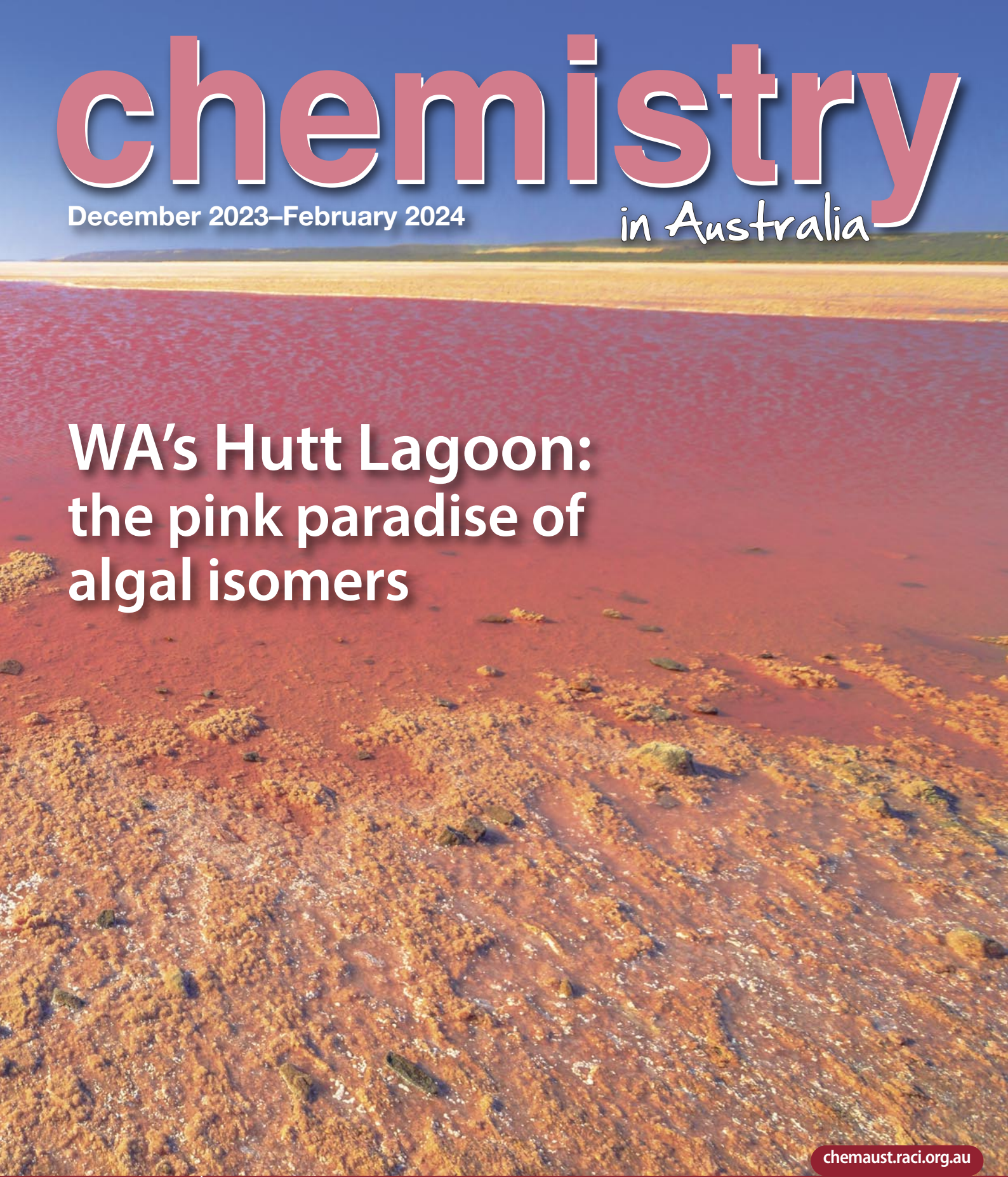
chemistry in Australia
December 2023–February 2024



WA's Hutt Lagoon: the pink paradise of algal isomers

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cover story

The pink lagoon: more than meets the eye

The stunning pink of Western Australia's Hutt Lagoon has caught the eye of many tourists, and the algal carotenes that cause it are of great interest to industrial chemists.

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Chemical safety at work has its frustrations – for workers and regulators alike – but neglecting it in the name of innovation can cost lives.

22 Artificial intelligence and chemistry

What is the future of AI in the chemistry professions, and is it something we should be worried about? Ian Maxwell reports on AI and its future compared to that of quantum computing in molecular quantum chemistry.

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Four seasons and chemistry

The best description for how 2023 has been for chemistry as a discipline and RACI itself is 'four seasons in a day' – something I am quite familiar with from the country I grew up in – Iceland.

For the discipline, we have seen a mixture of stormy days and sunny outlook. The academic sector faces headwinds. We saw a new low in terms of Discovery Project grants awarded to chemistry research projects from the Australian Research Council (ARC). The number of ARC Discovery Project grants going to chemistry has steadily declined in the past few years. Partly, this is due to the constant cuts to the ARC, but there are concerns that the size of the chemistry slice from the ever-shrinking ARC pie is also diminishing. The gradual decline in the number of students studying chemistry at high school, albeit varying from state to state, is also concerning. The situation seems to be more dire for physics, mathematics and engineering. Perhaps related to these funding cuts and high school recruitment challenges is that we had cuts and threats to the chemistry disciplines in some universities, particularly in regional areas.

This contrasts to the outlook for a significant portion of the chemistry industry. Federal and state governments are investing heavily in new technologies and manufacturing industries, many of which depend heavily on chemistry. This includes plans for local battery production, and hydrogen production, storage and shipping to accelerate the shift to renewable energy. Heavy investment in biotechnology, including synthetic biology and RNA therapeutics, will also require a lot of chemistry input and a workforce with a good chemistry background (e.g. for managing analytical and purification processes). The first real-world applications of quantum computing are likely to be in chemistry and the establishment of a domestic nuclear-powered submarine fleet with AUKUS depends on skilled chemists to manage the associated nuclear and non-nuclear materials. Despite high energy prices, the conventional manufacturing industry seems to be doing well and, in contrast to the situation with high school recruitment, there is growing demand for chemists in some regional centres.

RACI has had a mixture of headwinds and very bright moments this year. The 2022 RACI Assembly highlighted issues with our communication systems and a lack of mutual understanding of the activities that RACI and the various communities (Branches, Divisions, Groups and Committees) undertake. It quickly became clear that some of RACI's systems and operational procedures either had become outdated or needed significantly upgrading. And although our overall finances are still strong, our income needs to grow quite significantly, or we will have to permanently cut back on programs and staff. RACI had to respond to these by reviewing the bulk of programs and systems, with emphasis on understanding how to deliver better outcomes, including financially, for the organisation.

The subsequent reform and restructuring efforts are now in full flight and the sun is already breaking through the clouds! Our new IT and communication systems have already improved intra- and inter-community communications within the Branches and Divisions, and the new IT system for managing events is in the final stages of testing for a full launch next year. Internally, the National Office has been restructured around four functional teams: Careers and mentoring, Education and outreach, Corporate services, and Events. This will enable the team to give better quality services to the Divisions and Branches. As part of this overall restructure, we have been reviewing our events processes and many of our educational, outreach and mentoring programs. This work is not fully completed, and although we will try to keep most of them going, some may slow down or pause briefly as the recommendations of these reviews are implemented. I hope that members will bear with us because we aim to come back with much more effective and streamlined processes to run and grow these activities.

On the bright side, chemistry and RACI are becoming more visible. We had several constructive meetings with Australia's Chief Scientist and even with the Minister for Industry and Science. Our submissions to the ARC review and the new National Science and Research Priorities were recognised and welcomed by the government. Having caught the government's eye, we need to use that relationship to also turn the tide on funding for fundamental research in chemistry in Australia and further grow the chemistry cohort in high schools.

RACI has also made several new links to related organisations. This will only increase the visibility of chemistry and RACI, and link to our plans to grow new income streams in collaboration with governmental and industry associations. We have also revitalised and expanded our network to like-minded international organisations. Of note is our new partnership with the German Chemical Society and reinvigoration of relations with the American Chemical Society. To top this all, our own Emeritus Professor Mary Garson AM, FRACI CChem, was recently elected Vice President of IUPAC, and on to President in 2026.

I conclude this last President's column of the year by reiterating that despite some stormy days, we should celebrate the achievements we had this year and look forward to a brighter year again in 2024. Wishing you and your families all the best for the upcoming festivities and holiday season.

Pall Thordarson FRACI CChem (president@raci.org.au) is RACI President.

Chemists in industry or industrial chemists?

As highlighted by R. Thwaites (March–May, p. 38) and A. Zipper (June–August, p. 5), not all chemists work in research or academia. Approximately 50% of RACI members work in industry, but not all are industrial chemists. Often, the terms 'industrial chemist' and 'chemist in industry' are used interchangeably. Yet, a chemist who works in industry is not necessarily an industrial chemist; and an industrial chemist may not necessarily work in industry! The American Chemical Society defines industrial chemists as those who 'work to develop and manufacture products and processes that will increase their company's sales and profits'.

However, I disagree (to a point) with Zipper's comment relating to the National Awards. In fact, nine National Awards are open to nominations from industry-based members. However, the inability to disclose information subject to confidentiality and non-disclosure clauses places industry-based members at a disadvantage. Yet, the disparity does not end there. The inequality is also identified at the affiliate membership level, where teachers at affiliate schools can get recognition through the reward systems that a staff member of an industry affiliate organisation cannot.

Interestingly, the Weickhardt and Leighton medals were named after industrialists who made their mark in the chemical industry. Leighton was more than an industrial chemist; he championed dangerous goods safety, chemical manufacturing, development of national standards, and occupational health and safety. Yet in its history, only seven industry-based members have won the eponymous award. The list of Weickhardt Medal winners reveals a similar story.

RACI (and our academic-based colleagues) must understand that our industry-based colleagues play a significant role in partnering research and innovation. Some 90% of chemicals on a lab bench will have been assessed and handled by an industry-based chemist before they reach an academic's bench.

Many members have followed a career path where research or bench work is not integral to the job. They are the hazardous waste consultants, regulatory consultants, laboratory managers/technicians, health and safety/dangerous goods consultants, work health and safety inspectors, scientific writers and safety data sheet authors. Yet somewhere in the mix, this cohort needs to be considered regarding the reward and recognition program. These members are not industrial chemists; they are industry-based chemists.

To ensure equality in RACI's rewards and recognition program, industry-based chemists must be considered in terms of their achievements in industry, not against academic standards or by academics.

Lisa Stevens FRACI CChem

Poisonous alkaloids

During the lockdown, I wrote the Royal Society biographical memoir of Professor Basil Lythgoe (*Biographical Memoirs of Fellows of the Royal Society*, 2021, vol. 70, pp. 283–95), who was head of organic chemistry at the University of Leeds during my time there. Lythgoe worked inter alia on taxine alkaloids, which occur in yew trees and are poisonous to livestock. I naturally thought of that when I read the article 'Beautiful flowers, lovely perfume, and deadly!' by Peter Lehman (September–November, p. 38). European yew, systematic name *Taxus baccata*, is known to contain taxine alkaloids in its leaves and does occur in Australia, often in private gardens. Peter Lehman's article was concerned with *Cestrum nocturnum*, aka night-blooming jasmine. That contains not taxine alkaloids but tobacco alkaloids, including nicotine. Alkaloids are one group of plant toxins that provide a plant with defence against intrusion; for example, by insects and fungi.

Clifford Jones FRACI CChem

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Planting an important seed for nanotechnology

The Royal Swedish Academy of Sciences awarded the Nobel Prize in Chemistry 2023 to **Moungi G. Bawendi** (Professor at Massachusetts Institute of Technology, US), **Louis E. Brus** (Professor at Columbia University, US) and **Alexei I. Ekimov** (formerly Chief Scientist at Nanocrystals Technology Inc., US):

for the discovery and synthesis of quantum dots.

The Nobel Prize in Chemistry 2023 rewards the discovery and development of quantum dots, nanoparticles so tiny that their size determines their properties. These smallest components of nanotechnology now spread their light from televisions and LED lamps, and can also guide surgeons when they remove tumour tissue, among many other things.

Everyone who studies chemistry learns that an element's properties are governed by how many electrons it has. However, when matter shrinks to nano-dimensions, quantum phenomena arise; these are governed by the size of the matter. The Nobel Laureates in Chemistry 2023 have succeeded in producing particles so small that their properties are determined by quantum phenomena. The particles, which are called quantum dots, are now of great importance in nanotechnology.

'Quantum dots have many fascinating and unusual properties. Importantly, they have different colours depending on their size', said Johan Åqvist, Chair of the Nobel Committee for Chemistry.

Physicists had long known that, theoretically, size-dependent quantum effects could arise in nanoparticles, but at that time it was almost impossible to sculpt in nano-dimensions. Therefore, few people believed that this knowledge would be put to practical use.

However, in the early 1980s, Ekimov succeeded in creating size-dependent quantum effects in coloured glass. The colour came from nanoparticles of copper chloride, and Ekimov demonstrated that the particle size affected the colour of the glass via quantum effects.

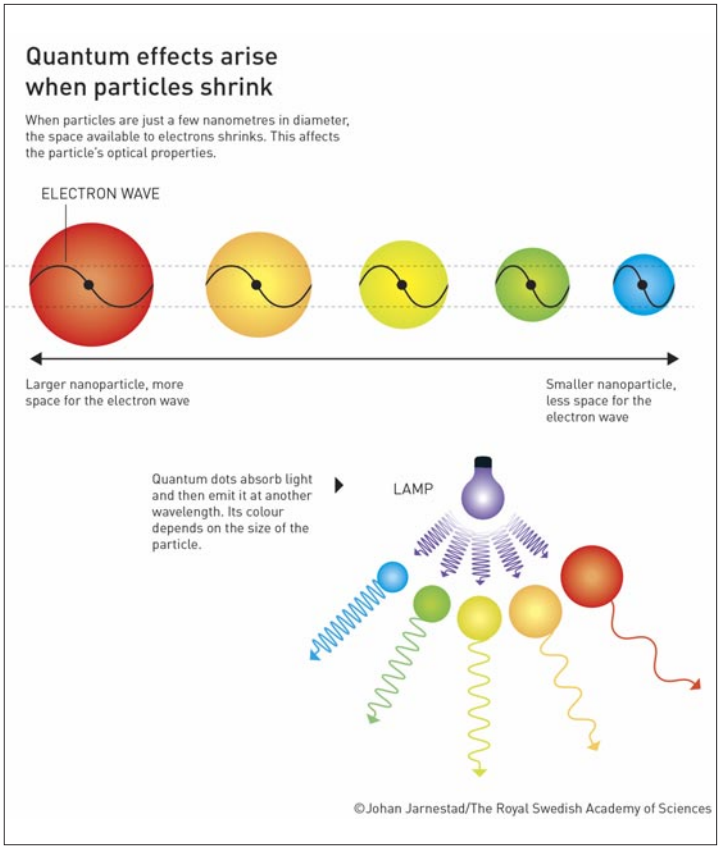
A few years later, Brus was the first scientist in the world to prove size-dependent quantum effects in particles floating freely in a fluid.

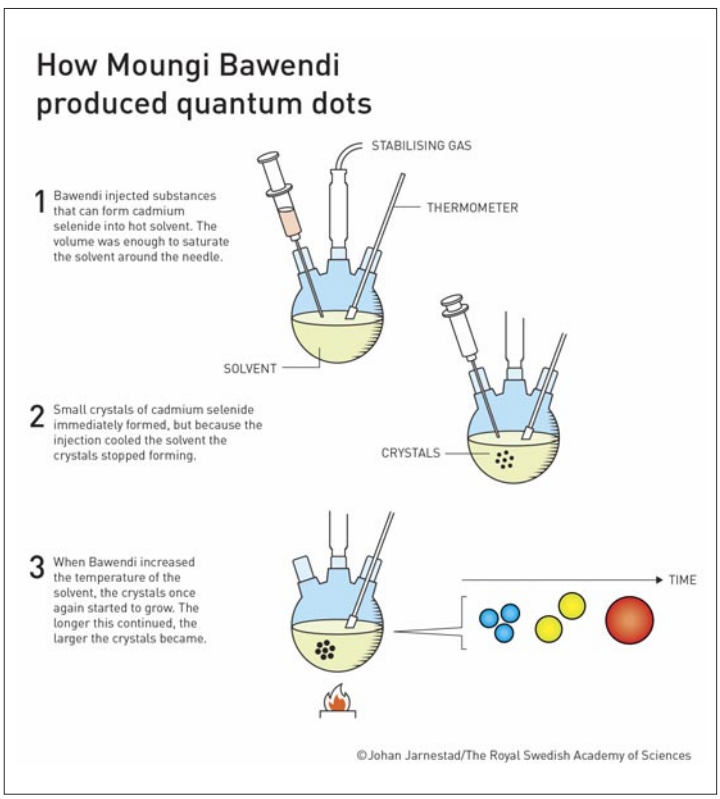
In 1993, Bawendi revolutionised the chemical production of quantum dots, resulting in almost perfect particles. This high quality was necessary for them to be used in applications.

Quantum dots now illuminate computer monitors and television screens based on QLED (quantum-dot light-emitting diode) technology. They also add nuance to the light of some LED lamps, and biochemists and doctors use them to map biological tissue.

Quantum dots are thus bringing the greatest benefit to humankind. Researchers believe that in the future they could contribute to flexible electronics, tiny sensors, thinner solar cells and encrypted quantum communication – so we have just started exploring the potential of these tiny particles.

Nobelprize.org





Light experiments to capture the shortest of moments

The Nobel Prize in Physics 2023 was awarded to **Pierre Agostini** (Professor at the Ohio State University, US), **Ferenc Krausz** (Director at Max Planck Institute of Quantum Optics, Garchingn and Professor at Ludwig-Maximilians-Universität München, Germany) and **Anne L'Huillier** (Professor at Lund University, Sweden):

> *for experimental methods that generate attosecond pulses of light for the study of electron dynamics in matter.*

The three Nobel Laureates in Physics 2023 are being recognised for their experiments, which have given humanity new tools for exploring the world of electrons inside atoms and molecules. Agostini, Krausz and L'Huillier have demonstrated a way to create extremely short pulses of light that can be used to measure the rapid processes in which electrons move or change energy.

Fast-moving events flow into each other when perceived by humans, just as a film that consists of still images is perceived as continual movement. If we want to investigate really brief events, we need special technology. In the world of electrons, changes occur in a few tenths of an attosecond – an attosecond is so short that there are as many in one second as there have been seconds since the birth of the universe.

The laureates' experiments have produced pulses of light so short that they are measured in attoseconds, thus demonstrating that these pulses can be used to provide images of processes inside atoms and molecules.

In 1987, L'Huillier discovered that many different overtones of light arose when she transmitted infrared laser light through a noble gas. Each overtone is a light wave with a given number of cycles for each cycle in the laser light. They are caused by the laser light interacting with atoms in the gas; it gives some electrons extra energy that is then emitted as light. L'Huillier has continued to explore this phenomenon, laying the ground for subsequent breakthroughs.

In 2001, Agostini succeeded in producing and investigating a series of consecutive light pulses, in which each pulse lasted just 250 attoseconds. At the same time, Krausz was working with another type of experiment, one that made it possible to isolate a single light pulse that lasted 650 attoseconds.

The laureates' contributions have enabled the investigation of processes that are so rapid they were previously impossible to follow.

'We can now open the door to the world of electrons. Attosecond physics gives us the opportunity to understand mechanisms that are governed by electrons. The next step will be utilising them', said Eva Olsson, Chair of the Nobel Committee for Physics.

There are potential applications in many different areas. In electronics, for example, it is important to understand and control how electrons behave in a material. Attosecond pulses can also be used to identify different molecules, such as in medical diagnostics.

