

# chemistry

August 2017

in Australia

## Stowaways: managing the burden of ballast water



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August 2017



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## From the President

On 22 April this year, a March for Science was held in 600 cities worldwide in attempts to have scientists of all disciplines recognised for what they do and to ensure science is funded to required levels. There were 12 sites in Australia, including Townsville where I attended along with several hundred interested scientists and the public. While this event may have sprung to life after science funding cuts in the US and was initially a political protest, organisers began to realise the weight behind the scientific movement worldwide and it morphed into a rally for recognition.

The March for Science was a global event bringing together people from all walks of life who say we need more evidence and reason in our political process. Public discovery, distribution and understanding of scientific knowledge as crucial to the freedom, success, health and safety of life on this planet was championed.

March for Science is a non-partisan group, marching to promote stable public science funding, open communication of science, evidence-based policy, and greater scientific literacy and education in critical thinking.

The aims of the march were around fostering a flourishing culture of robust scientific pursuit, ensuring that the knowledge gained through science is used for the public good, and improving the public's relationship with the scientific process and a universal literacy in science.

Among its endeavours, March for Science Australia calls for world-class science education and teaching of critical thinking skills in Australian schools, and a well-informed community. March for Science supports initiatives to promote:

- broad public knowledge and discussion of scientific work and science education that teaches children and adults to think critically, ask questions and evaluate truth based on the weight of evidence
- open communication
- decision-makers genuinely considering all the available evidence when formulating policy
- long-term public investment in scientific research by the Australian government, to provide researchers with the stability needed to plan and execute large-scale projects
- investment in basic research as a matter of priority.

There has been a shift in recent years towards a focus on commercialising research. This is an essential area but cannot come at the expense of basic, or 'blue-sky', research (research for which the applications are not immediately obvious).


Anyone who values the role of science in society was encouraged to take part in the March for Science.

The RACI was reasonably quiet during this March for Science campaign. While we do not want to get heavily involved in the politics of other countries, I believe the RACI should be the voice of chemistry in Australia. Scientists have struggled for so long to ensure funding investments are made to support their endeavours, and this campaign may be the start of something bigger for which I feel the RACI should have a voice.

The march is complete for 2017 and now there is a call to act on outcomes of discussions, workshops etc. held during the march. Look for 'March for Science' on Google, Twitter and Facebook. We should be supporting such ambitious activities around the globe and I encourage chemists and their science colleagues to get behind this movement.



**Peter Junk** FRACI CChem (president@raci.org.au) is RACI President.



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## Aberdeen alumni

I greatly enjoyed Ian Rae's piece in the June issue (p. 41) about Alexander Findlay and other chemists, having been associated with the University of Aberdeen. I might be able to add to its content by pointing out that James Clerk Maxwell (1831–79) was Professor of Natural Philosophy at Marischal College, Aberdeen, at the time of its merger with King's College to form the University of Aberdeen. He is remembered and honoured as a physicist, but his endeavours did take him into physical chemistry. The best-known example of this is the Maxwell distribution, which every chemistry student is taught about in the physical chemistry component of his or her course.

I experienced quite a surge of nostalgia when I saw the photograph of Marischal College in Ian's article, having memories of visits there for two reasons: examination invigilation and degree ceremonies. Nowadays, only one wing of Marischal College is used for university purposes. The rest comprises the Aberdeen City Council Headquarters, an arrangement that has been in place since 2011.

Clifford Jones FRACI CChem

## Soil lead levels

The work done by the Macquarie University team on lead concentrations in Sydney backyards (June p. 34) is an admirable example of chemistry being applied for the public good. However, it seems Mark Taylor's team might be misapplying the soil Health Investigation Levels (HILs) listed in the *National Environment Protection (Assessment of site contamination) Measure 1999* ('the NEPM'), which sets the standards for conducting contaminated site investigations in Australia (it was updated in 2013). They write of the '300 mg/kg Australian health guideline' for lead in soil. The value of 300 mg/kg is the HIL applicable for low density housing and other sensitive sites (e.g. primary schools, childcare centres). However, the NEPM explicitly states: 'Investigation and screening levels are not clean-up or response levels, nor are they desirable soil quality criteria'.

The HILs were set on the basis of a number of assumptions about human exposures and the characteristics of the contaminant in solution. These include: home-grown fruit and vegetables represent less than 10% of the total amount consumed; the lead in soil is only 50% bioavailable; and a blood lead concentration of 10 µg/dL is the target that should not be exceeded. The NHMRC has more recently revised this last value to 5 µg/dL. These are among the range of factors to be considered if lead (or other contaminant) concentrations exceed the relevant HIL.

The NEPM provides additional guidance about how the HIL values should be applied. It suggests that where a HIL is exceeded, the 95% upper confidence limit of the mean concentration, the standard deviation of results, and the maximum concentration also be considered. Under some circumstances, it may be acceptable to allow soil with

individual sample concentrations up to 250% of the HIL to remain on site. Therefore, in the data provided by Taylor's team, many of the soil samples taken in backyards and vegetable gardens, and with lead concentrations greater than 300 mg/kg, might be acceptable for on-site use.

The article is right to point out that that airborne lead and lead-based paint on the site can contribute to elevated lead concentrations in soil. However, caution also needs to be exercised in importing 'clean garden soil' into garden beds. Occasionally, these soils from garden suppliers have a proportion of sewage treatment plant sludge incorporated in the mix, and elevated concentrations of metals can be present.

Paul Moritz FRACI CChem



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Last year, an investigation by the US Chemical Safety Board warned that regulatory changes to date do not sufficiently empower the regulator to oversee industry efforts to prevent another disaster like the Deepwater Horizon rig explosion and oil spill in 2010.

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**Without CSB carrying out independent, non-judgemental investigations, US chemical and petrochemical industries would be without one of the key tools they need to reduce the risk of catastrophic accidents.**

Ian Whewell, former HSE director of offshore safety, US Health and Safety Executive

## US Chemical Safety Board faces uncertain future

Under US President Donald Trump's proposed 2018 budget, the world's only independent body dedicated to investigating chemical-related industrial accidents would be abolished. A story in *Chemical & Engineering News* ([bit.ly/2rRSygE](http://bit.ly/2rRSygE)) revisits why the US Chemical Safety & Hazard Investigation Board was initially created, its accomplishments and what experts say about its potential demise.

Jeff Johnson, a special correspondent to *C&EN*, notes that the board – also known as the Chemical Safety Board, or CSB – was called for in the 1990 legislative overhaul of the Clean Air Act. But the board lacked the necessary support from presidents George H.W. Bush and Bill Clinton, so industrial chemical accident investigations were delegated to other agencies. But stalled investigations into a 1995 explosion at a New Jersey facility that killed five workers and destroyed surrounding businesses led to pressure from unions, community groups, the state's governor and a senator to fund the CSB. In 1998, the board opened its doors.

Since then, the CSB has investigated some 130 accidents, and has produced more than 90 accident reports and about 40 safety videos. The board has positively influenced industrial and chemical safety in the US and elsewhere, industrial accident experts told *C&EN*, and with a budget that has never exceeded \$12 million in any given year, they say that's a good deal.

American Chemical Society

## Changes to NHMRC funding announced

The National Health and Medical Research Council (NHMRC) has announced changes to its grant funding program that supports Australia's health and medical researchers. The NHMRC's restructured program will include four types of grants, and limits will be placed on the number of grants an individual researcher can apply for or hold. Assessment of Investigator Grants and Synergy Grants will focus mainly on track record, and assessment of Ideas Grants will focus primarily on the science, innovation and significance of the proposed research.

National Health and Medical Research Council

**I am encouraged that assessment of some grants under the new arrangements will be blinded to gender, age, career stage and institution.**

Andrew Holmes FRACI CChem, President, Australian Academy of Science



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## IChemE Safety Centre to publish insight in Health and Safety Body of Knowledge



Pam Pryor and Trish Kerin at ICHEM's annual safety conference, Hazards Australasia 2016.

The Institution of Chemical Engineers (ICHEM) Safety Centre and the Safety Institute of Australia have published two new chapters in the Occupational Health and Safety Body of Knowledge ([www.ohsbok.org.au](http://www.ohsbok.org.au)). The launch followed 18 months of collaborative working, aimed at closing the knowledge gap between health and safety professionals and process safety engineers.

Completed by a cross-discipline team of both ICHEM Safety Centre (ISC) members and Safety Institute Australia (SIA) members, the chapters were launched in April. They focus on process hazards in the chemical industries, and process safety management respectively.

There were 178 workplace safety incidents reported in Australia last year according to SafeWork Australia. Seventeen of these occurred in the process industries, which includes chemicals, oil and gas, pharmaceutical production and food production.

ICHEM Safety Centre Director, Trish Kerin, hosted the launch with a webinar entitled 'An Introduction to Process Safety'.

'The collaboration between ISC and SIA has been a positive step in closing the gap between process safety and more generalist health and safety roles ... A basic knowledge of

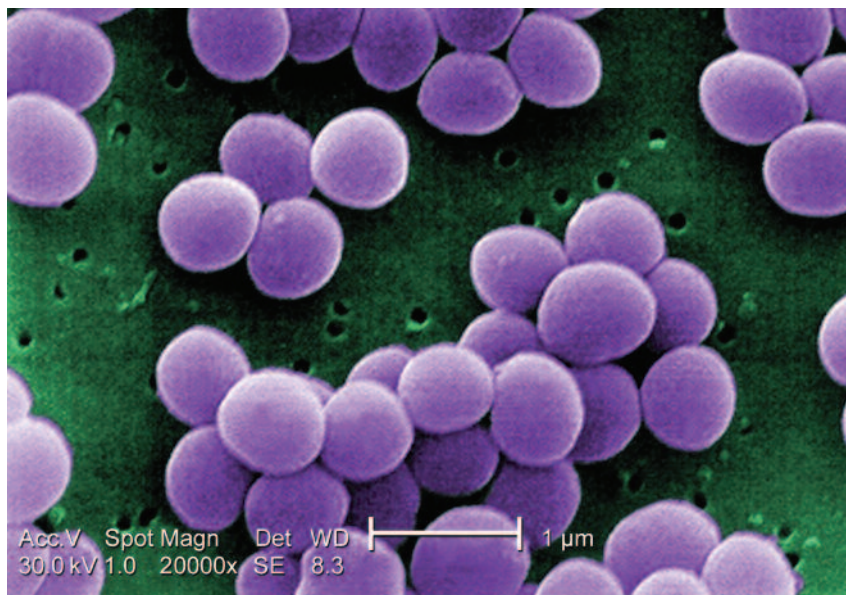
process safety is essential to improving your safety competencies more generally, whether you work in the process industries or not.'

Pam Pryor, Registrar of the Australian OHS Education Accreditation Board, custodian of the OHS Body of Knowledge, said, 'These new chapters are a fantastic addition to the Body of Knowledge. The evidence is clear; all health and safety generalists should have a basic knowledge of process safety, particularly when they are operating in high-risk environments. I am confident that this development will be essential to closing the current gap of knowledge, and in turn reduce the number of incidents, not only in Australia, but on a global scale.'

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Institution of Chemical Engineers

## Atomic-level motion may drive bacteria's ability to evade immune system defences



A scanning electron micrograph of *Staphylococcus aureus*. The scientists conducted their experiments on *S. aureus*, a common cause of skin, sinus and lung infections.

Janice Haney Carr, Centers for Disease Control and Prevention/Wiki

A study from Indiana University, USA, has found evidence that extremely small changes in how atoms move in bacterial proteins can play a big role in how these microorganisms function and evolve.

The research, published in *Proceedings of the National Academy of Sciences* (doi: 10.1073/pnas.1620665114), is a major departure from prevailing views about the evolution of new functions in organisms, which regarded a protein's shape, or 'structure', as the most important factor in controlling its activity.

'This study gives us a significant answer to the following question: How do different organisms evolve different functions with proteins whose structures all look essentially the same?' said David Giedroc, Lilly Chemistry Alumni Professor, who is senior author on the study.

The study also provides new insights into how microorganisms respond to their host's efforts to limit bacterial infection.

'What we've shown is atomic-level motional disorder – or entropy – can impact gene transcription to affect the function of proteins in major ways, and that these motions can be "tuned" evolutionarily', said Daiana A. Capdevila,

a postdoctoral researcher in Giedroc's lab, who is first author on the study. 'This may allow bacteria to rapidly evolve new ways to overcome medical treatment since atomic motions can be optimised for function more easily than a physical structure.'

In the battle between bacterial infection and modern medicine, she said a key step is 'mapping' the enemy's territory. Unravelling the molecular structure of proteins that trigger the mechanisms that thwart the human immune system informs the design of new drugs. However, this approach is based on the assumption that a protein's shape fundamentally controls its behaviour.

It also assumes proteins are rigid. The new study shows protein function is better understood by studying the structure's internal atomic motion.

Specifically, Giedroc and colleagues analysed the protein CzrA that controls how bacteria regulate zinc levels, an important ability that provides microorganisms the power to resist the human immune system. Zinc regulation allows the body to fight off infection by

either flooding invaders with zinc, causing cellular death or completely starving them of the element, which also kills infectious agents.

Through the use of NMR spectroscopy, the scientists measured the movement of atoms in CzrA and identified those most affected by zinc. They then 'swapped' these atoms with different amino acids and found that the protein almost completely lost the ability to regulate zinc levels in cells. The experiment revealed unexpected areas on the molecule that appeared to play a role in zinc regulation, despite their physically distant location on the protein 'map.'

