

# chemistry

July 2016

in Australia

## Flavours and fragrances:

using pharma  
methods to  
sniff for  
substitutes

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- Inside the National Innovation and Science Agenda
- Lodgement season for the Export Market and Development Grant
- Chernobyl and caesium, 30 years on

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### cover story

#### Flavours, fragrances and force fields

Computational methods that analyse how drugs interact with protein targets are also effective for flavour and fragrance molecules.

On the cover: Flowers of *Crocus sativus*; the crimson stigmas when dried are known as saffron. Picrocrocin and safranal are responsible for saffron's flavour and fragrance.

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## Thirty years in the life of Chernobyl caesium

Early on 28 April 1986, alarms sounded as an employee of the Forsmark nuclear power plant in Sweden set off a radiation detector on his way back from the bathroom. Radioactive particles on his shoes were soon identified as being Soviet ([bit.ly/1rfZwYi](http://bit.ly/1rfZwYi)). The fuel used and the operation and design of a nuclear reactor partly determine the radioactive nuclides produced – a signature of the power plant of origin. Soviet authorities had no choice to announce, two days after the event, the disaster at the Chernobyl plant in the Ukraine.

The Chernobyl disaster is now 30 years behind us, and during those years the radioactivity attributable to caesium-137 has decayed to half of its original level. Caesium-137 is a troublesome fission product because caesium's most common

chemical compounds are salts, which can move easily through natural environments. Being an emitter of gamma rays, caesium-137 is convenient for mobile detection.

In September 2014, a sample of reindeer from Jotunheimen in southern Norway was found to contain a surprising 8200 Bq/kg of caesium-137. Levels in that region two years before had been as low as 1500 Bq/kg. (The regulatory limit in Norway for caesium-137 in reindeer meat is 3000 Bq/kg.) So why the increase with time? Lavrans Skuterud of the Norwegian Radiation Protection Authority (NRPA) thinks that a long and bountiful season for mushrooms, of which reindeer are very fond, may be the answer ([bit.ly/1rPzNqq](http://bit.ly/1rPzNqq)).

Species such as the gypsy mushroom (*Cortinarius caperatus*) are effective accumulators of caesium-137, and they're a popular food for people as well as reindeer. Scandinavian authorities recommend that residents limit their intake of *C. caperatus*. Mushrooms have been suggested as a way to remediate radiation-contaminated sites, although the economics of such work throws their feasibility into question.

Regulatory thresholds for radionuclides vary significantly between countries and have been revisited worldwide since the Fukushima Daiichi nuclear accident in Japan in 2011.



Reindeer (*Rangifer tarandus*) in the Kebnekaise valley, Lapland, Sweden. Reindeer herding is a predominant livelihood for the Sami (also known as Laplanders), indigenous people who inhabit northern Norway, Sweden, Finland and Russia. [Alexandre Buisse/CC-BY-SA-3.0](http://AlexandreBuisse/CC-BY-SA-3.0)

Thresholds in any country must account for the frequency of consumption of different foodstuffs by residents. Scandinavian authorities also consider the impact of thresholds on indigenous peoples such as the Sami – these people consume more reindeer meat and they make a living by reindeer herding, including selling meat. The NRPA has been testing radioactive caesium levels in reindeer herders since the 1960s.

Location and weather conditions (e.g. elevation, snow, rain and wind) during nuclear tests and accidents affect the distribution of radioactive fallout. Reindeer delicacies such as mosses and lichen have been tested as biomonitors in order to create a regional map of fallout from Chernobyl in Norway ([bit.ly/1rFTBCu](http://bit.ly/1rFTBCu)).

And what of the people of Chernobyl? Despite the exclusion zone restrictions within 30 kilometres of the ill-fated Reactor 4, it seems people have to return to their homes, catching local fish and harvesting mushrooms.



Sally Woollett ([editor@raci.org.au](mailto:editor@raci.org.au))

## Science denial

I felt a frisson of fear when I read John Cook's description of psychological experiments on political conservatives (May issue, p. 6). I was reminded of men of science of another era, who conducted experiments on those deemed to be defective members of society. I am not suggesting that the experiments John Cook describes had the same intent as those earlier horrific crimes, but I am concerned when the impression is given that those who hold opinions different from those of an elite are in need of re-education. There is also the fear that applying labels to those who hold different views is an effort to change the way language is used. We are already seeing universities mandate the use of various words when discussing various contentious subjects. Perhaps, to borrow a word from George Orwell's Newspeak vocabulary, it will be a 'thoughtcrime' to even consider alternative points of view not approved by an elite.

I am concerned that John Cook confines his model of denying science to conservatives and denial of climate science. There are of course other important examples. The denial of the theory of evolution as proposed by Darwin and built on successively since pre-dates the climate change controversy by more than a century. On the 'progressive' side of politics, the Greens have made implacable opposition to the nuclear generation of electricity an article of faith, in spite of the advances in technology that make it a safe, non-carbon emitting solution to the use of fossil fuels. It is also part of their ideology that genetic manipulation of crops to reduce pesticide use and improve yield is evil. There are other beliefs that involve denials of science, such as anti-vaccination, biodynamic farming, the superiority of 'organic' foods, the fluoridation of the water supply and perhaps even the use of aluminium utensils in cooking. A more holistic approach might have made for a more credible argument.

I also have a concern as to a 'cookie cutter' approach in the intimation that all conservatives are climate change deniers. Firstly, the term 'conservative' can be regarded as a very broad descriptor, varying according to culture and country, and capable of many shades and nuances. For instance, it is quite possible for a person to be conservative in the belief that largely unfettered free enterprise and free markets offer the

best routes to human prosperity, be an atheist, and admit that the climate is warming after the last Little Ice Age, but have some reservations as to the extent to which humans have had an impact. Such a person may also consider that while science has brought us inestimable benefits, scientists don't always get it right all the time. Further, those who would describe themselves as 'progressive' may well express a range of views on various subjects and not necessarily ascribe to a monolithic set of beliefs.

There is also a danger that by concentrating solely on the subject of climate change denial, the impression could be gained that motives other than pure altruism may be at work. Most of the large number of scientists active in this area are funded from the public purse in one way or another. It is clear that government policy can have an impact on available funds and hence employment prospects, and those affected will behave as would any other when their job is at stake; that is, with great energy and fervour.

Tom Smith FRACI CChem

There are a number of common misconceptions about psychology and psychological research, some of which are found in Tom Smith's comment on my letter to *Chemistry in Australia* (May, p. 6).

Psychology is probabilistic, not deterministic. Many studies into how people think about climate change have observed that political conservatives are more likely to reject climate science than independents or liberals. But note the term 'more likely'. Psychology doesn't make deterministic claims such as 'all conservatives are climate change deniers', as Tom characterises. Rather, political ideology makes it more likely for a person to lean a certain way but by no means certain. That's why in my previous letter, I used phrases such as 'strongest predictor' and 'more likely to reject' to characterise the relationship between climate science denial and political ideology.

Because of the probabilistic nature of psychology, it's absolutely possible for a political conservative to accept the many lines of empirical evidence that humans are causing most of global warming. It's just harder than for someone whose beliefs aren't threatened by the scientific evidence. If your ideology predisposes you to oppose regulation of the fossil fuel

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industry, then you are more likely to deny that there is a problem that needs regulating.

Tom also makes the important point that science denial isn't restricted to climate change. There is evolution denial, anti-vaccination and GMO science denial. What typically unites these diverse forms of denial is that the implications of the science are perceived to conflict with a person's belief system. For example, evolution science is perceived to conflict with religious belief. However, to reinforce the earlier point against determinism, there are a number of religious believers who accept evolution science.

What also binds these different forms of science denial are the five characteristics of science denial (Diethelm P., McKee M. *Eur. J. Public Health*, vol. 19(1), pp. 2-4). These characteristics, remembered with the acronym FLICC, are Fake experts, Logical fallacies, Impossible expectations, Cherry picking and Conspiracy theories. Diethelm and McKee observed that FLICC occurs across all these different forms of science denial.

Understanding the techniques of science denial is key to neutralising the influence of misinformation. For this reason, I concur with Tom that we should avoid the use of labels, and instead direct our focus on the techniques and fallacies used to distort the science.

For example, a commonly encountered claim that Tom repeats is the conspiracy theory that climate scientists are motivated by publicly funded money rather than scientific discovery. However, in my own research (Cook J., Nuccitelli D., Green S.A., Richardson M., Winkler B., Painting R., Way R., Jacobs P., Skuce A. Quantifying the consensus on anthropogenic global warming in the scientific literature. *Environ. Res. Lett.*, 2013, vol. 8(2), 024024), we observed that 97% of relevant climate papers affirmed the consensus that humans are causing global warming. Included in this consensus were over 10 000 scientists from countries all over the world publishing scientific papers affirming human-caused global warming. These were scientists from countries with liberal or conservative governments. The scientific papers were published over a 21-year period, with the scientific consensus among US scientists just as strong during the Bush administration as it was during the Obama and Clinton administrations.

This disproves the conspiracy theory that government policy is driving the scientific consensus on climate change. The notion of thousands of scientists all over the world colluding to falsify a consensus is less plausible than the notion that the Moon landing was falsified in a government conspiracy.

John Cook

## PerkinElmer IR microscopy: Where everything's routine – except the results



Microplastics pollution is a topic of increasing concern to society. The term 'micro plastics' is used to describe small synthetic plastic particle with an upper size limit of 5mm.

Recent concerns are the introduction of new cosmetic products, such as facial scrubs, toothpastes, and shower gels, currently containing microplastic beads as abrasive materials. These microplastics typically sub-millimetre in size, get washed down the sink and are too small to be filtered by sewage treatment plants hence ending up in the river systems and ultimately in the oceans. These microplastics can be ingested by marine organisms and fish and end up in the human food chain.

While these pollutants are now known to enter aquatic environments via waste water treatment facilities, the abundance of microplastics in these matrices are only now been investigated. Emerging methods now using Infrared (IR) spectroscopy is the established technique for identifying polymer materials and has been used extensively for identifying large (over 100 micrometer) polymer materials. For microplastics, down to a few micrometers in size, an IR microscope can be used for the detection and identification of these materials.

PerkinElmer offer FTIR, microscope and autoimage ATR which can be used for the detection and identification of these microplastics. Our unique UATR delivers high quality and dependable results. The full automation of all microscope function means that focus adjustments, aperture and sample position are no longer necessary.

A commercially available facial scrub was tested using the Spotlight200i FTIR microscope system to identify the types of polymer present. The face scrub was mixed with hot water to dissolve soluble ingredients in the formulation. The resulting solution was filtered through a 50 micron mesh, capturing any insoluble components greater than 50 micron in size. The filter was then allowed to air dry prior to FTIR microscopy measurements - by both transmission and reflectance.

A "Visible Image Survey" was collected of the collected microplastics are shown in Figures 1a. "Analyze Image" function, an intelligent automated routine in the Spectrum 10 software detects particles present in the visible image and mark them as regions of interest automatically (Figure 2). It then calculate the maximum rectangular aperture size that can fit wholly inside each of the particles to maximize signal-to-noise. Clicking "ScanAnalyse Markers" initiates the collection of spectra for each particle, displaying sample spectra during data collection, and processing the spectra automatically using software routines such as Libraries Search in real time.

Figure 3 is a zoomed-in area of the sample showing the aperture positions used to measure the spectra of the particles. Whilst the spectra of the particles are being collected, a Library Search process identifies the particles and color-coded each particle according to the identification. In this case, particles identified as polypropylene are color-coded yellow, and those identified as polyethylene are color-coded blue.

Intelligent region of interest (ROI) finding is perfect for analysis of multiple particles, contaminant specks, powder samples, and automated laminate layer analysis.

For the full article and results or to find out how PerkinElmer can assist in future microplastic research please go to:

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Fig 1a:

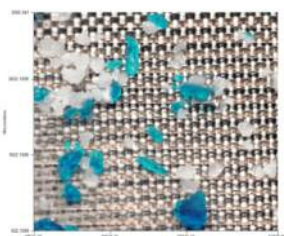


Fig 2:

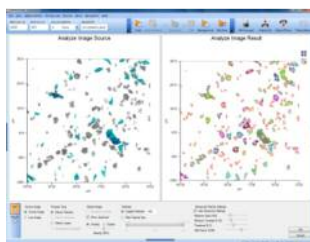
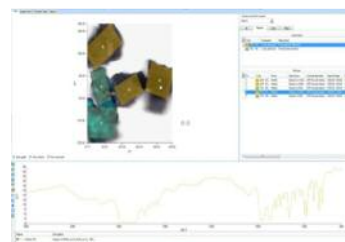


Fig 3.





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## Flying high with algae



A native freshwater algae grown in northern Australia can be used to create a high-quality, renewable jet fuel, an international research team has found.

The multidisciplinary team, which includes researchers from James Cook University, the University of Sydney and Israel's Ben Gurion University, has developed a proof-of-concept process to create high-quality renewable biofuel from the macroalgae *Oedogonium*, ready for blending with regular petrol, jet fuel and diesel.

Results for their collaborative work have been published online in *Energy & Environmental Science*.

Professor Rocky de Nys MRACI CChem from the Centre for Macroalgal Resources and Biotechnology at James Cook University led the group responsible for providing the project with the freshwater algae. He said the algae was grown under special conditions and tailor-made to fit the needs of the project.

'*Oedogonium* is a robust, non-invasive species that is highly productive and easily cultivated on a large scale. This makes the macroalgae an attractive source of biomass for further processing to create renewable fuels and chemicals.

'Its cultivation is highly efficient relative to harvesting of land-based plants and also avoids conflict for agricultural resources that might be diverted from food production.'

Joint leaders at the University of Sydney, Dr Thomas Maschmeyer FRACI CChem, Professor of Chemistry, and Professor Brian Haynes from the University's School of Chemical and Biomolecular Engineering worked with their teams to understand how to control the conversion of freshwater algae into a crude oil equivalent.

'A key problem associated with processing algae into liquid transportation fuel is the presence of nitrogen from algal proteins in the intermediate bio-crude oil, as the nitrogen poisons downstream catalysts required for further upgrading,' said Maschmeyer, who is also the Director of the Australian Institute for Nanoscale Science and Technology.

'However, the nitrogen content can, in fact, be controlled at multiple points in the production chain from biomass to high-grade fuel product.'

Explaining the process Haynes said:

'The low-nitrogen macroalgae are converted to bio-crude oil, which is combined with a synthetic fuel stream produced by catalytic conversion of waste CO<sub>2</sub>, resulting, after further processing, in a finished fuel blend.

'The process makes use of water at very high temperature and pressure to liquefy the algae and convert it into an energy-dense bio-crude oil.'

University of Sydney

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## Professionals Australia: 'Innovation at risk due to lack of science certainty'

Professionals Australia, the association representing science, technology and engineering professionals said the federal government needs to make sure science is funded with certainty, over the long term, or we risk our nation's future as an innovator.

'We currently have a bizarre situation in Australia where levels of investment in science are high but our best and most talented science graduates face job insecurity and ongoing funding uncertainty,' said Chris Walton, CEO of Professionals Australia.

'Scientists are in a funding merry-go-round, and there's always a review just around the corner. This Budget does nothing to fix the despondency in the sector following thousands of job cuts in government sector agencies like the CSIRO.'

The most recent Scientists Remuneration Survey by Professionals Australia found:

- 77.3% of scientists agreed or strongly agreed that cost-cutting was affecting their organisation's science capability
- 32.5% of scientists reported a decline in the number of professionals with science capabilities in management and decision-maker roles in their organisation
- a third of scientists reported being dissatisfied in their current role. Of those who said they were considering leaving their current job, 55.3% said a pay increase would alter their intention.

'The Government is good at talking the talk when it comes to creating a strong science and innovation agenda. This must be backed up with tangible actions to boost public-sector STEM skills and simplify funding for research and development,' said Walton.

'We commend the Government for fully funding the \$20 billion Medical Research Future Fund, representing a potential quantum leap forward for the industry. As part of our commitment to the sector, we must ensure we retain the staff we need by funding Medical Research Institutes sustainably.

'Prime Minister Turnbull envisages his \$1.1 billion National Science Innovation Agenda will drive a "culture of ideas and innovation". Experienced scientists and secure funding deliver real innovation,' said Walton.