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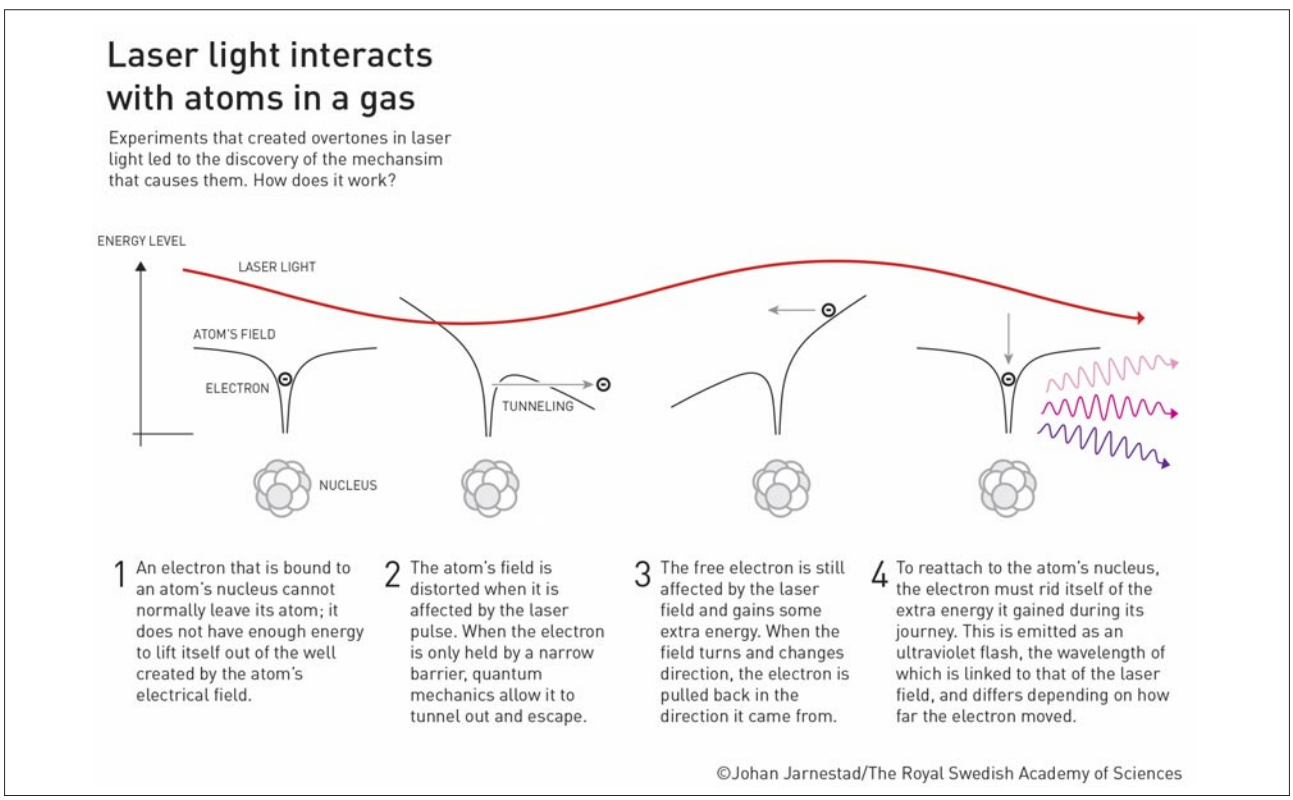
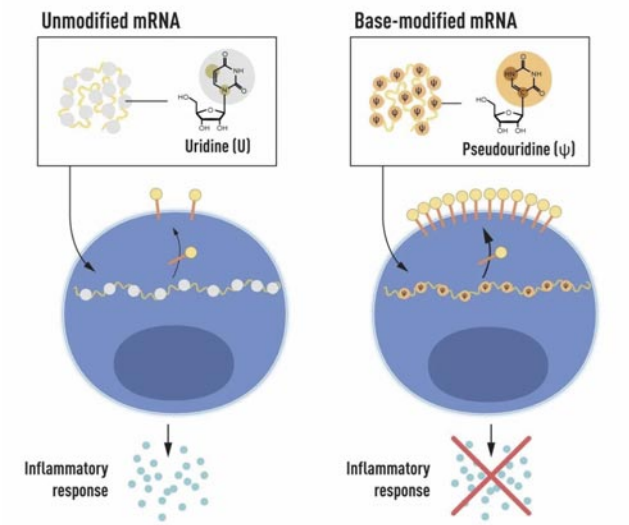


mRNA vaccines for COVID-19



mRNA contains four different bases, abbreviated A, U, G and C. The Nobel Laureates discovered that base-modified mRNA can be used to block activation of inflammatory reactions (secretion of signalling molecules) and increase protein production when mRNA is delivered to cells. © The Nobel Committee for Physiology or Medicine. Ill. Mattias Karlén

The 2023 Nobel Prize in Physiology or Medicine was awarded jointly to **Katalin Karikó** (Professor at Szeged University, Hungary, and Adjunct Professor at Perelman School of Medicine at the University of Pennsylvania, US) and **Drew Weissman** (Roberts Family Professor in Vaccine Research and Director of the Penn Institute for RNA Innovations, US):

> *for their discoveries concerning nucleoside base modifications that enabled the development of effective mRNA vaccines against COVID-19*.

The discoveries of this year's laureates were critical for developing effective mRNA vaccines against COVID-19 during the pandemic that began in early 2020. Through their groundbreaking findings, which have fundamentally changed our understanding of how mRNA interacts with our immune system, the laureates contributed to the unprecedented rate of vaccine development during one of the greatest threats to human health in modern times.

Producing whole virus-, protein- and vector-based vaccines requires large-scale cell culture. This resource-intensive process limits the possibilities for rapid vaccine production in response to outbreaks and pandemics. Therefore, researchers have long attempted to develop vaccine technologies independent of cell culture, but this proved challenging.

Genetic information encoded in DNA is transferred to messenger RNA (mRNA), which is used as a template for protein production. During the 1980s, efficient methods for producing mRNA without cell culture were introduced, called in vitro transcription. However, in vitro-transcribed mRNA was considered unstable and challenging to deliver, and in vitro-produced mRNA gave rise to inflammatory reactions.

These obstacles did not discourage Hungarian biochemist Karikó. During the early 1990s, when she was an assistant professor at the University of Pennsylvania, she remained true to her vision of realising mRNA as a therapeutic.

Karikó and colleague immunologist Drew Weissman noticed that dendritic cells recognise in vitro-transcribed mRNA as a foreign substance, which leads to their activation and the release of inflammatory signalling molecules. They wondered why the in vitro-transcribed mRNA was recognised as foreign while mRNA from mammalian cells did not give rise to the same reaction. Karikó and Weissman realised that some critical properties must distinguish the different types of mRNA.

Karikó and Weissman knew that bases in RNA from mammalian cells are frequently chemically modified, while in vitro-transcribed mRNA is not. They wondered if the absence of altered bases in the in vitro-transcribed RNA could explain the unwanted inflammatory reaction. To investigate this, they produced different variants of mRNA, each with unique chemical alterations in their bases, which they delivered to dendritic cells. The results were striking: the inflammatory response was almost abolished when base modifications were included in the mRNA. Karikó and Weissman immediately understood that their discovery had profound significance for using mRNA as therapy. These seminal results were published in 2005.

In further studies published in 2008 and 2010, Karikó and Weissman showed that the delivery of mRNA generated with base modifications markedly increased protein production compared to unmodified mRNA. The effect was due to the reduced activation of an enzyme that regulates protein production. Through their discoveries that base modifications both reduced inflammatory responses and increased protein production, Karikó and Weissman had eliminated critical obstacles on the way to clinical applications of mRNA.

Interest in mRNA technology began to pick up, and in 2010, several companies were working on developing the method. Vaccines against Zika virus and MERS-CoV were pursued; the latter is closely related to SARS-CoV-2. After the outbreak of the COVID-19 pandemic, two base-modified mRNA vaccines encoding the SARS-CoV-2 surface protein were developed at record speed. Protective effects of about 95% were reported, and both vaccines were approved as early as December 2020.

The impressive flexibility and speed with which mRNA vaccines can be developed pave the way for using the new platform also for vaccines against other infectious diseases. In the future, the technology may also be used to deliver therapeutic proteins and treat some cancer types.

Several other vaccines against SARS-CoV-2, based on different methodologies, were also rapidly introduced, and together, more than 13 billion COVID-19 vaccine doses have been given globally.

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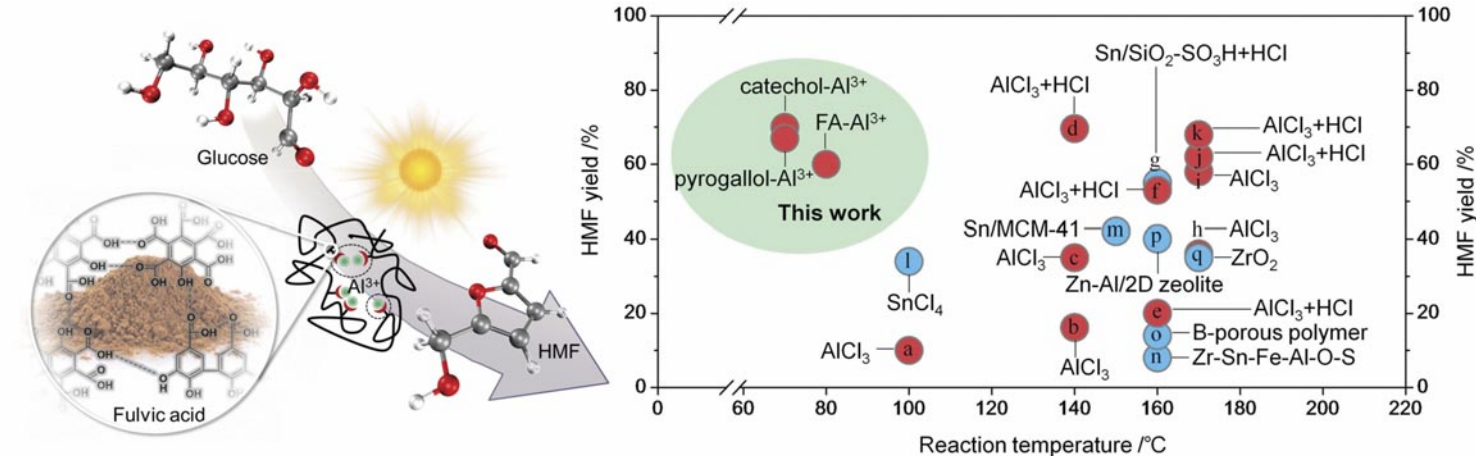
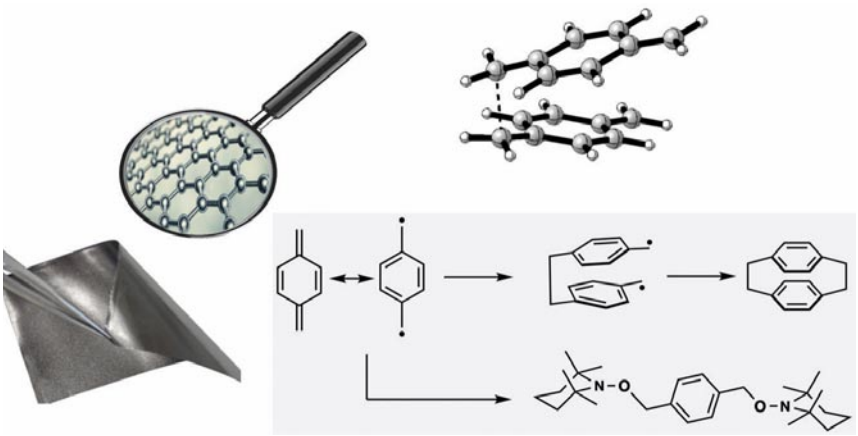
A novel approach to photocatalyst development



5-Hydroxymethylfurfural (HMF) holds significant importance as a fundamental platform chemical, paving the way for the development of a sustainable, environmentally friendly fine-chemical and pharmaceutical industry rooted in biomass resources. Achieving cost-effective HMF production from readily available C6 sugars necessitates mild reaction conditions and the use of efficient catalysts derived from abundant natural sources. Recently, researchers from the Queensland University of Technology, Inner Mongolia Minzu University (China), Hunan University (China) and the University of Sydney have found that, when employed in appropriate ratios, Al^{3+} ions and fulvic acid (FA), a class of naturally occurring compounds found in soil, peat and coal, exhibit remarkable light-absorption properties and significant photocatalytic activity for HMF production (Tana T., Han P., Brock A.J., Mao X., Sarina S., Waclawik E.R., Du A., Bottle S.E., Zhu H.Y. *Nat. Commun.* 2023, **14**, 4609). This innovative approach enables the efficient conversion of glucose to HMF in a one-pot reaction, achieving approximately 60% HMF yield at a moderate temperature of 80°C. This work demonstrates photocatalyst development from an unconventional source, thereby advancing the practical application of photocatalysis.

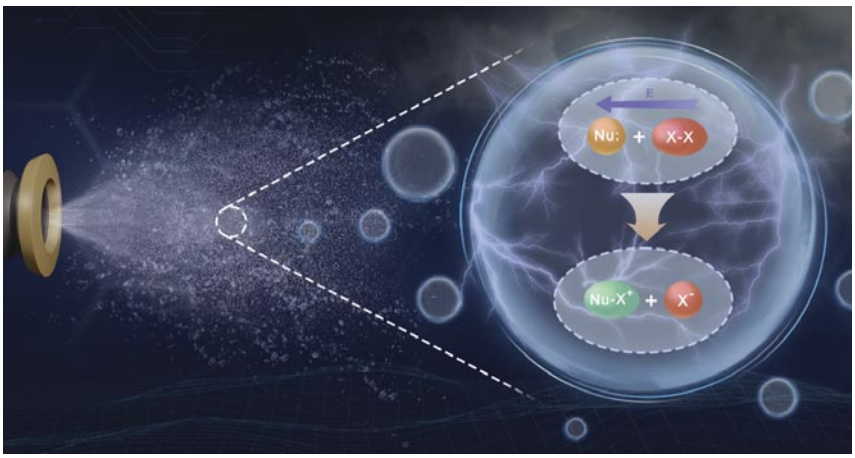
Unveiling the hidden diradical character of quinonedimethides



Initiation of radical reactions by non-radical species usually requires light, heat or catalysts such as N-heterocyclic carbenes. *para*-Quinonedimethide, the simplest structural subunit in graphene, is an important and rare exception. Scientists from Flinders University and the Australian National University have recently provided the first experimental and theoretical proof that its dimerisation occurs by a radical mechanism, and can be harnessed to initiate radical processes under mild conditions in the dark (Pei Z., Magann N.L., Sowden M.J., Murphy R.B., Gardiner M.G., Sherburn M.S., Coote M.L. *J. Am. Chem. Soc.* 2023, **145**, 16 037–44). They also explained why tetracyanoquinonedimethide, an important and closely related derivative, does not react in the same way. The work has broad fundamental importance for understanding and harnessing diradical reactivity in synthesis, and for understanding the structure–reactivity properties of nanographenes.

Electric fields on water microdroplets catalyse chemical reactions

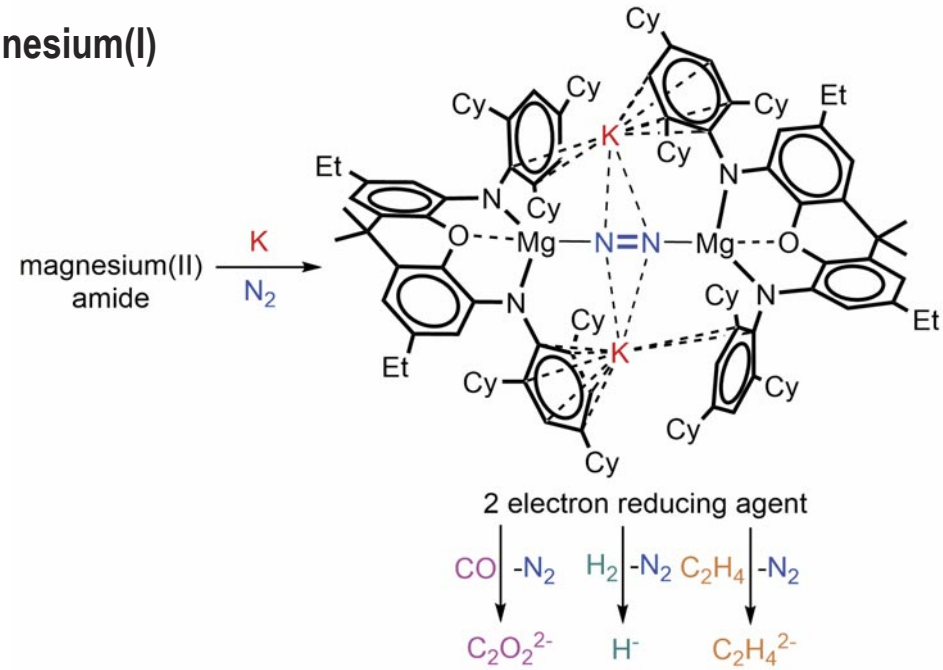
Electric fields show great promise as 'chemical-free' catalysts for synthetic chemistry due to their ability to offer precise control of reaction selectivity, orthogonal modes of activation and tremendous acceleration of reaction rates. However, methods for scaling up electrostatic catalysis beyond single-molecule experiments have thus far remained elusive. Water microdroplet chemistry offers a potential solution to this problem due to the high electric fields that are known to exist at the air–water interface. Recently, researchers from Flinders University and Nankai University (China) have demonstrated that the electric fields in sprayed water microdroplets can promote the reactions of nucleophiles such as pyridine and quinuclidine with molecular bromine and iodine (Zhu C., Pham L.N., Yuan X., Ouyang H., Coote M.L., Zhang X. *J. Am. Chem. Soc.* 2023, **145**, 21 207–12). The reactions occur in microseconds in microdroplets – orders of magnitude faster than in the bulk solution. Density functional theory calculations confirm that the reactions become barrier free as a result of the interfacial electric fields. Based on the success of these reactions, it is anticipated that microdroplet chemistry will become widely used as a practical platform for scaling electrostatic catalysis.



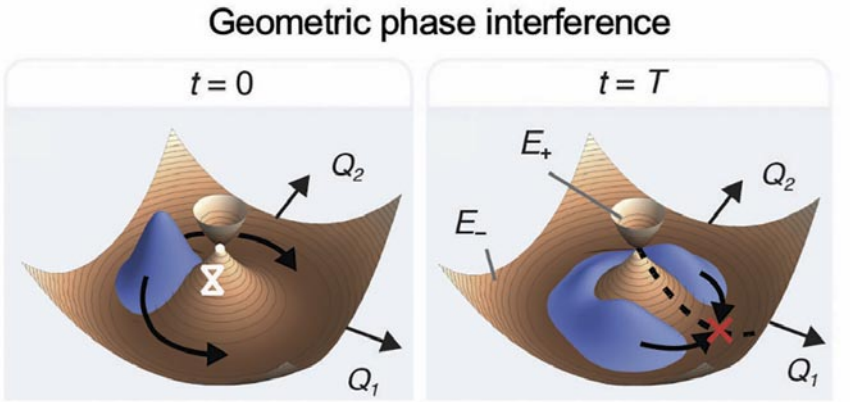
Reprinted (adapted) with permission from Zhu C., Pham L.N., Yuan X., Ouyang H., Coote M.L., Zhang X. High electric fields on water microdroplets catalyze spontaneous and fast reactions in halogen-bond complexes. *J. Am. Chem. Soc.* 2023, **145**, 21 207–12. Copyright 2023 American Chemical Society

Fixing nitrogen with magnesium(I)

The activation of dinitrogen (N_2) by transition metals is central to the production of NH_3 by the highly energy-intensive Haber–Bosch process. Although progress has been made towards more sustainable homogeneous activations of N_2 with d- and f-block metals, fixation of N_2 with main-group metals is essentially unknown. In an extension of their work on the activation of typically inert substrates (e.g. CO, H_2, C_2H_4) with magensium(I) compounds, the group of Cameron Jones at Monash University has reported an unprecedented activation of N_2 with a magnesium complex (Mondal R., Evans M.J., Rajeshkumar T., Maron L., Jones C. *Angew. Chem. Int Ed.* 2023, **62**, e202308347). Reduction of an extremely bulky magnesium(II) amide with potassium at room temperature under one atmosphere of N_2 leads to the double reduction of the diatomic molecule. Density functional theory calculations by collaborator Laurent Maron at the University of Toulouse (France) show that the cooperative heterometallic reduction proceeds via a transient anionic magnesium(I) radical. The formed magnesium complex of N_2^{2-} readily reductively activates CO, H_2 and C_2H_4 in reactions in which it acts as a masked dimagnesium(I) diradical. The synthesis of value-added compounds (including organo-nitrogen molecules) with magnesium–N_2 systems is currently being explored.