'There's no way anyone could have predicted these areas played a role in zinc regulation by simply looking at the protein structure,' Giedroc said. 'Once you know where these "hot spots" are located, however, it's theoretically possible to design a small molecule or drug to produce the same effect as our amino acid-swapping experiment – that is, to essentially shut off the protein.'

In fact, this is one of the main concepts behind a powerful new class of drugs called 'allosteric drugs', so named because they're designed to affect areas on a protein – called allosteric sites – that enhance or regulate the primary function of the protein, such as zinc binding, without directly targeting the part of the protein that controls the primary function.

'This is really about thinking about the functions of proteins in the context of a network – not simply targeting a single strategic point but rather looking at the system holistically,' Giedroc said. 'And this particular study shows the most effective way to gain this deeper knowledge requires going beyond the molecular level in proteins to understand how atomic motion plays a role in function – after which you can start applying that knowledge to designing more effective drug-based therapies.'

Indiana University



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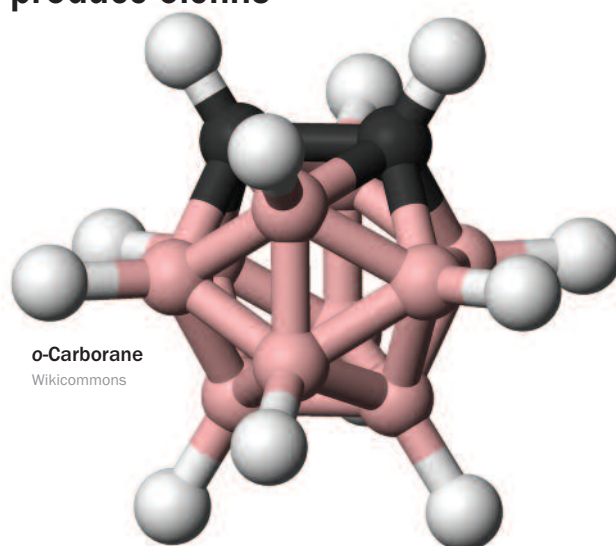
## A more energy-efficient catalytic process to produce olefins

Research at the University of Pittsburgh, USA, into a more energy-efficient catalytic process to produce olefins could influence potential applications in diverse technology areas from green energy and sustainable chemistry to materials engineering and catalysis.

‘Carboranes: the strongest Brønsted acids in alcohol dehydration’ (*Catalysis Science & Technology*, doi: 10.1039/C7CY00458C) was authored by Giannis Mpourmpakis, assistant professor of chemical and petroleum engineering, PhD candidate Pavlo Kostetsky and undergraduate student Nicholas A. Zervoudis.

‘Carboranes are one of the strongest known acids, but little is known about how these molecular catalysts can dehydrate biomass-derived alcohols’, Mpourmpakis explained. ‘Our computational research not only detailed the mechanism under which alcohols dehydrate on these catalysts, but most importantly we developed linear relationships between the energy input needed to observe dehydration of alcohols and the alcohol characteristics.’

According to the paper, ‘these obtained relationships are especially relevant to the field of solid acid catalysis, a widely studied area with a vast range of industrial applications, including the formation of olefins (polymer building blocks) from biomass-derived alcohols as well as fuels and chemicals from sugars and polyols’. The group’s research focused on



o-Carborane  
Wikicommons

primary, secondary and tertiary alcohols, and revealed the slope of linear relationships depending on the reaction mechanism.

‘This research is important because now experimentalists have a way to identify the reaction followed when different alcohols dehydrate’, Mpourmpakis said. ‘Because this process involves biomass-based production of polymers, we can potentially create a more sustainable and energy-efficient process.’

University of Pittsburgh

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## New projects at UWA: mine tailings and groundwater

Research that aims to reduce the risk of mine tailings failure and a project to improve understanding of the ecology and hydrology of streams in arid areas are two new research projects at the University of Western Australia to receive Federal Government funding.

Professor Andy Fourie, from the School of Civil, Environmental and Mining Engineering, and his team will use a \$630 000 grant plus \$720 000 cash and \$540 000 in-kind support from partner organisations to develop techniques to predict and mitigate the risk of failure in mine tailings storage facilities.

Dr Pauline Grierson and Dr Greg Skrzypek, from the West Australian Biogeochemistry Centre within UWA’s School of Biological Sciences, will use a \$620 000 grant plus \$400 000 cash and \$800 000 in-kind support from partner organisations.

They will work with researchers from Rio Tinto and the National Centre for

Groundwater Research and Training at Flinders University to investigate how surface groundwater affects the ecology of ephemeral streams, with a focus on the Pilbara region of northwestern Australia.

‘Findings from the study will be used

in conjunction with monitoring programs to help prevent and mitigate unwanted environmental outcomes of mining and other land management on groundwater resources and ecological values of these important ecosystems’, Dr Grierson said.

University of Western Australia

Ephemeral stream in the Hamersley Range, in the Pilbara region.

Alexandra Rouillard



# Middle East's first synchrotron opens in Jordan



Infrared beamline scientist Dr Gihan Kamel checks particle analysis data at SESAME International Research Centre, Jordan. Dean Calma/IAEA

SESAME, the Middle East's first major international research centre for science application research, was inaugurated on 16 May. It will see scientists from across the region and beyond work side by side in researching the peaceful uses of nuclear technology. The International Atomic Energy Agency (IAEA) has been closely associated with the project and is an observer on the SESAME council.

The facility will foster innovative scientific and technological research in areas ranging from biology, archaeology and medical sciences to studying the basic properties of materials science, physics, chemistry and life sciences.

'This centre, it is hoped, will also prevent and reverse the "scientific" brain drain and encourage scientists to contribute to the development of the people of the region', said Khaled Toukan, Chairman of Jordan Atomic Energy Commission. As a scientific and cultural bridge between diverse societies,

this centre of excellence is open to all scientists from the Middle East and elsewhere, he added.

SESAME is modelled on CERN (European Organization for Nuclear Research) and was developed under the auspices of the United Nations Educational, Scientific and Cultural Organization (UNESCO).

Scientists and engineers from Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the Palestinian Authority and Turkey – the current members of SESAME – have been involved in the preparatory work at the facility since 2004.

At the heart of the facility is a Synchrotron-light for Experimental Science and Applications (i.e. SESAME), which is capable of generating intense light beams for advanced scientific and technical research. It belongs to the family of synchrotron facilities.

'SESAME is an achievement both in terms of science and international

relations and its success is due to the interest and confidence of all involved', Toukan said. 'The support provided by the European Commission, as well as various international and national laboratories and organisations including the IAEA is well recognised.'

As a first step towards commissioning this synchrotron facility, the precise testing and circulation of the beam light in the 'storage rings' has been successfully achieved in the 2.5 GeV (gigaelectronvolt) compact high-performance light-source machine. The aim of this Centre is to have 24 beamlines covering a wide range of scientific applications. Two of these beamlines – the infrared and the XRF (X-ray fluorescence) – have been installed and are ready for producing photons.

The multipurpose infrared beamline will be used for a number of applications such as biological and materials science studies.

The facility will enable visiting scientists, including university students and researchers, to participate in experiments on synchrotron radiation sources, analyse the data obtained and acquire and share scientific expertise and knowledge, Toukan said.

The facility's managers plan to take up joint projects with other international synchrotron radiation laboratories to develop and improve features of beamlines around specific scientific research projects, as well as undertake projects involving SESAME members in areas such as environmental and cultural heritage studies tracing the origin of materials.

The IAEA has helped in the successful commissioning of the SESAME magnets, hands-on training in areas such as beamlines technology, installation, and testing of equipment in a high performance synchrotron radiation research centre, Toukan said.

International Atomic Energy Agency



## International prize for PhD student

Research into canola processing and the effect on bioactive components in the oil has earned a Charles Sturt University (CSU) PhD student international recognition.

Ms Clare Flakelar MRACI (pictured with her award), who is a member of the Graham Centre for Agricultural Innovation, was presented with a student excellence award at the American Oil Chemists' Society conference in Florida, USA.

Her research examines how canola oil processing affects the concentration of bioactive compounds.

'Many bioactive components in canola oil are linked to beneficial health effects', Flakelar said. 'For example, commercial canola seed contains lutein, a bioactive compound with the potential to prevent macular degeneration.'

'But these components, particularly carotenoids, tocopherols and sterols, are reduced or eliminated entirely during current commercial oil production.'

'My research involves assessing the behaviour and influence of certain factors on these bioactive components, primarily the effects of genotype, the storage of seed and oil, and the processing from seed to oil.'

'My goal is to provide industry with

some of the information they need to pursue the retention or enhancement of bioactive compounds in end-product oil for consumer health benefit.'

Flakelar said it was a thrill to be presented with the award and to present her research at the conference.

Her research is supervised by Associate Professor Paul Prenzler from CSU's School of Agricultural and Wine Sciences.

'This award is open to postgraduate students from all over the world,' Prenzler said. 'Not only is this award well

deserved for Clare's hard work, but it also shows that the Graham Centre has the capacity to undertake world-class research in oils chemistry.'

'Clare has already published her work in some of the best food chemistry journals, and there are more high-quality papers to come. On top of this academic success, she has developed strong links with oil processors in Australia who are very excited about the possibilities her research opens up to develop new products.'

Graham Centre for Agricultural Innovation



## New Crayola blue inspired by discovery of YInMn pigment

Crayola is introducing a new blue crayon colour inspired by the discovery of a 'new to the world' blue pigment. YInMn Blue, the vibrant pigment discovered in 2009 by chemist Mas Subramanian and his team at Oregon State University, is the inspiration behind Crayola's newest crayon colour.

On 1 July, Crayola released the top five blue crayon colour names. Consumers can vote for their favourite colour and view the real-time, daily voting results at [Crayola.com/NewColor](http://Crayola.com/NewColor). Voters will be entered for a chance to win one of six grand prizes of an all-expense paid trip for four to the Orlando Crayola Experience and a daily prize of the award-winning Crayola Air Marker Sprayer.

Crayola will unveil the new blue crayon colour name and the six grand prize winners in early September 2017.

Crayola



## Plutonium discovery lights way to clean up nuclear waste

Plutonium has long been part of many countries' nuclear energy strategies, but scientists are still unlocking the mysteries behind this complicated element and seeing how they can use heavier nuclear elements to clean up nuclear waste.

Now, new research by Florida State University Professor Thomas Albrecht-Schmitt shows that plutonium doesn't exactly work the way scientists thought it did. The findings will contribute to his team's efforts to develop technologies to clean up nuclear waste. The work was published in *Nature Chemistry* (doi: 10.1038/nchem.2777).

Albrecht-Schmitt and a team of researchers have been studying plutonium for almost two decades to understand how it behaves chemically, and how it differs from lighter elements such as iron or nickel. To Albrecht-Schmitt's surprise, a plutonium-organic hybrid compound that his team assembled in the lab behaved much like compounds made with lighter elements.

'What makes this discovery so interesting is that the material – rather than being really complicated and really exotic – is really, really simple', Albrecht-Schmitt said. 'Your imagination goes wild, and you think: "Wow, I could make that class of compound with many other types of heavy elements". I could use other heavy elements like uranium or maybe even berkelium.'

The team observed that electrons were shuttling back and forth between two different plutonium ions.

The movement of electrons between two positive ions is an action that typically happens between ions of lighter elements such as iron, which is why lighter elements are often used in



Thomas Albrecht-Schmitt is the Gregory R. Choppin Professor of Chemistry at Florida State University. Bill Lax/Florida State University

biology to accomplish chemical reactions.

Albrecht-Schmitt said his team immediately realised there was something unique about the compound they had engineered in the lab simply because of its colour.

'Plutonium makes wild, vibrant colours', Albrecht-Schmitt said. 'It can be purple, it can be these beautiful pinks. It can be this super dark black-blue. This compound was brown, like a beautiful brown chocolate bar. When we saw that colour, we knew something was electronically unusual about it.'

Albrecht-Schmitt's work is part of his lab's overall mission to better understand the heavier elements at the very bottom of the periodic table. Last year, he received \$10 million from the Department of Energy to form a new Energy Frontier Research Center that will focus on accelerating scientific efforts to clean up nuclear waste.

'In order to develop materials that, say, trap plutonium, you first have to understand at the most basic level, the electronic properties of plutonium', Albrecht-Schmitt said. 'So that means making very simple compounds, characterising them in exquisite detail and understanding both experimentally and theoretically all of the properties you're observing.'

Albrecht-Schmitt and his research team have conducted similar work on the elements californium and berkelium.

Florida State University

## EPP Group reacts to impending US withdrawal from Paris Agreement

US President Trump's decision to withdraw from the Paris Agreement on fighting climate change has been met with regret by the EPP Group in the European Parliament.

'Trump's decision is a sad one, but I am certain that the Paris Agreement and the worldwide efforts to fight climate change will survive Donald Trump. Europe and the rest of the world need to give a strong signal. We need to fulfil our commitments and continue the international process on climate mitigation. At the same time, it is more important than ever to protect European industry when it produces to the best possible environmental standard', said

Peter Liese MEP, the EPP Group's Spokesman on Environment and Health.

'Trump's decision cannot be legally binding before 2020. Who knows if President Trump will still be in office at that time? Many parts of the United States, for example California, will still continue to reduce greenhouse gas emissions. The European Union and all the other partners in the agreement are committed to continuing with their commitments and the international process despite Trump's decision', said Liese.