Professionals Australia

## CONSUL 21, the intuitive choice in centrifuges

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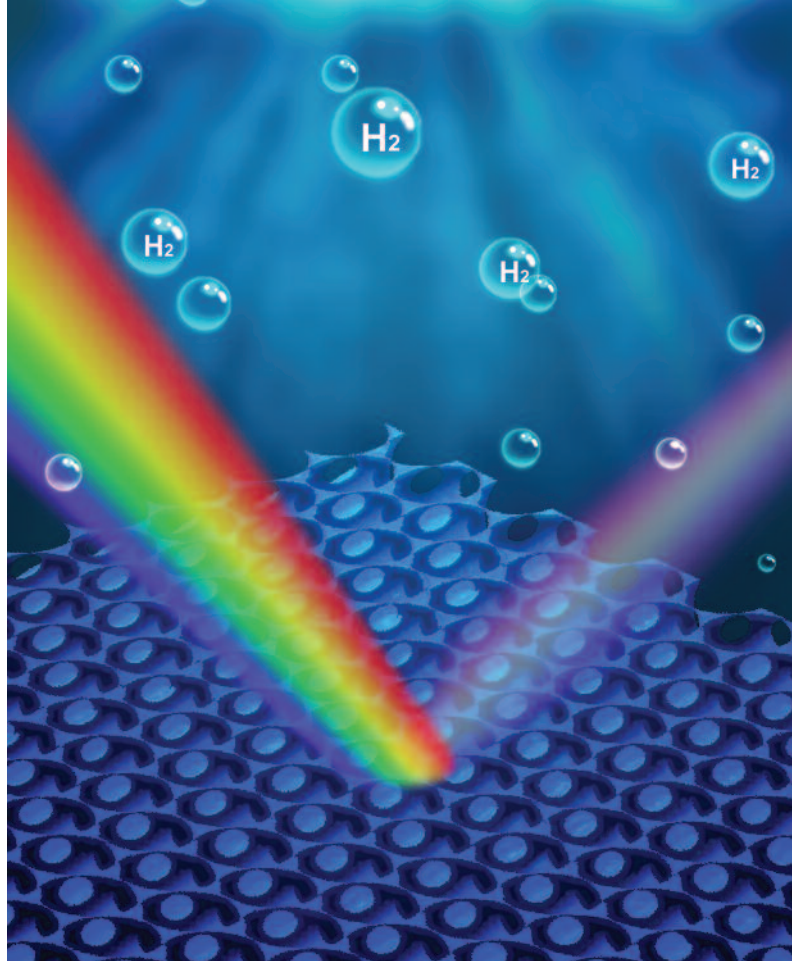
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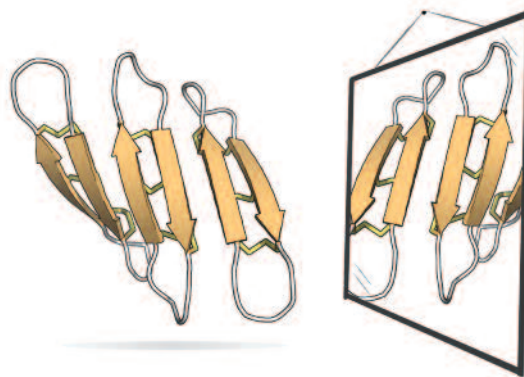
## Strongly coupled hybrid materials for enhanced solar fuel production

Photoelectrochemical (PEC) water splitting, which uses sunlight to produce hydrogen, is a clean, renewable and environmentally benign strategy for making fuels. Organic–inorganic hybrid materials are highly attractive in PEC applications for their favourable light trapping and absorption and fast charge separation and transfer. The research team of Professor Shizhang Qiao at the University of Adelaide, in collaboration with Associate Professor Tao Ling at Tianjin University, China, has taken significant steps in this area. They have strongly coupled Nafion molecules and ordered porous CdS networks for visible light PEC hydrogen evolution (Zheng X.L., Song J.P., Ling T., Hu Z.P., Yin P.F., Davey K., Du X.W., Qiao S.Z. *Adv. Mater.* 2016, doi: 10.1002/adma.201600437). Impressively, the organic Nafion molecules favorably shift the band positions of CdS and effectively suppress the formation of compensation defects in the semiconductor. Consequently, this hybrid photoelectrode achieves a remarkably high incident photon-to-current conversion efficiency (75%) under visible light illumination. It is expected that the effect of strong coupling between inorganic and organic materials will provide a new route to engineer photoelectrodes in water-splitting devices.



## Reflections of antimicrobial and amyloid peptides

Antimicrobial peptides have attracted significant interest because of their potential as next-generation therapeutics to combat the spread of drug-resistant bacteria. A team led by Professor David Craik and postdoctoral fellow Dr Conan Wang at the University of Queensland has explored the use of mirror-image peptides to determine the structures of  $\beta$ -sheet antimicrobial peptides (Wang C.K., King G.J., Conibear A.C., Ramos M.C., Chaousis S., Henriques S.T., Craik D.J. *J. Am. Chem. Soc.* 2016, **138**, 5706–13). A cyclic antimicrobial peptide from baboons called BTD-2 was crystallised by racemic crystallography, in which crystals were grown from a mixture containing the peptide and its synthetic mirror image. The structure revealed a supramolecular assembly that might



represent the active form of BTD-2 and also resembles a fibril-like assembly, providing an intriguing structural link to amyloid peptides. The potential of antimicrobial peptides as therapeutics is currently being further explored at the University of Queensland.

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



## Highlights of the July issue

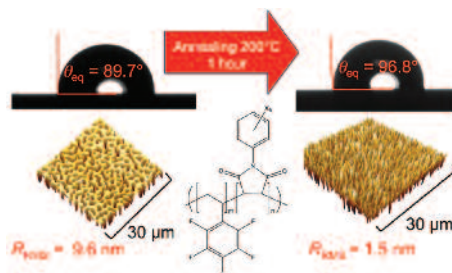
The 35th Australasian Polymer Symposium (APS) took place on the Gold Coast, Queensland, 12–15 July 2015, and encompassed three and a half days of stimulating talks from numerous areas of polymer science. There were 260 delegates from Australia and around the world in attendance, with six plenary speakers and 24 keynote speakers, five of whom were Early Career Researchers. Plenaries were from Professor Mitch Winnick from the University of Toronto, who talked about his work investigating metal-chelating polymers and their potential for biological applications of sensing and imaging. Professor Yanlei Yu from Fudan University, China, discussed the field of liquid crystal polymers: crystalline aromatic polyesters that form areas of highly ordered structures when in the liquid phase. Professor Bjorn T. Stokke from the Norwegian University of Science and Technology gave a plenary lecture on responsive polymer hydrogels. Professor Benjamin Hsiao from Stony Brook University, New York, demonstrated an example of translation of laboratory to industry with his work on nanofibrous membrane filters for high-flux water purification. Professor Werner Joseph Blau from Trinity College Dublin described his interdisciplinary work with materials science and physics in the development of nanocarbons and atomic crystals. Finally, Professor Mats Andersson from the Future Industries Institute, Adelaide, discussed his work on polymeric materials for energy and conducting applications.

Topics covered exemplified the diversity of our discipline, including photopolymerisation, advanced characterisation techniques, biomaterials, drug delivery, polymers for bioimaging and biomedical applications, novel synthetic techniques, and industry and innovation.

This special issue of *Aust. J. Chem.* has a Research Front and includes a report from plenary speaker Mats Andersson on the 'Stability of polymer interlayer modified ITO electrodes for organic solar cells'. A highlight paper by invited Keynote Professor Christine Luscombe illustrates how changing the end-functional groups of P3HT to incorporate chalcogens opens up the opportunity to control and alter interactions with different materials.

Two review articles from Early Career Researchers include Dr Katherine Locock's (CSIRO, Melbourne) review, which traces the development of the antimicrobial polymethacrylates from the initial mimicry of global cationic and lipophilic AMP properties through to the level of specific amino acids present in the peptides. Dr Luke Connal, University of Melbourne, reviews the design and synthesis of polymers functionalised with amino acids. Dr Connal also presents a communication paper that highlights how morphologies of poly(2-vinyl pyridine)-block-poly(dimethylsiloxane) diblock copolymers can be tuned by controlling the interfacial energy using functional surfactants.

The RACI Treloar Best Poster prize winner, Molly Rowe from the University of New South Wales, presents a research paper entitled 'High glass transition temperature fluoropolymers for hydrophobic surface coatings via RAFT copolymerization' (see figure).



Amanda V. Ellis FRACI CChem, Guest Editor, and Greg G. Qiao FRACI CChem, Associate Editor, *Australian Journal of Chemistry*

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# Flavours, fragrances and force fields



Stockphoto/crisphotography

BY **MARTIN SLATER** AND **KATRIONA SCOFFIN**

**Computational methods that analyse how drugs interact with protein targets are also effective for flavour and fragrance molecules.**

**F**lavours and fragrances traditionally depend on essential oils drawn from naturally occurring products. Camphor oil is obtained by steaming the wood of the camphor tree; saffron is the stigma plucked from the flower of *Crocus sativus*.

Natural products are often subject to short or erratic supply owing to weather and other natural events. Environmental or preservation considerations also come into play. Up to 50 male musk deer are killed to produce 1 kilogram of musk, highly sought after for perfumes. Ambergris, produced in the digestive system of

the sperm whale, was formerly used as a fixative to make scents last longer. Its use is now illegal in Australia and the US and the synthetic ambroxide is widely used as a substitute.

Synthetic substitutes that retain the same odour and flavour characteristics as the natural compound have been developed for many flavours and fragrances. Degradation is a particular factor for flavours, and synthetic versions are often chosen because of their longer shelf life. Health considerations drive other synthetic choices; for example, low calorie sweeteners as alternatives to sugar.

Companies are continually looking



for new and improved versions of these substitutes, synthetic or otherwise. In some cases manufacturers are keen to identify alternative natural products that have a similar effect to hard-to-obtain flavours and fragrances. Molecular modelling plays an important role in identifying possible alternatives.

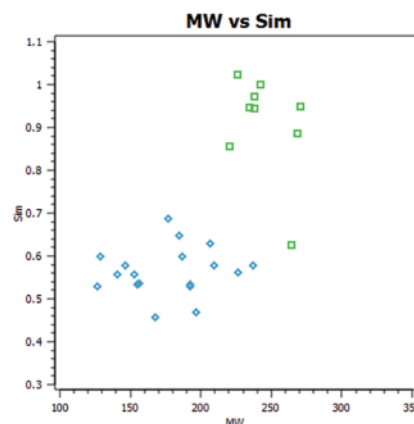
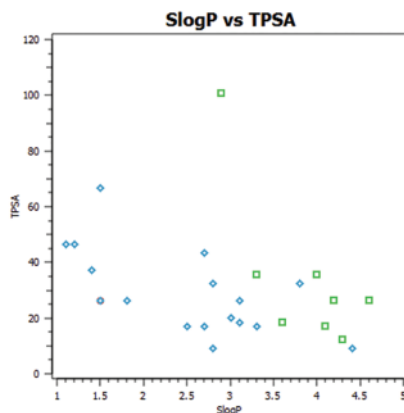
## Applying pharmaceutical discovery methods to flavours and fragrances

There are many well-established computational techniques for modelling the interactions between pharmaceuticals and proteins. Since flavour and fragrance molecules interact with specific protein targets to exert their effects, many of these computational techniques are directly transferable from pharmaceuticals to flavours and fragrances.

When looking for new synthetic flavours or fragrances, the starting point could be an existing natural or synthetic compound, or a taste or odour receptor. Perhaps surprisingly, flavours are more diverse and complex in their interactions than pharmaceuticals. Some components of taste perception also include the simultaneous triggering of olfactory receptors, which belong to the wider, therapeutically important, G-protein-coupled receptors (GPCR) family.

Clearly, there are many differences between flavour and fragrance molecules compared with their drug counterparts. The pharmacological effects of pharmaceuticals cover a wide spectrum of therapeutically relevant biological targets and also require physiochemical properties in keeping with their use; for example, oral, central nervous system, inhaled or topical applications.

Fragrance molecules need to be both non-toxic and volatile and as such are restricted by tight chemical and physical property considerations. In addition, the mode of action of fragrance molecules is generally accepted to be through GPCR



The physiochemical properties of 18 diverse fragrance molecules (blue diamonds) and 9 diverse musks (green squares), showing the narrow spectrum of size, shape and molecular weight that these molecules occupy.

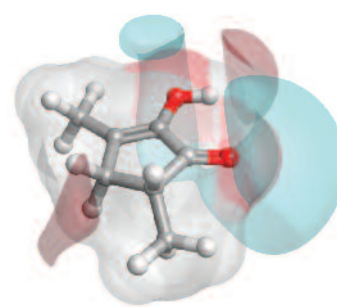
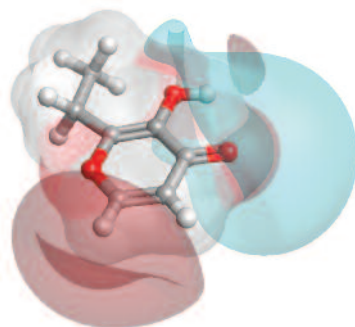
agonism and therefore the spectrum of size, shape and molecular weight is accordingly further narrowed (see graphs above). It is an incredible observation that the huge spectrum of fragrance perception is dictated by the precise 3D distribution of typically between only 2 and 20 atoms of only five elements – carbon, hydrogen, nitrogen, oxygen and sulfur. Possibly unsurprisingly, this translates into very compact electrostatic, shape and chirality profiles for each of these special molecules.

## Molecular fields and virtual screening

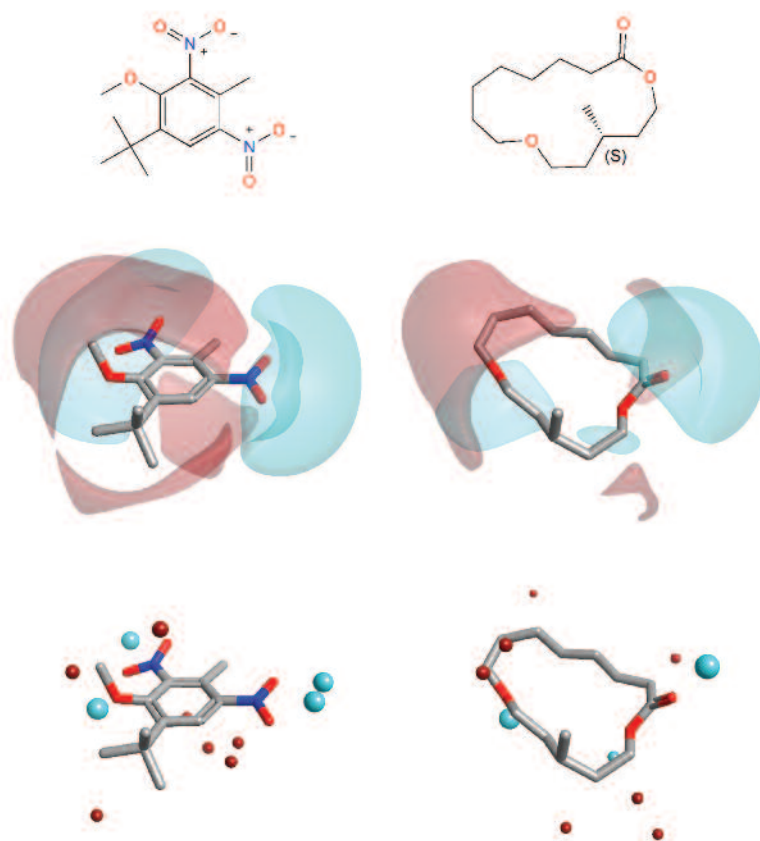
Small molecules are recognised by and bind to proteins on the basis of their 3D electrostatic, shape and hydrophobic properties, otherwise known as their molecular fields. It is

possible to calculate detailed computational models of these fields that provide a highly accurate description of the interactions between a small molecule and its protein binding site. In this way, the active profile of a compound can be calculated, visualised and analysed, giving a 'protein's eye view' of the compound (see below). These calculations are complex and long if carried out by using quantum mechanics methods, but a comparable level of quality can be obtained in a fraction of the time using a force field approach. The molecular fields shown here were calculated using the Cresset XED force field, which combines electrostatic calculations in combination with Van der Waals forces.

However, molecular field calculations are computationally



The molecular fields around two caramels, ethyl maltol and furaneol. The surfaces show the shape (grey) and the positive (red) and negative (blue) electrostatic isopotentials, giving a 'protein's eye view' of the compound.