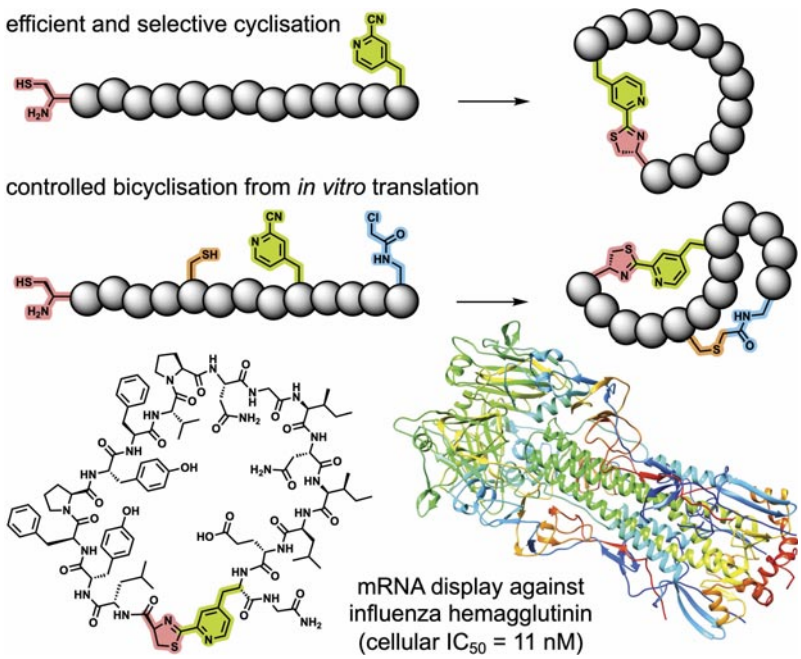


Observing ultrafast chemical dynamics



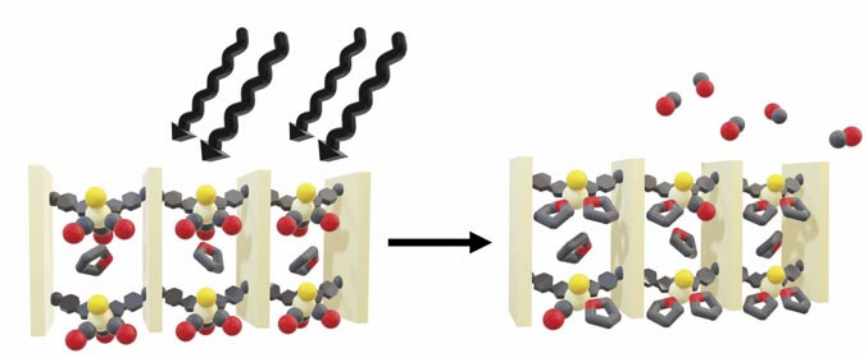
Chemical processes such as light harvesting, photocatalysis and chemical reactivity are often governed by conical intersections, points where two electronic states have the same energy. By acting as funnels between electronic states of molecules, conical intersections allow rapid and efficient relaxation during chemical dynamics. In addition, when a reaction path encircles a conical intersection, the molecular wavefunction experiences a geometric phase, which can affect the outcome of the reaction through quantum-mechanical interference. These processes happen at ultrafast time scales, making them particularly difficult to directly track during chemical experiments. Researchers at the University of Sydney have used a programmable trapped-ion quantum simulator to access ultrafast time scales and directly observe the geometric phase interference created when a molecular wavefunction encircles a conical intersection (Valahu C.H., Olaya-Aguedelo V.C., MacDonell R.J., Navickas T., Rao A.D., Millican M.J., Pérez-Sánchez J.B., Yuen-Zhou J., Biercuk M.J., Hempel C., Tan T.R., Kassal I. *Nat. Chem.* 2023, **15**, 1503–8). This is the first direct observation of interference due to geometric phase and achieves a key milestone towards reliable simulation of chemical processes using quantum computers. Further development of this quantum technology could accelerate discoveries across industrial fields, including materials science, catalysis, atmospheric science, combustion, pharmacology and energy conversion and storage.

A new tool for peptide drug discovery



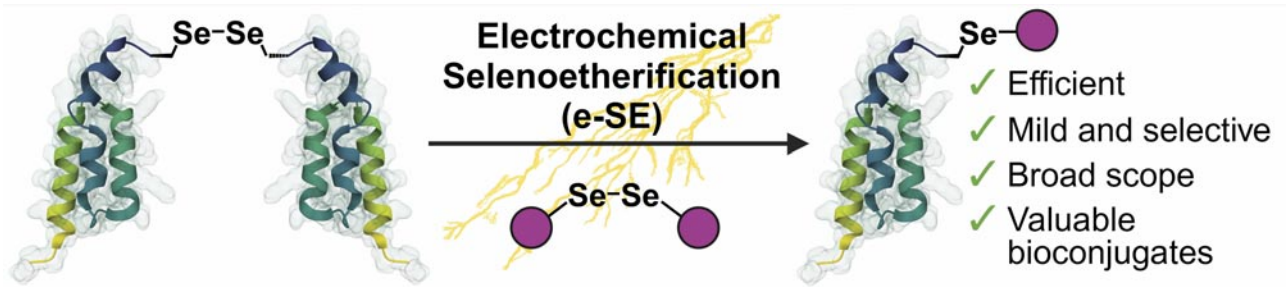
Thanks to their unique position between conventional small molecules and large antibodies in terms of size and properties, peptides are gaining growing attention in drug discovery. Macrocyclic peptides are particularly promising drug candidates due to their superior activity and stability compared with their linear counterparts. An international team led by Christoph Nitsche from the Australian National University and Seino Jongkees from Vrije Universiteit Amsterdam (The Netherlands) has reported a new approach for the identification of mono- and bi-cyclic peptides from genetically encoded libraries (Liu M., Morewood R., Yoshisada R., Pascha M.N., Hopstaken A.J.P., Tarcoveanu E., Poole D.A., de Haan C.A.M., Nitsche C., Jongkees S.A.K. *Chem. Sci.* 2023, **14**, 10 561–9). The strategy utilises the nitrile–aminothiol click reaction, specifically involving a cyclocondensation between 2-cyanopyridine and N-terminal cysteine initially reported by Nitsche for peptide macrocyclisation in 2019. Because cyanopyridine reacts selectively with the N-terminus, an additional cysteine residue in the peptide chain can be employed for in vitro translation of bicyclic peptides. The team showcased the utility of this technology by discovering a macrocyclic peptide that targets haemagglutinin of the influenza A virus, a protein responsible for facilitating viral entry into host cells.

Impact of porosity in solid-state Mn(I) carbonyl photochemistry



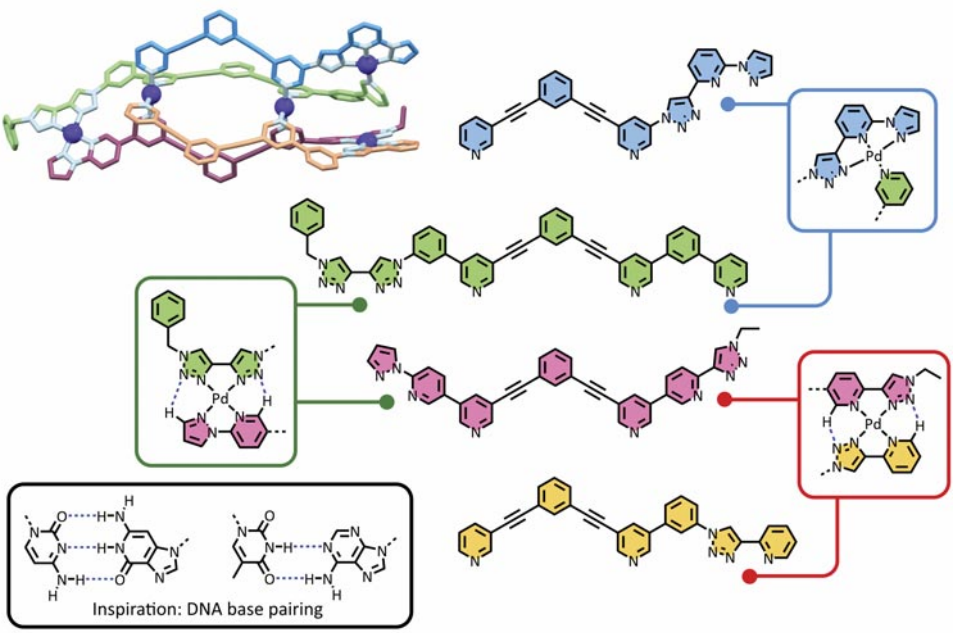
A recent collaboration between researchers at the University of Adelaide, the University of Nottingham (UK) and the University of Birmingham (UK) has shown novel photochemistry for a metal carbonyl complex anchored within a permanently porous metal–organic framework (MOF) (Young R.J., Huxley M.T., Wu L., Hart J., O'Shea J., Doonan C.J., Champness N.R., Sumby C.J. *Chem. Sci.* 2023, **14**, 9409–17). The work used time-resolved spectroscopic and X-ray crystallographic techniques to examine the photochemistry of a MOF-supported Mn(I) carbonyl complex under visible and UV irradiation. The results revealed the sequential photo-induced loss of all three carbonyl ligands, which were subsequently replaced by solvent. These findings highlight significant differences in the photochemistry of MOF-supported Mn(I) carbonyl complexes compared with typical solid-state or solution behaviour. These disparities have implications for applications that employ analogous complexes as photocatalysts or solid-state photoCORMs (photo-activated carbon monoxide releasing molecules). The work further validates the emerging role of MOFs as porous, crystalline matrices within which chemical transformations can be followed in the solid-state. The in crystallo environment of the MOF pores offers a unique opportunity to apply classical solid-state techniques in a local chemical environment more akin to the solution phase.

Electrifying polypeptide modification



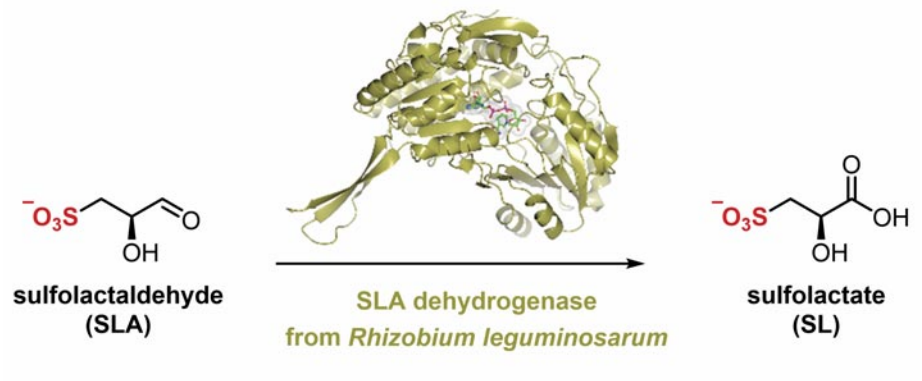
New strategies for the site-specific modification of peptides and proteins are in high demand for applications in fundamental research and therapeutic development. Electrosynthesis, having experienced a recent surge in interest, has emerged as an attractive strategy for facilitating such selective transformations under mild reaction conditions. Now, a research team from the University of Sydney, collaborating with researchers from the Australian National University and Colorado State University (US), have developed a mild and selective electrochemical method for late-stage polypeptide modification (Mackay A.S., Maxwell J.W.C., Bedding M.J., Kulkarni S.S., Byrne S.A., Kambanis L., Popescu M.V., Paton R.S., Malins L.R., Ashhurst A.S., Corcilius L., Payne R.J. *Angew. Chem. Int. Ed.* 2023, doi.org/10.1002/anie.202313037). Termed electrochemical selenoetherification (e-SE), the strategy uses the unique reactivity of selenocysteine (often called the 21st amino acid) to generate stable selenoether-linked bioconjugates from corresponding diselenide starting materials, with formal extrusion of a single selenium atom. The team demonstrated that e-SE could be used to modify leuprolide, an FDA-approved cancer drug, and to rapidly construct a library of anti-HER2 (anti-human epidermal growth factor receptor 2) affibody (antibody-mimicking protein) conjugates. Affibody conjugates bearing complex cargoes were used for in vitro imaging and targeting of HER2-positive breast and lung cancer cell lines.

Metallo-supramolecular cages made of different low-symmetry ligands



Self-assembled cages represent an easy route to synthetic structures that can rival the size of biological machinery such as peptides and proteins. But they have been hampered by their high symmetry, meaning that they do not exhibit the structural diversity of natural molecules that gives them their high specificity and selectivity for molecular targets. Two approaches have arisen to try to circumvent this issue: incorporating different ligands into a structure to form heteroleptic cages, and using the same low-symmetry ligand to form homoleptic cages. Chemists from the Australian National University and the University of Adelaide have reported the first example that unifies these two approaches (Preston D., Evans J.D. *Agnew. Chem. Int. Ed.* 2023, doi.org/10.1002/anie.202314378). They took inspiration from the hydrogen-bonding complementarity between bases in DNA to develop ligands with ancillary Pd(II)-binding sites that exploit the square planar four-coordinate geometry of Pd(II) to pair on the basis of denticity (monodentate to tridentate or bidentate to bidentate) and hydrogen-bonding capability between ligands (acceptor/acceptor to donor/donor or acceptor/donor to donor/acceptor). Using this approach, they were able to generate a lantern-shaped cage with four different low-symmetry ligands with positional and orientational control.

Decoding the secrets of organosulfur catabolism



Organosulfur compounds are important reservoirs of sulfur in the biosphere. Yet little is known about the enzymes that form and degrade organosulfur compounds. Researchers at the University of Melbourne, the Walter and Eliza Hall Institute, and York University (UK) have revealed the structure and mechanism for the enzyme that makes the short-chain organosulfur compound sulfolactate (Li J., Sharma M., Meek R., Alhifthi A., Armstrong Z., Madiedo Soler N., Lee M., Goddard-Borger E.D., Blaza J.N., Davies G.J., Williams S.J. *Chem. Sci.* 2023, **14**, 11 429–40). They studied a sulfolactaldehyde dehydrogenase from a soil bacterium originally isolated in western New South Wales. Enzyme kinetics gave evidence for the order of substrate binding, which supported structural studies using cryogenic electron microscopy to determine the 3D structure of the enzyme in a complex with nicotinamide cofactor. This work provides a detailed molecular view of a key enzyme in the organosulfur cycle.

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.

The pink lagoon

More than meets the eye

Aerial view of Hutt Lagoon, Western Australia.

Jennifer Martin/iStockphoto

BY **ALF LARCHER**

The stunning pink of Western Australia's Hutt Lagoon has caught the eye of many tourists, and the algal carotenes that cause it are of great interest to industrial chemists.

This story begins with a chance meeting with three Japanese tourists in Geraldton, in my home state of Western Australia. We met on a family holiday to the north-west of WA, and they had something quite specific on their itinerary. These three young women were determined to see a natural marvel that obviously we didn't appreciate, having whizzed straight past the turn-off on our way back to Perth. They unfolded a map, pointed to the location of the nearby pink lake and looked at us questioningly. Despite the last stretch to their destination being a long bush-lined road off the main highway and prone to prancing kangaroos between dusk and dawn, they were undeterred. You could see in their eyes that they would do whatever it took to see the pink lake.

The pink lake that these tourists were determined to visit is 100 kilometres north of Geraldton and officially known as Hutt Lagoon. The town of Port Gregory is nestled on its shores, hosting coachloads of international tourists who view the lake by walking, four-wheel-drive and aerial tours. As well as being a tourist drawcard, the pink lake is the site of one of the world's largest producers of β-carotene.

Hutt Lagoon – halophile haven

Hutt Lagoon is 12 kilometres by two kilometres and shallow (less than one metre), and classed as a hypersaline evaporative birrida. Birridas are bodies of water that have been isolated over geological time as sea levels decreased. It was an estuary of the nearby Hutt River that became isolated from the sea between coastal dunes during this process. The lagoon receives water from natural rainfall and, because it is below sea level, it also receives marine water by subsurface flow. The salinity range of Hutt River is 3–7 g/L, whereas that of Hutt Lagoon is up to 320 g/L (the range for seawater is 33–37 g/L).

Despite their harshness to 'normal' life, saline lakes such as Hutt Lagoon host a variety of salt-tolerant (halophilic) organisms, including crustacea, bacteria and microalgae. Both bacteria and algae can generate pink-red colours in the water, but a delicate balance of water salinity and quality, sunlight and water hydrology optimises the growth of the main actor that causes the pink colour of Hutt Lagoon, the alga *Dunaliella salina*.

A microalga's metabolic trick

Pink, orange and red lakes and even red snow have been the object of wonder for centuries, with biblical references in which red-coloured waters are compared to blood: 'To the Moabites across the way, the water looked red – like blood' (2 Kings 3:22). It was not until the development of microscopes in the late 16th century that microscopic life was observed and the mystery behind the colour began to be understood.

Prompted by an invitation from the Académie des Sciences in Paris, French botanist Michel Félix Dunal reported what he called *Haematococcus salinus* and *Protococcus* in the salterns of Montpellier, France. This study, published in 1838 in *Annales des Sciences Naturelles; Botanique*, is the first known to identify the alga that now carries Dunal's name.

Algae are often described in negative terms – think garden pond slimes and toxic algal blooms. But they are vital to marine food webs as well as consuming carbon dioxide and producing oxygen. Algae are simple, non-flowering and typically aquatic plants of a large group that includes the seaweeds and many single-celled forms. Algae contain chlorophyll but lack true stems, roots, leaves and vascular tissue.

D. salina, of the phylum Chlorophyta, is a unicellular, photosynthetic microalga with a distinguishing feature of not having a rigid cell wall. Its chloroplasts, where photosynthesis takes place, are cup shaped. Its cells (each of which is 5–25 micrometres) are ovoid, and each is capable of motion due to two long thin flagella. The cells can 'swim' using the flagella with a 'breaststroke'-type action. *D. salina* is usually green but develops its red colour with increasing salinity and sunlight, which is often present in saline lakes in arid environments. The alga develops a pink colour to absorb the high-intensity light present as a photoprotective response to chloroplast damage. The compounds that give *D. salina* its pink-red colour under stressful conditions are a complex mixture of carotenes. The main carotene synthesised is β-carotene, which the alga achieves, amazingly, by decomposing its green chlorophyll. Levels of 14% dry weight of β-carotene in *D. salina* have been reported.

D. salina can survive in saline environments because of another metabolic trick: it synthesises glycerol, maintaining an intracellular glycerol concentration so that the osmotic pressure is higher than the extracellular pressure. This permits the alga to take up water even when growing at high salt concentrations.

Pink lakes change colour naturally with the seasons (rainfall and sunlight), but changes can also be a sign of *D. salina*'s sensitivity to urbanisation, salt mining and pollutants such as pesticides and heavy metals. An example is the 'former pink lake' near the southern WA town of Esperance, in which only the faintest hint remains of its former intense pink colour. Its demise is the object of much study, and a feasibility study of the lake prepared for the Shire of Esperance in 2020 concluded that removal of too much salt has reduced its salinity to a level where *D. salina* cannot thrive (see executive summary in bit.ly/3tTv0JI). The levels of the alga in this lake have been compared to those in Hutt Lagoon, with the lagoon having 45 times more cells of *D. salina* per millilitre (p. 20 of feasibility report). The nearby bubble-gum pink Lake Hillier, which is on an island and only accessible for tourist viewing by plane, with aerial tours being available for tourists, is now even more prized and protected by Esperance locals. Although algae are present, recent research indicates the colour is mainly due to the bacterium *Salinabacter ruber*, which is also able to produce carotenes as photoprotective compounds. Such algal and bacterial halophiles are studied by extremophile scientists to try to predict, among other things, forms of extraterrestrial life.

Not many species of *Dunaliella* produce β-carotenoids, and those that do tend to be green in less saline environments.
CSIRO ScienceImage

Carotenoids – more than just a pretty colour

Carotenoids are present in fruits and vegetables, algae and bacteria, and their isoprenoid subunits form a 40-carbon tetraterpenoid backbone. The series of conjugated double bonds is responsible for the molecule's strong colour: it absorbs light in the blue part of the spectrum (~0.4–0.5 micrometres). The yellow-orange vegetables and fruits are generally α- and β-carotene rich, while lycopene is responsible for the bright red of tomatoes. Carotenes have many biological functions in humans, who

BASF's β-carotene production facility at Hutt Lagoon. Chris Gordon/iStockphoto

François Boucher (1703–1770). ***Madame de Pompadour*** **1759. Oil on canvas, 91 × 68 cm** Wallace Collection

In the early 19th century, pink was considered masculine because it was a variation of red and thus warlike. Later in the century, it became fashionable to differentiate babies' gender by clothing. The French led this trend, favouring pink for girls due to their penchant for a rather stunning 18th century portrait by François Boucher. Painted in the flamboyant rococo style, it featured the highly influential Madame de Pompadour, official mistress of King Louis XV.

cannot synthesise them. Most importantly, carotenoids are classed as a provitamin A, being converted to vitamin A in the body. Vitamin A is important for normal vision, the immune system, reproduction, and growth and development. The global market for all carotenoids is in the order of US$2.0 billion, promoted by the growing consumer demand for naturally grown products in foods and dietary supplements.