As for the reform of the European Emissions Trading Scheme (ETS), Liese insists that companies producing

according to the best technology are not burdened by the EU ETS. 'I sincerely hope that the Council adopts the amendments that the European Parliament already adopted with a broad majority. We have to consider further action such as a border tax adjustment if the measures are insufficient. If US companies now benefit because they have no more climate obligations, such a measure should not be ruled out', the EPP Group MEP concluded.

EPP Group

**Editor's note:** The EPP Group (European People's Party group) is the political group in the European Parliament comprising deputies (MEPs) from the member parties of the European People's Party.



# With more light, chemistry speeds up

Light initiates many chemical reactions. Experiments at the Laser Centre of the Institute of Physical Chemistry of the Polish Academy of Sciences (IPC PAS) and the University of Warsaw's Faculty of Physics have for the first time demonstrated that by increasing the intensity of illumination, some reactions can be significantly faster. Here, acceleration was achieved using pairs of ultrashort laser pulses.

In order to thoroughly investigate the nature of the processes involved, ultra-short consecutive pairs of laser pulses were used, and an increase in the rate of reaction between the molecules was observed by up to several dozen per cent. The observations of the Warsaw scientists have been reported in *Physical Chemistry Chemical Physics* (doi: 10.1039/c6cp08562h).

'Our experiments provide fundamental knowledge about the physical processes that are important for the course of important light-induced reactions. This knowledge can potentially be used in many applications, especially when dealing with high-intensity light sources. These include, among others, various microscopic imaging techniques, ultra-fast spectroscopy as well as photovoltaics, particularly if light-focusing devices such as solar collectors are used', said Dr Gonzalo Angulo (IPC PAS).

In light-induced reactions, a photon with the appropriate energy excites a molecule of dye. When there is a molecule of quencher near the excited molecule, an interaction takes place: there may be a transfer of energy, an electron or a proton, between the two reactants. Reactions of this type are common in nature. A good example is electron transfer in photosynthesis, which plays a key role in the formation of the Earth's ecosystem.

A factor that can influence the acceleration of reactions is the intensity of the light that initiates them. In order to study the nature of the processes taking place, the Warsaw chemists used laser pulses lasting femtoseconds instead of the traditional continuous stream of light. The energy of the impulses was adjusted so that, under their influence, the dye molecules moved into the excited energy state. The pulses were grouped in pairs. The interval between pulses in a pair was several dozen picoseconds (trillionths of a second) and was matched to the type of reacting molecules and the environment of the solution.

'The theory and the experiments required care and attention, but the physical idea itself is quite simple here', noted Jadwiga Milkiewicz, a PhD student at IPC PAS. 'In order for the reaction



Some chemical reactions can be accelerated by increasing the intensity of illumination – this has been demonstrated by researchers from the Institute of Physical Chemistry of the Polish Academy of Sciences in Warsaw. IPC PAS, Grzegorz Krzyzewski

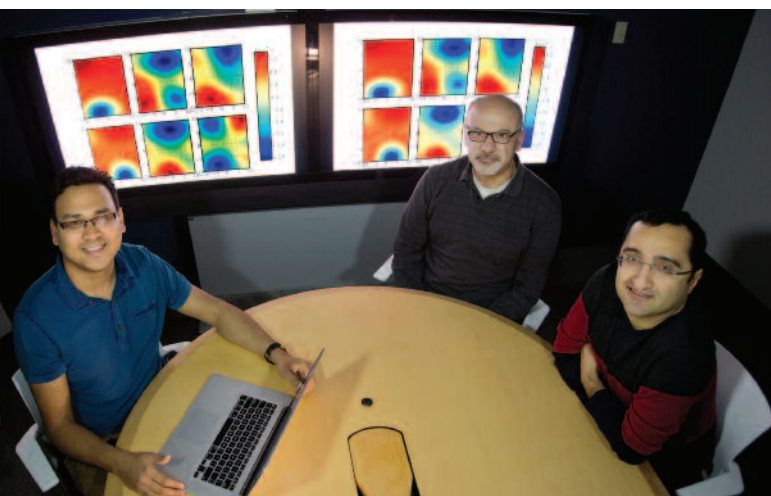
to occur, there must be a molecule of quencher near the light-excited dye molecule. So, if we have a pair of molecules that have already reacted with each other, this means that they were close enough to each other. By increasing the number of photons in time, we thus increase the chance that if, after the reaction, both molecules have managed to return to their ground state, the absorption of a new photon by the dye has the potential to initiate another reaction before the molecules move away from each other in space.'

The course of reactions in solutions depends on many factors such as temperature, pressure, viscosity or the presence of an electric or magnetic field. This research has proved that these factors also influence the acceleration of the chemical reaction that occurs with an increased intensity of illumination. Under some conditions, the acceleration of the reaction was unnoticeable; under optimal conditions, the rate of the reaction increased by up to 25–30%.

'In our experiments so far, we have concentrated on light-induced electron transfer reactions; that is, those which change the electrical charge of the molecules. However, we do not see any reason why the mechanism we have observed could not function in other variations of these reactions. So, in the near future, we will try to confirm its efficacy in energy transfer reactions or in reactions involving also proton transfer', said Angulo.

Institute of Physical Chemistry of the Polish Academy of Sciences

## Maths techniques to improve computational efficiency in quantum chemistry



Sandia National Laboratories researchers Prashant Rai (left), Habib Najm (centre) and Khachik Sargsyan discuss mathematical techniques used to study the behaviour of large molecules at quantum scale. Dino Vournas

Researchers at Sandia National Laboratories in the US have developed new mathematical techniques to advance the study of molecules at the quantum level. Mathematical and algorithmic developments along these lines are necessary for enabling the detailed study of complex hydrocarbon molecules that are relevant in engine combustion.

Existing methods to approximate potential energy functions at the quantum scale need too much computer power and are thus limited to small molecules. Sandia researchers say their technique will speed up quantum mechanical computations and improve predictions made by theoretical chemistry models. Given the computational speed-up, these methods can potentially be applied to bigger molecules.

Sandia postdoctoral researcher Prashant Rai worked with researchers Khachik Sargsyan and Habib Najm at Sandia's Combustion Research Facility and collaborated with quantum chemists So Hirata and Matthew Hermes at the University of Illinois. Computing energy at fewer geometric arrangements than normally required, the team developed computationally efficient methods to approximate potential energy surfaces.

A precise understanding of potential energy surfaces, key elements in virtually all calculations of quantum dynamics, is required to accurately estimate the energy and frequency of vibrational modes of molecules.

'If we can find the energy of the molecule for all possible configurations, we can determine important information, such as stable states of molecular transition structure or intermediate states of molecules in chemical reactions', Rai said.

Initial results of this research were published in *Molecular Physics* (doi: 10.1080/00268976.2017.1288937).

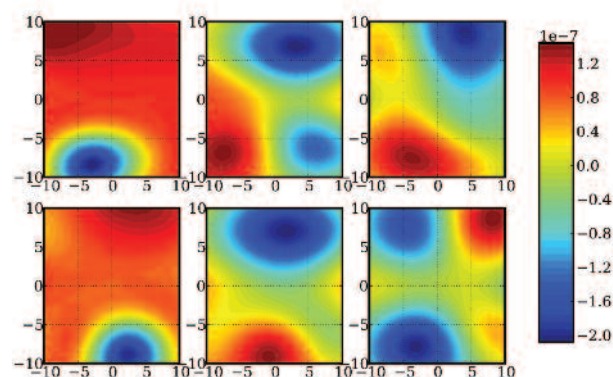
'Approximating potential energy surfaces of bigger molecules is an extremely challenging task due to the exponential increase

in information required to describe them with each additional atom in the system', Rai said. 'In mathematics, it is termed the curse of dimensionality.'

The key to beating the curse of dimensionality is to exploit the characteristics of the specific structure of the potential energy surfaces. Rai said this structure information can then be used to approximate the requisite high dimensional functions.

'We make use of the fact that although potential energy surfaces can be high dimensional, they can be well approximated as a small sum of products of one-dimensional functions. This is known as the low-rank structure, where the rank of the potential energy surface is the number of terms in the sum', Rai said. 'Such an assumption on structure is quite general and has also been used in similar problems in other fields. Mathematically, the intuition of low-rank approximation techniques comes from multilinear algebra where the function is interpreted as a tensor and is decomposed using standard tensor decomposition techniques.'

The energy and frequency corrections are formulated as integrals of these high-dimensional energy functions. Approximation in such a low-rank format renders these functions easily integrable as it breaks the integration problem to the sum of products of one- or two-dimensional integrals, so standard integration methods apply.



A depiction of random two-dimensional slices of a 12-dimensional function for determining energy and frequency corrections of a formaldehyde molecule. Sandia National Laboratories

The team tried out their computational methods on small molecules such as water and formaldehyde. Compared to the classical Monte Carlo method, the randomness-based standard workhorse for high-dimensional integration problems, their approach predicted energy and frequency of water molecules that were more accurate, and it was at least 1000 times more computationally efficient.

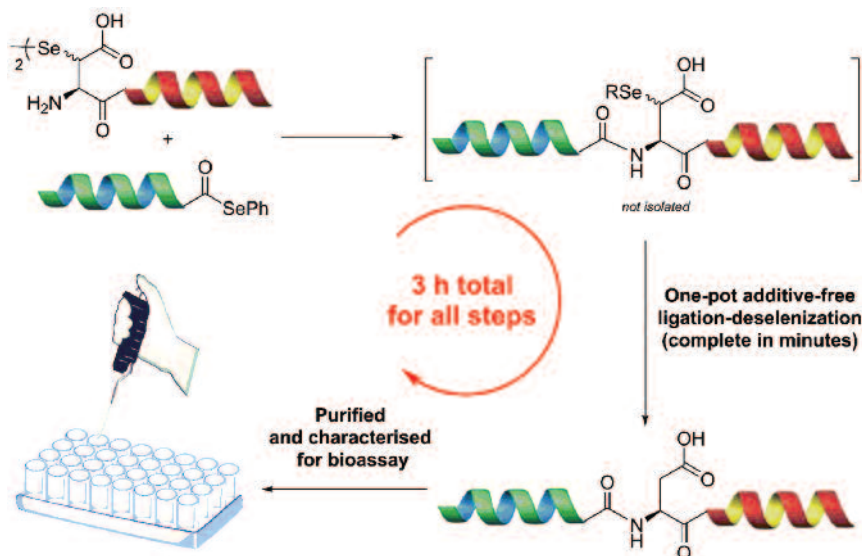
Rai said the next step is to further enhance the technique by challenging it with bigger molecules, such as benzene.

Sandia National Laboratories



## Fast route to tailor-made proteins

A renaissance in the use of large polypeptides and proteins as therapeutic agents has led to significant interest in synthetic technologies to rapidly and efficiently access these biomolecules. Peptide ligation methods have revolutionised protein science and provided an avenue to make polypeptides and proteins with tailor-made modifications to maximise specificity and activity or to probe biological function. One of the key problems remaining in the field is that it still takes an unacceptably long time to synthesise a given protein. Professor Richard Payne and co-workers at the University of Sydney have recently described the development of a one-pot ligation–deselenisation technique at aspartate and glutamate residues that enables the synthesis of native proteins with unprecedented speed (Mitchell N.J., Sayers J., Kulkarni S.S., Clayton D., Goldys A.M., Ripoll-Rozada J.,



Pereira P.J.B., Chan B., Radom L., Payne R.J. *Chem* 2017, **2**, 703–15). The key feature of the method is that both the ligation and deselenisation reactions proceed rapidly and cleanly within minutes and are compatible for use in one-pot synthesis. The team demonstrated the utility of the technique

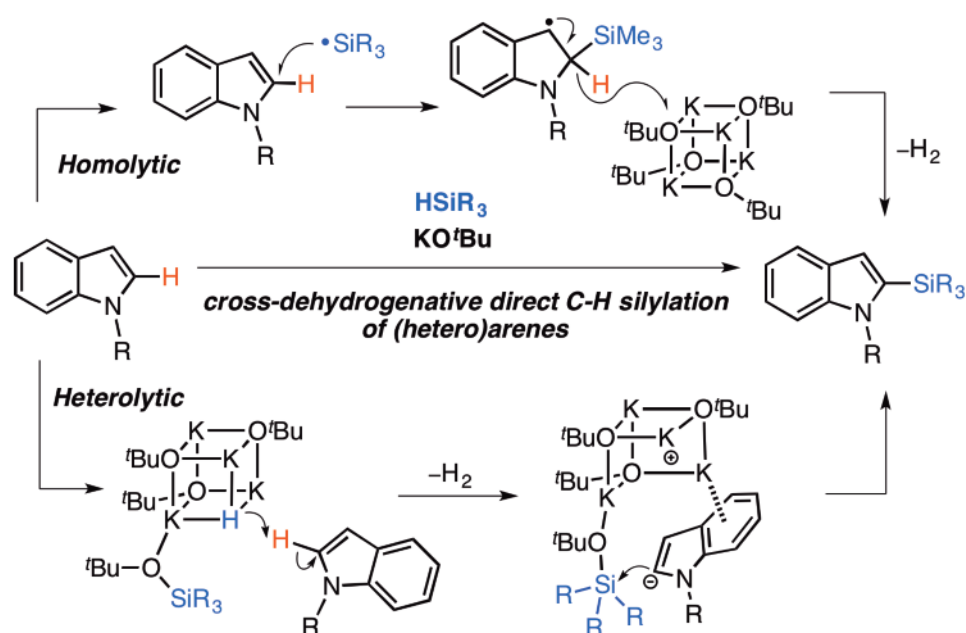
by synthesising several protein targets, including three tick-derived thrombin inhibitors that could be assembled, purified and isolated for biological interrogation within a few hours. The method serves as a powerful means to access synthetic proteins, including therapeutic leads.