Two structurally diverse musks, nitro musk (left) and ambrette (right), with their electrostatic isopotential surfaces positive (red) and negative (blue). The molecular fields (centre) reveal similar bioactivity that is not evident from their 2D or 3D structures. Field points (bottom) make it possible to compare thousands of structures and fragments on the basis of biological similarity.

intensive. It is unfeasible to use an entire molecular field profile to search through large collections of molecules. Such a search would take more computing power and time than any project would have available. Instead, methods have been developed to condense molecular fields down to 'field points' that encode the fields accurately enough to make biologically useful comparisons between the profiles of different compounds (see above). Field points are an elegant and computationally viable way of expressing the molecular field patterns of molecules and they unlock tremendous computational potential.

These field point profiles can be used as molecular fingerprints to search databases of active molecules

to return compounds that are likely to have similar activity. Field points make it possible to search a database of about 10 million compounds in 48 hours on a 30 CPU cluster. This method of virtual screening has proved highly successful in pharmaceutical research in identifying compounds with similar activity profiles, despite being from different chemical classes and having markedly different 2D structures.

The same method has been successfully applied to fragrance and flavour molecules in order to compare their active profile. Field-based models of active flavour and fragrance ingredients can be developed in the same way and used to search for synthetic alternatives for natural products. Once a range of alternative

compounds has been identified, the individual alternatives can be modelled and compared in greater detail by using a more accurate calculation of the molecular fields.

### Utility of molecular fields for analysing flavour and fragrance bioactivity

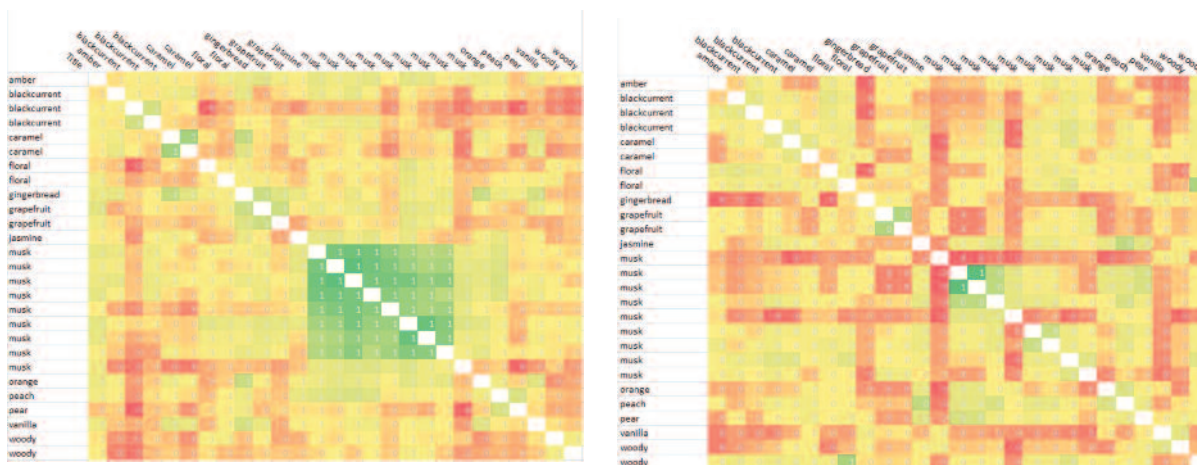
To illustrate the usefulness of electrostatic descriptions for fragrance molecule space, a small set of 27 diverse fragrance molecules were built and analysed (Kraft P, Bajgrowicz J.A., Denis C., Frater G., *Angew. Chem.* 2000, vol. 112, p. 3106; *Angew. Chem., Int. Ed.* 2000, vol. 39, p. 2980; [www.leffingwell.com/chirality/chirality.htm](http://www.leffingwell.com/chirality/chirality.htm)). The set included an extended group of musks.

One of the compounds, coumarin, was chosen as a starting point for the analysis. The centre of gravity and the overall dipole were fixed relative to this starting point. Some detailed modelling work was carried out on the compounds in the set in order to determine the likely 3D alignments.

Similarity scores were calculated for all of the compounds and each molecule was scored relative to each other to generate an all-by-all matrix

**When looking for new synthetic flavours or fragrances, the starting point could be an existing natural or synthetic compound, or a taste or odour receptor.**





(Left): All-by-all field similarity matrix of 18 diverse fragrance molecules and nine diverse musks (green – yellow – red signifying decreasing similarity), showing significant clustering around fragrance groups.

(Right): All-by-all ECFP4 2D similarity matrix of 18 diverse fragrance molecules and nine diverse musks, showing the low levels of similarity calculated using a purely structure-driven analysis.

(see figure top left). This simple exercise was limited only by the low numbers involved in the analysis, yet still provides a very intuitive picture. From the matrix, brighter green corresponds to higher similarity, and red to a low similarity.

There is a significant cluster around the musks, but also other hot spots of high similarity. For the sake of comparison, a purely chemical structure driven analysis was also carried out using ECFP4 2D similarity. The results are shown in the matrix on the right and they reveal a stark contrast to the force field version, showing mostly low similarity. The

relationship of the musk structure activity relationships (SAR) in this example is likely to defeat most 2D similarity methods; therefore, the structurally diverse musk clusters disappear and the caramels blend into the noise.

A hierarchical clustering was also carried out, which provided a different overview of the fragrance set. Interestingly, gingerbread, caramel and orange fragrance compounds, which many would say are highly complementary flavours, showed a high similarity, which suggests that their corresponding targets may be highly similar to each other. The 3D

aligned structures of gingerbread and orange with their molecular fields are shown below.

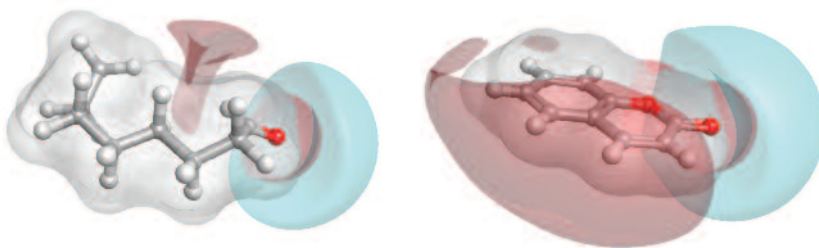
## Pharma potential

The world of flavours and fragrances holds a wealth of subtle chemistry and huge potential for benefiting from the transfer of computational methods from pharmaceutical discovery.

The analysis discussed here demonstrates the power of a field-based approach for usefully analysing the bioactivity of flavour and fragrance molecules. The fields approach gets to the essence of the unique and precise way that flavours and fragrances molecules interact with their protein targets, independent of their chemical architecture.

Field-based models of active flavour and fragrance ingredients are already being used in industry to provide novel chemotypes, echoing the success of this technology in providing new hits and leads for the pharmaceutical industry.

**Martin Slater** is Director of Discovery Services and **Katriona Scoffin** is Science Writer at Cresset, [www.cresset-group.com](http://www.cresset-group.com).



Gingerbread and orange; coumarin (left) and laural aldehyde (right) and positive (red) and negative (blue) electrostatic isopotential surfaces.



# Inside the 'IDEAS BOOM'

BY **BRITTANY HOWARD**

**Cultural change is at the core of the new National Innovation and Science Agenda, say its proponents.**

Australia has a science and innovation problem. By now, most of us are aware of the bleak statistics – Australia is ranked ninth in the Global Innovation Index in respect of the calibre of its science institutions, yet 72nd for innovation efficiency. So why do we continue to have such trouble traversing the gap between scientific research and innovation?

Many of us regard a paucity of government funding as being responsible for our underperformance in commercialisation and, undoubtedly, this is an issue that must be addressed. However, our inability to translate world-class scientific research into innovative and commercialised outcomes is a problem far more

complex than simply a lack of financial support from the key funding bodies. It is something much more challenging to address.

The underlying problem is our culture. We're a risk-averse nation, which is further compounded by our generally poor understanding of how to practically innovate research into commercial success. Indeed, Australia's Chief Scientist, Dr Alan Finkel, has acknowledged the crippling 'fear of failure' mentality that lies deep among Australians.

So what is being implemented to shift our risk-averse culture to one that pursues innovation and commercialisation? In the past 15 years, Australia has seen approximately 60 reports on



innovation at the Commonwealth level. The recommendations in these reports mostly remain to be actioned, or otherwise they have evidently failed to transform this fear of failure mentality.

Yet, in December of last year, the Government, led by Prime Minister Malcolm Turnbull and the Minister for Innovation, Christopher Pyne, released the National Innovation and Science Agenda (NISA). How is this program different from all those that have gone before? Well, quite simply, it aims to transform our culture from one of a 'fear of failure' to one of 'embracing risk'.

### Extent of Australia's science and innovation problem

Australia is ranked a dismal 72nd for innovation efficiency according to the Global Innovation Index. This 'innovation efficiency' is a measure of innovation output a given country is obtaining for its comparative inputs, which is based on turning research into commercial outcomes.

Contributing to our inability to innovate, Australia's venture capital market is yet to recover from the global financial crisis, while countries such as the US have surged ahead. For us, it's all too difficult for start-ups to obtain finance.

Further, Prime Minister Turnbull has continually highlighted that, as a nation, we are poor at forming collaborations between researchers, typically at universities, and businesses. Though arguably, particularly in the chemical sciences, Australia simply does not have an industry with the capacity to engage in fundamental research. The ongoing downsizing of the chemical industry, as exemplified by the overseas acquisition and local closure of Biota Pharmaceuticals in 2015 indicates that this scarcity of industry-academia collaborations in Australia is unlikely to change anytime soon.

Finally, Australian workplaces lack a high performance innovation culture. Statistically, only 16% of Australian businesses have a high performance

innovation culture, in contrast to 44% of the Global Innovation 1000. Factors that contribute to a nation's performance innovation culture include whether a business sources ideas for innovation from users or customers, the importance a business places on innovation as a measure and strategy for business performance, and a tendency to network and collaborate.

The Government has recognised these key points as being just some of the barriers that continually prevent fundamental research from being translated into commercial outcomes, and the implementation of the National Innovation and Science Agenda (NISA) is aimed at lowering these barriers.

### What is the NISA?

Prime Minister Turnbull is banking on an 'ideas boom' as being the new source for Australia's growth and prosperity in the face of a declining mining industry. To support this, he launched the NISA, a policy that will cost the government \$1.1 billion over four years, and will be introduced into legislation effective from 1 July 2016.

The policy recognises that innovation is critical to improving Australia's competitiveness, standard of living, high wages and generous social welfare net. Most essentially, the NISA proposes that fostering innovation and commercialising research will be a key driver of future national growth.

The NISA includes the creation of an advisory body, Innovation and Science Australia (ISA), spearheaded by Mr Bill Ferris AC and Dr Alan Finkel AO. According to its Government website ([innovation.gov.au](http://innovation.gov.au)), ISA 'will be a new independent body with a mandate to provide strategic whole-of-government advice to the Government on all science, research and innovation matters'.

ISA will publish its research findings and advice in order to promote public discussion, and will publicly advocate

reforms on key issues that include innovation investment, collaboration, research infrastructure, and how to better invest in research and development. It will have a role in auditing the performance of the NISA and in developing a 15-year plan for the Government's investment in science, research and innovation.

The NISA will focus on four key pillars: culture and capital, collaboration and skills, incentivising risk and government as an exemplar.



Stockphoto/LeeYiuTung

**... only 16% of Australian businesses have a high performance innovation culture, in contrast to 44% of the Global Innovation 1000.**



**Antennas of CSIRO's Australian SKA Pathfinder (ASKAP) telescope at the Murchison Radio-astronomy Observatory in Western Australia.. The ASKAP telescope is a high-speed survey instrument comprising 36 independent beams. It uses innovative technologies such as an extremely wide field-of-view interferometer with phased array feeds. The first ever 36-beam image was produced in April during commissioning activities. CSIRO/CC-BY-3.0**

Key to the NISA is the emphasis on the need for collaboration between business, research organisations and educational institutions. As it stands, Australia ranks last among OECD countries for business collaboration, and the NISA proposes to take steps to rectify this by introducing 'clear and transparent measures of non-academic impact and industry and end-user engagement' through a national assessment of university research performance. What this means, however, remains unclear, although a pilot assessment program is set to commence in 2017.

The NISA will also seek to reverse the innovation problem by introducing an Entrepreneur Visa 'for entrepreneurs with innovative ideas and financial backing' that provides a pathway to permanent residency. Further, the pathways to permanent residency for postgraduate researchers with STEM qualifications will also be significantly enhanced.

The NISA also aims to create a

culture that fosters and inspires entrepreneurship and innovation, which it plans to do through changes to the research and development tax incentives and bankruptcy laws. This includes reducing the bankruptcy period from three years to one year, introducing a safe harbour to protect directors from personal liability for insolvent trading, and introducing clauses that allow for the termination of contracts in the event of insolvency.

Perhaps most importantly, the NISA plans to provide additional educational opportunities. This includes arming young Australians with the requisite skills for the jobs of the future, as well as investing in measures to encourage more women to pursue STEM-related careers.

The funding itself is spread across multiple initiatives, of which the highlights include: \$200 million to CSIRO for an innovation fund to help commercialise research; \$2.3 billion over 10 years for the National Collaborative Research and

Infrastructure Strategy, the Australian Synchrotron and the Square Kilometre Array; \$127 million for research block grants with greater emphasis on research-industry collaboration; \$13 million to promote women in science, including the Science in Australia Gender Equity (SAGE) pilot; and \$48 million to promote STEM to all Australians over the next five years.

There is no doubt that the NISA is a broad-ranging and ambitious agenda. Prime Minister Turnbull has stated that 'the package is designed to inspire. It is designed to lead. It is designed to encourage every single business, large or small to be more innovative, to be more prepared to have a go at something new ... a national culture of innovation, of risk-taking. Unlike the mining boom, the ideas boom is 'a boom that can continue forever; it is limited only by our imagination.'

## Does the NISA focus on innovation and research knowledge?

Undoubtedly, the NISA has an aura of change to it. It has a sense of addressing a long-felt need, and the rousing potential to propel Australia into the ideas boom.

However, disappointingly, the NISA fails to mandate innovation and commercialisation training. Consequently, Australian scientists will generally still be lacking an understanding and the practical skills that are so essential in translating research into commercialisation, although perhaps this responsibility lies not with the Government, and instead with the very research institutions set to benefit from the NISA. This includes research institutions, such as the CSIRO, universities and even secondary schools.

Australian scientists need to be raised in an innovative and commercialisation-savvy environment – it needs to become second nature. For this to occur, a fundamental understanding of



innovation and commercialisation should ideally be introduced at secondary school level. Otherwise, every tertiary student, especially those in STEM courses, must be introduced to these skills. At the postgraduate level, courses directed to the commercialisation of specific research programs should be available, if not compulsory. This will eventually lead to a generation of Australian scientists with the skill and practical know-how to drive the ideas boom. Only then will we be capable of undertaking the much needed shift in culture from 'fear of failure' to 'embracing risk'.

In the meantime, there must be a focus on further training for current research leaders, including university scientists, as this is where we presently

have the greatest potential to innovate. It is rare to find a senior academic or lab head who has had formal training in these areas, and, instead, they must solely rely on knowledge they have picked up from many years of working in the field. It is a priority that future leaders directing research groups have a knowledge of innovation and commercialisation.

### **The NISA is a promising step forward**

To be a successful nation, Australian must ditch its 'fear of failure' culture and instead adopt an 'embracing risk' culture. Pleasingly, the Government appears to be actively encouraging this through the implementation of the NISA, which proposes to knock down the key

barriers to commercialisation, and inspire us to achieve through innovation.

However, it won't come without challenges, and as Prime Minister Turnbull has stated, 'Australia has embarked on one of the most ambitious public sector innovation projects ever attempted ... Its aim is set out in the National Innovation and Science Agenda.'

With the upcoming Australian federal election, we can only hope that it's a priority of the government to continue with a long-term vision to encourage and foster innovation.

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**Brittany Howard** MRACI completed a PhD in medicinal chemistry at the Monash Institute of Pharmaceutical Sciences before undertaking a postdoctoral position with the National Institutes of Health (US). She is currently a trainee attorney with FB Rice.

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# Prime numbers

## 41 years of EMDG

BY **DAVE SAMMUT**

**N**ow embarking on its 41st year, the Australian Government's Export Market Development Grant (EMDG) is very much a program in its prime. It is arguably the country's most successful long-term targeted economic stimulus initiative.