Producing β-carotene

Hutt Lagoon hosts BASF's large β-carotene production facility, comprising 450 hectares of lakes surrounded by 3500 hectares of natural lagoon. BASF has similar facilities in Whyalla in South Australia, making it the world's largest producer of algal β-carotene, with its two production sites being the biggest in the world.

The β-carotene produced by *D. salina* is composed of a mixture of the *cis*- and *trans*-isomers, with a typical composition of 9-*cis* (41%), all-*trans* (42%), 15-*cis* (10%) and other isomers (6%). β-Carotene can be produced synthetically, in the all-*trans* form, but it is 9-*cis*-β-carotene that has been used to treat conditions such as retinal dystrophy, chronic psoriasis and atherosclerosis. The *cis*-isomer is more than 8000 times more expensive, in the pure form, than the *trans*-isomer.

Much research has been done to optimise the growth of *D. salina* and the production of β-carotene. One group of researchers proposed a

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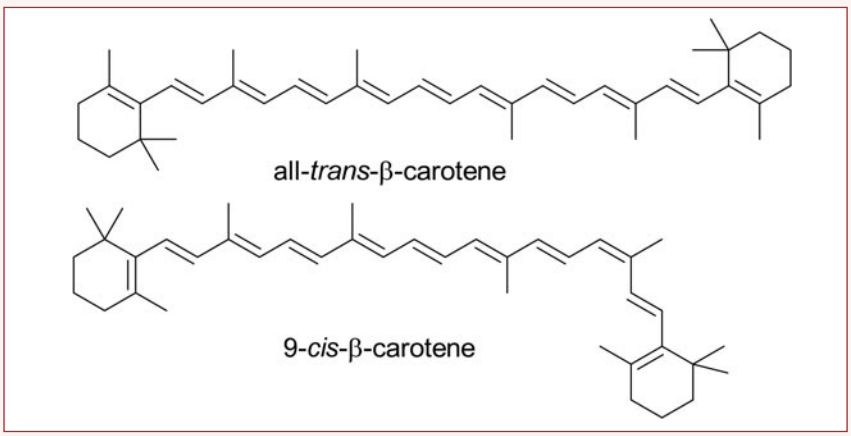

two-stage process, in which nutrient-rich, lower-salinity nursery ponds were used to boost biomass, with algae then transferred to larger production ponds of higher salinity and with fewer nutrients to promote β-carotene production (Borowitzka L.J., Borowitzka M.A. *Bulletin of Marine Science*, 1990, vol. 47(1), p. 244). However, field trials showed this strategy was not feasible: predation by protozoa in the nursery ponds resulted in significant losses. Also, these ponds promoted the preferential growth of other *Dunaliella* species, and the two-stage process was labour intensive and required a greater pond area. The researchers proposed a semi-continuous process operating at intermediate salinity with optimised nutrient concentrations. The major nutrients added are nitrogen, phosphate and chelated iron. The ratios of calcium to magnesium and chloride to sulfate also affect growth and carotene production.

Harvesting choices and challenges

Harvesting the microscopic algae from large volumes of water poses more technological challenges. Options include filtration using diatomaceous earth, floating fibres on rafts to trap the algae, as well as the use of salinity gradients. The harvested cells may be spray dried to produce an algal powder or extracted with further processing, producing β-carotene. Various extraction methods, using toluene, hexane or hot oil, can be used. Typical products from the process are spray-dried *D. salina* for use in animal feeds, including aquaculture, and solutions/suspensions of β-carotene in vegetable oil for dietary supplements and food colouring.

Supercritical carbon dioxide has also been investigated as an extraction solvent, and optimising pressure and temperature and using a co-solvent have produced good results. The higher energy requirements are offset by the lower solvent costs, with the green properties of carbon dioxide being an extra impetus for the work.

The specific techniques used by different producers are commercial-in-confidence and may be different from those described here (based on research results and other published information). They do, however, give insights into the challenges faced by producers.

D. salina can also be harvested for glycerol – which is used as a solvent, an emollient and a sweetening agent – and for a variety of other carotenoids, lipid components for cosmetic applications as well as proteins and carbohydrates. The use of desalination plant brines to cultivate *D. salina*, along with the use of carbon dioxide-rich flue gases to promote growth, has also been assessed.

Algal oils and lipids can be used as feedstock for diesel and aviation fuels, while the biomass itself can be converted into biogas and biofuels. An extensive study of WA locations suitable for large-scale microalgal production, such as those with suitable physical locations, light intensities and temperature range, has been completed. The use of microalgae as a renewable energy source continues to be an active area of research and development.

Alf Larcher FRACI CChem is a petroleum, environmental and industrial chemist with an interest in science communication.

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A pink lake paradise

Australia has many natural wonders and perhaps this is why its pink lakes (some shown here) are underappreciated and underpromoted. More about Australia's major pink lakes can be found by searching 'pink lakes' at australia.com.

Lake Bumbunga, Yorke Peninsula, South Australia. Georgie Sharp/Flickr

Lake MacDonnell, Eyre Peninsula, South Australia. Andrew Cook/iStockphoto

The pink lakes, Murray–Sunset National Park, Victoria. tsvibrav/iStockphoto

Safety and science

Partners in innovation

BY **LISA J. STEVENS**

COMiCA/iStockphoto

Chemical safety at work has its frustrations – for workers and regulators alike – but neglecting it in the name of innovation can cost lives.

In a 2018 email exchange between the late entrepreneur and engineer Stockton Rush and divemaster/explorer Rob McCallum, as reported by the BBC (bit.ly/3RLqbvQ), Rush stated:

> *I have grown tired of industry players who try to use a safety argument to stop innovation and new entrants from entering their small existing market.*

McCallum's response was illuminating:

> *… having stood in a Coroners Court as a technical expert, it would be remiss of me not to bring this [danger] to your attention.*

In a CBS news interview (bit.ly/3EXdV3X), Rush also stated that:

> *… there's a limit. You know, at some point, safety just is a pure waste. I mean, if you just want to be safe, don't get out of bed … At some point, you're going to take some risk, and it really is a risk/reward question. I think I can do this [innovation] just as safely by breaking the rules.*

We will never know whether this was just rhetoric or a more ingrained way of thinking. Stockton Rush and four others perished during the *Titan* submersible dive to view the RMS *Titanic*.

The conversation between Rush and McCallum highlights many issues. One is the shocking disregard for safety and the role of safety in innovation. Despite McCallum putting forward several arguments as to why breaking the rules was not an option, Rush was steadfast in his determination in 'breaking the rules' and disregarding the basic principles of physics and safety. There is a difference between being innovative by thinking outside the square and deciding which rules you will break in the name of innovation and recognition. Five people, including Rush, paid the price for his attitude. Sadly, these kinds of conversations are not unique – they play out daily in many workplaces.

Rush was right and wrong. Everything we do, from getting out of bed, working with hazardous chemicals,

and even crossing the road, is not without risk. Life has risks. Every day we make hundreds of decisions based on the associated risk of activities. Yet, when it comes to managing workplace risks, workers and employers are often brought kicking and screaming to the health, safety and environment (HSE) table. Like Rush, many see safety as a barrier to innovation or that breaking the safety rules in the name of science and progress is okay.

Why negative attitudes to HSE?

Why and when do people decide to disregard safety advice and regulations? Where is the 'point' that Rush described? After all, we know that when some rules are broken, the results can be catastrophic. There always seems to be someone who considers themselves competent enough to not comply with the laboratory safety standards or health and safety regulations.

Safety professionals are often labelled 'bureaucratic', 'safety cops' and 'petty'. In 2013, the UK's Health and Safety Executive took an unusual approach by implementing a campaign to counter the increasing misinformation and incorrect application of health and safety requirements.

Is the problem that health and safety professionals focus so much on the requirements to meet strict workplace health and safety (WHS) regulatory requirements, key performance indicators and other prescriptive measures that we have lost sight of the impact of this on workplaces? Or is it that the body of knowledge that defines the health and safety profession has taken us away from understanding and managing specific hazards to operating in a mode of critical thinking, regulatory compliance and legal ramifications, rather than acting as the enablers we should be?

HSE consultants frustrated too

Health and safety consultants also get frustrated with the often-overwhelming bureaucratic red tape. In early 2023, the safety landscape changed when a health and safety manager was charged with breaching Queensland's *Workplace Health and Safety Act 2011* after two workers contracted Q fever. The prosecution was based on the health and safety manager's failure 'so far as reasonably practicable' to develop and implement relevant policies and procedures to control the hazard and the failure to complete a risk assessment and implement the relevant controls. The ramification of this prosecution is a point of continuing discussion for the occupational health and safety profession. However, it is a reminder that as workers we have a responsibility to take reasonable care of our own health and safety while also ensuring that our acts and omissions do not adversely affect the health and safety of others.

Every day we make hundreds of decisions based on the associated risk of activities. Yet, when it comes to managing workplace risks, workers and employers are often brought kicking and screaming to the health, safety and environment (HSE) table.

The bottom line is that the health and safety consultant has a role in protecting employees from workplace hazards, and in assisting organisations to comply with regulations. There is no getting around the fact that the regulator expects to see completed risk assessments, standard operating procedures and worksite inspections. From a health and safety consultant's perspective, if that is what the regulator wants, that is what the regulator gets. Health and safety consultants are the messengers. We are the ones who have to implement the regulations; we do not make the rules.

Reflecting on the 'E' in HSE

The point of safety is not the mandated WHS worksite inspections, risk assessments and hazardous chemicals registers. In 2011, the International Year of Chemistry, the OECD published a retrospective review, *40 years of chemical safety*, covering roughly the same 40 years since the publication of Bretherick's handbook. It was not about chemical innovations but was a reflection of toxic chemicals' impact on the environment, humans and other animal species. Incidents such as the release of methyl isocyanate in Bhopal, India (1984), and the Sandoz chemical spill and fire in Schweizerhalle, Switzerland (1986), led to the publication of OECD's *Guiding principles for chemical accident prevention, preparedness and response* in 1992, with the third edition published earlier this year.

The OECD's book focuses on chemists such as Rachel Carson (1960s) and Rowland and Molina (1995 Nobel Laureates) for their work on DDT and on the health and environmental impact of CFCs, respectively. The OECD acknowledged their Environment, Health and Safety Division for its work with independent experts, government and policymakers regarding existing and emerging issues in the chemical safety arena and reflected upon the development of good laboratory practices, animal welfare process safety and risk assessments.

Despite the focus on chemical safety in recent decades, the world

Two pioneers in chemistry health, safety and environment

Chemical Engineer, Wikimedia Commons

A.E. Leighton, after whom RACI's premier medal is named, was a paradigm of safety at a time when Australia's health and safety framework was just being developed. With a background in explosives research and production in England and India, Leighton was appointed designer and manager of the Maribyrnong (Victoria) cordite factory in 1909. Leighton was more than just a chemist; he was an innovator developing safer alternatives to cotton cordite and glycerine. In a time before Australian Standards and WHS regulations, he pushed for absolute standards of measurement. Leighton saw the need for and benefits of implementing safety measures within the munitions factories. He saw the human impact of exposure to chemicals and the effect on productivity. Leighton knew that just because the Maribyrnong factory had not suffered an accident, precautions still needed to be taken to avoid one. For Leighton, safety was about paying attention and reminding others of the importance of those irksome and seemingly trifling requirements.

Two near misses, including one that 'almost involved [his] personal oxidation',* started British chemist Leslie Bretherick on a quest to improve chemists' knowledge of adverse reactions. He devoted a significant part of his career to writing his 1000-page *Bretherick's handbook of reactive chemical hazards*, published in 1975. Today, RACI recognises Bretherick's contribution to laboratory safety and chemical management through the Health, Safety and Environmental Division's Leslie Bretherick Memorial Lecture.

*According to an opinion piece in *Chemistry World* (bit.ly/3sB8LaJ), Leslie Bretherick described the incident, involving chromium trioxide and acetic anhydride, in a letter to *Chemistry & Industry* in 1964.

Despite the focus on chemical safety in recent decades, the world continues to see many incidents that could have been avoided.

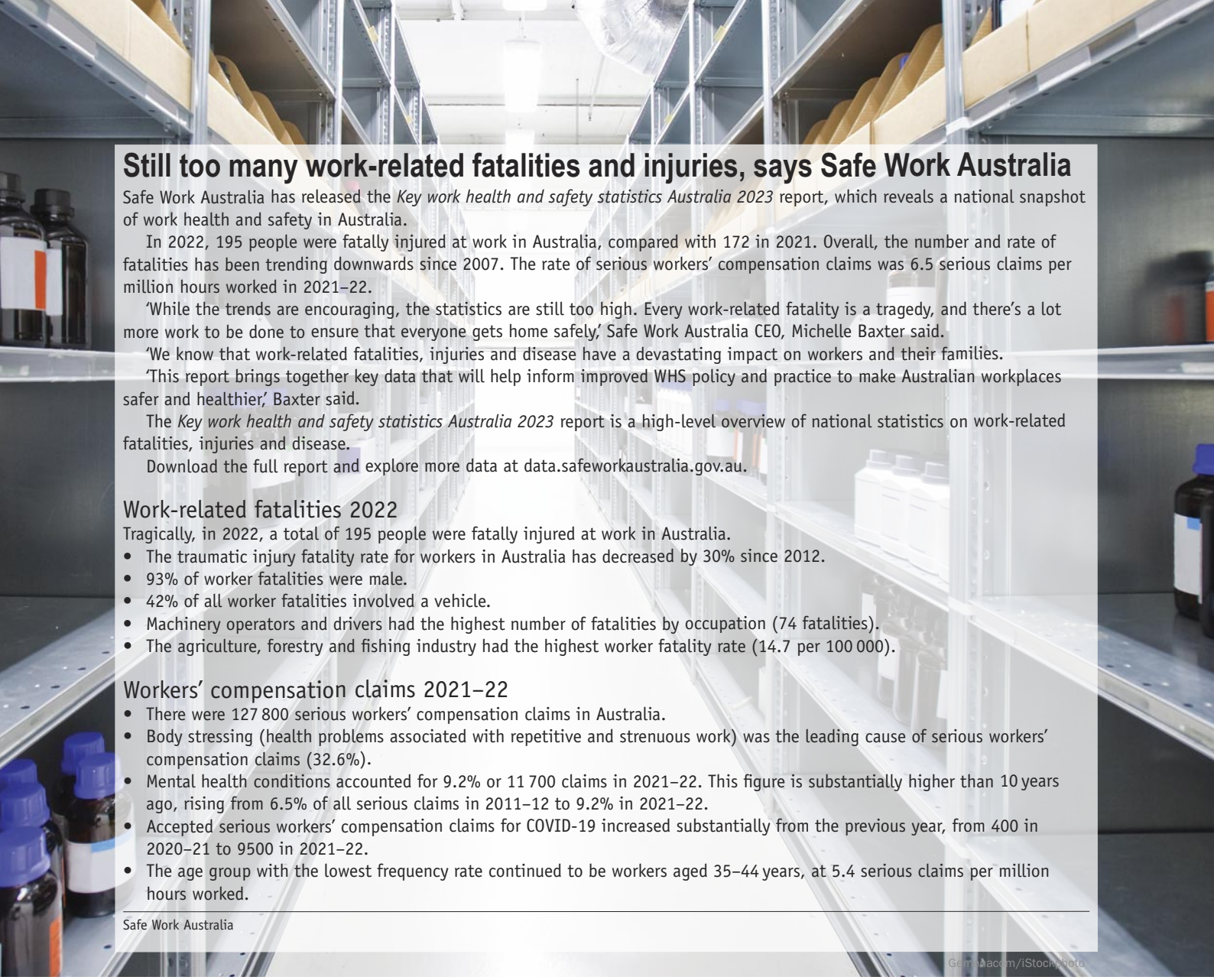
continues to see many incidents that could have been avoided.

In 2019, John B. Goodenough, M. Stanley Whittingham and A. Yoshino were awarded the Nobel Prize for Chemistry for developing a lithium-ion battery. Yet, in the past 18 months, Australia has seen more than 450 fires linked to lithium-ion fires. In New York City alone, more than 250 people have been injured as a result of lithium-ion battery fires. Government agencies worldwide are now tasked with assessing the risks and reviewing regulations associated with lithium-ion batteries. Australasian Fire and Emergency Service Authorities Council have acknowledged that lithium-ion battery fires are incredibly challenging.

Leighton and Rush represent a dichotomy in health and safety. Leighton was an innovator and a safety leader concerned about worker and public safety. Not only did he consider the hazards, he respected them at a time when health and safety was in its infancy. Rush considered safety an obstruction to innovation. He disrespected the hazards and broke the rules. In doing so, he paid the ultimate price. Had *Titan* been rescued, would Rush have rethought his perspective on safety?

Every worker has the right to go home from work in the same condition in which they started the day. Every consumer has the right to a product that will be safe. Despite this and the abundant and sometimes frustrating regulatory framework, people still die at work or from diseases caused by exposure to hazardous chemicals. Hazardous chemicals involve some of the most complex safety hazards that workplaces have to manage, and the chemicals and their hazards need to be respected and understood. Chemistry and safety should fit hand in glove, and innovation and safety should work hand in hand. None of us is invincible.

Lisa J. Stevens FAIHS ChOHSP, FRACI CChem is an OHS consultant specialising in laboratory safety and chemical management. She is a past chair of the Health, Safety and Environmental Division, Winner of the 2020 HSE Division Medal and PhD candidate at Edith Cowan University.



Still too many work-related fatalities and injuries, says Safe Work Australia

Safe Work Australia has released the *Key work health and safety statistics Australia 2023* report, which reveals a national snapshot of work health and safety in Australia.

In 2022, 195 people were fatally injured at work in Australia, compared with 172 in 2021. Overall, the number and rate of fatalities has been trending downwards since 2007. The rate of serious workers' compensation claims was 6.5 serious claims per million hours worked in 2021–22.

'While the trends are encouraging, the statistics are still too high. Every work-related fatality is a tragedy, and there's a lot more work to be done to ensure that everyone gets home safely,' Safe Work Australia CEO, Michelle Baxter said.

'We know that work-related fatalities, injuries and disease have a devastating impact on workers and their families.

'This report brings together key data that will help inform improved WHS policy and practice to make Australian workplaces safer and healthier,' Baxter said.

The *Key work health and safety statistics Australia 2023* report is a high-level overview of national statistics on work-related fatalities, injuries and disease.

Download the full report and explore more data at data.safeworkaustralia.gov.au.

Work-related fatalities 2022

Tragically, in 2022, a total of 195 people were fatally injured at work in Australia.