## Unusual C–H activation mechanisms

A versatile method for the direct C–H silylation of (hetero)aromatic compounds, developed by the Grubbs and Stoltz laboratories, makes use of potassium *t*-butoxide as a cheap, environmentally friendly catalyst (*Nature* 2015, **518**, 80–4). Exactly how this transition-metal-free transformation occurs has remained a mystery. Now, a team of chemists from the US, Germany and Australia propose two distinct mechanisms for the C–H silylation in back-to-back papers in the *Journal of the American Chemical Society* (*J. Am. Chem. Soc.* 2017, **139**, 6867–79; Banerjee S., Yang Y.-F., Jenkins I.D., Liang Y., Toutov A.A., Liu W.-B., Schuman D.P., Grubbs R.H., Stoltz B.M., Krenke E.H., Houk K.N., Zare R.N. *J. Am. Chem. Soc.* 2017, **139**, 6880–7). Unexpectedly, experiment and theory support both mechanisms: a homolytic pathway involving silyl radical addition followed by *ipso*-H abstraction and a heterolytic pathway involving heteroarene

deprotonation by a hydridic intermediate. Intriguingly, calculations reveal that a novel cubane-like KO<sup>t</sup>Bu/HSiR<sub>3</sub>-derived hydride may be involved in both

pathways. These studies point to useful new mechanistic paradigms for C–H activation by the environmentally friendly, earth-abundant KO<sup>t</sup>Bu.



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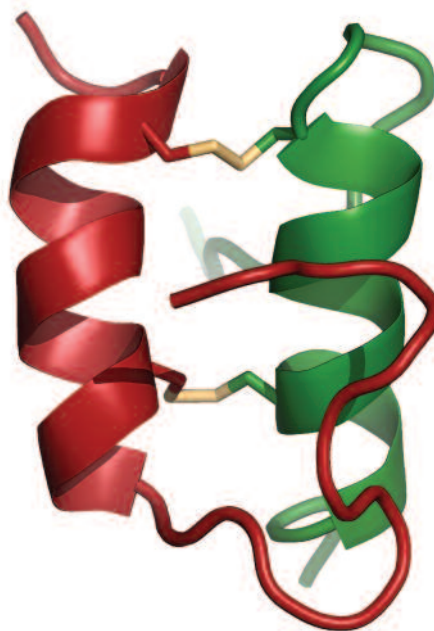
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## Why bull ant stings are painful



Venom-derived peptide toxins provide an abundant pool of molecules with diverse biological functions. Researchers from the University of Queensland, Monash University and the Kolling Institute of Medical Research have recently discovered a new pain-causing peptide ( $\Delta$ -myrtotoxin-Mp1a) from the jack jumper bull ant *Myrmecia pilosula* with very unusual structural and functional properties (Dekan Z., Headey S.J., Scanlon M., Baldo B.A., Lee T.-H., Aguilar M.-I., Deuis J.R., Vetter I., Elliott A.G., Amado M., Cooper M.A., Alewood D., Alewood P.F. *Angew. Chem. Int. Ed.* 2017, doi: 10.1002/anie.201703360).  $\Delta$ -Myrtotoxin-Mp1a is a 49-residue antiparallel heterodimeric peptide with a unique framework comprising two non-identical chains connected by two disulfide bonds. Remarkably, combining the individual synthetic chains resulted in the self-assembly of Mp1a without employing directed disulfide bond formation. 2D-NMR analysis revealed a well-defined and unique structure containing a pair of antiparallel  $\alpha$ -helices. Dual polarisation interferometry showed strong interaction with supported lipid bilayers and insertion within the bilayers of both mammalian and bacterial membranes. Mp1a also displayed broad-spectrum antimicrobial activity, with the highest potency against Gram-negative *A. baumannii* (MIC 25 nM). Injection of 10  $\mu$ M of Mp1a into the paws of mice elicited spontaneous pain and mechanical allodynia (pain caused by mild mechanical stimuli such as a light touch), indicating that the peptide is the probable cause of the bull ant's painful stings.

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



## Wiley and CAS to deliver advanced predictive cheminformatics capabilities to researchers worldwide

John Wiley and Sons, Inc. and CAS, a division of the American Chemical Society, have announced a partnership that will accelerate the evolution of predictive synthesis by enriching Wiley's ChemPlanner technology with the most accurate and complete chemical information from CAS.

Rapid advances in the fields of predictive analytics, artificial intelligence and machine learning offer tremendous opportunity to enhance the way scientific information is queried and analysed. ChemPlanner's state-of-the-art cheminformatics technology helps chemists find the best selection of diverse and viable routes for their synthesis, increasing their efficiency and creativity when developing new molecules.

As an innovative provider of sophisticated digital information solutions, CAS will enhance ChemPlanner with a wealth of additional reaction content and associated references, including reactions from patents. Integrating more than 10 times the reaction content and offering valuable new features suggested by current ChemPlanner users, including stereoselective retrosynthetic prediction and customisable relevance ranking, this powerful new version of ChemPlanner will be delivered exclusively in SciFinder<sup>®</sup>, a new research experience from CAS that exponentially elevates scientific discovery.

'The integration of the rich CAS content portfolio will greatly enhance the quality and scope of ChemPlanner's predictions, as well as the utility of the resulting synthetic routes to help researchers overcome synthesis challenges faster', said Dr Matthew J. Toussant, senior vice president of product and content operations, CAS. 'CAS has a strategic focus on leveraging emerging machine learning and predictive technologies to accelerate the pace of scientific research, and this is our initial step in that evolution.'

'Wiley is thrilled to collaborate with CAS and to make ChemPlanner accessible to hundreds of thousands of researchers worldwide', said Jay Flynn, SVP & MD, Research Publishing, Wiley. 'CAS is big data for chemistry, making this marriage of best-in-class content and technology a natural partnership. Our goal is to provide powerful, data-driven content that helps chemists solve global challenges.'

## Lean Laboratory webinar: optimising lab processes



Successful lean manufacturing principles are increasingly being adopted in the laboratory environment. The challenge is to understand how best to put Lean Laboratory into practice in a particular workplace.

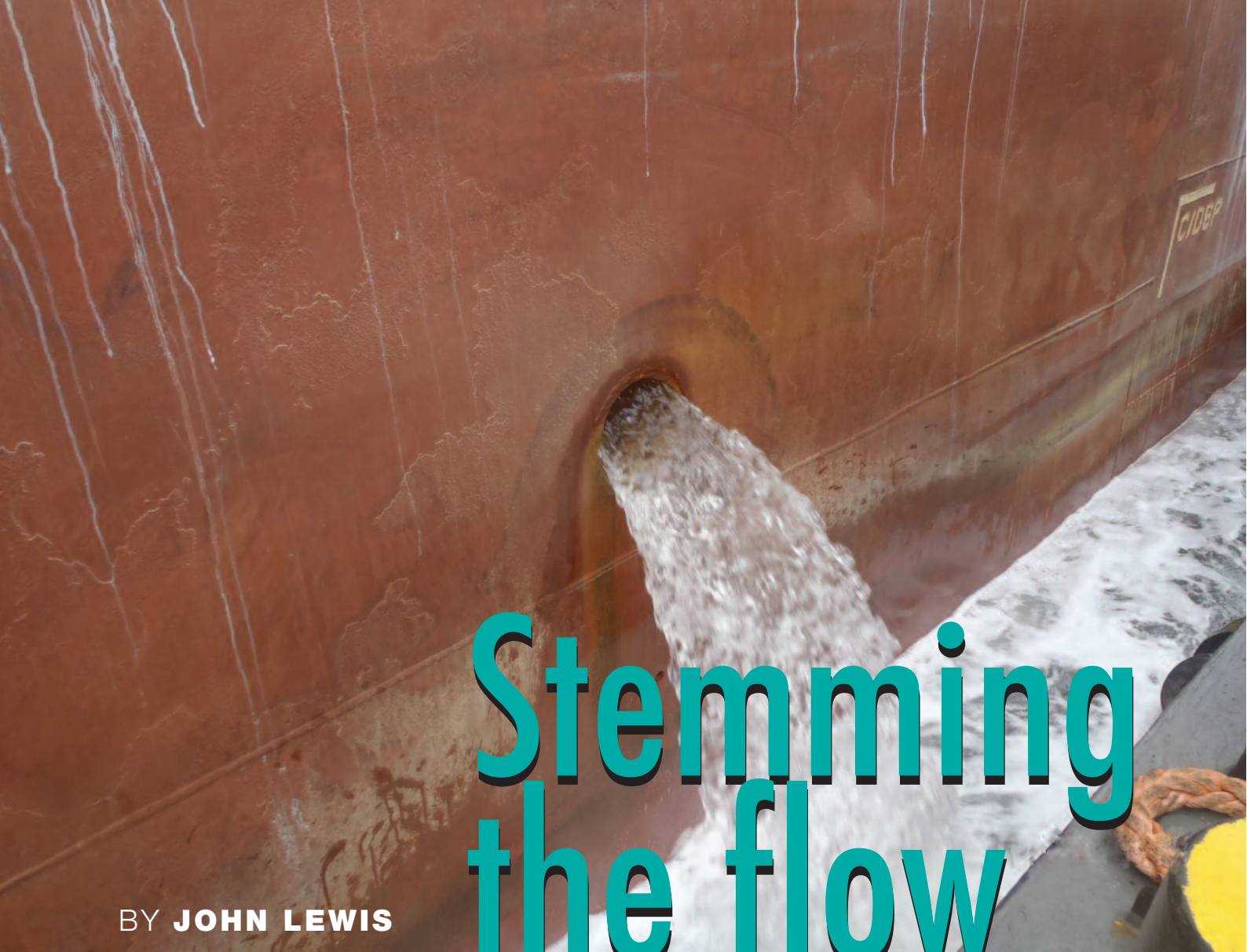
A two-part webinar series by METTLER TOLEDO, 'Employing a Lean Lab Approach to Optimize Lab Processes', co-presented by lean laboratory expert Erwin Studer, explains the concept of Lean Lab and how it can be applied to established laboratories or the design of a new laboratory. Lean methods help to ensure that laboratory processes are clearly defined, structured and controlled to deliver more consistent and predictable laboratory performance. This generates a detailed understanding of lab capacity and resourcing requirements and leads to a positive impact on lead time and costs, productivity and right-first-time.

Part 1 'Work Smarter, Not Harder' introduces the basic concepts of Lean Laboratory and explains the 10 areas to consider in assessment of the current status of a lab. These are used to guide the improvement of existing processes. It is often the simplest or smallest changes that can bring about the most significant improvements.

Part 2 'Improve Productivity' goes deeper into value stream mapping and performance management. Advice is given on how to identify value-adding or unnecessary steps in a workflow, using the example of sample preparation for analysis. This allows participants to identify the issues that could have the biggest impact on improving lab productivity. Measuring the impact using a number of key performance indicators is also discussed.

Watch these recorded webinars now at [www.mt.com](http://www.mt.com) (click on Events & Expertise).

For more information, visit METTLER TOLEDO at [www.mt.com](http://www.mt.com).



# Stemming the flow

BY **JOHN LEWIS**

**An international convention for managing ships' ballast water to prevent the arrival of invasive marine species is about to come into force.**

**T**he diversity of marine ecosystems evolved, not just by the physico-chemical characteristics of regional water bodies, but also by the biogeographic isolation of coasts by oceans and seas. From the time mariners first set to sea, their vessels became a vector for the global distribution of species, both intentionally, for example food crops and domestic animals, and accidentally, for example terrestrial weeds and rodents. Introductions of alien species in the marine environment are often less obvious, but ships have facilitated the movement of species for centuries. A survey of alien marine species in Port

Phillip Bay, Victoria, in 1999 documented 160 species considered likely to be alien, which represented 13% of the known marine flora and fauna in the bay.

Although some marine aliens were known to have been in Australia since gold rush times, the evidence suggested a new pulse of arrivals in the latter decades of the 20th century. Of particular concern in the 1990s was the arrival and rapid population growth of a number of species, including the Northern Pacific seastar (*Asterias amurens*) in Hobart's Derwent River and Port Phillip Bay, the Asian kelp (*Undaria pinnatifida*) in southeastern Tasmania and Port Phillip Bay, and the black-striped mussel



(*Mytilopsis sallei*) in Darwin Harbour. There were also concerns about the movement of toxic dinoflagellates – microalgae that can bloom to cause ‘red tides’ that can lead to paralytic shellfish poisoning from eating mussels and oysters that have fed on these algae.

Ballast is used in ships to provide stability and to compensate for weight changes in cargo loads, and from fuel and water consumption. In the days of sail, rocks collected from seashores were commonly used as ballast but, with the introduction of steel-hulled ships, ballast tanks for holding seawater ballast became the norm. Ballast water is taken aboard as ships unload, and discharged as ships load. With Australia's trading patterns, bulk carriers that export raw materials such as coal, iron ore, oil and gas would discharge ballast in the Australian ports of call, and container ships and vehicle carriers that import manufactured goods would take up ballast prior to departure.

In the late 1980s, Australia, together with Canada, raised concerns on ballast water at the International Maritime Organization (IMO) Marine Environment Protection Committee and, in 1991, the committee adopted the non-mandatory International Guidelines for preventing the introduction of unwanted aquatic organism and pathogens from ships' ballast water and sediment discharges. Continued review of the issue consequently led the IMO to adopt the legally binding International Convention for the Control and Management of Ships' Ballast Water and Sediments ('the BWM Convention') on 13 February 2004.

