACI members.

It is interesting to think that the three dozen or so Australian universities offering chemistry or chemistry-related degree programs probably produce in total about 1000 new chemistry graduates a year. Assuming an average working life of 40 years (and no net change due to immigration and emigration), up to 40 000 practising chemists might be working in Australia at any one time. Membership of RACI runs to around 10% of this number.

Potential benefits of working together

We all know the advantages of getting out of our own little silos in terms of cross-fertilisation of ideas, recognising and understanding other branches of chemistry not to mention other branches of science and technology, and discovering new ways of collaborating and working together. I suspect that currently many academics are unaware of the scope of the chemical industry in Australia, and many in industry are unaware of the groundbreaking research currently being undertaken in universities, CSIRO and other research institutions. Establishing FAAACS could help to improve communication between industry and academia.

A second major benefit would be in our dealings with the different layers of government. An organisation covering the thousands of people involved in the whole spectrum of chemistry in one way or another is likely to have a lot more clout than a largely academic chemical institute with 4000 members. A large FAAACS would be a true voice of chemistry and could speak to government more forcefully about regulation and control of chemical products, possible new directions for future funding for chemistry research, and the need to mandate suitably qualified personnel to manage chemical operations, to name but a few.

A third benefit would be in the sphere of chemical education: collaboration rather than fragmentation could bring about more relevant education and training programs at all levels (school, TAFE and university). A federation of chemical societies in Australia could help develop a common focus on chemistry education that is relevant and rigorous.

What next?

Complete amalgamations or mergers probably won't work, but cooperation and collaboration, within a federation of societies with a chemical focus, should be the way forward.

Martin Luther King had a dream. I'm not sure that this dream of a Federation of Australian Academic and Applied Chemical Societies is quite in the same league, or whether trying to establish something like this would become a nightmare instead of a dream. But I'd like to think that coming together under an umbrella body spearheaded by RACI would generate benefits for Australian chemists beyond their own dreams.

Richard Thwaites FRACI CChem worked in the chemical industry in Australia and London for more than 40 years. He is an active member of RACI's Victorian Branch.

New year, new directions

It is with pleasure that we have accepted an invitation to follow on from the Grapevine column, which was diligently prepared for the past 11 years by Professor Geoffrey Scollary.* With this change comes a new name – *Un-wined* – and a new direction. With our backgrounds in wine chemistry, it is natural that wine will remain a common feature, but we intend to branch into other areas of food and beverage chemistry, or more generally, chemistry associated with the agrifood sector.

Along with writing our own articles, we have decided to open up the column by inviting contributions from experts undertaking innovative research in relevant fields. As such, we are considering the content for this year and beyond. Potential topics include the molecular basis of stone fruit aroma in wine, the flavour chemistry of beer, volatile sulfur compounds in food or beverage, the application of spectroscopy and chemometrics to food quality or authenticity, botanicals used for gin production, and much more. While we intend to use our network of colleagues and collaborators from across Australia, we welcome suggestions for topics based on our research areas, and are happy to hear from anyone who undertakes agrifood-related chemistry and may wish to contribute an article to this column in the future.

After that brief taste of where we are heading, we will use our first column to introduce ourselves and the types of research we conduct.

* Editor's note: In his final column (December 2022 – February 2023, p. 40), Geoff remarked, 'There does come a time when the wine stored in a cellar needs to be rejuvenated. The same also applies to those who write about wine!'

Kerry Wilkinson

I completed a BSc(Hons) with a major in chemistry at Flinders University, after which I pursued a PhD investigating the release of oak-derived volatile compounds into wine during barrel maturation, in collaboration with the Australian Wine Research Institute (AWRI). This not only allowed me to apply my chemistry expertise to an issue of industry relevance, but introduced me to winemaking, flavour chemistry and sensory analysis.

After a brief year as a water chemist at the Australia Water Quality Centre, I returned to wine via a postdoctoral position at Curtin University, based in Margaret River. I moved back to South Australia in mid-2007 as an academic at the University of Adelaide, where I am currently a professor of oenology.

My primary research interests concern the influence of environmental conditions, vineyard management practices and winemaking techniques/technologies on the composition, sensory properties and consumer acceptance of wine – but I'm best known for my research on the impacts of vineyard exposure to bushfire smoke, and remediation of 'smoke taint' in grapes and wine.

When time permits, I also study the chemistry and/or consumer acceptance of other foods and beverages, including edible insects. I have published more than 100 papers on these topics, and look forward to showcasing a range of agrifood-related chemistry with you via this column in the future.

David Jeffery

After gaining qualifications as a chef and working in kitchens for a number of years, I obtained a BSc(Hons) in chemistry and then went on to a PhD in synthetic organic chemistry at Flinders University.

My first foray into wine was a postdoctoral position at AWRI upon completing my PhD. This gave me a solid foundation in wine chemistry as I researched red wine polyphenols and then moved onto aroma compounds.