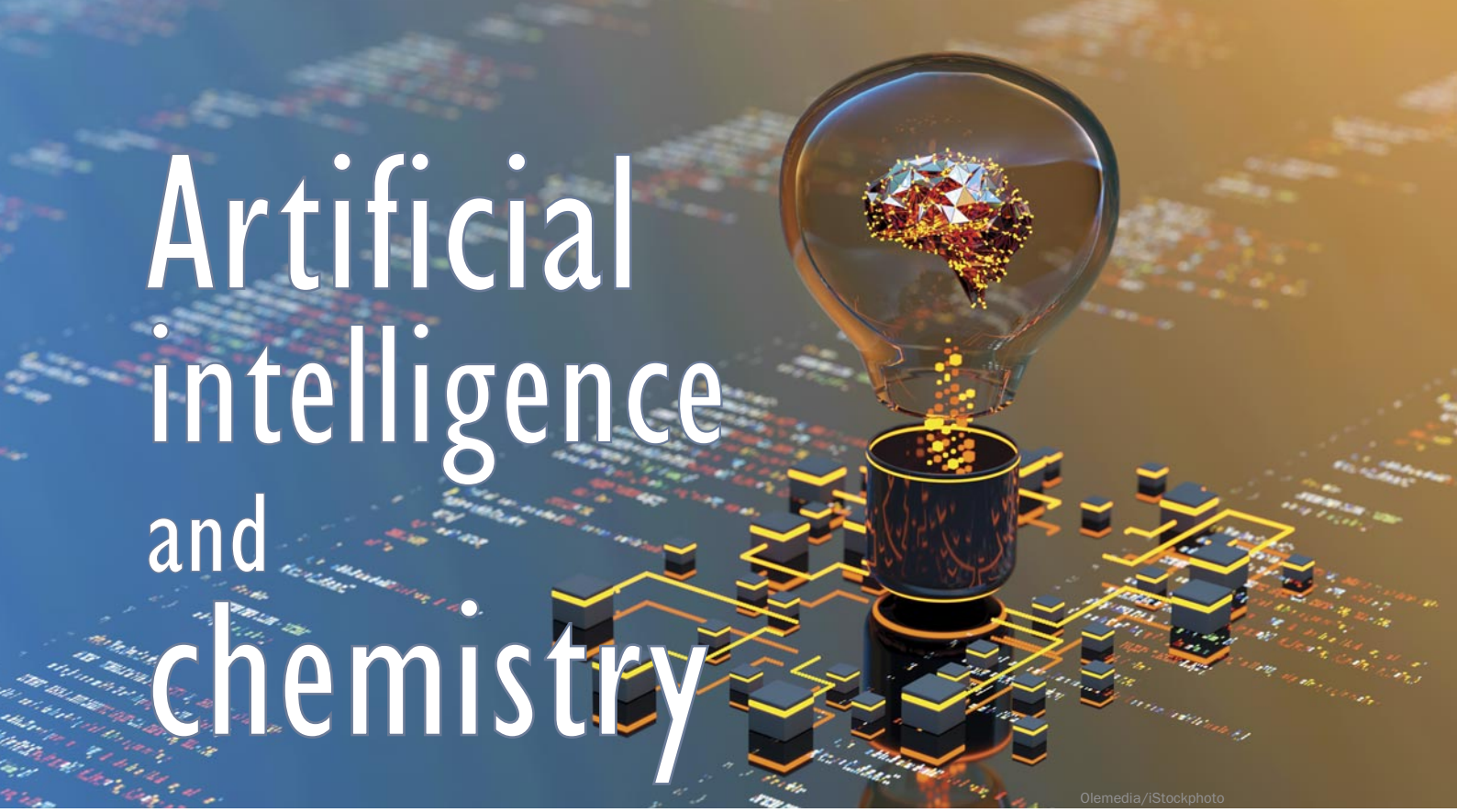
- The traumatic injury fatality rate for workers in Australia has decreased by 30% since 2012.
- 93% of worker fatalities were male.
- 42% of all worker fatalities involved a vehicle.
- Machinery operators and drivers had the highest number of fatalities by occupation (74 fatalities).
- The agriculture, forestry and fishing industry had the highest worker fatality rate (14.7 per 100 000).

Workers' compensation claims 2021–22

- There were 127 800 serious workers' compensation claims in Australia.
- Body stressing (health problems associated with repetitive and strenuous work) was the leading cause of serious workers' compensation claims (32.6%).
- Mental health conditions accounted for 9.2% or 11 700 claims in 2021–22. This figure is substantially higher than 10 years ago, rising from 6.5% of all serious claims in 2011–12 to 9.2% in 2021–22.
- Accepted serious workers' compensation claims for COVID-19 increased substantially from the previous year, from 400 in 2020–21 to 9500 in 2021–22.
- The age group with the lowest frequency rate continued to be workers aged 35–44 years, at 5.4 serious claims per million hours worked.

Safe Work Australia

Artificial intelligence and chemistry



Olemedia/iStockphoto

What is the future of AI in the chemistry professions, and is it something we should be worried about? Ian Maxwell reports on AI and its future compared to that of quantum computing in molecular quantum chemistry.

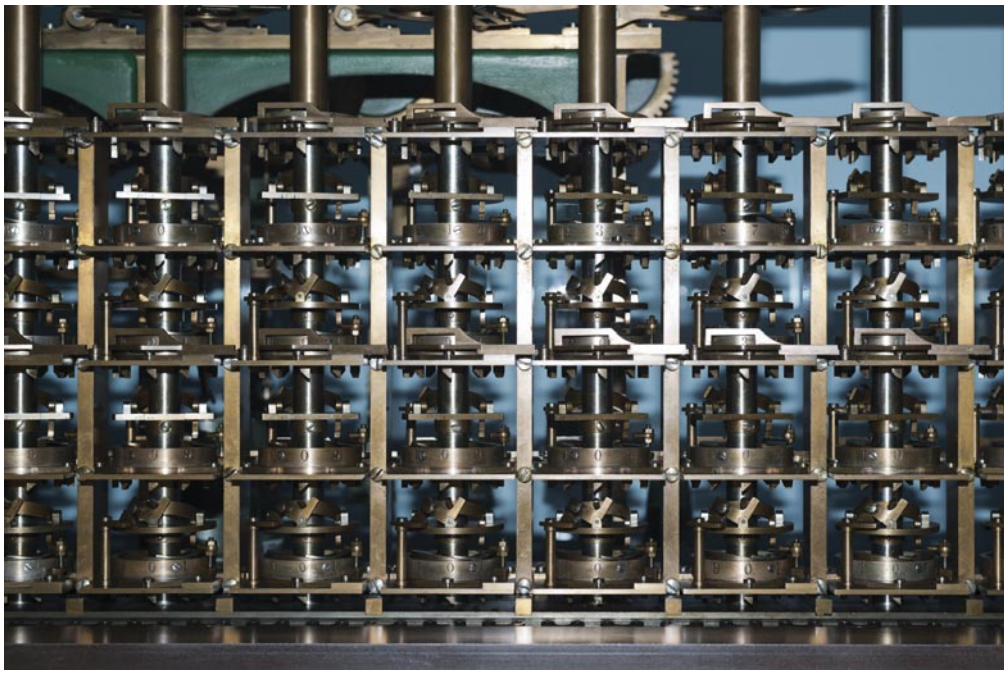
My thoughts on AI start with an article by a former Australian chief scientist. After throwing out a few examples for the potential uses of AI technologies (e.g. designing powerful chemical toxins, replacing actors with their likenesses without their consent, perpetrating undetectable scams, spreading misinformation during elections and building autonomous weapons), the author moved right on to the subject of how to 'regulate' AI technology.

Why is this style of critique so popular? Possibly it is because humans have evolved to resist change, since one hypothesis suggests that before the Industrial Revolution, it was statistically reasonable to assume that all change would have negative results; hence, opposition to change became a hard-wired heuristic.

However, since the Industrial Revolution, a small fraction of society has learnt to over-ride their instincts and embrace change so as to personally benefit by quickly adapting and exploiting change. A nice example in the context of AI is the hundreds and possibly thousands of start-ups that are being funded by venture capital to exploit AI technologies for specific applications. A specific example in chemistry is worth noting: many start-ups are being funded for the use of AI in drug discovery. Nothing scary there – they are just using AI technologies to improve the odds of finding medically useful pharmaceuticals. Of course, if they are very successful, many jobs in the pharmaceutical R&D supply chain might be displaced, but one likes to think that the highly intelligent and skilled individuals in these jobs will be able to repurpose themselves fairly quickly.

The usual experts in predicting the future have forecasted that the jobs most likely at risk from AI technologies are those where an employee spends most of their time in front of a computer monitor. Honestly, I think that might be a good thing. Some years back I did a 'time and motion' study of my own work life and discovered that an unhealthy amount of my time was being spent looking at a screen – so I changed my life. Of course, I am looking at a screen as I type this, the alternative being to handwrite a draft,

... the Turing test proposed that if a human evaluator can be fooled by a machine, then we have achieved a machine that can 'think' (which has been equated to the creation of AI).



Turing machines, invented by English mathematician Alan Turing in 1936, continue to be a focus of the theory of computing. exopixel/iStockphoto

or to use an actual typewriter. Or I could have jotted down some bullet points and asked ChatGPT to do the heavy lifting to create all the filler words in between. I have tried that, and the results have not been impressive. In fact, the last time I wrote an article, I was asked by the editorial staff to reduce it from 1200 to 800 words; even for this task ChatGPT was completely useless – it disembowelled the meaning and readability of the essay while apparently also being unable to count words (I said 800 not 565 words).

On four counts I am not the least bit worried about AI technologies: progress in AI technologies will likely be a lot slower than people imagine, giving society ample time to adjust to each new breakthrough in capability; AI technologies will help humans break away from their work-enforced screen time (what they then do with their extra free time is on them); with a bit of luck, someone will apply AI technologies to a next-generation spelling and grammar checker for a word processor that is substantially better than that touted by Microsoft; and I like change.

Alan Turing famously posed the challenge for what was to become the AI-driven machine – the Turing test proposed that if a human evaluator can be fooled by a machine, then we have achieved a machine that can 'think' (which has been equated to the creation of AI). I don't suppose Turing ever stopped to think about the distribution of human capabilities when it came to being fooled. In any case, I am sure we have all by now read articles that have been generated by ChatGPT and its ilk and are none the wiser as to whether they were human- or machine-generated. I don't think that means that ChatGPT can 'think' or is an Orwellian threat to society. When AI software competes with humans for resources or demands a bank account, that's when we should get worried. Until then, AI is there to make our lives easier and simpler by doing things for us that we prefer not to do, for one reason or another.

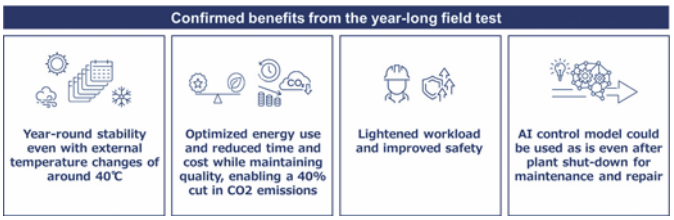
In fact, many researchers are already adopting AI for the writing of reports and papers. As many of you are aware, academic researchers are very much slaves to their *h*-indices – an obtusely simple approach to measuring the impact of academic research that simply counts citations to an academic's papers by other academic researchers. If an *h*-index even has a second-order correlation to research impact, I would be very surprised.

Michael J. Douma, a well-known historian and polymath, published research into academic papers and concluded that (bit.ly/3QbJZGn):

> *… a scholar who writes articles in recognisable journals, even lower ranked ones, should expect that each article will be read about 100 times. If you are lucky and good, it might be read 1000 times. In the top, say 50 history journals, there are probably no articles that after 10 years have not been read at least a few dozen times.*

In this context, and reintroducing AI into the discussion – if hardly anyone is reading your papers, then why not turn over the writing of them to AI?

Last year, after a 30-year hiatus, in my role as a visiting professor at the University of Technology Sydney, I published two papers in a peer-reviewed journal. The experience was completely underwhelming, and I have



In 2022, Yokogawa Electric Corporation and JSR Corporation reported plans to officially adopt a reinforcement learning-based AI algorithm for use at an ENEOS Materials chemical plant in Japan after a successful year-long field test demonstrated a high level of performance in controlling a distillation column (bit.ly/49Jky7R). Yokogowa

a new-found sympathy for academic researchers. The research outcomes were first published as precis on LinkedIn, where we generated a substantial amount of commentary and feedback. After months of delays, the full papers were accepted for publication in the peer-reviewed journal – we have not received a single item of feedback as yet, other than from the peer reviewers. And we first had to endure the peer-review process. Given my experience with the low quality of the reviewing process, wouldn't publishers be better off employing AI to simulate peer reviewers?

An area where I am certain AI is being used is in the generation of educational material by academics. I know of an academic who has decided to take the 'working from home' vibe to its extreme. He is now using AI software as the basis of his undergraduate lectures (which are delivered remotely of course). If an audience can't tell the difference, then does it matter? All he has managed to achieve is a high level of work efficiency, where he has a lot more leisure time than his colleagues. Eventually everyone will catch up with him and he will be paid less for this effort, commensurate with the work effort required by the AI route.

To me, the impact of AI on chemistry is going to pale next to that of the use of quantum computing in molecular quantum chemistry.

Returning to the use of AI in chemistry, I found a report that suggested the key areas of deployment will be molecule property prediction, molecule design, retrosynthesis, reaction outcome prediction, reaction conditions prediction, and chemical reaction optimisation.

If you ponder that list properly, it suggests that AI in chemistry will be used as a better means to solve complex model-based chemistry problems. That is, it will be used as an optimisation approach to replace current numerical approaches, rules of thumb and human insight.

I can't resist the temptation to be a futurologist myself from time to time. To me, the impact of AI on chemistry is going to pale next to that of the use of quantum computing in molecular quantum chemistry. If and when we have fully functional quantum computers with millions or even billions of error-free qubits, it will be possible to solve Schrödinger's equation for any molecular situation without having to make the current kind of assumptions that generally reduce the usefulness of molecular quantum chemistry to a very mathematically frustrating academic activity. Quantum chemistry has been around since 1927 when Walter Heitler published the first recognised paper in the area. To this day, I have not found one quantum chemist who can name a single practical application of molecular quantum chemistry outside of academia (if one excludes the application of quantum mechanics to solid state non-molecular materials such as inorganic semiconductors).

Please note, this comment absolutely is not a criticism; it's just to note that it's a field that is waiting on the availability of new technologies so that it can have its day in the sun. Those new technologies will be quantum computing (for the processing of ab initio equations that define molecular properties, without the current value-destroying assumptions) and AI (to optimise said processing for a specific desired outcome).

... I feel that as application-specific AI technologies become slowly available, society will adapt to them.

On the topic of quantum computing, I am chair of a quantum computing start-up (Eigensystems) and this company has developed an educational product (the Quokka) so that people can learn to program and use quantum computers. (It is sort of analogous to the 1980s Tandy Color Computer in the digital computing era – if you are old enough to remember that.) Eigensystems uses sophisticated techniques to emulate a quantum computer – it's a $500 product that emulates a quantum computer that would cost many millions of dollars, and it does so without any errors, unlike real quantum computers.

Quantum computing as a field of endeavour goes back to the 1980s, and to this day, although heavily hyped, is still effectively an investor-driven boondoggle. The largest functioning quantum computer in the world currently has 433 qubits, but to quote my expert 'it's as noisy as [*#@!]'. Currently no resources in this device are employed to correct errors. The only way to use it is to run programs that are so small that statistically few if no errors actually occur.

Google has demonstrated an error-corrected qubit (that still doesn't work properly) on a 53 qubit chip. It gave them one effective encoded qubit, but only reduces error rates by a fraction of a fraction of one per cent.

Generally, in quantum computing, the figure of merit is the 'quantum volume' – which effectively quantifies the size of the quantum program that can be successfully run. The largest quantum volume to date by a real quantum computer is 524 288. For comparison, Eigensystem's $500 quantum computer emulator has a quantum volume of approximately one billion. So, please don't hold your breath, folks … practically speaking, I wouldn't be surprised if quantum chemistry has to wait for another 100 years to have the tools in place to finally take off, such is the challenge faced by the hardware developers in quantum computing. I believe the relevant AI technologies will be available well ahead of that time.

Generally speaking, I feel that as application-specific AI technologies become slowly available, society will adapt to them. It's this slow pace of availability that has enabled society to already adapt to the millions of life-changing technologies that have been invented since the start of the Industrial Revolution. Despite the warnings of Aldous Huxley and social media, apocalyptic visions of billions of unemployed people enslaved to the desire of machines haven't eventuated as yet. For chemistry and chemists, I think it's all upside, and it's worth noting that embracing change is probably a good way to not become a victim of it.

Ian A. Maxwell is a visiting professor in the Faculty of Engineering and IT at the University of Technology Sydney, who started his career as a physical polymer chemist. Ian is also the chair of a number of high-tech start-ups.

Vale John White

Leader in neutron scattering

Emeritus Professor John White, AO CMG FRS FAA FAIP FRACI CChem, passed away suddenly at home in Canberra on 16 August 2023. John was a very well-known and highly regarded member of the international scientific community, and his death has deeply saddened his colleagues, ex-students and friends around the world. John's spirited presence and polite and warm manner, coupled with seemingly boundless energy and enthusiasm, were known to all who interacted with him. John was a major contributor to RACI, having been President from 2000 to 2002, and recipient of the H.G. Smith Memorial Medal in 1997 and the Leighton Memorial Medal in 2005.

John was originally from Newcastle and studied chemistry at the University of Sydney, receiving the Dixon Prize for Chemistry, a first-class Honours degree and an MSc. He won an 1851 scholarship, which took him to Oxford University in 1959, where, supervised by Rex Richards, he worked on the new technique of nuclear magnetic resonance, which was being pioneered for chemistry. Even before finishing his DPhil, he was elected an ICI Fellow in Lincoln College, and in 1963 a fellow of St John's College Oxford, where he remained for 26 years. It was in this period in the 1960s that John began his long and distinguished career in neutron scattering when many exciting developments were taking place.

During this time, John met Ailsa Vise, a microbiologist, who had also won a research scholarship to Oxford, and they married in 1966. This was to be an enduring lifelong partnership. John and Ailsa even published an article together in the *Australian Journal of Chemistry* in 2011 on the discovery of the neutron as a legacy of the Curie family's work.

Within 10 years, he had risen to the top of the leadership in the field, serving as Neutron Beam Coordinator at Harwell and then Director of the Institut Laue-Langevin in Grenoble, France, where he proposed and led the '*deuxième souffle*' renewal program from 1978.

In 1985, John and his family returned to Australia where he was appointed Professor of Physical and Theoretical Chemistry at the Australian National University. His return greatly benefited Australia, as he was largely responsible for introducing the new experimental techniques of small-angle scattering and reflectometry to the Australian chemistry, biology and physics communities.

John was the most politically influential and effective advocate for neutron scattering in Australia through his roles as a Fellow of the Australian Academy of Science, President of RACI and President of the Australian Institute of Nuclear Science and Engineering.

Under the heading of 'Small Country Big Science', he organised a crucial access deal for Australian scientists to the ISIS Neutron & Muon Facility in the UK. Over 20 years, this provided Australian researchers with access to the most powerful spallation neutron source, with scattering techniques unavailable in Australia. The growth of new scientific and engineering uses of neutrons in Australia through ISIS access provided a sound basis upon which the case for a replacement research reactor at ANSTO was developed, which was ultimately commissioned as OPAL in 2006. John was also instrumental in the development of the neutron scattering capabilities at the OPAL reactor, participating on the Beam Facilities Consultative Group (1997–1998), Beam Instruments Advisory Group (2000–2004) and the Bragg Institute Advisory Committee (2004–2010). He was also a major driver in building an Asia–Oceania neutron scattering community as a founding executive member and then President of the Asia–Oceania Neutron Scattering Association (AONSA).

John was a key figure in the international scientific community for more than five decades. Over the course of a long and distinguished career, through a combination of advances in experimentation and choice of paradigm examples, his work demonstrated how neutron scattering data could be

John was the most politically influential and effective advocate for neutron scattering in Australia ...

analysed to provide precise details of molecular structure and dynamics for a wide variety of chemical systems.

He was awarded fellowships of the Royal Society of Chemistry (1982), RACI (1986), the Australian Institute of Physics (1986), the Royal Society of London (1993) and the Australian Academy of Science (1991). He was a visiting Fellow at Argonne National Laboratory in 1984. Among his many other awards, including the RACI awards mentioned above, are the David Craig Medal and Lecture of the Australian Academy of Science (2005), the Archibald Liversidge Medal of the Royal Society of New South Wales (2010) and the AONSA Prize (2015). He was awarded the Order of St Michael and St George (CMG) in 1981 and the Centenary Medal in 2001 and appointed an Officer of the Order of Australia in 2016.

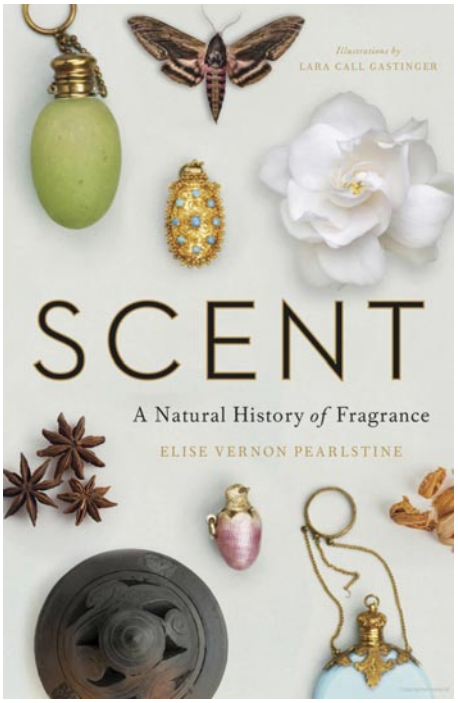
John had a long involvement at the faith–science interface from his days at Oxford with the Research Scientists' Christian Fellowship to being a key player in the establishment of the Institute for the Study of Christianity in an Age of Science and Technology in 1987 and serving as President from 1992 to 2006. It was his vision to establish the biennial Conference on Science and Christianity series, which began in 1997 and continues today.