The BWM Convention included a two-stage introduction of management measures: first, up until at latest 2016, ships would be required to meet a ballast water exchange standard (Regulation D-1), then, after this, ships would have to meet a ballast water performance standard (Regulation D-2). Regulation D-1 required ships on

international voyages to exchange ballast water taken up in ports with open ocean water with an efficiency of at least 95% volumetric exchange. Regulation D-2 requires ships to have a ballast water treatment system installed that will ensure that ballast water discharged contains:

- less than 10 viable organisms per cubic metre greater than or equal to 50 micrometres in minimum dimension
- less than 10 viable organisms per millilitre less than or equal to 10 micrometres in minimum dimension
- indicator microbes concentrations as a human health standard of:
  - toxicogenic *Vibrio cholera* less than one colony-forming unit (cfu) per 100 millilitres
  - *Escherichia coli* less than 250 cfu per 100 millilitres
  - intestinal enterococci less than 100 cfu per 100 millilitres.

As with all IMO conventions, entry-into-force of the BWM Convention would be 12 months after a required minimum number of IMO Member States ratified the Convention and, for this Convention, the requirement was not less than 30 States, the combined merchant fleets of which constituted not less than 35% of the gross tonnage of the world's merchant shipping. Acceptance of the convention by States was slow, and the requirement was only met in September 2016, so the date for entry-into-force of the convention is 8 September 2017. However, it should be noted that ballast water discharge from international ships arriving in Australian ports has been managed since 2001 under the Australian Ballast Water Management Requirements that require deep ocean ballast water exchange.

Meeting the D-2 standard for ballast water treatment systems (BWTS) is challenging because of factors including the range of organisms to be rendered non-viable, the volume of water to be treated, the water

## Ballast water is taken aboard as ships unload, and discharged as ships load.



(top) The Northern Pacific seastar (*Asterias amurensis*) and (bottom) the Asian kelp (*Undaria pinnatifida*) arrived in Australia in the 1990s and quickly established themselves.



A container ship berthing at Swanston Dock in the Port of Melbourne. Ballast water, and sometimes unwanted marine species, are discharged from a ship as it loads.

chemistry and quality, which may encompass salinity ranges from freshwater to fully marine and high water turbidity, and that the standard is a discharge standard, meaning that organisms are not able to regrow in the tanks during the voyage. The IMO requires that a commercially developed BWTS is approved by a flag administration in accord with IMO guidelines that require land-based testing ship-board trials and, for systems using active substances, approval of environmental impact of discharged ballast water by the Marine Environment Protection Committee. At the end of 2016, some 68 systems had received type approval certification in line with IMO requirements, 30 of which made use of active substances.

Treatment systems generally include a two-stage process: physical solid-liquid separation to separate suspended solid material, including larger organisms from the intake water, then disinfection to kill or inactivate microorganisms.

The physical solid-liquid separation phase can employ hydrocyclone separation or surface filtration, sometimes with upstream addition of chemical flocculants or coagulants to increase the efficiency of particle separation. Filtration systems can use discs or fixed screens with automatic backwashing. The hydrocyclone system of high-velocity centrifugal rotation can be more effective than filtration.

Disinfection can involve physical methods, or the addition or generation of active substances. Physical methods include UV irradiation, cavitation, deoxygenation and heat. UV irradiation is a widely used method for

**Treatment systems generally include a two-stage process: physical solid-liquid separation ... then disinfection**

industrial and municipal water treatment. A technological challenge for UV application was the need for water clarity to enable UV penetration through the full treatment pipe or vessel diameter. However, this has been overcome in the development of some systems through effective filtration of water prior to the disinfection stage. Ballast water can also be passed through the reactor during deballasting, but without the need for filtration, to kill any organisms that may have regrown during the voyage.

Deoxygenation of the water will kill organisms within several days, but there is a heightened risk of anaerobic corrosion of tank walls by sulfate-reducing bacteria, the human health risk of the deoxygenated tank head space if hatches are opened, and the environmental risk from the release of large volumes of deoxygenated water into a recipient water body. Cavitation, generated ultrasonically or by gas injection, disrupts organism cell walls but has been found to require





A small container ship under way off Singapore. Singapore is the second largest container port in the world (behind Shanghai), and Melbourne is the largest in Australia.

additional treatment systems downstream for total efficacy. Heat has limitations in the requirement for the lethal temperature to be maintained over an extended period of time and the risks that sub-lethal temperatures could enhance bacterial growth.

Chemical disinfection using oxidising biocides is the other widely used approach, with different systems using chlorination, electrochlorination, chlorine dioxide, ozonation, paracetic acid and/or hydrogen peroxide. As is the case for UV radiation, chlorination systems are widely used for the treatment of municipal and industrial waters. In natural waters, the biocidal effect is achieved by a sodium hypochlorite solution producing different oxidising compounds. Free chlorine, or free available chlorine, is present as an equilibrium mixture of hypochlorous acid and hypochlorite ions, which are both oxidants, but the latter is far less effective than the former. For ballast water treatment, sodium hypochlorite can be generated electrochemically directly from

seawater or, in freshwater or low salinity waters, from stored brine.

Ozone is a stronger oxidant than chlorine and can decompose high molecular weight organic substances to produce low molecular weight compounds such as aldehydes and carboxylic acids. Ozone decomposes rapidly with a half-life in pure water of a few hours, but with a half-life of minutes in raw water due to reaction with organic matter.

A drawback of both chlorination and ozonation systems is the formation of by-products that can include halogenated methanes, hydrocarbons, amines, acetonitriles etc. The risks of residual oxidants in discharge ballast water causing environmental damage in the receiving waters can require neutralisation of residual chemicals prior to discharge, which can be achieved, for example, by dosing with sodium bisulfate.

An added complication for the installation of a BWTS is that the US Coast Guard has set more stringent standards than the IMO on the

performance of a BWTS and US-type approval of systems is required for ships operating in US waters. The US Coast Guard regulations require compliance at the first dry-docking after 1 January 2016 and at delivery for new builds. However, the first US-type approval of a BWTS was not issued until December 2016 and only two more systems have been approved since.

With entry-into-force of the BWM Convention, ships not already fitted with a ballast water treatment system will be required to do so by 2021. Estimates of the number of ships needing retrofit BWTS installations over the next five years vary from 35 000 to 120 000 ships. One calculation based on the lower number, and an estimate that there are 250 shipyards worldwide capable of doing the work, results in each yard having to install a system every 16 days. Installation of a BWTS can cost up to US\$5 million per ship.

Quite a task ...

**John A Lewis** is Principal Marine Consultant, ES Link Services Pty Ltd, Castlemaine, Victoria.



**Dave Sammut** was thrilled to share a set with two of his science heroes while filming experiments for the RACI Centenary project 100 Reactions in 100 Days.

**F**rom the youngest age, I loved what science had to offer me. Beyond learning, science was inspiration, and imagination. The RACI's Centenary project '100 Reactions in 100 Days' has allowed me to fulfil the dreams of a little boy who sat glued to the television through the peak of the *Curiosity Show* years (see box). As it was for so many budding scientists of my generation, hosts Dr Rob Morrison and Dr Deane Hutton (pictured above) fanned the flames of my early science interest.

#### The project

Led by Dr Nathan Kilah of the University of Tasmania, the RACI's 100 Reactions in 100 Days seeks to create engaging YouTube content for the newest generation of scientific minds. The videos are being created by RACI scientists around Australia, often just with webcam and smartphone.

It's an opportunity for our members 'to celebrate the centenary, to highlight your work, and to demonstrate your outreach abilities to a global audience'. Aiming at a wide audience,



the project invites members to create videos up to five minutes long, 'with a focus on inspiring engagement and enthusiasm for chemistry' ([www.raci.org.au/raci-news/100](http://www.raci.org.au/raci-news/100)).

From the first email invitation to members, I was enthusiastic about the project. I put the resources of the team at my organisation, DCS Technical, behind it, and we got to work on developing our contribution to the project.

My starting point was to reach out to Dr Rob Morrison. Rob had written some columns for *Chemistry in Australia* a few years ago (2009–2012). At the time, I had sent Rob a 'fan boy' email, and he had been generous enough to reply.

Rob responded to my invitation immediately and enthusiastically, on behalf of both himself and Deane. I was transported. The idea that I could collaborate with my childhood heroes was a gift to my younger self that I would never have dared to dream of.

## Creating content

In consultation with Nathan Kilah (keeper of the master list of experiments, to minimise duplications), we prepared a list of 10 experiments for the project. There are so many experiment options that are interesting and highly visual, and I was delighted with Rob and Deane's idea to reprise a couple of the experiments from the *Curiosity Show* days.

We eventually settled on experiments with acid–base chemistry (dissolving egg shells, and creating 'rubber bones'), gases (helium and liquid nitrogen) and a couple of spectacular flame experiments with hydrogen generation and firework chemistry. The full set is available on the RACI's YouTube channel.

We reached out to other scientists and institutions, to see who wanted to collaborate. So many people have put up their hands to volunteer space, resources and support, it was gratifying to receive such enthusiasm –

with that enthusiasm all the greater when we mentioned Rob and Deane's involvement.

The challenge was not in finding support, but in finding mutually compatible dates to bring all the offered resources together. It was a logistical exercise, but eventually the team was brought together for two days of filming in May 2017.

## The shoot

The team and I went a bit overboard. If we were going to film with the professionals, then we were going to try to make a professional showing of ourselves. As we say in 'the biz' – do not try this at home.

The shoot, involving about 10 people, was organised for three locations over two days: the National Measurement Institute and Fledge Innovation Labs at the joint CSIRO site at Lindfield, New South Wales, and at University of Technology, Sydney.

Our volunteer video professional brought enough cameras so that we would shoot everything simultaneously – the wide shots, the

'talking head', the close-ups, even a 'go pro' camera taped to the ceiling. That made filming considerably simpler, because we didn't have to repeat the reactions to get the different views. There was lighting. There were microphones. It was an electricity utility's dream.

For each experiment, we started with a series of rehearsals, testing the sequence and timing of the actions, and giving the camera crew an

**The challenge was not in finding support, but in finding mutually compatible dates to bring all the offered resources together.**

## Curiosity Show

*Curiosity Show* was a seminal Australian science-based program broadcast from 1972 to 1990, and it now lives on at YouTube.

The *Curiosity Show* website states that the show '... was a nationally broadcast science and technology television program for young people, including segments on natural history, astronomy, music, technology and puzzles. It is remembered for its emphasis on how to make working machines and models from everyday materials around the home. More than 500 programs were produced, with a total of around 5000 segments.'

The show could be likened to the American series *Mythbusters*, with fewer explosions and more science. Anecdotally, the creator of *Mythbusters*, producer Peter Rees, was a fan of *Curiosity Show* during his formative years growing up in Sydney.

After the end of *Curiosity Show*, Rob and Deane have continued to be active in science communications, with extensive science writing and speaking engagements that continue to this day.



*Curiosity Show* in the 1970s.

opportunity to adjust and optimise their shots and angles. Then being relatively well prepared, we could film most of the experiments in just a couple of takes.

And so filming began. Deane was the first on the schedule, and hearing him say the immortal words 'Why did this happen? I'm glad you asked!' was a nostalgic thunderbolt.

Even though we were relatively well organised, the filming of each 3–5-minute video took more than an hour. And that was when everything went well. We lost quite a bit of time on the first day of the shoot when things went awry.

In shooting the fireworks chemistry video, we made a last-minute decision with our hosts to change the order of filming. It seemed a good idea to use

the darker of two rooms available to us, to better bring out the visuals as we discussed the way different metals are used to generate colours in fireworks. Rob was using cornflour as the carrier, then mixing various metal powders and 'puffing' them into a flame. The resulting flash was spectacular, with a small associated puff of smoke and dust. It was all safe and benign, but hindsight provides wonderful clarity, and in hindsight the better-ventilated room would have been the better choice.

We'd made it through the rehearsal and most of the filming. As Rob opened his mouth to say the final line in the script '... and now we'd better stop, before we set the fire alarms off', the wailing began. I'd like to take this opportunity to reiterate our apology to

the professional scientists of NMI and CSIRO for the interruption to their day.

Throughout the shoot, it was wonderful to see how many established scientists clustered outside at each location, whispering excitedly while waiting for an opportunity to say hello and 'thanks for everything you did'. Rob said that it can be a little sobering when a middle-aged person enthuses about what a fan they were as they grew up, but there were plenty of examples of that during the two days of filming. The sense of fun and the underlying admiration were abundantly evident throughout the experience.

The highlight for me was the opportunity to actually get on camera with my heroes. My acting was terrible. I forgot my lines. I stood there

**Dr Rob Morrison filming at the National Measurement Institute.**







Dr Deane Hutton preparing to film at Fledge Innovation Labs, with Dave Sammut just happy to be there.

grinning like an idiot, just thrilled to be there. And I don't mind any of that. I was living the dream. So where do I audition for *Mythbusters*?

### Getting involved

I've written this piece because I'd like to encourage you to create something of your own, and because it was so much fun to do that I just have to tell *somebody*.

RACI members around Australia still have time to get involved. 100 Reactions in 100 Days will be extensively promoted during National Science Week (12–20 August), with some awards for the best student film. Please contact Nathan Kilah ([nathan.kilah@utas.edu.au](mailto:nathan.kilah@utas.edu.au)) to talk about ideas.