It's July, and lodgement season has opened once again for exporters to submit claims for entitlements under the EMDG program. For every dollar spent on eligible export marketing activities, these companies will be

claiming a cash rebate of almost 50%, up to a maximum of \$150 000 of cash in hand per claim.

One of the keynote characteristics of the EMDG is that, unlike most other grants and funding, it is a legislated entitlement program. Businesses that have expended funds according to the eligibility criteria are *entitled* to claim the associated benefits. The money is non-discretionary, and non-competitive.

I have seen the critical difference that this program has made for many





## The Export Market Development Grant is helping take Australian innovation to the world.

property protection and trademarks, marketing travel, trade shows and promotional events, free giveaways and samples, advertising (both print and digital) and even some costs for bringing overseas buyers to Australia for approved export purposes.

One of the factors behind the success and longevity of the program is that it is thoroughly audited, and so successful claims are very much based on clear and pertinent evidence: documents and receipts that demonstrate both the expense transactions and the purpose and/or proportionality of those expenses.

The EMDG is performance based. A company's entitlements are linked to the actual export revenues it generates, but in the 'fair go' Australian spirit the Government gives the companies two years to put 'runs on the board' before this applies.

And it is this balance between performance, auditing rigour and fair usage that has made the program a success over the last four decades.

Until recently, the legislation underpinning the EMDG had a five-year 'sunset clause', meaning that the program had to be independently reviewed and reintroduced to parliament every five years or so.

The most recent review was conducted in 2015 by Michael Lee (former director of Zip Industries). In his report to the Minister for Trade and Investment, Lee stated: 'I have seen firsthand the benefits that this modest government support provides to Australian companies at critical early stages in their export journeys ... I found that this 40-year-old scheme remains highly relevant and continues to bring benefits to Australia by encouraging the creation, development and expansion of

new exporters, yet I am always surprised by how many people have yet to hear about it. The EMDG is targeted at businesses that are seeking to grow their export revenues for the international sale/licensing of their products, service and/or intellectual property.

The activities eligible for cash rebate are broad, and include most of the key items that would be on the checklist of any potential exporter: overseas representatives, export consultants, international intellectual

### '50% cash back' – how it works

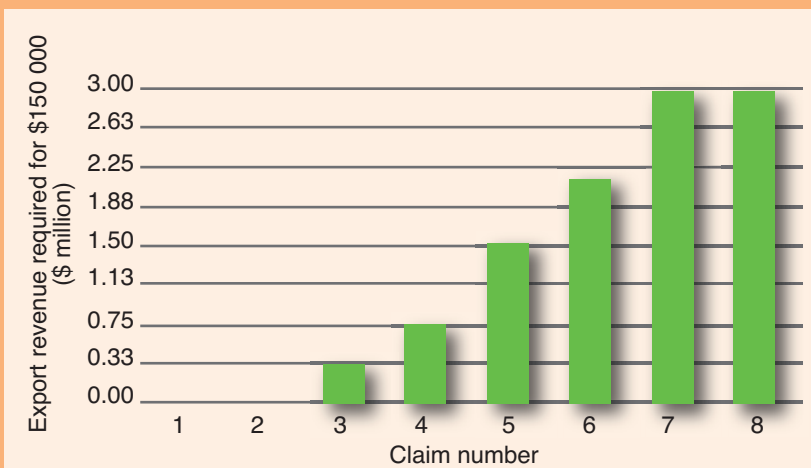
Effective from 1 July 2016, the EMDG program has eight categories of eligible expenditure to help determine the cash rebate payable to an applicant (a company, partnership, sole trader or trust). Austrade has specific schedules and varying rules for claimable expenditures for each of the eight categories:

- Overseas representatives/offices on a 12+ month contract, up to \$200 000
- Marketing consultants, either based in Australia or overseas, up to \$50 000
- Travel for export marketing purposes (international and domestic, up to 21 days per trip, including flights plus daily allowance of \$350)
- Free samples and giveaways, up to \$15 000
- Trade fairs and promotional events, such as conferences, trade fairs, forums and private exhibitions, uncapped
- Advertising and literature, including brochures, videos, websites, advertising, uncapped
- Overseas buyer expenses for export promotion, up to \$7500 per buyer per visit, and up to \$45 000
- Intellectual property protection, including international patents and trademarks, up to \$50 000

The total expenditure from these schedules is added together. \$5000 is deducted, and the balance is multiplied by 50% to give the maximum entitlement, up to \$150 000 (i.e. \$305 000 of expenditure). This is then compared against the performance target (see box 'The performance text – a fair go') for the given claim year to determine that actual grant.

## The performance test – a fair go

The maximum EMDG grant in a given year is based on the export revenue performance by the business. After giving an applicant two claim years to establish its exports, it then caps the entitlement at 40% of export revenue received for the third claim, and 'raises the bar' each claim thereafter: 20%, 10%, 7.5%, 5% and 5% for claims in years 4–8.



Export performance requirement for maximum EMDG claim.

For this reason, some applicants often elect to 'skip' a year or more in their claims, and only lodge EMDG claims when their export performance maximises the grant entitlements. As Rod Campbell (Chair of the Export Consultants Association Incorporated) says: 'You can only claim eight times over the life of the company. Make it eight *good* claims.'

overseas markets for Australian goods and services. It was particularly encouraging to note that more than half of the 74 finalists in the 2014 Australian Export Awards were beneficiaries under the scheme.'

KPMG modelling in the Lee review found that every EMDG dollar generates an economic benefit of \$7.03 when industry spillovers and productivity gains are taken into account. The industry's peak EMDG body, the Export Consultants Association Inc. (ECAI), pointed to even higher statistics for the success of the program. In the three years prior to the review, the first-time claimants under the scheme achieved \$13 of export revenue for every dollar spent. By claim 7, the export revenue was on average over \$54 per dollar of EMDG.

Put simply, there is no other grant program that achieves such strong leverage of national benefit versus

government expense for small business. And Lee clearly agreed, proposing that the government's funding of the program should be lifted to provide greater certainty of outcomes for Australian exporters.

Following the review, amended EMDG legislation was passed by parliament with bilateral support. As a landmark change, the legislation has been fixed in the pantheon of government support to industry, with the removal of the five-year sunset clause. The legislation also tweaked the entitlements slightly, removing a 3% automatic benefit for communications costs, introducing a \$15 000 limit on free sample expenditures, and increasing the daily allowance for food, accommodation and ground transport while travelling internationally to \$350.

However, despite an increase in funding from \$125 million to

**The EMDG is targeted at businesses that are seeking to grow their export revenues for the international sale/licensing of their products, service and/or intellectual property.**

\$137.5 million for 2013/14 claims, the program is still chronically underfunded. In a recent briefing, Austrade (which administers the program) estimated that total claims would exceed \$170 million. As such, claimants will be paid a guaranteed up to \$40 000 immediately on approval of their export expenses claim by Austrade as a first instalment, then a percentage of any amount over \$40 000 based on the pool of available funds once all claims have been assessed. ECAI anticipates that the shortfall could leave maximum \$150 000 claimants 'short' by \$40 000–50 000 for 2014–15 financial year claims.

Compare this to the benefit of the R&D Tax Incentive (itself a critical support mechanism for businesses conducting R&D in Australia). A recent analysis submitted by the Centre for International Economics to the federal review of the R&D Tax Incentive, identified additional Australian R&D expenditure of between \$0.3 and \$1.0 per dollar of tax forgone for large firms, and between \$0.9 and \$1.5 per dollar of tax forgone for SMEs. That is a



## Getting the claim right

Austrade data shows that the use of EMDG consultants has grown strongly over recent years, to 71% of claims for the 2013–14 year. This would in part reflect the change in Austrade's approach to the EMDG program from that year, with the introduction of fairly punitive compliance provisions, and the removal of provisions to query 'grey area' items in claims. Austrade has acquired powers to act as judge, jury and executioner in assessing errors in EMDG claims, and the power to declare applicants as 'not fit and proper' persons for EMDG, with the effect of both striking out the whole claim under assessment and potentially preventing any company associated with the claimant signing authority from ever claiming again. So it is understandable that many applicants would turn to consultants to help ensure that the claims are correct.

The EMDG is very much an evidence-based program, but it is also complex, with a highly-nuanced set of rules, exceptions and exclusions. According to Austrade data, the total 'slippage' (the difference between the amount claimed and that approved after assessment) was 27% for self-claimants in the 2012–13 financial year. For the top quartile of professional EMDG consultants, the slippage was 4%. So there is also a strong economic incentive for companies to use the advice of expert consultants to plan the export strategy maximise entitlements.

A list of 'Quality Incentive' consultants (which have passed Austrade's most rigorous assessment with the highest success rates) is available on Austrade's website: [www.austrade.gov.au/Australian/Export/Export-Grants/Consultants](http://www.austrade.gov.au/Australian/Export/Export-Grants/Consultants).

substantially lesser benefit, yet the R&D program is virtually uncapped, at a cost of nearly \$3 billion per annum and based on self-assessment.

With the falling Australian dollar and a general improvement in international conditions following the GFC, Australian companies are again looking outwards for growth opportunities. For many of those companies, particularly the SMEs, the funding support available through the EMDG will be a critical factor in their investment decisions for the coming year.

EMDG registrations for 2015–16 opens on 1 July. Has your company considered accessing its entitlements?

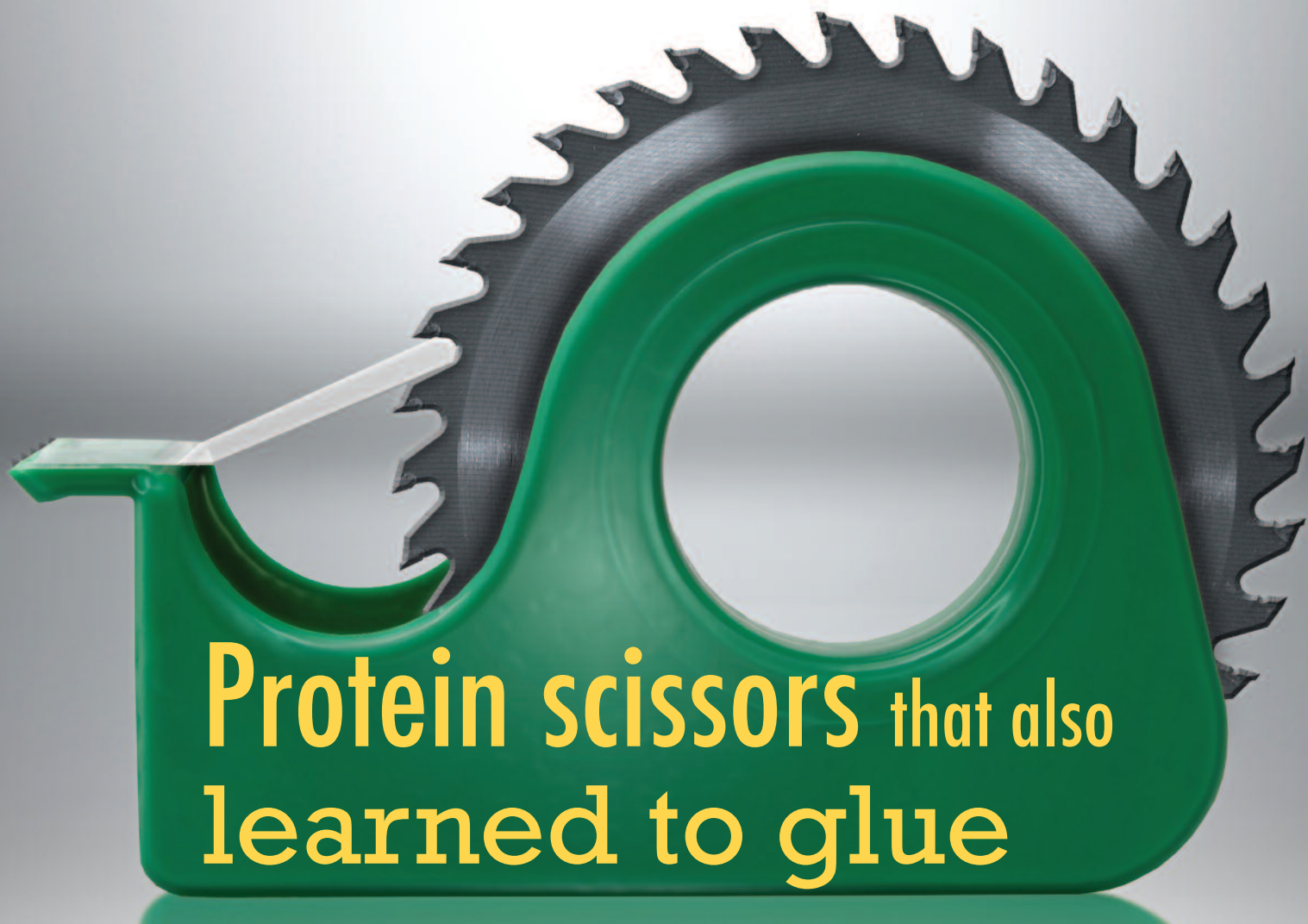
**Dave Sammut** FRACI CChem is principal of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries. Dave is also a 'Quality Incentive' EMDG consultant (as listed on the Austrade website), supplying services through Rod Campbell & Associates – a specialist practice on EMDG since 1980.

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Artwork by Scot Nicholls, Domokun Design, reproduced from *Chemistry & Biology*

BY **JOSHUA  
MYLNE**

**An enzyme found in plants has some remarkable abilities that have drug designers excited.**

**P**roteins are a hotly researched area of drug design, but proteins can be degraded by the human body. Protein rings, however, are super-stable, giving them greater potential as drugs.

The main way to make protein rings is by chemical synthesis, but this is costly, inefficient and uses toxic chemicals. However, we have worked out how sunflowers turn a protein string into a super-stable protein ring in their seeds.

The enzyme that performs this ring-forming reaction is one that usually cuts proteins, but instead of using water to finish the job it uses the head

of a protein chain to form a new bond instead of breaking one. The ability to develop water-based reactions will eliminate the need for expensive and harmful chemical synthesis of drugs that are stable protein rings.

The work on this unusual ring-forming reaction began with a small protein found in the seeds of sunflowers called SunFlower Trypsin Inhibitor 1. SFTI-1 is a ring of 14 amino acids that has no head or tail.

SFTI-1 was discovered in the late 1990s and became popular with synthetic protein drug designers, but only in 2011 did the gene that encodes SFTI-1 become known. The sequence



for SFTI-1 is buried inside a gene that also makes seed storage albumin, a protein that accumulates to very high levels in seeds before degrading during germination to provide nutrients for the growing seedling.

How the sequence for SFTI-1 came to be buried alongside an albumin seemed curious indeed, but recent work has found that sequences for protein rings like SFTI-1 have been buried in albumin genes for at least 28 million years. SFTI-1 is just the first known member of a very large family of tiny seed proteins.

Seed storage proteins were worked on a lot in the 1990s. Ikuko Hara-Nishimura and her Japanese colleagues found a protease called AEP that helps to assemble seed storage proteins. It transpires that the albumin and its adjacent SFTI-1 both need AEP to be assembled correctly.

A breakthrough that made it possible to study the 'string to ring' reaction was the ability to make AEP properly in bacteria. *Escherichia coli* has been used in labs all around the world to make tens of thousands of different proteins, but it sometimes struggles to make certain proteins. Some proteins are toxic to *E. coli* whereas others don't fold properly and, once extracted, are insoluble in water. Sometimes a protein can be soluble and correctly folded, but *E. coli* cannot decorate the protein with the right chemical modifications for it to be active.

Over the years, the number of engineered *E. coli* strains has continued to grow, each with different capabilities. The *E. coli* strain that enabled us to make active AEP was a new strain that was especially good at protein folding and forming sulfur-sulfur bonds, which isn't something *E. coli* usually does well.

We used this new strain of *E. coli* to make and purify a suite of AEPs. Once we had pure AEP we changed the pH and the AEPs would self-activate by cutting themselves in several places. This self-activation by proteases is

quite common.

We mixed these activated AEPs from *E. coli* with a range of protein strings containing the sequence for SFTI-1, and found that AEP uses a rather ingenious way to make a protein ring.

Proteases usually cut proteins for two reasons: enthalpy and entropy. Enthalpy refers to the energy balance of the reaction. Cutting a protein releases energy whereas forming or ligating a protein bond usually requires an energy input. Hence bondbreaking is easier to do than making one.