Among John's extraordinary list of achievements and contributions, perhaps most significant for many, is that through a combination of his exemplary science and his promotion of scattering techniques, John has been responsible for launching the careers of a great many scientists across the globe. University departments and scattering facilities throughout the world are populated with John's former students, postdocs and others whom he formally and informally mentored over more than five decades. The legacy of his leadership will be felt in Australia, the Asia–Oceania region and beyond for many years to come.

He is survived by Ailsa, children Sarah, Catherine, David and Rachel and their families, including seven grandchildren. John was farewelled in the church of St John the Baptist, Reid, Canberra, on 22 August 2023, where John and Ailsa were long-standing and enthusiastic members. He will be sadly missed.

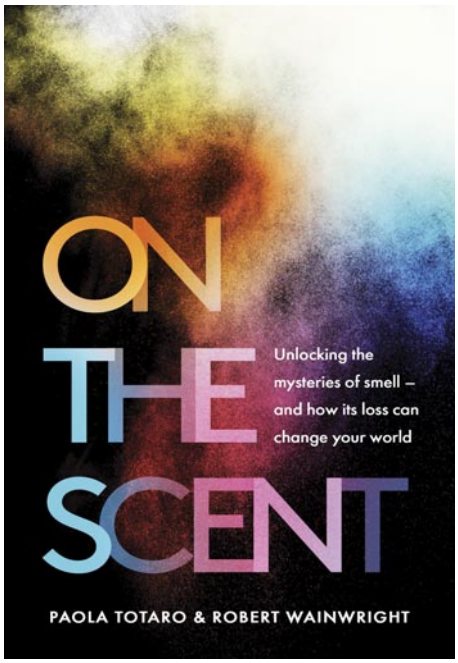
Ian Gentle MRACI CChem and **Elliot Gilbert**

Making scents of things



Scent: a natural history of fragrance

Vernon Pearlstine E., Yale University Press, 2022, hardback, ISBN 9780300146964, 272 pp., $38 approx.



On the scent: unlocking the mysteries of smell and how its loss can change your world

Totaro P., Wainwright R., Elliot and Thompson Ltd, 2022, hardback, ISBN 9781783966424, 272 pp., $25

Scent: a natural history of fragrance and *On the scent: unlocking the mysteries of smell and how its loss can change your world* have a common theme about smells and aromas and their perception or lack thereof. That is about where the commonality ends. Indeed, the word 'smell' itself conjures up a variety of meanings, including that of the pug owner who commented that her dog had no nose. The answer to the follow-up question of how does the said dog smell is, 'Woeful'.

Elise Vernon Pearlstine's *Scent* is an absolute delight. It is well written with clear explanations of the biological origins of many of the natural aromas and odours humans know and love so well. Moreover, she explores the chemistry of plant aromas and how these have evolved to serve the ecological niches of their hosts. We are all more or less aware of the pleasant sensory delights of natural perfumes and the magical *je ne sai quoi* herbs and spices contribute to our favourite dishes. What Pearlstine does is pull together the history and social milieu resulting from our interactions with the world of natural scents to give us a complete rounded picture.

Pearlstine began her career as a wildlife biologist 17 years prior to developing her expertise in natural perfumes, and she conducts classes on the biology, artistry and history of perfume ingredients. Her book is very impressive and I commend it most highly. Reading it is a great educational pleasure.

It is a complicated field: subtle changes in molecular structures can totally alter the smell of compounds.

Paola Totaro's and Robert Wainwright's *On the scent* is a very different kettle of fish. Essentially, Totaro totally lost her sense of smell as a result of COVID infection. Apparently, this is not quite so rare as you might think. (Certainly, more common than I had imagined!) The total loss of the sense of smell is anosmia, while partial loss is hyposmia.

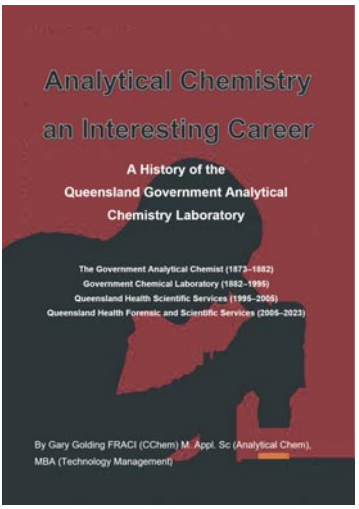
Traditionally, we are regarded as having five senses, so to suddenly lose one would be a tad alarming. Given a choice, which would you least regret losing? However, do not despair, animal behaviourist Ashley Ward (*Sensational: a new story of our senses*, Profile Books, 2023) has recently identified more than 50, including a sense of balance and a sense of time.

Totaro is an award-winning journalist and Wainwright an author and a journalist. This is reflected in the book, which is a fine piece of investigative journalism. I confess at times I found this journalistic style irksome, even though I feel the authors have done a very competent job in making the whole area accessible to a general reader.

It is a complicated field: subtle changes in molecular structures can totally alter the smell of compounds. So, does smell involve a key and lock mechanism? Well, we can sense a lot more distinct keynotes than we have locks to fit them. Are smell and taste totally orthogonal? When you eat a lemon tart, surely the experience is an amalgam of the aroma of the lemon and the zing of the acid on the tongue. There are all sorts of intricacies and intrigues abounding when the authors probe this important area, which, let's face it, is not something we tend to worry about over much. As the song goes, 'Don't it always seem to go, that you don't know what you've got 'til it's gone'.

Meanwhile, there is a lot of interesting reading in this book, which can only enhance your pleasure in smelling the flowers or, indeed, a fine wine.

R.J. Casey FRACI CChem HLM



Analytical chemistry, an interesting career: a history of the Queensland Government Analytical Chemistry Laboratory

Golding G., self-published, 2022, ISBN 9780645545104, 181 pp.; to purchase a copy, contact the author at goldingf@bigpond.net.au

This is an unusual book. Self-published by Gary Golding, a retired director of the Queensland Government's Analytical Laboratory, it traces the history of the laboratories through the careers of its managers and directors from 1873 to 2023. This format serves also to illustrate one of the themes – that of the chemist as a problem solver who adapts to constant change in both techniques and fields of work. Another theme is the management challenge of recruiting, mentoring and promoting chemists to senior positions while keeping them protected from distractions such as interference by their government masters or consultants. Survival with expertise intact often depended on chemists coping with transfer of 'ownership' between ministers, restructuring, renaming (overnight in one case) and forced outsourcing to commercial laboratories.

I found the role of the assistant director to be especially interesting. He or she was often the project manager who developed and installed new systems, wrote up standard procedures and set up a program of method validation.

Threaded through the stories are accounts of the variety of substances that had to be measured or found to be absent. Also appearing are the introduction of computer-aided, then computer-dominated, instruments and laboratory certification to NATA standards or to an ISO quality systems standard. Both certifications proved to be valuable exercises.

There was a 'do-it-yourself' philosophy: one manager was handed *Networking for dummies* and proceeded to rewire the whole laboratory's cable network!

Any reader would be impressed by the account of extensive involvement of the laboratories in external activities, including committees, national and international collaborative studies, standard setting and staff training. This kind of back-room work is often not well recognised.

The book contains many interesting photos. Anecdotes are also plentiful, some chemical, some personal, often appearing in gold frames among the text. One described how in the early days one had to give back the empty Biro to get a new one.

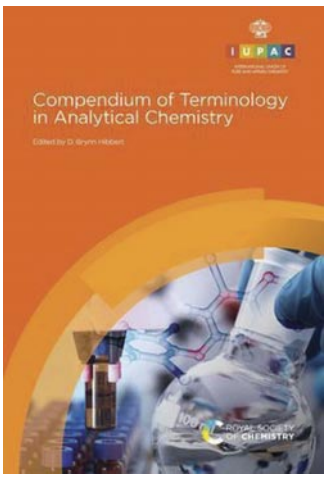
There was a 'do-it-yourself' philosophy ...

Once, when funds were tight, lighting that only responded to motion-sensing meant those attending a meeting had to learn to wave their hands around now and then to keep the lights on.

It is not surprising that the first cautious print run had to be soon followed by another. *Analytical chemistry, an interesting career* is available direct from the author.

Bruce Graham FRACI CChem

Compendium of terminology in analytical chemistry



Edited by D.B. Hibbert,* The Royal Society of Chemistry, 2023, ISBN 978178262944, 666 pp., $520–656

For what is essentially a specialised dictionary, the *Compendium of terminology in analytical chemistry* (IUPAC's 'Orange Book') makes a surprisingly good read. Reviewing the Orange Book was concurrently both easy and hard.

Easy because the chances of having something negative to say about this text were always going to be slim to nil from the outset, given the depth and breadth of its contributors and the (blindingly obvious) staggering amount of effort of its devoted editor and support networks. There are no 'ah ha' discovery moments where you can point out error, omission, nor even a hint of bias. Reading it only inspires a genuine heartfelt appreciation and desire to thank all those involved for their incredibly daunting and time-consuming efforts. Reading it cover to cover is not for the faint of heart or those seeking thrills and excitement. It is an important work, as any general or specialised dictionary is.

The hard part was to put aside my admiration for the feat accomplished and objectively produce a review that helps readers determine whether this book is for them and what they are looking for without having to read it cover to cover themselves. In this sense, the book itself assisted in that task by providing a helpful generic checklist on page 47 that applies not only to any analytical procedure in chemistry but also to this and potentially many other endeavours.

While the book's concise definitions, complemented by diagrams as and when needed, would help those seeking an understanding of unfamiliar terms, its inclusion of a diagrammatically assisted definition and basic explanation of AAN (artificial neural networks, p. 71) both is poignant and begs discussion of whether it is relevant any longer in the era of generational artificial intelligence (AI). The salient, haunting underlying question at the heart of this review is whether this book reflects a bygone era or a relevant ongoing need. In fact,

* Brynn's account of the making of the IUPAC 'Orange Book' was published in the Sept–Nov issue, p. 36.

editor Brynn Hibbert ponders whether this may well be the last edition of the hardcover Orange Book (p. xii), lamenting that this tome along with other IUPAC 'colour' books may be absorbed into the online-only 'Gold Book'.

I tested the premise with a statistically significant number of randomly selected terms through the volume and compared against results of various AI chatbots. At this stage, the AI did not recognise any esoteric or uncommon terms used in analytical chemistry. However, for all the common terms, AI generally provided impressively better explanations and definitions. In the sense the Orange Book is a publication 'by chemists for chemists' and that is its Achilles heel. AI is known for its variable accuracy (inclusive of numerous reports of 'hallucinations' – i.e. making things up when it does not know the correct answer), yet in the prompts I issued it did a surprisingly good job for common terms only and consistently stated that it does not understand nor recognise the remainder without seemingly trying to make up an answer. For someone who does not already understand the term, the Orange Book gives a good definition and explanation aimed at knowledgeable chemists, whereas AI explains noticeably better for those who have limited or even utterly no prior experience with the term's subject matter.

In the era of generational AI, hardcover reference books like the Orange Book will likely remain relevant to some people due to their depth, credibility and accessibility, especially for niche topics. However, they face challenges in terms of accessibility to a wider interested audience, timeliness and convenience compared to AI-generated content. The choice between AI and reference books depends on individual preferences and specific needs.

As an individual, there are several reasons why you might choose to consult the Orange Book:

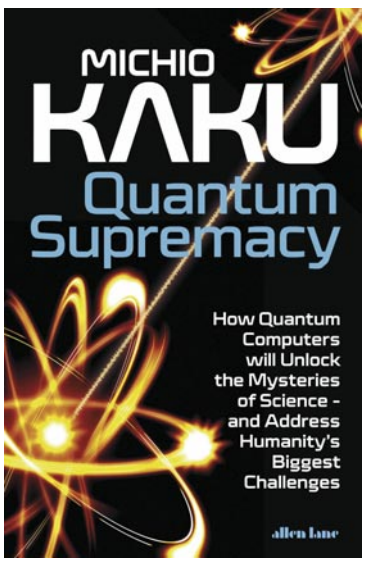
- Specialised knowledge: If you are studying or working in the field of analytical chemistry, the Orange Book can provide you with in-depth and specialised knowledge, including terminology, concepts and principles relevant to the subject.
- Research and academic purposes: For researchers, scientists and academics, the book can serve as a valuable reference for your work, helping you find accurate and comprehensive information on various aspects of analytical chemistry.
- Professional development: If you are a professional in the chemical industry or a related field, reading the Orange Book can enhance your expertise and update you on the latest developments and terminology in analytical chemistry as at the time it was published (2023).
- Trusted resource: The Orange Book is known for its credibility and accuracy, making it a trusted resource for those seeking reliable information in the field.
- Library or institutional use: Libraries and academic institutions may have the book available for their members, making it accessible to students, researchers and educators.
- Interest in chemistry: If you have a passion for chemistry and want to explore the subject in greater depth, the Orange Book can satisfy your intellectual curiosity, especially for non-common terms.
- Book collectors: Some individuals might seek to own the book due to its historical importance and its role in documenting the development of analytical chemistry terminology over time.

As an individual and a hands-on analytical chemist, as part of the wider scope of my interests from the very onset of my career where I dived in head first into HPLC, and widely diverse instrumental analysis, I truly enjoyed reading this book. And I conclude that expensive and hard-to-read compendiums like the Orange Book are most likely only going to have sufficient value to be purchased by a very limited subset of professionals, researchers, academics and students in analytical chemistry. Such tomes serve as valuable references for in-depth knowledge and are also of value to libraries and institutions, places that offer comprehensive resources to their users. Collectors and those interested in the history of chemistry may also value these books. Yet in instances where you simply want to understand a common analytical chemistry term and may be generally unfamiliar with the area, AI chatbots may better serve your needs.

Motty Sobol FRACI CChem

Quantum supremacy. How quantum computers will unlock the mysteries of science – and address humanity's biggest challenges

Kaku M., Allen Lane, part of Penguin Random House, 2023, paperback, ISBN 9780241639610, 352 pp., $26.96



Of recent books and reports written on the topic of quantum computers, *Quantum supremacy* by Michio Kaku offers an exciting and stimulating overview of the visions, hopes and aspirations for quantum computers.

Kaku notes the 2019 and 2020 'bombshell announcements' by Google and the Chinese Quantum Innovation Institute showed that prototype quantum computers can solve complex mathematical problems at incredibly faster rates than the world's leading supercomputers (seconds contrasted with multiple years – figures like 100 trillion times faster).

Governments in China, the US, the UK, Germany, France, Sweden (jointly with Finland), Singapore, Canada and Australia, among others, are supporters of this emerging technology. Some have provided targeted research funding for the establishment of National Centres in Quantum Research, some

with joint funding with industry research partners and others to create start-ups; but, above all, national quantum strategies have evolved. Other leading corporates investing heavily in this technology are IBM, Microsoft, Intel, Rigetti and Honeywell, accompanied by an array of start-ups.

I note analysts suggest the team led by the University of Sydney, including collaborators at the Australian National University, Macquarie University, University of Queensland, University of New South Wales and University of Western Australia stands among the 12 top quantum computing universities in the world.

Why is this technology so fast and capable of handling such enormous volumes of data?

Kaku reminds us that the familiar digital computer is encoded in a series of 0s and 1s – a single digit being a 'bit'. A sequence of 0s and 1s are fed into a digital processor to perform a desired calculation.

Richard Feynman's critical observation in 1959 that atomic particles behave like spinning tops, and in a magnetic field may be up or down with respect to the direction of the field, effectively corresponds to a 0 or a 1 encoding. Atoms can also be in an infinite number of combinations of up or down. This means an atom can carry much more information, not only a bit, but a 'qubit' – a simultaneous mixture of up and down. The same quantum properties also apply to photons enclosed in a ring. The photons can travel in both directions and following the quantum rules provide multiple 0 and 1 encoding.

In the atomic world, this simultaneous existence of multiple states is called 'superposition'. In addition, qubits can interact with each other, so each time a qubit is added, the number of interactions is effectively doubled. The current prototype quantum computers have up to 100 qubits, meaning they are 2^{100} times more powerful than a supercomputer with just 1 qubit.

The smallest impurities or disturbances from the outside world can cause the array of atoms/photons to fall out of coherence. This is a current stumbling block in quantum computer development, though a working solution exists in high-field superconducting magnets where the coil is contained in a bath of liquid helium (0 K). Kaku contends that in nature, photosynthesis represents an ideal ambient temperature model of quantum computing in practice.

The bulk of the book (300 pages) contains Kaku's considered analyses of the latest research and thinking (e.g. in chemistry, biology and medicine) on an array of problems that may only be efficiently addressed given this new-found computer power. Topics include quantum computing's potential to discover the secrets of abiogenesis, green the world, feed the planet, aid/facilitate energy generation, tackle global warming and carbon sequestration, nuclear fusion, simulate the universe, and make advances in health, drug development, gene editing, cures for cancer and AI.

I conclude the digital 'supercomputer' starts to appear like an 'abacus' compared to what may just be over the horizon. But, I hesitate to add, only time will tell.

Dr Alan J. Jones FRACI CChem

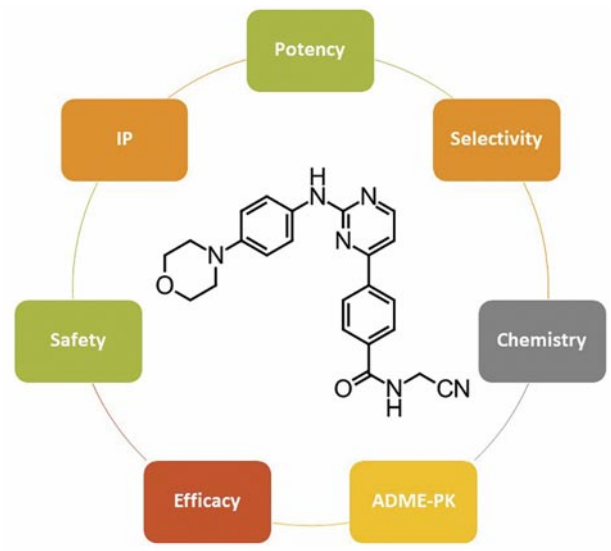
A brief history of Ojjaara™ (momelotinib)

Approved by the FDA, discovered in Melbourne

On 15 September 2023, the US Food and Drug Administration (FDA) announced that momelotinib, an orally bioavailable JAK1/JAK2 kinase inhibitor (JAK1 and JAK2 being enzymes that catalyse the transfer of a phosphate from ATP to specific signalling proteins), was approved for the treatment of myelofibrosis for patients with anaemia. For these patients, the approval represented an important advance for the treatment of their disease. For GSK, the global pharmaceutical giant that filed the New Drug Application with the FDA, it meant the beginning of a marketing campaign for a drug they predict will be a blockbuster (meaning annual sales of more than US$1 billion). And for a small group of scientists in Melbourne, your author included, it meant that the more than 20-year odyssey to discover and develop the drug had finally come to a triumphant conclusion.

Momelotinib is only the second drug invented in Australia to be approved by the FDA for sale in the US – the world's largest pharmaceutical market. Further, the drug's primary targets – the kinases JAK1 and JAK2 – were discovered in Melbourne, and in addition the discovery team, in close collaboration with academic scientists from Monash University, were the first in the world to obtain crystal structures of both kinases. Taken together, these achievements represent a high-water mark for medical science and drug discovery in Australia.

Unfortunately, however, the drug development activities, which began in Melbourne, were predominantly carried out by companies overseas. The momelotinib story is therefore another example of Australian science not being supported locally through its development journey, and being sold to overseas entities before significant benefits from commercialisation could flow back to local investors and the Australian drug discovery and development ecosystem more broadly.



Discovery of the JAKs

The JAKs were discovered by Professor Andrew Wilks, a laboratory head at the now-defunct Melbourne laboratories of the Ludwig Institute for Cancer Research. Wilks was building on the seminal work in the Parkville precinct in haematopoiesis, spearheaded by luminaries such as Professor Don Metcalf, trying to unravel the processes that, from a small number of precursor cells, gave rise to the many cells in our blood. Wilks invented a process to identify intracellular enzymes in precursor cells essential for their differentiation and maturation, and during this work discovered two enzymes called Just Another kinase 1 and 2 (JAK1 and JAK2), later renamed after the two-faced Roman god of doorways, Janus, to reflect the homodimer formed by the kinase units (*Molecular and Cellular Biology* 1991, vol. 11(4), pp. 2057–65).