Here is what I learned during filming.

- You don't have to do a full professional shoot. A webcam or mobile phone is fine.
- Planning is critical. From location, to resources, to script, know what you intend to do and what's required.
- Pay attention to lighting. Have enough natural and warm light to bring the video to life.
- Ideally, have a reasonably uncomplicated backdrop. Try not to make the shot too 'busy'.
- Eliminate background sound and distractions.
- Have a rehearsal, and run through the experiment a few times so that the whole crew is familiar with the sequence.

- Consider mixing up your views – close up, wide, 'talking head', overhead, whatever makes the final product more dynamic and interesting.
- Even basic editing takes a lot of time – hours per minute of video – but the results are definitely worthwhile.

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**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. Special thanks to Dr Rob Morrison and Dr Deane Hutton, DCS Technical Pty Ltd, Fledge Innovation Labs, National Measurement Institute, Samantha Ohlsen Photography, University of Technology Sydney and Warren Lewington.

# Phytochemistry of Australian plants

## A new database

BY **DAVID COLLINS**  
**AND DONALD MCGILVERY**

The creators of a new phytochemical database describe its development and their continued efforts to cover the many thousands of Australian plant species.

Phytochemical studies of Australian plants increased markedly in the early 1940s, during World War 2, when it became important to search for new sources of potentially useful drugs. A significant outcome was the large-scale production of the anti-seasickness compound hyoscine (a tropane alkaloid), which was isolated from the Australian plant *Duboisia myoporoides*. Hyoscine was used during World War 2 on the Australian, British and American warships.

After the war, what became known as the Australian Phytochemical Survey was intensified by CSIR (later CSIRO). Several chemists were employed full-time on this project. Chemists in Australian universities also became actively involved in what became a major collaborative effort – the collection and identification of

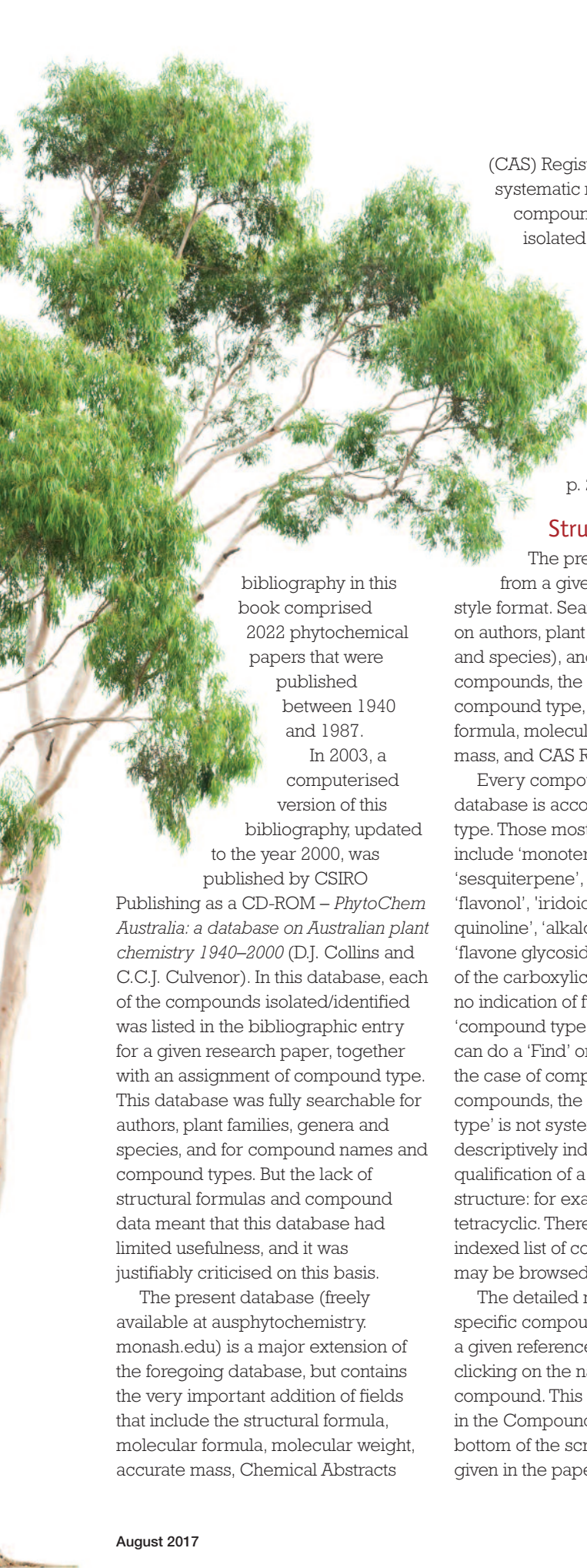
plant species being organised and provided by CSIRO. The involvement of CSIRO in the survey ceased in the mid-1970s, and since that time there has been relatively less phytochemical work done by chemists in Australian universities.\*

Details of the outcome of the Australian Phytochemical Survey were published in the book *Plants for medicines: a chemical and pharmacological survey of plants in the Australian region* (D.J. Collins, C.C.J. Culvenor, J.A. Lamberton, J.W. Loder and J.R. Price, CSIRO Publishing, 1990). 'In the Australian region' refers to the fact that several of the plant species studied were collected in New Guinea. The

\*For a historical account of the Survey, see Price J.R., Lamberton J.A. and Culvenor C.C.J., 'The Australian Phytochemical Survey: Historical Aspects of the CSIRO Search for New Drugs in Australian Plants', *Historical Records of Australian Science*, 1993, vol. 9, pp. 335–56.







(CAS) Registry Number, and systematic name of every compound that has been isolated from/identified in Australian plants. All of these items are fully searchable. Given the history described above, only research papers published since 1940 are included (see box, p. 28, for other criteria).

### Structure and content

The presentation of the data from a given reference is in card-style format. Searches may be made on authors, plant names (family, genus and species), and on compounds. For compounds, the search options are compound type, name, molecular formula, molecular weight, accurate mass, and CAS Registry number.

Every compound entered in the database is accorded a compound type. Those most frequently found include 'monoterpene', 'sesquiterpene', 'triterpene', 'flavone', 'flavonol', 'iridoid glycoside', 'alkaloid quinoline', 'alkaloid indole' and 'flavone glycoside'. With the exception of the carboxylic acid group, there is no indication of functionality in the 'compound type' – for example one can do a 'Find' on 'triterpene acid'. In the case of complex polycyclic compounds, the assigned 'compound type' is not systematic, but descriptively indicative by the qualification of a recognisable sub-structure: for example, alkaloid indole, tetracyclic. There is an alphabetically indexed list of compound types that may be browsed.

The detailed molecular data for a specific compound that is listed within a given reference may be accessed by clicking on the name of that compound. This updates all of the data in the Compound Details box at the bottom of the screen: the name as given in the paper, molecular formula,

molecular weight (four decimal places), accurate mass (four decimal places), CAS Registry number, systematic name as given by SciFinder, and structural formula. All of these criteria are individually searchable; for example, one can 'Find' all of the compounds in the database with a chosen molecular formula. One can also do a 'Find' on the numerical value of molecular weight, or accurate mass, provided that four decimal places are used. It should be noted that because of the relatively recent revision of atomic weights, the molecular weight for a given molecular formula will differ in the third and/or fourth decimal places for entries made in the database before and after that revision. A 'Find' on an accurate mass value would usually be more appropriate.

bibliography in this book comprised 2022 phytochemical papers that were published between 1940 and 1987.

In 2003, a computerised version of this bibliography, updated to the year 2000, was published by CSIRO

Publishing as a CD-ROM – *PhytoChem Australia: a database on Australian plant chemistry 1940–2000* (D.J. Collins and C.C.J. Culvenor). In this database, each of the compounds isolated/identified was listed in the bibliographic entry for a given research paper, together with an assignment of compound type. This database was fully searchable for authors, plant families, genera and species, and for compound names and compound types. But the lack of structural formulas and compound data meant that this database had limited usefulness, and it was justifiably criticised on this basis.

The present database (freely available at [ausphytochemistry.monash.edu](http://ausphytochemistry.monash.edu)) is a major extension of the foregoing database, but contains the very important addition of fields that include the structural formula, molecular formula, molecular weight, accurate mass, Chemical Abstracts

**The database ... contains the very important addition of fields that include the structural formula, molecular formula, molecular weight, accurate mass, CAS Registry Number, and systematic name of every compound that has been isolated from/identified in Australian plants.**

## Present content

The database contains information from 8446 scientific journal articles, and includes data for 14 656 different chemical compounds. These compounds have been isolated, identified and characterised from 10 450 different species of Australian plants. These numbers will grow automatically as new data is recorded. Given some 20 000 vascular plant species have been identified in Australia, and several thousand lower plants (2000 algae and lichens; 550 ferns; 1000 mosses; and 11 800 fungi), there is much more work to be done!

## Future data acquisition

Data acquisition will continue, and the updated version will be continually available online. Several mainstream phytochemical and related journals are scanned regularly for new data, but we are aware that there must be many more relevant references, especially by international chemists, that are yet to be found and 'extracted'. New data (relevant references) is also acquired by SciFinder searches on arbitrarily chosen plant species, or on specific senior authors known to be active in phytochemical research.

We welcome advice of errors and omissions, so that the appropriate corrections and additions can be made. A Send Comment button is available on the HELP page at [ausphytochemistry.monash.edu](http://ausphytochemistry.monash.edu).

**David J. Collins** FRACI CChem compiled the phytochemistry database and is Honorary Adjunct Senior Research Fellow, School of Chemistry, Monash University.

**Donald C. McGilvery**, who developed the database, is Lead Operator, Australian Synchrotron.

## Criteria for database inclusion

- 1 Only research papers published since 1940 are included.
- 2 The designation 'Australian plant' is based on two major publications. One is the *Census of Australian vascular plants*, by R.J. Hnatiuk, Australian Government Publishing Service, 1990 (Number 11 of *The Australian flora and fauna series*, produced by the Bureau of Flora and Fauna, Canberra). The other botanical authority used is the set of volumes (36 published so far) in the series *Flora of Australia*. In addition to the strictly indigenous flora, the foregoing volumes also include some overseas plants (names marked with an asterisk in the above publications) that have been naturalised in Australia: such plants are included in this database.  
Many of the plants that are indigenous in northern Australia are also indigenous in some other countries, particularly in Asia, including India, Japan and China, but also in other countries. Most of the recent studies on 'Australian plants' are by chemists working in those countries. We are aware that many more relevant phytochemical studies by international chemists have yet to be found and included. This is being done progressively by the arbitrary choice of plant species for systematic searches using SciFinder. Also, because many of the species of *Eucalyptus* have been adopted and cultivated by other countries, most of the recent work on the eucalypts is by overseas chemists. There is an ongoing search for relevant papers of this type that have yet to be included.
- 3 Papers that primarily describe pharmacological studies are not generally included, but papers that describe both the isolation and the results of pharmacological studies of biologically active compounds are relevant, and are included.
- 4 Phytochemical work described in patents is not included – only studies published in scientific journals are included in this database.
- 5 In those studies where several species of a given genus are examined, only the data for the Australian species is included.
- 6 In publications that describe the isolation/characterisation of compounds from more than one plant species, the compounds are not ascribed to a particular species. One needs to consult the paper for that detail.
- 7 In the case of essential oil analyses, the arbitrary choice has been made to include only those components that constitute 1% or more of the oil. Specific percentages are not given, but components of 20–40% are given an asterisk, those of 40–80% are given a double asterisk, and those of more than 80% are given a triple asterisk. One can do a find, for example on 1,8-cineole\*\*\*, to find all of the plants that have given essential oils rich in that compound.
- 8 The compound names entered into the database are usually those used by the author(s) of a given paper, except for the occasional correction of a typographical/spelling error. The result is that some compounds will be found under different names. This particularly applies to variability in the derivatisation of trivial names – especially in the naming of glycosides. For example, quercetin 3-*O*- $\alpha$ -D-glucopyranoside will also be found as quercetin-3-glucoside, quercetin-3-*O*-glucoside, isoquercetrin etc. For each of these entries, the Compound Data File contains the systematic name as given by SciFinder – namely, 2-(3,4-dihydroxyphenyl)-3-( $\beta$ -D-glucopyranosyloxy)-5,7-dihydroxy-4*H*-1-benzopyran-4-one.  
The duplicates/replicates of a given compound may be found by doing a 'Find' with the CAS Registry Number.
- 9 Articles that review the phytochemistry of specific species or genera are included in the database, but the numerous compounds listed in the review article are not included in the database entry. All of the compounds included in such a review should be found in the database entries for the various original research papers. Reviews are included primarily for their bibliographic value.
- 10 Papers that only report total group analyses – such as 'total phenolics' or 'total alkaloids' – are not included; only papers that report specifically identified compounds are included.
- 11 Papers that describe experiments on the tissue culture of plants are not included.





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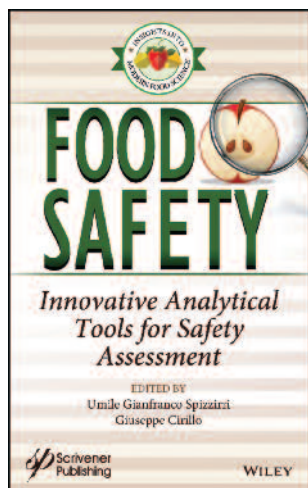
## Is your home and contents insurance up to date?

It is around this time of year that many people tackle the task of the half yearly clean! If you are taking the time to do a clear out, it is also a great opportunity to review your contents insurance to ensure it is up to date and covers all of your possessions.