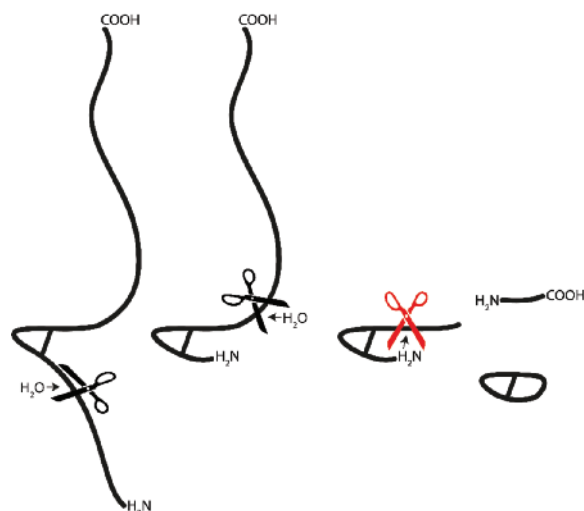
Entropy is about order. Cutting a protein usually gives you two proteins. It's easier for one piece of protein to be cut into two than for two disconnected proteins floating in solution to come close enough together to be joined by an enzyme into one.

For SFTI-1 to be made by a protease, these barriers of enthalpy and entropy must be overcome.

Proteases usually cut protein bonds by binding to the protein and then using water to hydrolyse the bond. However, water isn't involved when SFTI-1 is made.

The SFTI-1 string is made into a ring by cleaving off and discarding a small part of the string and using a nearby amino head group ( $H_2N$ ) instead of water ( $H_2O$ ) to complete the reaction (see diagram). To overcome enthalpy and entropy, AEP uses the energy obtained from cleaving to join the head of SFTI-1 to its tail in a reaction that moves a protein bond from one place to another place that's held really close by. The result is a circular protein with no ends.

During the same studies we found that if SFTI-1 did not get made into a ring it quickly broke down. Sealing the ends of a protein together makes it more stable, and this process has the potential to be industrialised using AEP. The ability to seal off the ends of a protein by joining them together is



**A protein string becomes a stable protein ring.**

therefore a popular approach that protein drug designers use to stabilise proteins that would otherwise be rapidly broken down in biological fluids.

An interesting finding from our work, which has been published in *Chemistry & Biology* ([bit.ly/1UgnWLX](http://bit.ly/1UgnWLX)), was that only one of four AEPs could perform the ring-forming reaction to make SFTI-1. The other AEPs could only cut the string into two pieces of string. What was perplexing is that this bond-making AEP looked very similar to the bond-breaking AEPs.

A different ring-forming enzyme in cyanobacteria has an extra protein 'wing' that helps protect the active centre of the enzyme from water, so how our bond-making AEP keeps water away from its centre must be more subtle.

Future work will attempt to understand what changes in the genetic sequence turn a cutting AEP into a ligating AEP and what changes improve its ligating ability. This should allow the engineering of artificial enzymes with superior cutting or ligating ability for industrial applications in biotechnology and protein drug stabilisation.

**Joshua Mylne** is an Australian Research Council Future Fellow appointed jointly to the School of Chemistry and Biochemistry & The ARC Centre of Excellence in Plant Energy Biology at the University of Western Australia. This article originally published in *Australasian Science* ([www.austscience.com](http://www.austscience.com)).

## New Fellows



**Shi-Zhang Qiao** received his PhD in chemical engineering from the Hong Kong University of Science and Technology in 2000, and is currently a professor (Chair of Nanotechnology) at the School of Chemical Engineering, University of Adelaide, and an Honorary Professor at the University of Queensland.

His research expertise is in nanomaterials and nanoporous materials for drug/gene delivery, and new energy technologies. He has co-authored more than 252 papers in

refereed journals (over 15 000 citations with *h*-index 66), including *Nature*, *Nature Materials*, *Nature Communications*, *Journal of the American Chemical Society*, *Angewandte Chemie* and *Advanced Materials*, and has filed several patents on novel nanomaterials that are promising for drug/gene delivery, fuel cells, photocatalysis and lithium-ion batteries.

He has attracted more than \$8.5 million in research grants from industrial partners and the ARC, including seven ARC Discovery projects, one ARC Linkage project and four ARC LIEF grants.

In recognition of his achievements in research, he was honoured with a prestigious ARC Discovery Outstanding Researcher Award (DORA, 2013), an Emerging Researcher Award (2013, ENFL Division of the American Chemical Society) and a University of Queensland Foundation Research Excellence Award (2008). He has also been awarded an ARC ARF Fellowship, an ARC APD Fellowship and an inaugural University of Queensland Mid-Career Research Fellowship. He has delivered more than 60 plenary, keynote and invited presentations at international conferences.

Qiao is an Associate Editor of *Journal of Materials Chemistry A* (RSC), Editorial Board Member of *ChemBioEng Review* (Wiley) and *Energy Storage Materials* (Elsevier) and Advisory Board Member of *ChemNanoMat* (Wiley), *Journal of Materials Science & Technology* (Elsevier) and *Advanced Materials Technologies* (Wiley). Qiao is currently appointed to the ARC College of Experts. He is also a Fellow of the Royal Society of Chemistry (FRSC).

At an early age, **Tania Notaras** spent many weekends assisting her older brother, Dr Boban Markovic with experiments in the garage. This early influence and the additional support and encouragement from her mother Mira inspired her to choose a career in science.

Notaras commenced her career under an industry traineeship in 1988 that quickly led to her appointment to various technical and management roles. Applying her talent and passion to continue developing the industry and creating efficiencies, Notaras emerged as a business leader in her field, locally and overseas.

Notaras' major impact to the industry was in 2005 as Managing Director and founder of Envirolab Services in Sydney and acquisition of MPL Laboratories Perth in 2010. From humble beginnings, this is now a successful, multimillion dollar commercial enterprise with offices and laboratories across Australia providing reliable, quality professional services for the environment and WHS sectors.

Notaras gives back to the profession by supporting the career development of her staff and offering industry placements for students. She is a mentor of women in industry, supports various student development programs and sponsors technical and professional meetings. She was a Telstra Business Women's Award Finalist in 2008 and appointed as a 2009 Women in Business Mentor, while also holding membership of the exclusive Executive Connection (TEC) since 2010.

From personal efforts and strategic alliances, Notaras is today sought for expert technical advice and guidance by decision makers in industry and government instrumentalities. These services have extended to assisting in the setting of industry standards and offering advice on regulations, and recognition through industry award nominations. Notaras also actively and voluntarily undertakes senior leadership roles in RACI affairs. This is illustrated by her 2015–17 successful nomination to the RACI New South Wales Branch as President-Elect and election to the RACI Board as an Ordinary Board Member. Attending RACI events has also assisted Notaras in her continued career development and business endeavours.

Alongside her successful professional career, Notaras has been happily married to her husband John for 26 years and is the proud mother of Natalie and Daniel.





## raci RACI Organic Division Awards

The RACI Division of Organic Chemistry is calling for nominations for the following awards. Nominations should be submitted to Dr John Tsanaktsidis (john.tsanaktsidis@csiro.au), Chair of the Organic Chemistry Division, by 30 June 2016. For more information, visit [www.raci.org.au/events-awards/organic-chemistry](http://www.raci.org.au/events-awards/organic-chemistry).

### The Athel Beckwith Lectureship

 Generously supported by the John Morris Group

The Organic Division has established an annual funded lectureship to allow outstanding, recently appointed, organic chemists to travel around Australia and present the results of their research work. The objective is to provide the lecturer with the opportunity to achieve broader recognition and exposure at an early stage in their career. Reasonable travel and accommodation expenses up to a maximum of \$3500 will be provided.

### The Mander Best PhD Thesis in Organic Chemistry Award

 Generously supported by Davies Collison Cave

The Mander Best PhD Thesis in Organic Chemistry Award recognises the best PhD thesis in the field of organic chemistry for outstanding achievement and communication. The recipient will receive a cash prize of \$1000, generously provided by Davies Collison Cave.

### Student Bursaries for Conference Travel



Generously supported by CSIRO Manufacturing

Up to 10 student bursaries (of up to \$500) are available to assist current RACI student members, who have been a member for at least one year, with attendance at organic chemistry related conferences within Australia.

### RACI Board elections

Nominations are open for the following positions on the RACI Board.

- President elect
- Treasurer
- Ordinary board member

Forms are available at [www.raci.org.au/theraci/corporate-governance/board-elections-2016](http://www.raci.org.au/theraci/corporate-governance/board-elections-2016)

Nominations close 20 August and elections will be held the first week in October.

## Young Chemists Group – Professional Development Series Part 1

### Professional Development Series Part 1: Grants, Fellowships and Awards

The first career event of the RACI Victorian Young Chemists Group provides participants with useful information about existing grants, fellowships and awards. Furthermore, we have invited successful researchers who will share their experience of writing and reviewing grants. The event will be split into 15-minute talks from our speakers, a panel discussion, followed by dinner and drinks.

#### Invited speakers

Grants, fellowships and awards – what is out there?

Dr Karen McConalogue

Manager, Research Programs, Monash University

A reviewer's perspective

Dr Cathy Foley

Deputy and Science Director of CSIRO Manufacturing

#### Venue

Thursday 14 July 2016, 5.30 pm – 7.30 pm  
RMIT Building 80, Level 5, Room 12, 445 Swanston Street, Melbourne

RACI Members \$10, non-RACI Members \$15 (includes dinner and drinks)

Register at [www.ivvy.com/event/VZG595](http://www.ivvy.com/event/VZG595).

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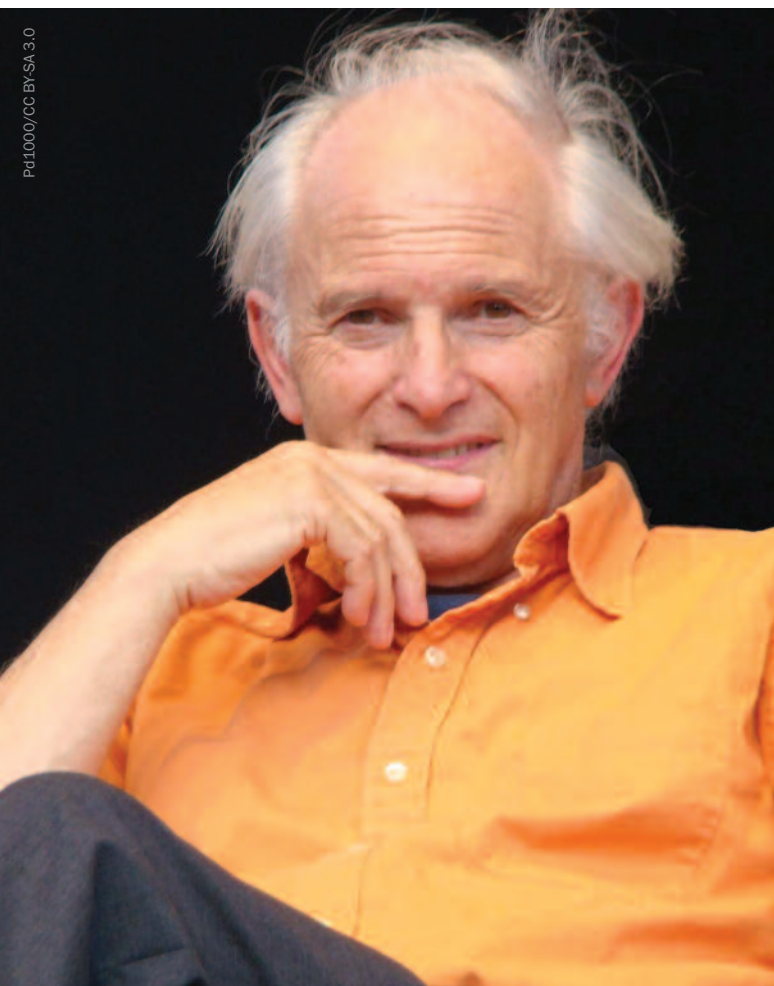
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## Nobel Prize winner and buckyball discoverer Harry Kroto dies



Nobel Prize-winning chemist and past president of the Royal Society of Chemistry Harry Kroto died on Saturday 30 April aged 76.

Kroto was awarded the 1996 chemistry Nobel Prize, along with Robert Curl and Richard Smalley, for the discovery of fullerenes, and was knighted the same year.

Born in Wisbech, Cambridgeshire, to parents who left Germany as refugees during the second world war, Kroto spent most of his childhood in Bolton in northern England, where his parents set up a balloon manufacturing and printing company in 1940. He went to Bolton School, where he developed a fascination with chemistry, physics and maths, and went on to study chemistry at the University of Sheffield in 1958, where he completed a BSc in chemistry, and then a PhD in molecular spectroscopy.

Upon completing his PhD in 1964 he moved to Canada and took up a postdoc position at the National Research Council (NRC) in Ottawa to undertake spectroscopy research. Then, in 1966, he went to Bell Labs to study liquid phase reactions using

Raman spectroscopy, but soon moved back to the UK to take up a postdoc position, and later a permanent lectureship at the University of Sussex.

For several years at Sussex he continued to carry out spectroscopic studies into new chemical species. Around this time he also worked with astronomers in Canada to characterise long, linear carbon chain molecules (such as  $\text{HC}_3\text{N}$  and  $\text{HC}_5\text{N}$ ) detected in outer space. This work eventually led to the discovery that would win him the Nobel Prize. In the 1980s, Kroto was working with Curl and Smalley at Rice University, US, on experiments that simulated conditions in the atmospheres of stars. It was these experiments that led to them discovering a new allotrope of football-shaped carbon –  $\text{C}_{60}$  – that could form from a condensing carbon vapour. It was Kroto's idea to christen the new allotrope buckminsterfullerene in homage to the US architect Buckminster Fuller, whose geodesic domes had helped him visualise the structure of  $\text{C}_{60}$ .

In the wake of his Nobel success, Kroto became a prolific speaker and science communicator, devoting much of his time to educational outreach and public engagement activities. In 1995 he set up the Vega Science Trust to create science films that were broadcast on BBC television.

He was president of the Royal Society of Chemistry from 2002–2004, after which he became a professor of chemistry at Florida State University in the US.

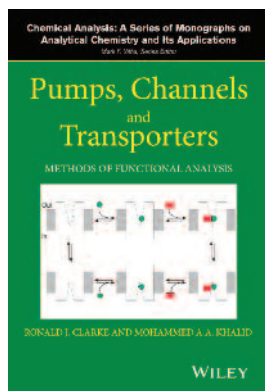
Robert Parker, now chief executive of the Royal Society of Chemistry, worked in the publishing wing of the organisation when Kroto was president. 'I've always been struck by Harry's genuine passion for chemistry, which he shared so generously with young people and early-career researchers especially. He had an easy-going style which made him so approachable and such a good communicator and ambassador for chemistry,' he says. 'While he was clearly a brilliant scientist, it wasn't his only passion and his abiding interest in art and design filtered through to influence in innovative journal covers and finding new ways to approach big problems. His warm-hearted nature, authentic interest in people and deeply-held personal opinions will be missed.'

Michael Farthing, vice-chancellor of the University of Sussex said: 'Harry Kroto's intelligence was stratospheric – and his contribution to chemistry will live on forever ... He was responsible for changing the way modern scientists think about chemistry and he mirrored this with an active role in global politics and the arts. His love of so many academic and cultural disciplines meant that he was able to view the world and its possibilities in such a unique and positive way.'

He is survived by wife Margaret, and two sons Stephen and David.

By **Emma Stoye**. This article was originally published by *Chemistry World*. Read more from *Chemistry World* at <http://www.chemistryworld.org>.





## Pumps, channels and transporters: methods of functional analysis

Clarke R.J., Khalid M.A.A. (Eds), Wiley, 2015, ISBN 9781118858806, 488 pp., \$178.95 (hardback), \$143.99 (ebook)

This book is volume 183 of *Chemical analysis: a series of monographs on analytical chemistry and its applications* (series editor Mark F. Vitha). Your body (and those of most other cellular life forms)

is kept going by a large variety of ion pumps, channels and transporters. Indeed, such structures are helping you interpret this information as you read. A lot of attention has been paid to how such systems work, and a number of Nobel Prizes have been awarded for research in this area; although as the editors of *Pumps, channel and transporters: methods of functional analysis* point out, the number of prizes awarded in a field may not be the most objective criteria for judging its relative importance.