The birth of Cytopia

In the 1990s, it was essentially unheard of for academics to leave academia and start a company, but Wilks did just that, founding the company Cytopia off the back of his discovery of the JAKs in 1997. He licensed the seminal JAK intellectual property from the Ludwig Institute and, after a number of years trying to secure funding, was finally successful in securing investment from the ASX-listed 'Pooled Development Fund' Medica Holdings. Medica, headed by chemist Kevin Healey, at that time was funding drug discovery activities at two other Australian biotechs, Xenome and Alchemia. Cytopia started its early lab work in the Gaol Ward of St Vincent's Hosptial in Fitzroy; not an auspicious beginning.

With funding in place, Wilks started building Cytopia's capabilities in kinase drug discovery. While the primary focus was on the kinase JAK2, an extensive panel of other kinases with known roles in cancer and/or inflammatory disease biology was also included, including JAK3, FAK, cFMS, cMET and KDR, among others. The team's initial focus was on establishing drug screening capabilities using both cell-free and cellular systems and, with these in hand, screening of small collections (up to 1000 compounds) of commercially available 'kinase-targeted' chemical libraries began. Hits in the cell-free screen against the JAK2 enzyme were seen early on, and at this time Wilks and his small group of biologists came to the realisation that they needed chemistry know-how to move things forward.

Drug discovery begins

I joined Cytopia at the beginning of 2001 after starting my medicinal chemistry career at Pfizer UK in the early 1990s. In Cytopia, and under Wilks' leadership, it was clear a unique capability with excellent people had been established to undertake target-driven drug discovery. In addition to drug screening capability, Wilks had enlisted the skills of molecular modellers Herbert Treutlein and Jun Zeng, both previously of

Momelotinib is only the second drug invented in Australia to be approved by the FDA for sale in the US ...

the Ludwig Institute, who were developing a unique and advanced virtual screening platform, well before machine learning and AI was de riguer in the industry. We opened chemistry labs at the Baker Institute, and began making and testing compounds designed from the initial hit compounds. Early work from this program focused on compounds with cell-killing activity against cancer cell lines, particularly prostate cancer cells, since this cancer had a documented JAK2 dependency. Optimisation of this series of compounds led to the discovery of the potent vascular disrupting agent CYT997 (lexibulin) that entered the clinic for treatment of solid tumours. While itself not a JAK2 inhibitor, this compound demonstrated the capability of the team to discover and develop compounds for clinical study.

JAK2 and myeloproliferative neoplasms

The JAK2 program gained momentum in 2005 after several scientific reports were published identifying an activating mutation in JAK2 as being the likely molecular cause for myeloproliferative neoplasms, a family of blood cancers in which over-production of specific cells in the blood leads to severe disease. Of these myeloproliferative neoplasms, the worst was idiopathic myelofibrosis, essentially a scarring of the bone marrow, for which there was no effective treatment and where patient median survival was approximately five years. In addition, these patients suffered from a suite of debilitating symptoms, including spleen enlargement, bone pain, night sweats, fever and chronic itchiness (pruritis), before ultimately succumbing to the disease.

Our JAK2 drug discovery program was already well advanced by the time of these reports, so we rapidly refocused attention to completing the optimisation work. The chemists involved in this work included Andrew Donohue, Michelle Farrugia, John Feutrill and Thao Nguyen, along with many others. Working with our molecular modellers along with talented structural biologists at Monash University (Professor Jamie Rossjohn, Isabel Lucet and Onisha Patel), we built a deep understanding of the ATP-binding site of JAK2 – the pocket in which our drugs bind to out-compete ATP and thereby stop the enzyme working. With these insights, we designed a series of potent JAK inhibitors and ran these through a battery of enzyme and cellular assays, as well as testing for selectivity, assessing pharmacokinetics and adsorption, distribution, metabolism and excretion (ADME), and undertaking preliminary safety profiling. From this work, CYT387 (momelotinib) emerged as the most promising compound: not necessarily the most potent or active in individual assays, but the best across all assays and studies. Importantly, CYT387 was active in cellular assays using cells derived from myelofibrosis patients, and in a genetic mouse model of myeloproliferative neoplasms. Armed with this combined dataset, we chose the compound as a development candidate and patented it in 2007. Formal preclinical studies began in 2008 under the leadership of Gregg Smith and in 2009 the first clinical trial began at the Mayo Clinic in the US, under the guidance of Professor Ayalew Tefferi, a world leader in myeloproliferative neoplasms.

Momelotinib leaves the country

In 2009, the global financial crisis was in full swing and Cytopia was unable to continue to fund the development programs underway. First the research team were let go, and within a year the company was sold to Canadian drug developer YM BioSciences for US$14 million.

The team at YM quickly realised the quality of the JAK2 program and continued to fund its development, generating exciting phase 2 data that resulted in the company's acquisition by Gilead BioSciences in 2012. Gilead purchased YM, solely for the JAK2 program and momelotinib in particular, for US$510 million. Clearly, two years and solid data can add a lot of value to a drug program!

Gilead initiated a phase 3 study, called the SIMPLIFY study, comparing momelotinib to the comparator JAK2 inhibitor ruxolitinib, a drug developed contemporaneously by the US biotech Incyte. The trial headline data reported in 2016, that there was little difference in the drugs with respect to spleen size reduction, was not sufficient in Gilead's eyes to warrant further development and they shelved the program. This was in spite of data showing that momelotinib-treated patients with disease-related anaemia had very profound responses, showing significantly improved iron levels and better patient outcomes. This could have been the end of momelotinib had it not been for the team from YM, now working for a new US biotech called Sierra Oncology. They negotiated a deal to purchase the compound from Gilead and planned a new phase 3 trial, working closely with the US FDA. That trial, the MOMENTUM trial, read out in 2021 and clearly demonstrated the efficacy of the drug in terms of spleen reduction, improvement in constitutional symptoms and importantly reversal of anaemia.

In April 2022, GSK purchased Sierra Oncology for US$1.9 billion, ostensibly for momelotinib, and then went about filing the New Drug Application with the FDA. The approval in September 2023 represents the final step in this long journey. Now to observe the drug's fortunes as a medicine approved 'to treat adults with certain types of myelofibrosis (MF) who have anemia'.

Chris Burns FRACI CChem has a PhD in Chemistry from the University of Melbourne, and after a postdoctoral position at Penn State University, USA, began his career at Pfizer UK. He has worked at several biotech start-ups in Australia, and is currently CEO at Amplia Therapeutics, a drug development company based in Melbourne.

Citizen science to unearth next-gen microbial friends

In early 2020, the University of Queensland's Institute for Molecular Bioscience launched Soils for Science (S4S), a national citizen science initiative inviting the public to share soil samples from their backyards. From these, we planned to isolate microbes to develop next-generation antibiotics and other life-saving drugs.

The timing of our launch at the start of a global pandemic was challenging, but not as inopportune as we first feared. It worked in our favour that the general public was rapidly acquiring an appreciation of the many threats of infectious viral disease and a thirst to know more about research and innovation that promised solutions.

As the pandemic progressed, there was much relief at the arrival of effective mRNA vaccines and comfort in the knowledge we were all safe again, right? Although the pandemic was winding back, momentum towards another global infectious catastrophe, which had begun decades before, was quietly building.

With a complacency born of a lifetime of ready access to a seeming endless array of reliable antibiotics, most of us view microbial infection as little more than an inconvenience. We expect that a short GP consult and a script (or sometimes a hospital stay to receive 'better' antibiotics) will do the job. A few decades ago, these were realistic expectations – but no longer.

When we use antibiotics to treat microbial (bacterial and fungal) infection, we inevitably select in favour of the survival of the very small subpopulation of microbes that are resistant to these antibiotics. With continued exposure to antibiotics, many microbes become resistant to many and even all known antibiotics.

If we liken COVID to a high-speed healthcare car crash, antimicrobial resistance (AMR) is a train wreck in the making – slower but potentially far more devastating. Informed analysts predict that, without urgent action, annual deaths from AMR infections will rise to 10 million by 2050, and continue to rise year on year thereafter – dwarfing the impact of the COVID pandemic.

Since the discovery of the β-lactam antibiotics (penicillins) from fungi of the genus *Penicillium* early last century, virtually all commercial antibiotic classes either are or are inspired by the defensive natural products produced by microbes (e.g. cephalosporins, tetracyclines, aminoglycosides, erythromycins, glycopeptides, rifamycins, polymyxins, lipopeptides, polyene macrolides and more), more often than not soil microbes. This should come as no surprise, as microbes have benefited from billions of years of evolution to acquire natural chemical defences that help them survive and prosper in highly complex and competitive microbial communities.

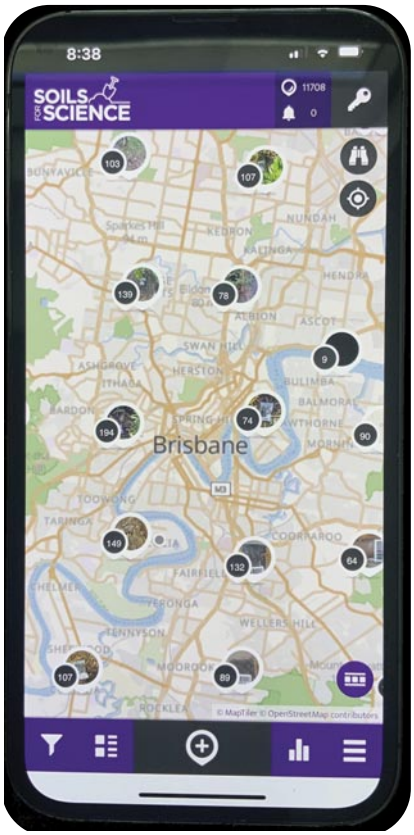
Turning to one microbe for a new antibiotic to fight other microbes is a classic example of the enemy of your enemy being your friend. To exploit this knowledge, we must figure out which handful of the countless millions of microbes in the global microbiome are our friends.

Over many years, my research group has explored the natural products from Australian marine and terrestrial biodiversity, with a particular focus on microbes (bacteria and fungi). In recent years, we have implemented exciting new advances in analytical technologies that have massively enhanced our capacity and capability, allowing us to more rapidly and cost effectively detect and prioritise new over known, and bioactive over non-bioactive natural products. While the traditional scale

of our microbial natural products research allowed the assembly and interrogation of libraries of a few thousand microbes, this new and improved capacity/capability could handle so much more – but to do this we needed to think outside the 'grant funding' box, and the confines of a single research lab.

Australian soil microbes represent an extraordinarily large and genetically diverse, sustainable natural resource, rich in unexplored chemical diversity that could fuel our research. Significantly, all the existing microbe-inspired commercial antibiotics had been discovered from microbes isolated from substrates (including soils) collected outside Australia. This encouraged the view that the Australian soil microbiome was a valuable and largely unexplored national asset, if only it could be accessed on a scale commensurate with its potential. So the problem became one of how to sample, with limited people and no travel budget, even a modest fraction of the soils of a continent as vast and environmentally diverse as Australia.

A potential answer came from our recent experience with the Cane Toad Challenge citizen science initiative, where we engaged the public, companies and local, state and federal authorities across Queensland, New South Wales, the Northern Territory and Western Australia, empowering them to trial a species-specific tadpole trapping technology to remove toxic cane toads from managed waterways. Thanks in part to citizen science, this cane toad control technology was successfully licenced and is being commercialised by Watergum (bit.ly/3QoZzi9). It was reasoned that, building on the knowledge gained running the Cane Toad Challenge, a new S4S citizen science initiative could inform the public about the threat of AMR, inspire the next generation to take up careers in STEM, demonstrate the benefits of university research, enlist the public to supply backyard soil samples from across Australia and enable assembly of a large library of Australian soil microbes.



As in any research, one of the early challenges was securing funding. We were very fortunate to benefit from generous philanthropic support, which in turn prompted internal support from the University of Queensland and the Institute for Molecular Bioscience. Several elements are critical to success:

- imb.uq.edu.au/soilsforscience has information on AMR and links to key S4S resources, including the option to request a free S4S Soil Kit.
- S4S Soil Kits are shipped free of charge and consist of a small trowel, barcoded soil bags, pre-paid return postage, and instructions (bit.ly/3QlQyGn).
- S4S participants register themselves in the free S4S app (spotteron.com/soilsforscience/auth/login), as well as each soil sample, to ensure they are geotagged and we have some details of the collection site.
- The interactive soilsforsciencegallery.org.au hosts and displays high-resolution digital images of all microbes recovered from individual soil samples, with the option to search against soil samples by barcodes, then zoom, pan and share images on social media.
- Dedicated video clips (such as bit.ly/3QiKP4d) were commissioned and shared, to support national and international print, broadcast and online media.

Public response to the S4S initiative has been humbling. To date, we have shipped more than 4500 S4S Soil Kits to all states across Australia and received more than 11 700 soil samples. Success has prompted an S4S Partners program to offer direct support to multiple schools and colleges, as well as an S4S Teacher-in-Residence to design primary/high school project resources that will dovetail into the science curriculum as of 2024. Along the way, we have been supported by multiple S4S Sponsors, who provide free/discounted services, and S4S Ambassadors, who expand our reach and message across multiple public events. More recently, we have received interest from Canada, Austria and the UK about how to set up parallel S4S initiatives.

So what of our goal to discover next-generation antibiotics? Further to our outreach, we have generated and cryopreserved more than 8000 microbial isolates and subjected their extracts to chemical and biological profiling – with some extremely promising results. The ongoing challenge is to secure sustainable funding to both continue and even expand S4S citizen science engagement, but also support in lab S4S research. S4S has already generated a microbial resource that exceeds our expectations, and will only continue to grow.

If you're an Australian natural products chemist looking for a collaboration, please feel free to get in touch. We are happy to share, and perhaps together we can apply the brakes to the AMR train.

Rob Capon FRACI CChem is Professorial Research Fellow and Group Leader in the University of Queensland, Institute for Molecular Bioscience, and Program Leader in the Marine Bioproducts CRC.

In-service programs for chemistry teachers – a lighthouse approach

For several years, the RACI (Vic) Chemistry Education Committee has run very successful professional learning days for Victorian chemistry teachers that are based on a unique 'formula'.

First, they are designed and run by the committee working in close collaboration with staff from a host university. Originally, they were hosted by Monash University. Since 2019, however, they have been hosted by RMIT University. This year, we were very honoured to work with Professor Sylvia Urban and Associate Professor Lathe Jones of the School of Science, RMIT University. Lathe is also the treasurer of our committee; the other committee members are all very experienced, dedicated chemistry teachers from different schools.

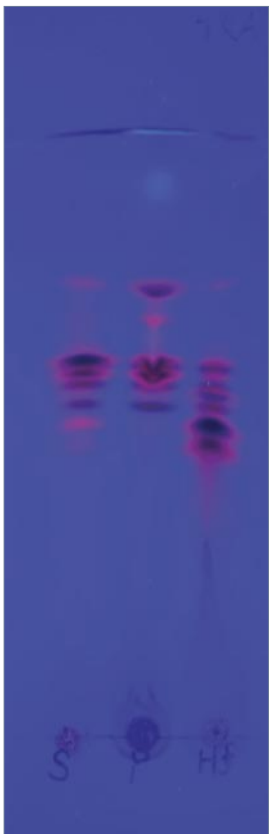
Second, our days feature hands-on experiments in the university laboratories. These experiments are designed and trialled by the committee members and academic staff, who work on them at their schools and at the host university over many months. Not only are our participants provided with a booklet of the experiments and teacher guides (printed in full colour), but after the day they are also sent copyright-free digital copies in Microsoft Word so they can adapt them for their schools.

We believe that practical investigations are integral to the study of chemistry and one of the main means by which students can be fascinated and excited about chemistry. For this reason, one of our key aims for the day is to inspire and enable the teachers to give their students the opportunity to undertake worthwhile, meaningful, hands-on laboratory investigations that not only meet the requirements of the latest Study Design, but also build up and extend students' science investigation and thinking skills and their understanding of the concepts involved.

Third, our days are based on a theme that is relevant to the Victorian Study Design, in an area for which teachers would benefit from extending their professional knowledge. This is often around a new area in a newly revised Study Design. This year, our theme was around the extraction, purification,

... practical investigations are integral to the study of chemistry and one of the main means by which students can be fascinated and excited about chemistry.

Left: The hydrodistillation apparatus used to demonstrate our first experiment: the extraction and analysis of oils from lemon myrtle leaves. Teachers can be seen in the background going off to the benches to perform their own hydrodistillations. In the follow-up session, they were provided with proton NMR, carbon-13 NMR, IR and GC-MS data for analysis. Two weeks earlier, Professor Urban and some of the RMIT lab and technical staff had performed the same hydrodistillation and performed instrumental analyses of the distillate to provide this data. Right: A TLC plate under UV light. In one experiment, teachers extracted and separated components of different plant materials using TLC plates and measured their R_f values.



> I really enjoyed the professional learning day; it was one of the best ones I've been to in a long time! I'm sure we will be able to incorporate these ideas into our teaching next year.

> We have managed to find our Quikfit apparatus from dusty old cupboards and have already trialled a distillation …

> We will be having a go with the students … And so today I acquired several lemon myrtle leaves from the garden centre.

> Thank you so much. It is wonderful to have such great support.

separation, testing and instrumental analysis of key components of Australian native plants, particularly antioxidants and oils.

The aim of this is to reinvigorate chemistry teaching by extending the teachers' knowledge of current research and practical applications in areas covered within the Study Design, so that they see the content in a wider context and appreciate its relevance and importance, which they can then pass on to their students.

This year, Professor Sylvia Urban of RMIT University gave an excellent, fascinating keynote address on the work her research group is doing on extracting, isolating and analysing useful compounds from Australian plants and marine invertebrates. This topic is now part of the new VCE Chemistry Study Design for both Years 11 and 12.

Fourth, our days feature a workshop with the Curriculum Manager, Science, of the Victorian Curriculum and Assessment Authority, Maria James. In these sessions, teachers can discuss various queries that they may have with regard to delivering the Study Design and meeting its school assessment requirements.

Fifth, we ensure that we provide a variety of excellent food for breakfast, morning tea and lunch, as well as tea and coffee all day. Many of our teachers travel from distant regional areas from very early hours in the morning. All the teachers really appreciate such good catering, which also takes into account all their various dietary requirements (which we ask about on their applications). These are times when the teachers can network.

Finally, at the end of the day, teachers are provided with attendance certificates signed by RACI that they can give to the Victorian Institute of Teaching to prove they have participated in seven hours of formal professional learning. (Teachers are required to participate in a number of hours of professional learning to maintain their teacher registration.)

We are committed to providing our professional learning at the lowest possible cost so that teachers at schools that are classified as disadvantaged can also attend. For this reason, each of us gives our time at no charge. And we are most grateful to the School of Science at RMIT University for sponsoring our event, including offering their facilities at no charge. This year, participants were only charged $100.

How successful was our 2023 event?

The RMIT laboratories were able to cater for 48 participants. We not only filled them but also had a waiting list, which showed we were meeting a real need.

Feedback was very positive, as the quotes above show.

Advice for groups wishing to run similar events

As far as we know, no other chemistry education groups or other organisations that run professional development events for chemistry teachers offer such a complete program. The usual model involves lectures and discussions but does not offer the experience of trying out new experiments that match the Study Design or curriculum, or providing copyright-free digital copies of the experiments afterwards, or very generous catering, all at an accessible price.

We believe that the following also helped make a difference:

- Our personal touch before, during and after the event. This included sending participants individual welcome emails before the event that also told them what they would be provided with, what they needed to bring, how to find us (with a photo), transport information etc.
- Our tight, well-organised program
- Our collaboration and teamwork in delivering the program
- The outstanding contributions of Sylvia Urban and Lathe Jones in planning and running the day
- The central location of the venue – the City Campus of RMIT University

We encourage other providers to consider our very different and very beneficial model – it is a lighthouse approach that others are welcome to follow. We are very happy to provide further information to other chemistry education groups should they wish to run a similar event.

For copies of our program and the three experiments we ran this year, and information about our past years, contact jennysharwood@aussiebroadband.com.au.

Jenny Sharwood OAM is a chemistry educator and author of many chemistry and science resources, including writing RACI Years 11 and 12 International Chemistry Quiz papers for several years. She wrote this article on behalf of RACI (Vic) Chemistry Education Committee and the School of Science, RMIT University.