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## Food safety: innovative analytical tools for safety assessment

Spizzirri U.G., Cirillo G. (Eds), Wiley, 2016, hardback, ISBN 9781119160557, 480 pp., \$321.95

The preface to *Food safety: innovative tools for safety assessment* announces that this is the first in a proposed series of compilations regarding food science in general. The present volume explores the use of modern techniques for the analysis of food constituents or contaminants or, in one case, deliberate

additives. It is not for the general reader, though each chapter introduction is itself excellent reading. Rather it suits those familiar with 'cutting-edge' methods and who wish to review their application to foods.

The book is well presented and, considering the authors are from 12 countries, only one of which has English as its first language, quite readable.

The book's editors hail from the Department of Pharmacy, Health and Nutritional Sciences at southern Italy's University of Calabria.

The introduction 'Food Analysis: a Brief Overview' walks the reader through available techniques and applications.

Chapter 2, the only chapter featuring deliberately added substances, deals with methods to detect and measure artificial (non-nutritive) sweeteners such as saccharin. Methods include sample clean-up, HPLC and capillary electrophoresis, the last able to detect four added sweeteners simultaneously. Considering the evident expertise of the authors, the overview would have benefitted from 'fleshing out' to greater depth.

Current official (US) methods for lipids are reviewed in Chapter 3, along with current advances in sample preparation, automation and detection. These include a section on infrared (FTIR) methods. The authors stress the importance (at least within the US) of AOAC methods; these, by definition, are well validated through sample exchange programs, an important feature where analyses do not have analytes with absolute values but depend in part on the methods themselves.

Chapter 4 covers analyses for substances that are markers for allergens present in foods. Here we enter the realm of the most modern analytical chemistry and biochemistry. Methods are chiefly immunochemistry, mass spectrometry and genomic amplification to detect and measure the protein, peptide or DNA markers of interest. An excellent final section explains the required parameters for method validation and an extensive table lists the allergens available to spike samples for this purpose.

Chapter 5 deals with methods to detect, identify and quantify characteristic fragments of genetically modified organisms (GMOs). The authors dedicate the first 12 pages to a

remarkably clear introduction to the history, scope of and need for GMOs and an introduction to the methods. The next 40 or so pages cover essentially 'textbook' DNA and protein-based methods, with some new twists, and the last ten pages cover newer, and an almost bewildering array of, biochemical methods. The most recent emphases are on speed of operation and the ability to detect multiple genetically modified elements: one GM corn variety has six different enhancements!

The analysis of antioxidant substances in foods is the subject of Chapter 6. Extraction methods are thoroughly examined; analysis is mostly by chromatography. A bibliography of 235 references up to 2015 provides an excellent base from which to explore the methodologies.

Chapter 7 features a useful overview of pesticide residues in food and food products and of appropriate analytical methods. For each step, the principle and its applications are given and examples provided. The range and complexity of methods for extraction, separation and detection is quite astonishing and all are well referenced. The emphasis is on modern techniques, especially those that are rapid. An interesting example is the use of a single hanging drop of solvent that is exposed, in a sealed chamber, to an aqueous liquid extract containing the desired pesticide. The drop is then withdrawn and injected into a GC for separation! So much for serial extractions in separating funnels!

Free amines as indicators of food spoilage are covered in Chapter 8. This chapter discusses chromatographic methods for identification and determination of biogenic amines in foods of animal origin. Free amines and amino acids are naturally present in foods, but amine concentration can increase due to the decarboxylation of amino acids by the action of microorganisms or from steps in food processing. Thus, if interpreted cautiously, free amine can be an indicator of food spoilage, particularly spoilage of animal products. The chapter discusses extraction and the applicable chromatographic techniques for particular food groups, and an extensive summary table is provided.

Food allergies are surprisingly common, requiring dependable and sensitive analytical methods for their detection and measurement, especially in regard to the cautionary labelling of foods. The authors of Chapter 9 compare protein-based methods (immunological assays) with extraction followed by mass spectrometry, the latter being far more specific, but expensive. They then discuss an alternative approach to assay for DNA markers using PCA, a very sensitive, though indirect, method.

Extensive tables list current methods using immunochemistry for detection and measurement as well as using immunosensors for detection only. The latter have the potential to enhance the speed of analysis (and therefore reduce analysis time) and are also discussed in Chapter 11. The field of immunochemistry is advancing very quickly, many of the references being dated 2005–2015.

Food-borne viruses are unwelcome visitors to the human body. Chapter 10 covers detection of food-borne viruses such as



norovirus and hepatitis A. Sensitive methods are needed here because the infective dose can be as low as ten particles. One current issue is how to distinguish infective from non-infective particles. Here, cell culture is the soundest method in principle but limited in range and often extremely difficult. So molecular methods, such as polymerase chain reaction to concentrate the analyte, are more often used. This chapter is very clearly written and generously referenced, the most recent item being dated 2015.

Chapter 11 covers biosensors in general. It explains that large-scale agriculture and processing have brought new safety concerns and with these the need for specific, sensitive and, if possible, rapid methods. Tables and detailed sections give methods where biosensors can be used to detect food components and contaminants. In these, recognition sites from organelles, cell receptors, enzymes and antibodies to tissues and even tailored molecules feed various transducers to deliver an electrical signal that can be measured. Biosensors may even appear in 'smart' packaging – packaging with built-in indicators for temperature or other indices of interest.


A final, short chapter reviews immunoassay methods in food analysis, though much of the detail appears in earlier chapters.

Overall, this is a potentially valuable reference tool, spanning a wide variety of analytical topics of interest to anyone working or planning to work at the leading edge of food chemistry or biochemistry.

Bruce Graham FRACI CChem

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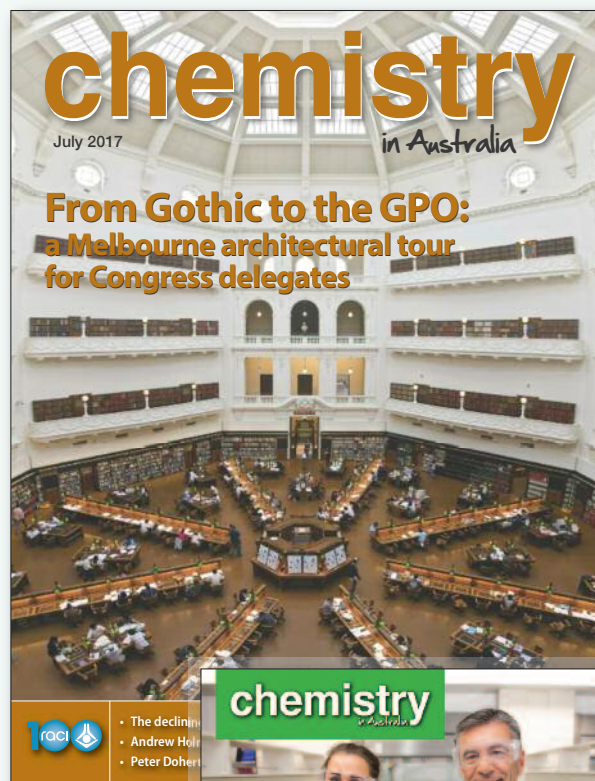
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## Australian ERA chemistry subdiscipline performances

The chemical sciences is one of 22 Fields of Research (FOR) assessed against world standard benchmarks as part of the Australian Research Council's Excellence in Research for Australia (ERA) exercises. Data are available from three exercises conducted in 2010, 2012 and 2015. Details of the exercises and primary data used are available from the ARC website ([www.arc.gov.au/era-reports](http://www.arc.gov.au/era-reports)). In the June issue (p. 38), the chemistry discipline performance was benchmarked against four other science FORs.

Universities report their research activities in eight four-digit chemistry subdiscipline categories, 0301–0307 (see table) and 0399. Category 0399 (designated 'Other Chemical Sciences') is a miscellaneous collection of data. This category has not been included in this comparative study because of variability in content sources between reports. All research outcomes are, however, included in any two-digit 03 chemical sciences figures presented.

Performance by subdiscipline and universities are rated on a scale of 1 to 5 – from well below to well above world standard. The number of universities submitting research for evaluation in each of the subdisciplines in 2015 is shown in the table along with the average national rating.

Some 26 of Australia's universities submitted chemical sciences research for evaluation. Physical and structural was the most widely researched subdiscipline. By contrast, theoretical and computational was actively researched in only five universities. Chemical sciences in aggregate and all subdisciplines, with the exception of organic, were assessed at above world standard (>4). The highest ranking was awarded to macromolecular and biomolecular at 4.75.

The aim of the presentation in the present report is to provide insight into the relative performance Australia-wide of the seven main subdisciplines using data from the 2015 and 2010 reports. Data on six parameters are reported to the ARC. Three have been evaluated here: the number of fulltime researchers (FTE) in the previous year, the research output over a six-year period and the research income over a three-year period. To simplify the presentation, the quantitative data for these parameters have been normalised to the performance for analytical. The relevant analytical chemistry values in the 2015 ERA report are: FTE 167.6, research output 1897.3, research income \$41.65 million. The corresponding 2010 values are: FTE 157, research output 1883, research income \$37.58 million. The values for the other disciplines may be obtained directly from the ERA reports or

derived using the analytical chemistry values and information in the graphs.

### Subdiscipline performances – 2015 ERA report

The analysis presented in the first graph reveals that the discipline of medicinal and biomolecular had the largest number of FTE researchers (57% more than analytical). Physical and structural, and organic also had more researchers than analytical. The smallest subdiscipline was theoretical and computational at less than half the researcher size of analytical.

Four subdisciplines have more research publications than analytical over the six years (2008–2013) covered by the report. Physical (at 90% more than analytical) ranks well ahead of all other subdisciplines. Five of the other six subdisciplines have a very similar total publication performance. Theoretical and computational is the exception, principally because it was assessed for only five universities.

Medicinal and biomolecular had the highest research income for the years 2011–2013, as well as the number of researchers. Its revenue was 86% more than for analytical. The strong revenue position was not mirrored in the research output. Physical and structural at 82% above analytical had a strong research output performance. The traditional areas of inorganic and organic received significantly less research funding than four other subdisciplines.

The data presented in the 2015 ERA report provide a valuable insight into the relative strengths of the various chemistry subdisciplines. Overall, medicinal and biomolecular and physical and structural are the strongest disciplines in terms of total number of researchers and total research income. Analytical, inorganic, organic and macromolecular and materials all are of comparable size. Theoretical and computational is by far the smallest of all the subdisciplines.

Research capacity of a subdiscipline is closely related to the number of researchers. It is useful therefore to examine the performances relative to this parameter.

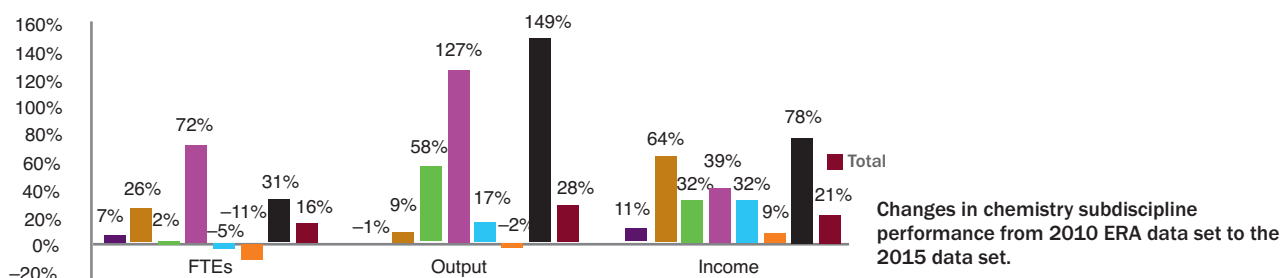
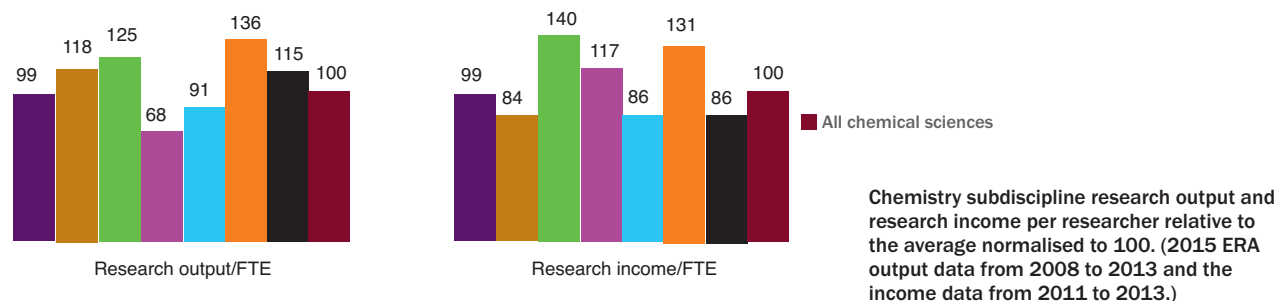
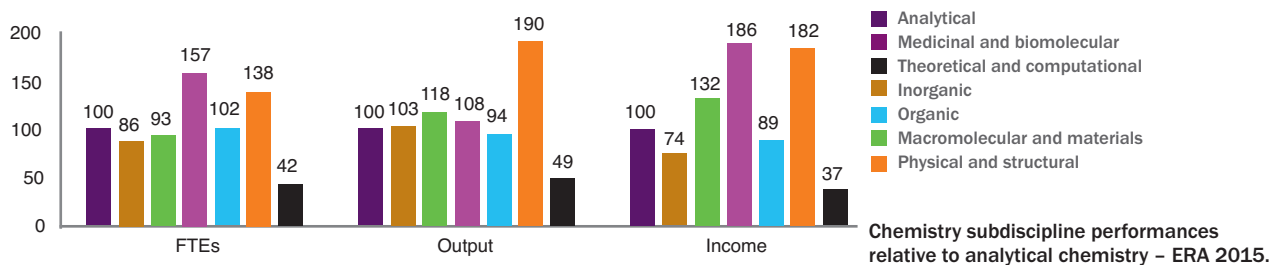
### Research output and income per FTE researcher – ERA 2015

The research output and the research income per FTE researcher are presented in the second graph. The data are normalised to the overall performance for the chemical sciences average set equal to 100. The actual chemical sciences value for the research output

Number of universities assessed and the average national ratings for the chemical sciences subdisciplines for the 2015 ERA exercise

	03 All chemical sciences	0301 Analytical	0302 Inorganic	0303 Macromolecular and materials	0304 Medicinal and biomolecular	0305 Organic	0306 Physical and structural	0307 Theoretical and computational
Universities assessed	26	16	13	16	12	11	20	5
Average national rating	4.25	4	4.15	4.75	4.08	3.55	4.55	4.6





per FTE is 11.5, while for the research income per FTE the value is \$251 300. Four of the seven subdisciplines have an output performance above the national average for the discipline, i.e. >100. Physical is the highest ranked subdiscipline at 36% above the average. Medicinal and biomolecular has the lowest output performance at 32% below the average even though it has an above average research income per researcher. Theoretical and computational now has a very competitive publication performance at 15% above the average.