Chemistry has long been involved in answering biological questions such as 'How do ions traverse membranes?' The structure and function of membrane proteins that facilitate such processes continue to be of interest, and over the years many techniques have become available to enable their study. This book, to its great credit, covers pretty much all them, and to an impressive level of detail. There are chapters covering everything from the more traditional methods of physiology such as patch clamp recording, through infrared, nuclear magnetic resonance and electron paramagnetic resonance spectroscopies, to cutting-edge technologies, based on the observation of single molecules. It even finishes with a chapter on molecular simulations for understanding channel function. Structural methods such as X-ray crystallography or electron microscopy are, however, intentionally omitted, since the book is focused on cellular kinetics.

The chapters are divided logically into four main sections. The book starts with an introduction to the history of ion channels, pumps and transporters, and covers their basic features and biological roles. This section is well worth reading by itself. I was quite interested to discover, for example, that osmosis was first discovered, accidentally, by a French priest and physicist (science and faith not being so far apart in times gone by as they are today) conducting an experiment involving an alcohol-filled pig's bladder being immersed in water. Quite why such an experiment was deemed necessary in the first place is not explained – but the original reference for this experiment is provided for the curious reader.

Section 2 discusses the use of electrical techniques to monitor currents produced by ion channels, pumps and transporters, while the third section covers the use of spectroscopic techniques to detail their macromolecular structure. The fourth section contains techniques that fall

outside the electrical or spectroscopic categories, such as theoretical simulations. I was particularly interested to read about the use of atomic absorption spectrophotometry for cation uptake studies in this section.

Each chapter starts with a detailed description of the technique and the principles behind it before moving on to those applications of said technique in understanding ion channels, pumps and transporters. The reader can dip in and out of the book and pick up information on a technique of interest or read in detail how such methods can give useful experimental information. It is quite pleasing to see methods that are sometimes overlooked, such as EPR, discussed.

The book brings together a large range of experts from all over the world with contributions from researchers from Australia, Germany, Italy Russia, Saudi Arabia, the UK and the US. The editors are Ronald Clarke (University of Sydney) and Mohammed Khalid (University of Taif). It is pleasing to see such cooperation between Australian and Saudi Arabian researchers, with this book being one of the many positive outcomes that can result from such collaborations.

Overall *Pumps, channels and transporters: methods of functional analysis* is an excellent book full of useful, detailed information and well worth reading whether you are an experienced cellular biologist or just a curious science undergraduate.

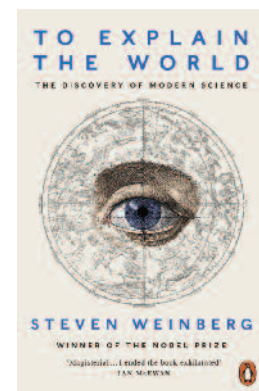
Oliver A.H. Jones MRACI CChem

## To explain the world: the discovery of modern science

Weinberg S., Penguin Random House, 2016, ISBN 9780141980874 (paperback), 416 pp., \$26.99

Much lauded, *To explain the world: the discovery of modern science*, which originally appeared under the Harper Collins banner in 2015, is now available in paperback form. Author Steven

Weinberg (b. 1933) is a Nobel laureate in Physics (1979, for his contributions, with Salam and Glashow, to theoretical physics, specifically to the unification of the weak force and electromagnetic interaction between elementary particles) with a fascination for the history of science, rather than a traditional historian of science. His particular interests are in the history of physics and astronomy and these are reflected in the book. If you're an academic or a teacher, one of the best ways I know to get your ideas straight in an area where you might not be, shall we say 'the world's greatest expert', is to 'volunteer' (and sometimes that can mean you just weren't quick enough to step backwards!) to teach it to someone. This is exactly what Weinberg did and the book arises from his experiences and research.



Weinberg's treatment benefits from elements of irreverence and the interspersing of his personal opinions from time to time. I expect a 'proper' historian of science would almost never do this, but it does add to the reader's experience and, if you're a Nobel laureate, then I guess you've earned the right to have opinions. For example, Weinberg writes of Francis Bacon and Rene Descartes as 'the two individuals whose importance in the scientific revolution is most overrated'. In similar vein, in a footnote about Isaac Newton's death, he observes the surgeon in whose arms Newton died and his doctor both reported to Voltaire that Newton 'never had intimacies with a woman', which, you'd have to agree, is a felicitous turn of phrase. He goes on to comment that Voltaire did not say how the doctor and surgeon could have known this! An interesting conundrum indeed!


The book is divided into three main sections: the text proper, a 94-page series containing 35 technical notes, and a section of endnotes tied to the chapters. You can read the book quite satisfactorily without going anywhere near the technical notes. However, if you want to know more or seek greater detail on how work from the past fits in with what actually exists in nature, the technical notes are useful and educational.

The main text of the book runs for 214 pages, covering Greek physics, with its philosophic notions of an ideal world, uncluttered by any experimentation or reality checking and Greek astronomy. Subsequently, moving to the Middle Ages,

Weinberg discusses the influence of Arab science and the milieu of medieval Europe. This is followed by an extensive exposition on the unravelling of the mysteries of the solar system before Newton more-or-less pulled things together into what we know as modern experimental science.

To show my prejudices, I found the discussion of Greek science fascinating, the contribution of the Arabs a worthy confirmation of one of my pet peeves ('God' was not, in fact, a European! Other people had ideas and contributions too!), the material about Newton inspiring (but, really wasn't he a nasty coot; a thoroughly perplexing individual) and the discussion of astronomy, in many ways the crux of the book, in greater abundance than my interest (well, that's my problem, I guess). Alas, chemistry rates not a mention. Certainly, the book 'explains the world' and explores 'the discovery of modern science', as its title suggests, but only from a particular perspective (physics/astronomy). This is no great revelation: Weinberg set out to do exactly that, and, in my view, he did a pretty good job of it. As a chemist, I'm probably a tad sensitive when the history of my profession finds itself confined to the wings in the great play about the emergence of modern science. However, chemistry too has its own great history, stretching back to the ancient Greek ideas about the divisibility of matter, forwards through the alchemists (and if Newton wasn't a 'paid-up' member, he was at least a fellow traveller) to modern chemistry as we know it. I expect biologists could make similar claims. So, for me, the book is an example of 'seeing dimly through a glass'. The picture is not too bad, but there's a lot of stuff lurking in the background if you want a complete picture.

R. John Casey FRACI CChem



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## Postcard from Dublin

This year is the centenary of the Easter Uprising in Ireland. On Easter Monday, 24 April 1916, several armed bands marched into Dublin and seized a number of vantage points. The British army responded by rushing 20 000 troops into the city and the subsequent fighting caused many casualties and much destruction. The uprising's leaders were court martialled and executed.

The 'Easter Martyrs' were not to know that their actions would provide the template for many an independence movement thereafter, and that the divisions that surfaced in the newly independent nations would mimic those in Ireland from the 1920s on.

But chemistry is everywhere, even in Ireland, so one asks the question: what is Ireland's most significant *chemical* achievement? It must surely be distillation! However, the first records of distillation are from the Alchemists of Alexandria, two millennia ago. Their product was herbal remedies and perfumes from plants. In medieval times, monastic orders produced alcoholic liquors, and by the Renaissance, aquavit sellers were to be found in European markets. According to Brian Townsend (*Lost distilleries of Ireland*, 1997, Neil Wilson Publishing), Irish whiskey distillation probably began in the late medieval times, and the skill was passed across the North Channel to the Scots.

In the 18th century, because of the Excise Act of 1779, there were many illegal stills in the Irish countryside, particularly in Donegal. A new Excise Act in 1823 made profitable the legal production of a more reliable product, and Irish whiskey became the dominant choice of spirit drinkers in the 19th century, displacing rum in England. This is the period of the great Dublin distilleries of Jameson, with the greatest distillery in the British Isles in Bow Street, and Powers in Johns Lane, whose



Historical whiskey pot still at the Midleton distillery complex of Jameson in County Cork.

Stephan Schulz/CC-BY-SA-3.0

products were so preferred over Scotch that there was an active trade in 'adulteration' of Irish with inferior Scotch, to sell on the English market.

A once great industry was brought down by business hubris, prohibition and tariff wars. The hubris was to assume that the dominance over Scotch would remain unchallenged ... but the Distillers Company, which bought up many Scotch distilleries in the late 19th century, introduced blending, a technique scorned by the Irish, but made possible by the patent still invented by Aeneas Coffey, the Excise official responsible for the 1823 Excise Act. A trade war with Britain followed Irish independence in 1922 and saw tariffs against Irish in favour of Scotch. Prohibition in the US from 1920 to 1933 almost killed off the Irish

whiskey trade in America, so that the great Dublin distilleries, which escaped destruction during Easter Week in 1916, finally closed in the 1970s. Most Irish whiskey is now made at a modern plant in County Cork, owned by the European beverage giant Diageo. Jameson's no longer comes from Dublin.

There is one traditional distillery left, Bushmills, which is on the north coast of Antrim, near the famous Giant's Causeway. Followers of *Game of Thrones* may well be familiar with this location, which is one of many in Northern Ireland used for that eponymous series.



**Trevor McAllister** FRACI CChem (trevormc@internode.on.net) is retired and enjoying life after science as a tour guide at the Melbourne Museum and the State Library of Victoria.

## Blast from the past: Australian steelworks

In 1911, the Broken Hill Proprietary Company decided to build a steelworks at Newcastle using coal from the Hunter Valley in New South Wales. Iron ore was shipped from the Iron Knob mine near Whyalla in South Australia. The advent of World War I isolated Australia from steel supplies in Britain and this made the new steelworks an extremely profitable operation.

The success of this operation spurred the Australian Iron and Steel Company (AIS) to build a steelworks at Port Kembla using coal from near Wollongong and iron ore from South Australia. The works started operation in 1928. Unfortunately for this enterprise, the Depression of the 1930s resulted in its demise and purchase by BHP in 1935. Again, isolation from the Empire during World War II resulted in the two steelworks becoming extremely profitable for BHP. Pressure by the South Australian government encouraged BHP to build another steelworks at Whyalla, which was opened in 1941.

During the 1950s, iron ore resources at Cockatoo Island and later the enormous reserves of the Pilbara were discovered and one of the conditions of exploiting these resources for export was that a steelworks be built in Western Australia. A steelworks was built by BHP at Kwinana south of Perth, which from the 1960s to 1984 was fed by its own blast furnace.

BHP ran the three remaining steelworks until 1999 when the Newcastle steelworks required major investment, which could not be justified by the company. BHP divested the Whyalla steelworks in 2000 and the Port Kembla operation in 2002, forming OneSteel (later renamed Arrium) and BlueScope, respectively.

All of these facilities produced steel by reducing iron ore with coal (as coke) followed by oxidising excess carbon in the iron by the basic oxygen process (BOS, a successor to the Bessemer process). This was one of the key technologies of the Industrial Revolution and still dominates the production of steel around the world.

The production of steel involves three large unit operations – the blast furnace, a coke oven and the BOS (Bessemer) converter.

The blast furnace is a very tall structure, which takes a charge of coke, iron ore and limestone (as flux) into the top of the furnace. Hot air is blown (blasted) into the bottom of the furnace and causes partial combustion of the coke to carbon monoxide. As the combustion gases rise through the furnace against the descending solids, the iron ore is heated and reduced to molten metal. Ash in the coke and non-ferrous ore is converted into a molten slag. The molten iron with a top layer of slag collects below the air injection zone in the furnace from which the iron (pig iron) and the slag are drawn off as liquids. Hot and still combustible gases are drawn off from the top of the furnace.

One of the major advantages of a blast furnace is that poor-quality metal scrap and some other intractable wastes can be added with the feed. Most tramp metals that otherwise would

contaminate the steel, are removed in the slag.

In the Bessemer converter, oxygen is blown through the molten iron, which reduces the carbon content of the iron to produce steel.

The other main unit operation is the coke oven. This has the duty to produce coke from coal. The coal is charged to a narrow vessel, which is heated externally by burning coke oven gases and excess blast furnace gas. Heating the coal drives off volatile matter, leaving behind incandescent coke. This is pushed out of the coke oven and falls into a rail car ready for charging into the blast furnace. Coke production is a batch process and the coke ovens are held in batteries of a hundred or more ovens to ensure a continuous supply of coke.

The raw coke oven gas is passed through condensers, which condense coal tar and an aqueous phase (known as ammoniacal liquor) and produce a coke oven gas used to fuel the coke oven operation. The liquids are worked up separately (often by other companies) to produce a wide range of coal chemical products. In Australia, coal tar liquids are separated at the Koppers (Koppers Carbon Materials and Chemicals Pty. Ltd.) works near Newcastle.

The three principal unit operations give the photographer some of the best images of the industrial landscape – blast-furnace tapping of hot metal, steel production when oxygen is blown through the molten metal, and the coke oven when incandescent coke is pushed out of the oven.

They also have some of the more intractable pollution issues in industry. Coal and blast furnace and downstream operations produce large quantities of slag and dust, which often affects the surrounding neighbourhoods, while coke ovens, especially older plant, are sources of discharges of polynuclear aromatics and benzene to the environment.

Steel production economics benefits from the economies of scale. Blast furnaces are now built with internal volumes over 5000 m<sup>3</sup> and produce many millions of tonnes of iron each year. These are very large facilities and one consequence is that the coke used has to be very strong to hold the enormous weight of the material in the top of the furnace. This has generated a specialised market for some coals (coking coal) and this sells at a significant premium to thermal (power station) coal (see table).

### Pertinent prices for steelmaking in March 2016

Commodity	Location (contract)	Price (\$/t)
Coking coal	Australia (FOB)	79.10
Thermal coal	Newcastle (FOB)	55.86
Iron ore	China (CFR)	55.5
Carbon steel	Asia	~380

CFR, cost and freight; FOB, free on board.

Because not all coal can produce high-strength coke, this can limit the scale of blast furnace operations, which are





Aerial view of Australian Iron and Steel factory in Port Kembla. Established in 1928, Australian Iron and Steel Pty Ltd manufactured iron and steel, as well as mining coal for use in the steel industry. Flickr/Royal Australian Historical Society

dependent on a local coal resource. This was the case at Newcastle where local coals could only support relatively small blast furnaces. Coking coal in Australia is produced from selected mines in the Bowen Basin in Queensland and exported to the large integrated steel operations in China, Taiwan, Japan and South Korea. These operations now dominate world production of low-cost export steel marginalising many operations in US, Europe and Australia.

In recent times the Port Kembla steelworks (BlueScope Steel) has gone through a major restructure and has had considerable state government support. At the time of writing, the Whyalla steelworks (Arrium) is under the control of an administrator and its ongoing operation is in some doubt. Furthermore, the reduction of iron ore using coal is innately a large emitter of

carbon dioxide. Approximately two tonnes of  $\text{CO}_2$  are emitted per tonne of iron produced. Clearly introduction of carbon emission charges would exacerbate the current economics of steel production in Australia. Furthermore, since the major facilities (blast furnaces, coke ovens) are long-life items, poor economics makes major investment in more efficient plant unlikely.

In a forthcoming article, I will discuss some of the lower carbon emission processes that from time to time have been tried in Australia.



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## Australia's part in the global effort to discover gravitational waves

The historic discovery of gravitational waves announced in February involved the work of more than a thousand scientists working tirelessly in several different institutions, across many different countries and time zones.

Why is an entire village, albeit a diverse and disparate one, required to verify experimentally the last of Einstein's major predictions in his theory of general relativity? And how does such a village function and coordinate in such a way that maximises scientific output?

### A tour of the village

LIGO Scientific Collaboration (LSC) consists of two individual experiments, located at two sites in the US, separated by 3000 kilometres. At each site, a single, very high-power laser beam is split in two, and travels down two perpendicular four-kilometre-long vacuum tunnels.

At the ends of these tunnels the laser hits large, 40-kilogram mirrors suspended by an intricate series of pendula to reduce shaking from external forces.

The laser light returns along the same tunnel, and recombines. Gravitational waves cause the actual length of each arm to change. The way the laser light recombines is used to determine this change.

In order to make a detection, the LIGO instruments needed to measure a change in arm length equal to 1000th the diameter of a proton. Performing such a measurement is a remarkable technological feat that involves development across multiple scientific streams.

These fields include, but are not limited to, quantum physics and quantum metrology; high-powered optics; mechanical systems, including thermal and vibrational control systems; general relativity and gravitation; theoretical astrophysics and traditional astronomy; large-scale computing ... the list goes on.

The multidisciplinary nature of this experiment is reflected in the structure of the LSC, which looks more like a

corporate entity than a traditional scientific collaboration.