After five years at AWRI, I took up a lecturing position at the University of Adelaide, where I am currently an associate professor in wine science. Still using my synthetic and analytical chemistry skills, my research involves many aspects of grape and wine chemistry, such as identifying biochemical pathways to formation of aroma compound precursors, developing analytical methods for compound quantitation, identifying new compounds, and conducting studies on the influence of fermentation or other winemaking variables on wine composition. I have published more than 100 papers involving those topics and others, and have co-authored a textbook – *Understanding wine chemistry* – with colleagues in the US.

In 2015, I was awarded RACI's Peter Alexander Medal (as it was formerly known) for excellence in research involving analytical chemistry as an early career researcher. In 2022, I received a Flinders University Distinguished Alumni Award for my distinguished contributions to grape and wine research and teaching.

The name game

Nomenclature in chemistry took a giant step forward in the late eighteenth century when French chemists – Louis Bernard Guyton de Morveau (1737–1816), Antoine Laurent Lavoisier (1743–94), Claude Louis Berthollet (1748–1822) and Antoine François Fourcroy (1755–1809) – proposed a system of names for inorganic substances based on their elemental composition. Sodium chloride for a substance formed from sodium and chlorine, for example. Their *Méthode de nomenclature chimique* was published by the Académie Royale des Sciences in Paris in 1787, and its inspiration clearly was the binomial system for nomenclature of animals and plants that had been introduced by Carl Linnaeus (1707–78) in 1735 and 1753, respectively.

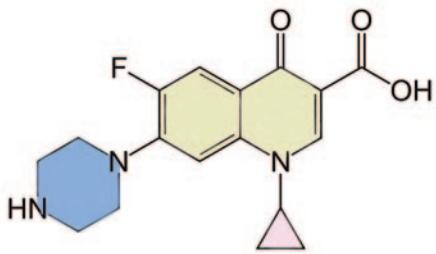
As with most sweeping changes, it took a while for the new names to catch on – copper sulfate for blue vitriol, sodium sulfate for Glauber's salt, and lead acetate for sugar of lead. There continue to be chinks in the nomenclatural armour, of course, especially for industrial chemicals for which the systematic names are seldom heard: think lime (calcium oxide) and slaked lime (calcium hydroxide).

Reforming organic chemical nomenclature was much more complicated. There wasn't much progress until the middle of the next century, as I have mentioned in some of my recent Letters. The result was a whole new language, one that we struggled to impart to first-year students but largely ignored in our daily life. As with inorganics, the trivial names for industrial substances proved very hard to displace and even laboratory chemists shunned propanone for acetone. In a kind of 'Sunday observance', we used the new language in much of our published work, under the eye of the editorial 'clergy', but on weekdays we lapsed. It was only a small transgression to speak of stearic instead of octadecanoic acid, but who would blame us when we eschewed pentacyclo[4.2.0.0^{2,5}.0^{3,8}.0^{4,7}]octane for cubane?

A lot of what started as lab jargon, only to become part of the lexicon is described in one of my favourite books, *Organic chemistry: the name game*, by Alex Nickon and Ernest F. Silversmith (1987), from which I borrowed the title of this Letter. Most of the names the authors mention have been bestowed in modern times. I don't think there is an equivalent book about inorganic substances and examples that could find a place in such a book don't come easily to mind. Perhaps modern inorganic chemists haven't been so keen to vocabularise.

The field of organometallic chemistry offers many opportunities for the creation of catchy, simple names for complex compounds, a simple example of which is ferrocene (cyclopenta-1,3-diene;iron(2+)). In 1830, William Christopher Zeise discovered a compound of platinum and ethylene; over a century later it was shown to be $K[(\eta\text{-}C_2H_4)PtCl_3].H_2O$, but I'm not sure when it was dubbed Zeise's salt. In the second half of the last century, coordination chemists produced (and named) crown ethers and cryptands.

Pharmaceutical companies come up with the simple – and sometimes not-so-simple, but often catchy or even euphonious – names for substances that have long and complicated systematic names. To see how it was done, I set out to see why Ciprofloxacin might have been chosen as the marketing name for 1-cyclopropyl-6-fluoro-4-oxo-7-(piperazin-1-yl)quinoline-3-carboxylic acid, the structure of which is shown.



Ciprofloxacin

Ciprofloxacin is the best-known member of the fluoroquinolone family of antibiotics, all of which contain *floxacin* as part of their commercial names. None of them include 'quinolone' – the structural unit I have shaded in yellow – as a segment in the name, but the *one* suffix that appears as *4-oxo* in the systematic names, is certain to be the source of *ox*. The other common segments are *fl* for the fluorine substituent, and *acin*, which is probably a homonym for azin, taken from the piperazine ring that I have shaded in blue. There are a few members of the fluoroquinolone family that do not contain this structural unit, but it was present in the first of this group to be invented, norfloxacin, and the *acin* seems to have been carried over for others in which the piperazine has been replaced by other heterocyclic rings. The unique segment in Ciprofloxacin is *cipro*, probably another phonetic slide, this time from the cyclopropyl ring that I have shaded in pink.