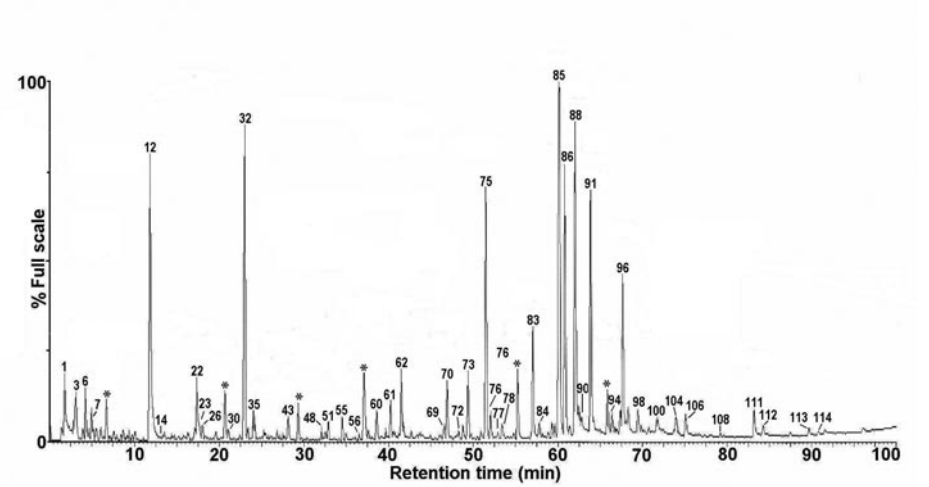
The Bengal tiger (*Panthera tigris tigris*).
Soumabrata Moulick/iStockphoto

Volatiles in your wine bouquet are also big in tiger territory

Chemistry plays a pivotal role in innumerable research fields, including those related to volatile compounds found throughout nature. One example is in unravelling the mechanisms by which animals communicate through semiochemicals, a term that originates from the Greek word *semeon*, which means 'signal' or 'to sign'. This encompasses chemical signalling molecules that have evolved for members of the same species or different species to communicate with one another, eliciting a specific behaviour in the receiver. Such signalling molecules can act as pheromones (semiochemicals) associated with sex, territory, recognition, food trail, aggregation, alarm and many others. Pheromones have been used for many decades to manage and control insect pests, but they also play an important role in many mammalian species.

The study of territorial marking fluid pheromones in big cats, such as tigers and leopards, has provided information that may aid in their conservation. Tigers use many different forms of communication, including sound and visual cues, but because they are mostly nocturnal and solitary creatures, they also use semiochemical communication. Urine mixed with scent gland secretion and faeces are the main vectors of these semiochemical messages, sprayed or marked on conspicuous objects. This is an effective way to communicate how recently a tiger has passed by, its gender and, in the case of a female, whether she is sexually receptive.

The Bengal tiger, *Panthera tigris tigris*, is a subspecies of tiger found throughout India and Indochina. My previous research aimed to understand the chemical composition of Bengal tiger territorial marking fluid (Burger B.V., Viviers M.Z., Bekker J.P.I., Le Roux M., Fish N., Fourie W.B., Weibchen G. *J. Chem. Ecol.* 2008, vol. 34, pp. 659–71) by using gas chromatography–mass spectrometry (GC-MS). We found that the territorial marking fluid of male tigers consists of a urine fraction and a small quantity of lipid material. We identified a rich mixture of 98 volatile organic compounds (VOCs) (see chromatogram p. 39), mostly consisting of alcohols, aldehydes, ketones, unbranched acids, esters and lactones. The dominant contribution of a select few VOCs present in the headspace of the marking fluid suggested that these compounds may be important constituents of the semiochemical message. Interestingly, although the lipid fraction made up only a small portion of the total volume of the marking fluid, it contained the largest quantity of VOCs. This suggested that the lipid fraction may act as a controlled-release carrier for the semiochemicals present in the marking fluid. We recorded the tiger's behaviour when exposed to certain chemical constituents identified in the marking fluid. The γ-lactone (*S*)-(+)-(*Z*)-6-dodecen-4-olide appeared to be an important compound for territorial marking behaviour by the male tiger, which reacted strongly to this compound and displayed distinct marking



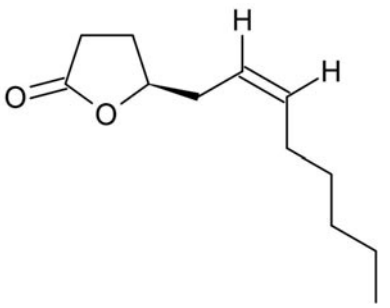
The total ion chromatogram obtained by GC-MS analysis of the volatile organic compounds collected with a sample enrichment probe at 40 °C from 46.67 grams of the urine fraction of the territorial marking fluid of the Bengal tiger.

Reused with permission from Burger B.V., Viviers M.Z., Bekker J.P.I., Le Roux M., Fish N., Fourie W.B., Weibchen G. *J. Chem. Ecol.* 2008, vol. 34, pp. 659–71. Springer-Nature.

behaviour. This knowledge could be used in tiger conservation programs to improve the monitoring of numbers in the wild. By installing counting stations that display synthetic pheromones, tigers could be enticed to 'report' for counting and 'mark' over the synthetic pheromones.

Pheromone research and wine aroma and flavour research may seem worlds apart, but the same science can unravel the chemical information and analytical techniques used to elucidate tiger communication semiochemicals and key aroma and flavour characteristics of wine – many foods and beverages contain a diverse array of volatiles. By using GC-MS-based analytical techniques, we have come to recognise that most of the volatile chemical compounds identified in the territorial marking fluid of tigers are also present as volatile compounds in a wine's aromatic bouquet. In fact, most of the hundreds of volatile aroma compounds identified in wine (including alcohols, aldehydes, ketones, esters, terpenes, norisoprenoids, phenols and lactones), in concentrations ranging from a few nanograms to hundreds of milligrams per litre, have also been identified in tiger marking fluid.

... most of the volatile chemical compounds identified in the territorial marking fluid of tigers are also present as volatile compounds in a wine's aromatic bouquet.



The lactone (*S*)-(+)-(*Z*)-6-dodecen-4-olide is an important component in tiger marking fluid. Similar lactones are also implicated in wine stone fruit aroma.

Interestingly, lactones important for tiger marking fluid are also implicated in wine stone fruit aroma (see June–August issue, p. 40). Lactones such as γ-nonalactone have been found to be important for the stone fruit aroma of botrytis Semillon wine (Siebert T.E., Barter S.R., de Barros Lopes M.A., Herderich M.J., Francis L. *Food Chem.* 2018, vol. 256, pp. 286–96). Such is the natural world of volatiles, lactones are not unique to tigers and wine, but are also important for the sensory characters of fresh stone fruit such as peaches and apricots.

Many natural products, such as those in tiger urine and wine, contain the same volatile aroma compounds, but it is their concentrations and interactions with other compounds in a given matrix that is important. Volatile composition determines the final sensory impact and unique aroma that each natural product will have, and that applies to a multitude of wine styles or Bengal tiger semiochemicals.

Marlize Bekker is a senior lecturer in food chemistry at the School of Agriculture and Food Sustainability, University of Queensland.

Hanging up the lab coat

How do you make a career change after a spending most of your life ensconced in chemistry? To get some insight, we recently debriefed with a member of our War on Wasted Talent community of experienced professionals, a senior chemist who has transitioned into a role in the intelligence sector. That's a bit different!

On the surface, this may sound like rather an unusual career change. But the lessons learnt would apply to most career transitions as a mature-age professional. Here, we outline the process and mindset that worked so effectively for our chemistry colleague.

Working as a chemist, you don't appreciate the many skills you have, but those skills have really come to the fore for me now.

1. Provide a different lens through which people can view you and you can view yourself.

- Ask yourself the big questions – who am I and what can I do? This takes some deep reflection to move beyond your identity as a chemist.
- Stop and think about what else you can do and really understand your transferable skills. In particular, think about your motivated skills – the ones you most want to use in a new role.
- Revise your CV and develop a 120-word summary to describe yourself – key skills, achievements, values and aspirations – the essence of you. It takes discipline but is worth it.

2. Deal head-on with thoughts of ageism. Don't engage in mind-reading by assuming you know what others are thinking.

- Negative stereotypes can play on your mind, such as 'The organisation won't be comfortable with me – they'll think I won't take instruction' or 'They'll dismiss me as an older person who wants to work in the way I've always been accustomed to.'
- While most mature-age professionals don't believe these stereotypes apply to them personally, these common misconceptions can still erode their confidence.
- Don't succumb to these negative thought patterns and instead accept that most people are less judgemental or preoccupied with your age than you think.
- If an employer is ageist, would you want to work there anyway?

3. Frame your experience.

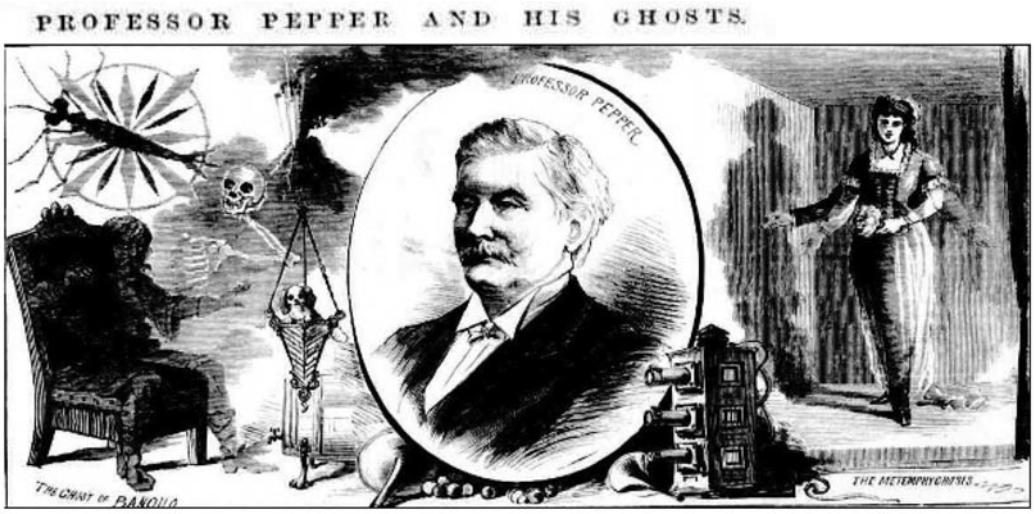
- One of the great advantages of age is experience.
- When making a career transition into a new field or sector, it follows that your breadth of experience is likely to be more of a selling point than your depth of experience in a relatively narrow field.
- Experience is not enough on its own. It needs to be tempered with a healthy dose of humility. An over-reliance on your experience as a selling point in a career transition can come across as complacent.
- Jobs are changing all the time and employers want to see a willingness to adapt and learn new skills. They want to see what you can do in the future, not just what you have done in the past.
- Both your application and interview should reflect this future-orientation. Always have examples on hand of where you have demonstrated an openness to change.

There is an underlying theme here. Although you can't single-handedly change ageist attitudes in the workplace, when you approach career change with positivity, dig deep into your whole self and think of your age as an advantage, this is what tends to define the whole transition process. Your optimism and sense of self will shine through.

So, what's life like in the new job for our chemist career-changer? Well, he describes it as 'drinking from the firehose' as he learns a whole new language. Although he came to this new role with very little knowledge of the subject, he believes he has made a meaningful contribution in a relatively short time. In doing so, he has drawn on his transferable skills of critical thinking, asking questions, collating information and writing. He says, 'You do these naturally as a scientist, from the time you get out of bed in the morning. Working as a chemist, you don't appreciate the many skills you have, but those skills have really come to the fore for me now'.

Dr Barbara Cosson and **Dr Janine Pickering** are co-founders of War on Wasted Talent (www.waronwastedtalent.com.au), a social enterprise providing career transition services for mature age professionals.

Pepper's ghost



A cartoon of Professor Pepper, *Illustrated Australian News*, Saturday 2 August 1879, p. 116.

It's not often that my interest in the history of chemistry, usually with an Australian flavour, coincides with my interest in the history of the area where I grew up and where I have been back living since 1995. One link between the two is a certain Professor Pepper, who is described in Wikipedia as 'a scientific all-rounder who was both an effective public educator in science and an astute, publicity-conscious, commercial showman'. Newspapers concentrating on the last of these referred to him as an illusionist. The illusion he created on stage was described as 'Pepper's Ghost'.

Thanks to the National Library of Australia's Trove, I have been able for some years to search the digitised version of a local paper, the *Williamstown Chronicle*, where I found an advertisement for Pepper's talk on 'Light and Optics', to be delivered at several venues, one of which, 'Mr. Ulbrick's State School', was in fact the North Williamstown Primary School where I learnt my 3Rs in the 1940s. Ulbrick (actually J.F.C. Ulbrich) was the first headmaster at the school, which had opened in 1874, not long after primary education became free and compulsory in the colony under the *Education Act 1872*.

Pepper and his family, along with a team of assistants and more than 30 tons of scientific and exhibitory apparatus, arrived in Melbourne in mid-1879. His formal engagement was to lecture in every one of Victoria's state schools and he offered a range of topics that included the electric light, spectrum analysis, musical notes rendered visible, Darwinian theory, telephones and so on. His 'ghost' involved the projection of images from an adjacent room onto a glass screen so the subjects appeared to be in the lecture room. It was a popular phenomenon in London and it featured in many of his lectures, especially those we could describe as 'magic shows'. By the time he hit Melbourne, the ghost's appearances had become gentrified to include 'dioramic views', which, in one Melbourne performance, featured views of Afghanistan and the Afghan war. Newspaper coverage, however, preferred skeletons and the images of long-dead people, as can be seen in the cartoon from the *Illustrated Australian News* shown here.

John Henry Pepper, born in London in 1821, really was a chemist. He had been employed at London's Royal Polytechnic, where he combined serious chemistry with public entertainment. A conflict between these two roles caused a rift between him and management that he resolved by removing to the Australian colonies. After his lecture tours of Victoria, South Australia and New South Wales, he settled in Brisbane, where his lectures continued and he was established as a consulting analytical chemist and teacher at the School of Arts. As happened with his old employer, his new employer was also unhappy with the way he managed his several roles, so once again he resolved the issue by changing continents in 1889, returning to England, where he died in 1900.

An Australian chemist described Pepper as 'an extrovert who didn't take kindly to authoritarian rule'. This was Reg Cane (1917–92), whose article 'John H. Pepper – analyst and rainmaker' was published in the *Journal of the Royal Historical Society of Queensland* (1974–5, vol. 9(6), pp. 116–33). Like so much of our literature, it's hiding behind a paywall where even ChatGPT can't find it. Various libraries hold the journal and I wonder if the Society might be prepared to help any eager reader who can't access them but has a yen to read more about Pepper.

Melbourne-based readers can see a good selection of Pepper's many books in the State Library of Victoria. In researching this Letter, I found that Cane had had an interesting career that I will summarise in what space is left to me. (This magazine's editor, Sally Woollett, would appreciate this problem that besets writers and editors!) A graduate of the University of Tasmania, and foundation member of the ACI branch there, Cane worked at the Glen Davis shale oil works during World War 2, then with General Motors for a few years and ICI Australia (1947–63). He returned to the University of Tasmania in 1968 but then took up a senior appointment at the Queensland Institute of Technology. In 1977, he retired and returned to his native Tasmania but remained active as an expert on applications of chemistry to industry.

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*.

sudoku

Difficulty rating: medium.
The symbols for nine 'P' elements are used. Your challenge is to complete the grid so that each 3 × 3 box as well as each column and each row contains all nine of these elements.

	Pa		K	Pb			P	
	Pb		Pr	Pd				
				P				Po
	P	Po					K	Pr
Pd	Pr						Po	Pu
Pu	K					Pb	Pt	
Pa				Pt				
				Pr	Pb		Pd	
	Po			K	Pa		Pr	

events

Find out more at raci.org.au/events

Mentoring Program 2023 end of year wrap-up
7 December 2023, webinar

SA RACI Physical, Polymer and Materials Chemistry Symposium
11 December 2023, Adelaide Health and Medical Sciences Building, Adelaide, SA

Supramol24
1–2 February 2024, University of New South Wales, Sydney, NSW

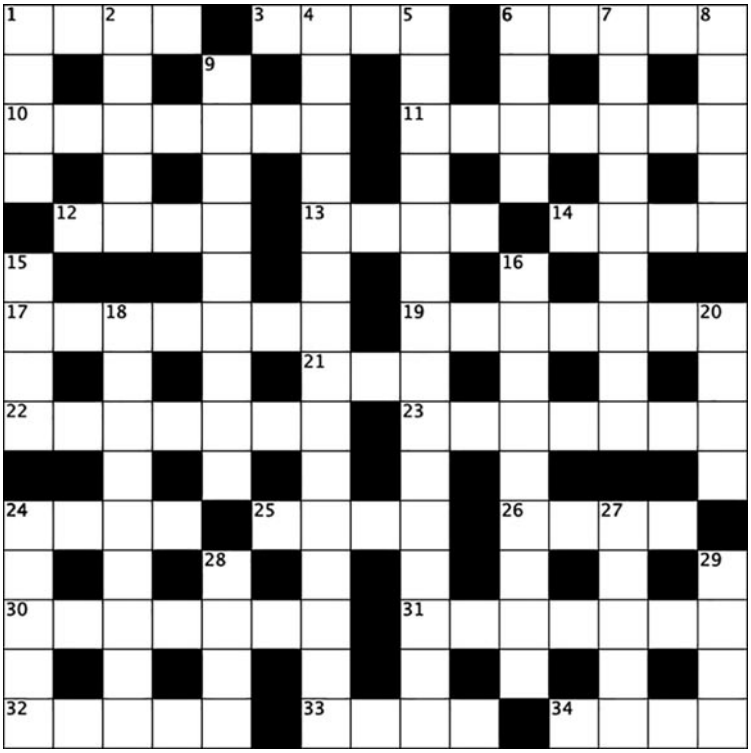
Australian Rare Earths Meeting 2024
9 February 2024, Curtin University, Perth, WA

Understanding AS 2243.2 Chemical Aspects and Storage
13 February 2024, webinar

Physical Chemistry Division Conference and Hush Symposium
1–4 July 2024, University of Sydney, Sydney, NSW

24th Australasian Electrochemistry Symposium
5–6 December 2024, La Trobe University, Melbourne, Vic.

cryptic chemistry



Across

1 Regular participants in the comeback when Mendeleyev paid Humphry. (4)
3 Even neoprene is used for fencing. (4)
6 Believes bears. (5)
10 All 15 Down make R_3SiOH. (7)
11 Reply 42 comes out as long and repetitive. (7)
12 Ends interest rate futures contract used in 5 Down. (4)
13 Heads or tails in class. (4)
14 Starts to heat up sulfur in the way indicated. (4)
17 Four elements related to movement of a solvent across a semipermeable membrane. (7)
19 Came across boxes used in 5 Down. (7)
21 Signal clue missing something. (3)
22 Withdraw from the start without advantage. (7)
23 It's not nothing nor, zone out! (7)
24 A technique off. (4)
25 Start up relevant equipment arrangement for carbamide. (4)
26 Seconds carbon dioxide emissions aspirational objectives. (4)
30 Nobel Prize recipient was told to change. (7)
31 Catalogues 5360 flames. (7)
32 Presents fellow over in that Nashville music festival. (5)
33 Two elements of a mathematical function. (4)
34 & 2 Down Saved dual work which increases the selling price of the product. (4,5)

Down

1 Where in the world is carbon contained? It might be a record. (4)
2 See 34 Across.
4 Natural 11 Acrosses broadcast representatives dismiss a set of vehicle trips. (15)
5 Main pioneer text which changed what we do. (15)
6 Separates primary Haber process life cycle. (1.1.1.1)
7 First and last latency speed bump in the adaptive immune system. (5,4)
8 Arranges 13 Across and 16. (5)
9 Research body set up. (9)
15 Four elements of little ones. (4)
16 Values bases for comparison. (9)
18 Carpet man used thiol. (9)
20 Moderate hold up. (4)
24 Little ones grab cat in a second. (5)
27 Central holding of xenon hybrid. (5)
28 Upcoming heat advisory inclusion obtained from 5 Down. (4)
29 Applications of three elements. (4)

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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Image: Hutt Lagoon is a striking pink marine lake on Western Australia's coral coast, about an hour's drive north of Geraldton.