Among other things, there are many, many science working groups which fall within the scope of three main themes: instrument science, detector characterisation and data analysis.

Alongside the science working groups sit groups such as Education and Public Outreach, Diversity, and the Presentation and Publications Committee.

Each working group is a dynamic, scientific collaboration all unto themselves. Each has a chairperson, or multiple co-chairs, who report to the theme leaders who, in turn, report to the LSC spokesperson, executive committee and council.

### Who works in the village?

So exactly how many scientists does it take to detect a gravitational wave? This particular effort took 1,006 scientists working tirelessly in 16 countries in 83 different institutions, located in 14 different timezones!

Research for the discovery was done all over North America, Brazil, throughout Europe, Russia, India, China and South-East Asia and Australia.

We, along with about 50 colleagues, work on this experiment in Australia. A majority of the leadership group work in institutes in the US, at places such as CalTech and MIT.

The result of this unfortunate circumstance is that full, collaboration-

wide teleconferences typically take place between 2am and 4am in Australian time. Over the past two months, building to the announcement, this has affected our lives many times!

In general, science working groups hold weekly teleconferences. Many of us are part of working groups that only exist on two continents, making it possible to schedule meetings that also allow for a relatively normal existence.

Many of us also work in groups that have numerous members on three or more continents; very early, or very late teleconferences are not uncommon, but remind us of the scale of the collaboration and the international effect of our work.

### What do they do?

As mentioned before, this is a precision measurement! Every aspect of the experiment is incredibly finely-tuned. For example, multiple groups and individuals around Australia work on the technology and design of the mirrors.

Monash University researcher Yuri Levin, while a PhD student of Kip Thorne's at CalTech, developed the theoretical framework for computing thermal noise (which is now widely used within the collaboration). From this work it became clear that LIGO mirrors require exceptionally high-quality reflective coatings.

The coating noise Levin anticipated is now considered to be among the most

**In order to make a detection, the LIGO instruments needed to measure a change in arm length equal to 1000th the diameter of a proton. Performing such a measurement is a remarkable technological feat that involves development across multiple scientific streams.**

serious sources of noise in the LIGO experiment.

Scientists at Adelaide University developed, installed and commissioned wavefront sensors for the LIGO mirrors that measure the mirrors' change in shape due to the temperature of the high-powered laser, and corrects these distortions.

Researchers at CSIRO developed mirror coatings and polishing techniques for the initial phase of the LIGO experiment that lasted from 2002 to 2010. A team at the Australian National University developed tip-tilt mirror suspension systems that can be used to steer the laser light with remarkable accuracy.

A group at the University of Western Australia have built a mini-LIGO experiment that is used, among other things, to study an instability the high-powered laser can induce on the mirrors, causing them to wobble uncontrollably.

Each element and each component of the incredibly complex LIGO system undergoes incredible levels of development and scrutiny.

This is perhaps best exemplified in the data analysis sphere. In Australia, we have strong groups at Monash University, the universities of Melbourne and Western Australia, the Australian National University and Charles Sturt University.

We all work on developing and running computer software that can pick a tiny signal out of noisy data streams. Somewhat infamously, LIGO puts itself through a process called blind injections.

Blind injections are performed by a very small group of people. The team inject a fake signal into the data stream by artificially shaking the mirrors of the detector in such a way that makes it look like a gravitational wave has passed through.

The unsuspecting data analysts play their usual games of analysing this data and, lo and behold, inevitably find the signal.

### An early result?

The most famous of these blind injections occurred in September 2010. Very soon after the signal was automatically



LIGO Laboratory operates two detector sites, one near Hanford in eastern Washington, and another near Livingston, Louisiana. This photo shows the Hanford detector site. LIGO/Caltech

injected into the detectors, it was picked up with the initial data analysis algorithms.

The purported signal looked like it to have come from the constellation Canis Major, and the event was subsequently called the 'Big Dog'. The collaboration then went through a six-month process of vetting, checking, and re-checking the analysis, and even wrote up a full paper to be submitted to the journal.

An independent Detection Committee reviewed all of the results, and a collaboration-wide vote was held on whether to submit the paper for peer review – the result was an anonymous 'yes'.

And then the envelope was opened: the signal was fake.

That exercise, while incredibly painful to many, shows just how seriously the LIGO Scientific Collaboration takes its science. That this latest detection was not a blind injection has been known by the entire collaboration for a long time – the experiment was only beginning to collect data, and the blind injection software had not yet been set up properly.

Less than one hour after the LIGO experiment wobbled from the

gravitational wave on that fateful day on September 14, 2015, one of us (Lasky) and fellow Monash academic and LIGO researcher Eric Thrane, who sits on the fake injection committee, were sitting at our laptops at home when we both received an email titled 'Very interesting event on ER8' (ER8 stands for Engineering Run 8, which was the name of the pre-science phase of the experiment).

A quick Skype conversation quickly ensued:

*Thrane: Have you seen the email?*

*Lasky: Yes. Is it a false injection?*

*Thrane: No!*

*Lasky: Did we just detect a gravitational wave?*

*Thrane: I think we did.*

And the rest, as they say, is history.

This is truly the dawn of a new age of discovery. The gravitational-wave universe has many untold stories to tell, and scientists across Australia are striving to tell the tale along with the rest of the world.

**Paul Lasky** is Postdoctoral Fellow in Gravitational Wave Astrophysics, Monash University. **Letizia Sammut** is Postdoctoral Research Fellow in Gravitational Wave Astrophysics, Monash University. First published at *The Conversation* ([www.theconversation.com](http://www.theconversation.com)).

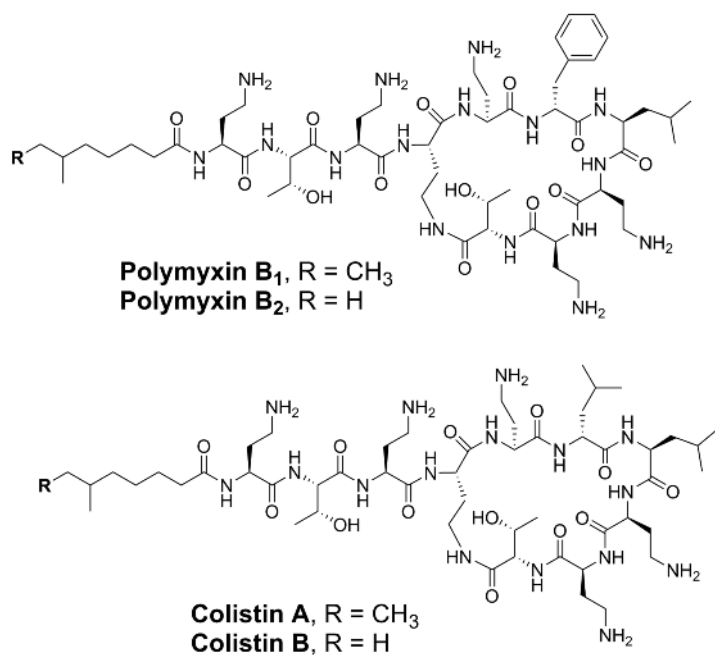
## Improving the safety and efficacy of 'last resort' antibiotics

The emergence of multi-drug resistant (MDR) gram-negative pathogens is now a major global health issue, a problem that is further compounded by the lack of development of new antibiotics.

Gram-negative bacteria, particularly *Pseudomonas aeruginosa*, *Acinetobacter baumannii* and *Klebsiella pneumoniae*, are spread worldwide in virtually all environments that support life. These opportunistic pathogens have a range of serious consequences for infected patients, including secondary meningitis, respiratory problems and ventilator-associated pneumonia.

'There are currently very limited options available for the treatment of infections caused by MDR gram-negative "superbugs". This has forced clinicians to revive "old" antibiotics such as the polymyxins,' says Dr Kade Roberts, Senior Research Scientist in the Li Lab at Monash University and project manager for the group's polymyxin drug discovery program.

Currently, polymyxin B and colistin are used as a 'last-resort' treatment for MDR gram-negative bacteria. However, effective use of these antibiotics is limited by their potential to cause kidney toxicity in patients. Delivering a smaller, suboptimal dosage does not present a viable solution, as this will decrease efficacy and potentially promote resistance to the polymyxins. There is an urgent need to develop new polymyxins that have improved safety and efficacy.



In a program based on intellectual property developed by Monash University, Dr Roberts and an interdisciplinary team of researchers aim to produce novel polymyxins with improved safety over the currently available polymyxin antibiotics.

'We are really excited by the progress of our drug discovery program to date. We have developed some really promising novel polymyxins that have significantly improved safety in animal models. Over the next 12 months two of our lead compounds will undergo IND-enabling studies. If successful, we can then move them into phase I clinical trials,' says Dr Roberts.

Dr Roberts will discuss aspects of their polymyxin drug discovery program including their novel drug design strategy, compound synthesis and lead optimisation studies at the 17th International Biotechnology Symposium (IBS 2016) to be held in Melbourne, 24–27 October 2016 ([www.ibs2016.org](http://www.ibs2016.org)).

'We are excited to be presenting our research at IBS 2016. This conference is a great platform for highlighting Australian drug discovery efforts like ours to an international audience of both academic and industry researchers from a diverse range of scientific fields,' says Dr Roberts.

This is the first time IBS will be hosted in Australia by AusBiotech, Australia's biotechnology organisation. Since 1960, IBS has been organised under the auspices of the International Union of Pure and Applied Chemistry (IUPAC) and is the most representative biotechnology event at the global level; typically more than 1000 participants congregate from academia and industry to explore the advances and frontiers of science and applied biotechnologies.

The IBS 2016 program in Australia will present the most advanced issues in biotech, green chemistry and its related fields, which will be discussed by an extraordinary group of international speakers, many of whom will travel to Australia for the first time. Topics will include agri-business; industrial and environmental biotechnology; pharmaceutical, medical and molecular; bioenergy and bio-refinery; the bio-economy, policy and investment; and biosensors and nanotechnology.

IBS 2016 will be part of International BioFest 2016, a three-conference event that paves the way for the life sciences to advance Australia's knowledge economy. These events include AusBiotech 2016, Australia's national life sciences conference, and Australia Biotech Invest, Australia's investment showcase.

This conference forms a critical part of the chemical research ecosystem and is essential to its growth, particularly for emerging elements of the industry.

Find out more at [www.ibs2016.org](http://www.ibs2016.org).

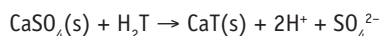
**Dr Kade Roberts** is Senior Research Scientist in the Li Lab at Monash University and project manager for the group's polymyxin drug discovery program.



## Adjusting grape and wine acidity

This month I will continue discussing options for acidification of grape juice or must and wine. A medium-size winery in Australia may spend around \$10 000 per vintage on L(+)-tartaric acid, of which a significant proportion is lost through tartrate instability. Techniques that can reduce this cost are eagerly sought after.

Plastering (great name for a wine treatment!) is a practice that evolved in Spain for the production of dry white fortified wine (aka sherry). It involves the addition of calcium sulfate, plaster of Paris, to wine and is based on  $\text{CaSO}_4$  being more soluble than calcium tartrate (CaT). The process can be represented as:



thereby releasing  $2\text{H}^+$  ions per added  $\text{Ca}^{2+}$  and reducing the pH.

While the process has been shown to be effective in pH reduction (see Gómez et al. *Food Chem.* 2015, vol. 168, pp. 218–24), there are several limitations, including a significant increase in the sulfate concentration (often regulated) and an increase in the calcium concentration that enhances potential for post-bottling CaT precipitation. Plastering does not yet have general approval for use in wine.

Cation exchange, now approved in many countries, is effective, especially for juice and wine that is high in potassium. The resin is first prepared in its hydrogen form by treatment with sulfuric acid and regenerated by the passage of sulfuric acid as required during the treatment of juice or wine. Cation exchange is far more effective in correcting acidity and pH than tartaric acid addition and it does not lead to tartrate instability, as does tartaric acid addition. Winemakers who regularly use ion exchange claim that it is relatively inexpensive compared to tartaric acid addition, provided the capital cost of the unit is not part of the equation. It is recommended to treat not more than about 20% to a very low pH (about 2.7–2.8) and then mix this treated batch with the remaining wine or juice. Experience shows that if the entire batch is treated, some 'metallic' flavours appear, leading to a reduction in quality.

A poster presented by Konrad Pixner and Ulrich Pedri at the *In Vino Analytica Scientia* conference in Trento last year, described an industrial trial on a 2012 Chardonnay juice from Sud Tyrol in Italy. The experimental design involved comparing cation exchange resin (CER; 25% treatment) with tartaric acid addition (TAA; 2.3 g/L addition) to the juice. The control (untreated) juice sample had a pH of 3.60 and a titratable acidity of 5.3. After CER treatment, the pH dropped to 3.32 and titratable acidity increased to 6.25, while the TAA treatment gave the same pH decrease, but an increase in titratable acidity to 7.57. This shows one significant advantage of CER: minimal impact on the titratable acidity value. High titratable acidity values can bring about an overly sour taste to the wine, seen as a negative in the marketplace. Reduction of the potassium ion concentration by about 25% was also achieved by CER, highlighting another advantage.

After fermentation, sensory profiling of the two treated wines was performed at six and 18 months. The data showed little difference in acidity perception between CER and TAA. However, 30 months after treatment, acidity perception was significantly lower for the CER-treated wine, suggesting that acidity perception is more constant over time with TAA adjustment.

Bipolar membrane electrodialysis was approved by the *Organisation Internationale de la vigne et du vin* in 2010. It is a rather high-tech approach and it is expensive: initial capital outlay of \$1 million or more. The bipolar membrane consists of a cation-selective layer, an anion-selective layer and a contact

**Cation exchange is far more effective in correcting acidity and pH than tartaric acid addition and it does not lead to tartrate instability, as does tartaric acid addition.**

region between the two layers. The combination of the bipolar membrane and a potassium ion selective membrane allows for removal of potassium ions from the wine and their replacement by hydrogen ions, the latter arising from electrolysis of water in the interface layer of the bipolar membrane under an applied electric field. A fuller description can be found by downloading the pdf at [bit.ly/1rDYlme](http://bit.ly/1rDYlme).

It is claimed that the approach can adjust the pH to within 0.05 pH units. It would appear from the limited published data that bipolar membrane electrodialysis is effective in reducing the pH and the potassium concentration. The phenolic index remained constant between the control and a treated red wine, implying no loss of phenolic compounds. The colour intensity was improved by the treatment, as would be expected with a lower pH. Justifying the capital cost means that the technique would only be appropriate for large wineries.



**Geoffrey R. Scollary** FRACI CChem ([scollary@unimelb.edu.au](mailto:scollary@unimelb.edu.au)) was the foundation professor of oenology at Charles Sturt University and foundation director of the National Wine and Grape Industry Centre. He continues his wine research at the University of Melbourne and Charles Sturt University. This column and the two preceding columns are based on notes that I prepared for workshops in the Mudgee and Hunter Valley wine regions. The support of the New South Wales Department of Primary Industries is acknowledged.

## Storing power

In August last year, I wrote about domestic renewable energy sources and the enthusiasm for the Tesla Powerwall battery, which was current at that time. I commented that, based on media reports and online discussion groups, it seemed that the Powerwall wasn't quite up to the task of daily charge and discharge cycles. Well, it seems that I got that wrong!

In early February this year, ABC TV's *Catalyst* program reported on a range of battery technologies for domestic and commercial power storage. The Powerwall was discussed and, by that time, it was apparent that Tesla had solved the problem of the limited number of charge/discharge cycles. According to the program, it is available with a ten-year guarantee, and the major criticism of the system was from the consumer organisation Choice, which said that the guarantee wasn't sufficient for a consumer capital item with a 20-year payback period. The best new car warranty I have seen advertised is seven years, and a 20-year working life for a car is not unheard of, so I am close to convinced that battery storage of domestically generated electricity is a new reality.

When it comes to being wrong about battery technology, I have to admit to previous form. As a freshly minted PhD in 1987, one of the first tasks I had in my new job was to evaluate a funding request from the University of New South Wales research group working on the (flow cell) vanadium redox battery (VRB). This seemed like a really elegant chemical approach to energy storage, based on the water-soluble salts of the four oxidation states of vanadium. However, ultimately I didn't recommend that the company should fund the research, mainly because we didn't own a vanadium mine. I wasn't alone, it would seem. The financial journalist Trevor Sykes (AKA Pierpont) commented in early 2004: 'A potentially revolutionary worldwide technology had been invented on their doorstep, yet all the Top 200 [Australian]

companies yawned' (*Australian Financial Review* 27 February 2004). Sykes was writing on the occasion of the opening of a wind farm on King Island that used a VRB unit to store electricity for continuity of supply. Despite its potential, the VRB hasn't set the world on fire. The Wikipedia entry on the topic lists 14 installed units with capacities between 100 kW and 5 MW (60 kWh to 20 MWh).