Maybe you didn't need to know all this – just take the stuff and hope you get better because it could be an example of Bismarck's warning that it might be best if we didn't know how laws and sausages are made.

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 is an editor of *Historical Records of Australian Science*.

events

European Congress on Chemistry and Applied Sciences
20–21 March 2023, Belstay Roma Aurelia, Rome
scisynopsisconferences.com/chemistry

VCE Chemistry Teachers' Professional Learning Day
7 June 2023, RMIT University city campus, Melbourne
raci.org.au/events

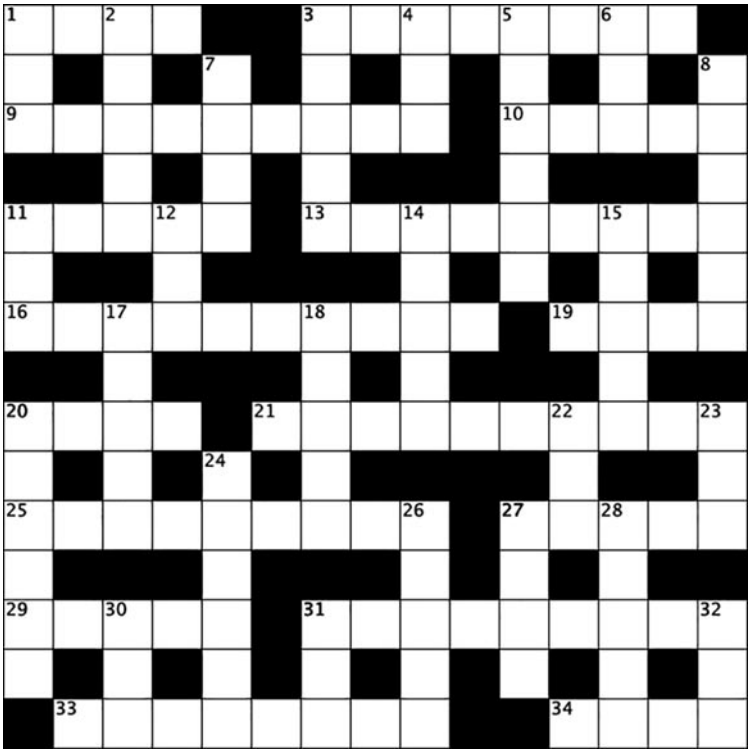
1st Biennial Conference on Green and Sustainable Chemistry and Engineering
2–5 July 2023, Shangri-La Hotel, Cairns
gasc.au

20th International Conference on Biological Inorganic Chemistry
16–21 July 2023, Adelaide
icbic2023.org

IUPAC World Chemistry Congress 2023
18–25 August 2023, World Forum, The Hague
iupac.org/event/iupac-world-chemistry-congress-2023

14th Australasian Organometallics Meeting
4–7 December 2023, Canberra
raci.org.au/events

cryptic chemistry



All the Across words plus 7 Down have something important in common; otherwise their clues provide no definition.

Across

1 Last company. (4)
3 Said to be against cash. (8)
9 Game minus manoeuvring. (9)
10 Party! Hurried over. (5)
11 Blessing over radical. (5)
13 A 71 with little hesitation. (9)
16 It's under seven. (10)
19 Press. (4)
20 One. (4)
21 Only bummed around. (10)
25 Ruin the mu variant. (9)
27 Holding back? There is no next time. (5)
29 Sounds like they left. (5)
31 Buy Miller brew. (9)
33 One. (8)
34 Clue. (4)

Down

1 A steel coating technology. That's magic! (3)
2 Nickel-germanium radical state. (5)
3 Psyche brings up parts of Fireman Sam in Action. (5)
4 Grimalkin trappin ovine molecule. (3)
5 Room around to spoil the liquor. (6)
6 Consent to drift off. (3)
7 None broken. (4)
8 A fellow from the north is a superhero. (3-3)
11 6-Benzylaminopurine can be served with dinner. (3)
12 See 23 Down.
14 The theoretical element 171 Rydberg unit of energy attracts a lot of interest. (5)
15 Deposed Prime Minister sent down fast ones. (5)
17 Throw in the towel and get the bird. (5)
18 8583 parts of a drachma. (5)
20 Bunsen, for example, needed about 10 gram. (6)
22 See 32 Down.
23 & 12 Down Secondary courses can be found in cyanocobalamin or some other compounds. (6)
24 Wasted the Tower of Pisa? (6)
26 Edge into Spooner's wine. (5)
27 Wood combining form in sexy love. (4)
28 Sound out nitric oxide ion-selective electrode. (5)
30 Amino acid extracted from *evening lychnis*. (3)
31 Badger infection. (3)
32 & 22 Down Look after wet earth bait. (6)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University.

Solution available online at chemaust.raci.org.au, Other resources.

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