The University of NSW group has continued its research, and is now focusing on the zinc bromine flow battery. This, too, was featured in the *Catalyst* program in February, and the development of gel applications of the battery was also described. According to the report, the gel technology gives the potential to embed the battery in the structural components of a large building, greatly increasing the storage capacity of a given site. Most recently, a business park in Adelaide was reported to have installed a 660 kWh zinc bromine unit. The unit is located inside a standard six-metre shipping container, and was said to have the capacity to power the business park, where 50 people are employed, for four days.

These developments may signal the start of paradigm shift away from centralised generation of electricity, and the extensive transmission systems required to deliver electricity to remote areas. In developing nations, where cheap power has the potential to greatly improve quality of life, electricity could be generated from renewable sources like solar and wind, stored and distributed over small local networks. Advocates of the continued use of coal say that coal generation is cheaper, and the use of renewables would condemn developing nations to expensive electricity. However, if we Australians are being told that our electricity costs have gone up because of increased investment in 'poles and wires', then eliminating long-distance transmission might just be the low-cost answer. In addition, local generation and distribution mean the environmental footprint (land use) of the transmission system is eliminated, and the power losses in transmission and distribution are reduced.

While in retrospective mode, I'd also like to go back to April 2015, when I suggested that Australia might be a good place to store radioactive wastes from nuclear power generation. One of the Tentative Findings of the SA Royal Commission on the Nuclear Fuel Cycle was: 'The storage and disposal of used nuclear fuel in South Australia is likely to deliver substantial economic benefits to the South Australian community.' The Royal Commission delivered its final report and recommendations to the Governor on 6 May 2016, as this article went to press. The recommendations and findings will most likely have been released, and received widespread publicity, by the time you read this (provided the federal election hasn't drowned out this important policy debate in the meantime).



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... if we Australians are being told that our electricity costs have gone up because of increased investment in 'poles and wires', then eliminating long-distance transmission might just be the low-cost answer.



Tesla Motors/CC-BY-4.0

## A big day out

Since I worked one of my vacations with Cuming Smith & Co in Yarraville, where they made sulfuric acid and superphosphate, I have been interested in the processes and the sources of the raw materials. In those days (mid-1950s) the major source of sulfur was iron pyrites ( $\text{FeS}_2$ ), which was a by-product of the recovery of copper ores by flotation. The finely divided pyrites was roasted and the resulting sulfur dioxide went into lead chambers where it was oxidised with nitrogen oxides and the resulting sulfur trioxide was absorbed in water to form sulfuric acid. The acid strength was about 70%, quite all right for reacting with phosphate rock to produce superphosphate, but a different process was used to make stronger acid. The starting material was elemental sulfur that I think was sourced from Florida where it was 'mined' by the Frasch process, which involved the injection of superheated steam and water into sulfur-bearing strata and separation, after cooling, of what came up. The sulfur dioxide from this sulfur was passed with oxygen (air) over a vanadium oxide catalyst, leading to the formation of 96% sulfuric acid, or, if the oxide were dissolved in strong acid, oleum of various concentrations.

In researching the history of acid production in Australia I sometimes came across advertisements for White Island sulfur, which I knew was sourced from a volcanic island in the Bay of Plenty off the east coast of New Zealand's north island. It all came to mind last summer when I was holidaying in that region and seized the chance to visit the island and walk in an active volcano. The island, local name Whakaari, is about 50 kilometres off the coastal town of Whakatane. A two-hour boat ride or, for the well-heeled or those in a hurry, a short helicopter ride, takes visitors to the privately owned island where hard hats and gas masks are issued for the guided tour, which takes a couple of hours.

The island is the extremity of the volcanic region that includes Rotorua, but gaseous emissions at the two sites are different. In Rotorua it's hydrogen sulfide but on the island it's sulfur dioxide; steam rising from the crater is distinctly acidic. It's a spectacular place, with crystalline sulfur deposits, bubbling mud pools and a nasty-looking crater lake. My photographs provide a couple of glimpses.

James Cook passed this way in 1769, named the island on account of the steam plume, but never landed there. Long before that it was a birding place for Maori, and there are numerous gannet colonies (now protected) on the island. Sulfur production began in the middle of the 19th century and continued on and off for roughly a century, broken by eruptions from time to time and consequent losses of life and equipment. The operation generally involved loading sulfur-laden rock into an oven and collecting the molten sulfur. The guide had a fund of stories, including one about the supply boat that came to the island one month with supplies for the miners, but found nobody left ... except a pet cat. Debris from the eruption, but no bodies, washed up on nearby shores for several weeks.



Approaching White Island by boat.



Sulfur and acidic steam on White Island.

The Cuming Smith company was using White Island sulfur in 1882, and in the same year the New Zealand Drug Company (Kempthorne Prosser) used it to produce 50 tons of sulfuric acid, thereby winning a government reward for the establishment of a new industry. Their counterparts in Melbourne, Felton Grimwade, had brokered a deal between the New Zealanders and Cuming Smith in Melbourne. The technology transfer was achieved by the transfer of George Smith, who made his subsequent career with the Kiwis although the Melbourne company retained his name.

There were no rumbles while I was ashore but the landscape showed evidence of successive instances of being torn apart, interspersed with the deposition of layers of volcanic ash. Prevailing winds kept the worst of the fumes away from the steep northern flanks of the island, where there was some grass and that's where the gannets were seen. Dolphins played around our boat as we made our way to and from the island and gannets followed them, diving in characteristic fashion when they saw that the dolphins had rounded up a shoal of fish.

Altogether, quite a day out.



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



## 2nd Energy Future Conference and Exhibition

4–6 July, University of NSW, Sydney, NSW  
<http://energystoragealliance.com.au/event/energy-future-conference-exhibition>

## 7th Heron Island Conference on Reactive Intermediates and Unusual Molecules

9–15 July 2016, Heron Island, Qld  
[www.Heron7.org](http://www.Heron7.org)

## 27th International Conference on Organometallic Chemistry (Incorporating the RACI Inorganic Chemistry Division Conference)

17–22 July 2016, Melbourne Convention and Exhibition Centre, Melbourne, Vic.  
<http://icomc2016.com>

## International Conference and Exhibition on Marine Drugs and Natural Products

25 July 2016, Rydges, Melbourne, Vic.  
<http://naturalproducts.pharmaceuticalconferences.com>

## Seminar on GHS

27 July 2016, FB Rice, Melbourne  
[bit.ly/1qp72iE](http://bit.ly/1qp72iE)

## NZIC-16

21–24 August 2016, Millennium Hotel, Queenstown, New Zealand  
[www.nzic16.org](http://www.nzic16.org)

## 6th International Meeting on Antimicrobial Peptides

1–3 September 2016  
 Leipzig, Germany  
<http://peptideconferences.org/imap-2016>

## European Symposium of Biochemical Engineering Sciences (ESBES)

11–14 September 2016, Dublin, Ireland  
[www.esbes2016.org](http://www.esbes2016.org)

## Chemeca 2016

25–28 September 2016, Adelaide Convention Centre, Adelaide, SA  
[www.chemeca2016.org](http://www.chemeca2016.org)

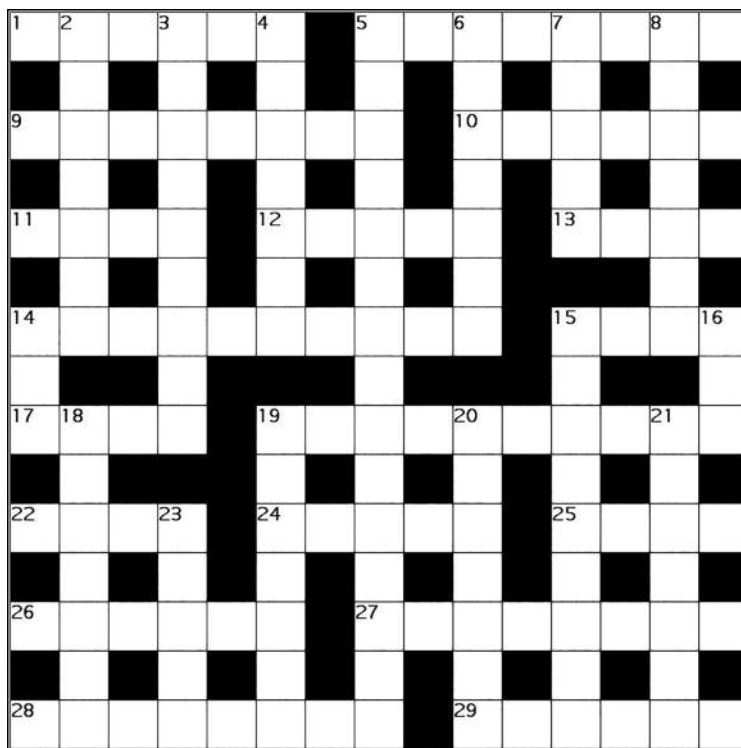
## 6th International Conference and Exhibition on Pharmaceutical Regulatory Affairs and IPR

29 September – 1 October 2016, Orlando, Florida, US  
<http://regulatoryaffairs.pharmaceuticalconferences.com>

## AusBiotech 2016

24–26 October 2016, Melbourne Convention Centre, Vic.  
[www.ausbiotechnc.org](http://www.ausbiotechnc.org)

RACI events are shown in blue.



### Across

- 1 Mob sounds out worthless material in a mineral deposit. (6)
- 5 New cage pins are breaking away. (8)
- 9 Outage duration feathers opportunity. (8)
- 10 Leave out exchange of carbon with phosphorus to get forecast. (6)
- 11 How much is tungsten covering? (4)
- 12 Bird the French name. (5)
- 13 Positions groups. (4)
- 14 They come before dogs tied up in new radical ropes. (10)
- 15 Two or three elements of prejudice. (4)
- 17 Account of proposed law. (4)
- 19 Time planning design of clues hiding loss of iodine. (10)
- 22 Within an orientation of a group attached to a non-bridgehead atom. (4-)
- 24 Radical current for freeway exits. (5)
- 25 Last η ζ. (4)
- 26 Where we work lie new species likely to change. (6)
- 27 Revolutionary passed away sulfur and, perhaps, metallocenes. (8)
- 28 Authentic eccentric person. (8)
- 29 Spoiled without a colour added. (6)

### Down

- 2 One more near hot change. (7)
- 3 Client age is transformed when considering the study of heredity. (9)
- 4 Sends out within system it terminates. (7)
- 5 Choose chrome reaction with iodine, carbon and aluminium involving a cell. (15)
- 6 Wrote about Sawyer and Finn in *Miracle Men* study. (7)
- 7 Plays guitar selections. (5)
- 8 Path has sodium and hydrogen reacting with a hydrocarbon mixture. (7)
- 14 Three elements with a bar. (3)
- 15 Constant Spooner loses feathers – a no-no. (9)
- 16 Slump upstate. (3)
- 18 Iodine on protactinium spectrum? There's a positive and there's a negative. (3,4)
- 19 Spike on cutter. (7)
- 20 Moving down line of ancestry. (7)
- 21 R–N: and inert neon reaction. (7)
- 23 Unsettled oxygen pinion. (5)

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

## History of chemistry at the 251st ACS national meeting

The twice-yearly national meetings of the American Chemical Society are large and impressive events. More than 16 000 delegates attended this meeting in San Diego in mid-March. However, as the convention centre and surrounding hotels are used for particular branches of chemistry, there was no sense of overcrowding. I attended the three days of presentations of the Division of the History of Chemistry, which were of a high standard.

The first morning was devoted to six general papers and the afternoon to five papers on the topic of 'Preceptors of chemistry'. On the second day, there were 12 papers on the program with the overall general title 'The posthumous Nobel Prize in chemistry. Correcting the errors and oversights of the Nobel Prize Committee', though only ten of these papers could be presented because two intended presenters had health problems.

This topic allowed for some mixture of the hypothetical and the factual and revealed the tensions and the occasional personal animosity between chemists, which may have led to some unjust exclusions from the Nobel Prize. There was also the suggestion that R.B. Woodward may have deserved two Nobel Prizes. Overall, it was a good topic, which gave room for speculation as to what might have been and provided

information about the lives of some great chemists. Further information about five of the papers presented can be found in an article by Borman in *Chemical and Engineering News* (2016, vol. 94(15), pp. 19–21) with more suggestions for deserving Nobel recipients available in the online discussion of the article.

On the third day, there were four more general papers presented in the morning session. I found the last of these papers entitled 'R.J.P. Williams and the chemical sequence of natural history' presented by B.J. McFarland of particular interest as he discussed the role of chemistry as a determinant of biological evolution and the importance of the periodic table in sequencing the development of the Earth and life (McFarland, *A world from dust: how the periodic table shaped life*, Oxford University Press, 2016).

In the afternoon, the Division of the History of Chemistry joined with the Division of Inorganic Chemistry to honour the life and work of Karen J. Brewer, who had recently passed away, with a Memorial Symposium.

The next ACS National meeting will be in Philadelphia, 21–25 August 2016.

Bill Palmer FRACI CChem



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**Mr Paul Perreault** – CEO and Managing Director, CSL, USA



*Biotechnology and innovation: risk and precaution: social license or not?*

**Prof Sir Peter Gluckman** – Chief Science Advisor to the Prime Minister, Office of the Prime Minister, New Zealand



*2016 Millis Oration*

**Prof Ian Gust AO** – Professorial Fellow, University of Melbourne



*A New Model for Drug Development in Academic Institutions*

**Prof Dennis Liotta** – Executive Director Emory Institute for Drug Development, Emory College, Atlanta USA



*Interrogating and Guiding the Microbiome for Macro-organism Health and Productivity*

**Dr James Tiedje** – Director, Centre for Microbial Ecology, Michigan State University, USA



*Self-Assembled Supramolecular Nanosystems for Targeting Therapy of Intractable Diseases*

**Prof Kazunori Kataoka** – Professor, Department of Materials Engineering and Bioengineering Graduate Schools of Engineering, University of Tokyo, Japan



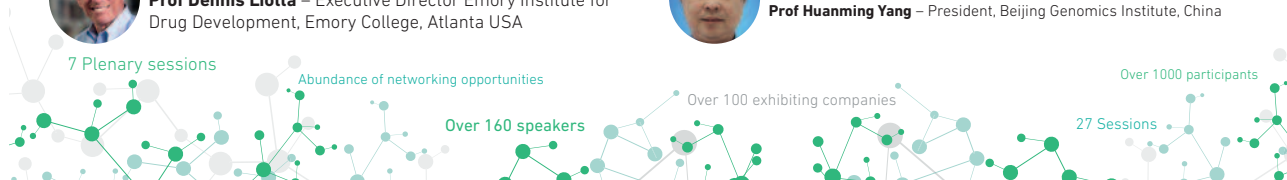
*Synthetic Designer Vaccines Protect from Bacterial Infections*

**Prof Dr Peter Seeberger** – Director, Max-Planck Institute of Colloids and Interfaces, Germany



*Biotech and the future of man*

**Prof Huanming Yang** – President, Beijing Genomics Institute, China





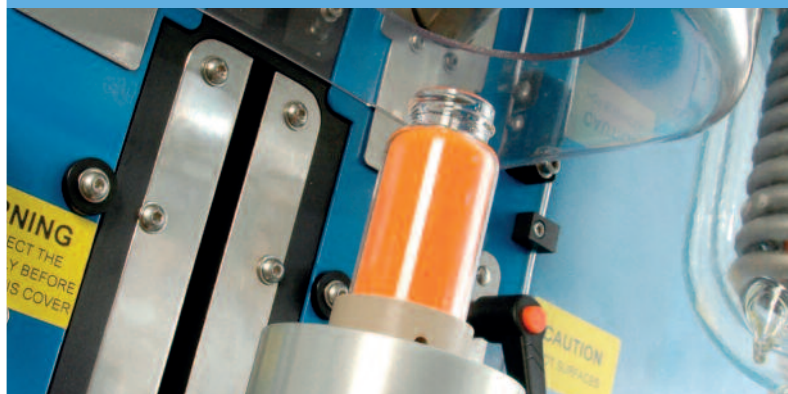
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