Macromolecular and materials is the best performing subdiscipline for research income per researcher, being 40% above the average. Physical and structural at 31% is also well above the average. Three subdisciplines – inorganic, organic and theoretical – are around 15% below the discipline average for research income. Organic is the only one of these three with an output performance below the average.

### Performance trend from 2010 to 2015 results

The percentage changes from the 2010 exercise to the 2015 exercise are presented in the third graph, again for the three main research parameters. Overall, the number of researchers engaged in chemical sciences research increased by 16%, while the research output grew by 28% and the research income by 21%. While these are encouraging figures, as discussed in the previous article, several other science disciplines have outperformed chemistry.

Medicinal and biomolecular reported the highest growth in FTE

researchers. Theoretical and computational was the most improved in publication growth and research income. Two areas, organic and physical and structural, had a decline in the number of researchers. Physical and structural, while remaining strong in absolute terms for the 2015 ERA report, actually declined in total research output and researchers. It also was the field with the least growth in research income. Interestingly, inorganic received a significant increase in research income (64%), evident in increased research numbers (26%), but not publications (9%) to the same extent.

The adverse timeline trend for physical and structural should be of concern because of its central importance to chemistry. Overall, it is the weakest subdiscipline in terms of its growth profile.

The ERA assessments provide one valuable measure of the international standing of Australian chemical sciences and its subdisciplines. Universities use these results when making strategic investment decisions to support chemical sciences research. The exercise to be held in 2018 will provide further insight into the relative trends between subdisciplines. Overall, the international standing of Australian chemical sciences is high; however, relative to the performance of other Australian fields of science, there is need for improvement. This situation was discussed in the previous article (June issue, p. 38).

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## Ships ahoy!

Every so often I hear or see something in the news media that makes me sit up and ask, 'Can that be right?'. That was my reaction to a recent breakfast radio report that stated that the 15 largest container ships contribute as much air pollution as all the cars in the world. The report went on to discuss emissions of sulfur and nitrogen oxides ( $\text{SO}_x$  and  $\text{NO}_x$ ) from marine diesel engines, and how these are influenced by fuel quality.

Sensing a factual disconnect, I delved a bit further, and found that this was old news, with numerous recurrences of the same story going back to the original in 2009. However, in the spirit of never letting the facts get in the way of a good story, the reprised stories had not kept abreast of changing circumstances. The original story was based on a set of assumptions about fuel quality and the fuel consumption rates of large and small diesel engines. It assumed that the sulfur concentration in marine diesel fuel was 4.5%. In 2009, this was the maximum concentration allowed by the International Maritime Organisation (IMO). The authors of the original article apparently assumed this to be the sulfur concentration in all marine fuels, even though a shipping company executive quoted in the article stated that the average for his fleet was 2.5%, and that 4.5% sulfur in fuel was rare. So, unless the 15 largest ships only used fuel at the maximum allowable sulfur content, the report was flawed from the outset.

In the intervening years, as the story was re-hashed in (at least) 2013, 2015 and 2017, the IMO has tightened fuel specifications, so that the maximum allowed sulfur content was 3.5% in 2012, with a projected limit of 0.5% in 2020. Also, over this period, cruise ship operators, and maybe other shipping companies, have installed caustic scrubbers on the exhaust systems of their ships. These remove  $\text{SO}_x$  and  $\text{NO}_x$  from the exhaust stream, and give a faint plume of steam from the exhaust stack.

These limits are considerably higher than the allowable amounts in automotive diesel fuel (10 ppm in Australia), and the original article did serve to highlight the disparity. However, by not keeping pace with the latest developments in fuel standards, those repeating the story did a disservice to the lay readership.

While it should be no surprise that marine diesel engines, operating 24 hours a day up to 280 days per year, and with power outputs multiples of automotive engines (cars and trucks), produce more emissions, the simple analysis used also overlooked the effect of concentration of emissions sources on overall air quality. The impact of a single ship on the high seas is less than the combined effect of a million motor vehicles concentrated in a megalopolis where millions of people are exposed to the high concentrations of atmospheric

pollutants. Also, pollutant concentrations determine the potential for acid rain. However, when ships are grouped together (much like cars and trucks can be), they can cause appreciable increases in concentrations. This is so on some of the major inland waterways around the globe, such as the Amazon and Volga rivers, and the North American Great Lakes. In the latter case, ships contribute to  $\text{SO}_x$  and  $\text{NO}_x$  concentrations in the airshed of the industrial heartland of North America, where they add to the emissions from motor vehicles and stationary sources.

Despite all this, ships still represent the most efficient means of transportation over large distances, with emission rates per kilometre tonne travelled (for all exhaust gases) well below land-based transport. The development of the shipping container in the 1950s made the movement of materials and goods more efficient, and was further enhanced by the use of ever larger cargo ships. Low-cost trade has become a reality and, with it, the breaking down of trade barriers such as tariffs and import quotas. Non-tariff trade barriers have also been attacked and reduced, although in some cases they still exist and are relevant and important.

Sometimes, an unintended consequence of free trade agreements is that technical standards have been relaxed or ignored in the process. In Australia in recent years, we have seen the importation of asbestos-backed floor tiles, lead-based paint in children's toys, building cladding that doesn't meet fire resistance standards, and faecal contamination in frozen berries. These incidents can be attributed to poor supervision of technical trade and quality standards and the lower costs of imported goods. So, while large efficient marine engines might be responsible for atmospheric pollution, they can also be indirect agents facilitating other potential health risks. But, just like the caustic scrubbers on the exhaust stacks, there are control measures, which, if used properly, can deal with risks such as these.



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## Are you prepared to collaborate?

Mary Turonek, Senior Associate, FB Rice



Collaboration is an essential element of technical innovation and successful commercialisation of technology. There are many challenges to collaboration between the industry and research sectors, not least the different commercial drivers at play. Ownership and management of intellectual property (IP) is one of them.

It is rare that parties commence collaboration empty handed. The existing IP inputs arising from work created prior to the collaboration may be defined as the Background IP.

A collaboration agreement needs to specify if Background IP will be used, the manner and purpose of its use and by whom. Additionally, the collaboration agreement should contemplate and make allowances for continuing reliance on the Background IP after the collaboration project has ended for teaching purposes, commercialisation of the project IP or improvements.

Typically, a licence to access or use Background IP will be granted by the owner to the other collaborators with terms that correspond with the collaboration agreement. The licensee(s) may also seek a warranty from the owner that it owns or has the right to make the Background IP available.

Therefore, in order to be 'collaboration-ready', research organisations need to perform internal due diligence to clearly articulate not only the scope of the Background IP but also their legal entitlement to own and use the Background IP.

This raises many questions that are best answered as early as possible. Most importantly, who has contributed to the Background IP and would they be entitled to co-ownership in their own right?

Under an employment contract, most research staff of universities and research organisations are required to automatically assign the IP they create to their employer. However, no blind assumptions should be made. Do contracts clearly spell out the assignment and/or scope of 'normal course of employment'?

Students or visiting researchers are unlikely to be bound in the same way as research staff. It is important to understand whether their participation gives them a claim to ownership of the Background IP or the IP that may be created during the collaboration. If this is the case, it would be prudent to negotiate an assignment of their IP as early as possible or prior to them making a contribution.

Do contracts with contractors (e.g. software developers, consultants) clarify ownership of any IP generated? Are licences from third parties required to use the Background IP?

Other important questions to address include: Is there any technology or highly sensitive information that needs to be ring-fenced and not distributed regardless of confidentiality agreements in place? Are there any legal obligations to third parties from past collaboration projects? Are there any possible conflicts that should be disclosed upfront?

The time expended in negotiating IP contracts (typically 10 months) is one of the deterrents for collaboration with Australian research organisations. Ensuring that your organisation is 'collaboration-ready' is one step towards becoming an attractive collaboration partner.

For more information, email [mturonek@fbrice.com.au](mailto:mturonek@fbrice.com.au).

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## The chemistry of everything

As a scientist primarily interested in the chemical and biological sciences, I find it hard to go outside and not be reminded of the sheer beauty and complexity of the natural world. Studying and understanding just a small fraction of its chemical processes gives me sheer and humbling joy.

James Kennedy, a chemistry educator in Victoria, shows just how chemically complex something simple can be in his series of ingredients lists for fruits. His ingredients list for a blueberry ([bit.ly/2r9chH4](http://bit.ly/2r9chH4)) contains around 80 different chemicals. James notes also that ‘thousands of minority ingredients including DNA have been omitted for brevity’s sake’.

The family holiday snap shown was taken recently on the west coast of Tasmania, in the little town of Queenstown. For a fun exercise, and hopefully without ruining the magic of the photo, I am going to describe some of the chemistry pictured. (Beyond, that is, the obvious chemistry between the two people on the left.)

### Clouds

Clouds are made up mostly of liquid water and ice, but can contain other chemicals. They are formed when the water level, temperature and pressure are just right. In Tasmania, we have a large hydroelectric system, which relies on rainfall. Rainfall, of course, requires the presence of clouds! Research in Australia has shown that it is possible to use a simple and readily

available chemical to assist in the formation of clouds, and increase rainfall over a target area. Known as cloud seeding, planes are used to disperse silver iodide, which promotes the formation of ice crystals and water droplets. This has been shown to be an effective technique in increasing rainfall, and importantly has been shown to be safe for humans and the environment. More information including links to research on cloud seeding can be found through the Hydro Tasmania website ([bit.ly/2qz7Cj3](http://bit.ly/2qz7Cj3)).

### Grass, gardens and plants

Researchers at Texas A&M AgriLife recently reported that the smell of freshly mown grass is due to a combination of chemicals released by the grass as a stress response. The grass is, essentially, yelling for help and activating its protective mechanisms to help it survive the trauma of being cut open ([bit.ly/2sk5S9L](http://bit.ly/2sk5S9L)). The researchers hope that they can learn more about drought tolerance of plants through studying this stress response.

The successful tending of a garden can require the tightest of chemical balances. As we well know, some undesirable plants will grow just about anywhere under the harshest of conditions. Some more ornate, delicate and desirable plants require the right acidity of soil, the right water levels, the right balance of nutrients, and so on.



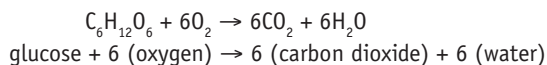


As biological systems, plants are incredibly complicated, but the reason they are green is quite simple. Most green plants contain green pigment molecules known as chlorophylls. The green colour is no accident: it is very much related to the function of the plant. Plants are green because they reflect green light, which is what you see, but they absorb other colours. The absorption of blue light by chlorophylls is what allows them to harness energy from the sun to allow the plant to produce food for itself, and survive.

## Car and train engines

Steam engines and typical car engines work by somewhat similar processes. Each involves the use of a fuel, which can be burnt, causing a release of energy that is then used to power the vehicle. When a fuel burns, it undergoes a combustion reaction. One example of a fuel that can be used to power a steam train is wood. Wood is primarily composed of cellulose, which in turn is composed largely of individual glucose molecules joined together in long branching chains. While wood is made of a lot of different chemicals that all burn in different ways, the combustion of glucose can be used as a model for understanding how combustion leads to energy production.

The overall chemical equation for the combustion of glucose is:



Described in words, one molecule of glucose reacts with six molecules of oxygen to form six molecules of carbon dioxide and six molecules of water. This reaction is exothermic – it releases energy.

## People

To try to describe every chemical process going on inside a person would be a near impossible feat. Here I want to describe only one aspect. There are few activities that humans spend

## Researchers at Texas A&M AgriLife recently reported that the smell of freshly mown grass is due to a combination of chemicals released by the grass as a stress response.

more time preparing for, planning for and money on than ... eating! One of the main reasons we eat is so that we have energy. Curiously, one of the main molecules used by our bodies to get energy from is glucose. Perhaps even more curiously, the overall chemical equation for the way our bodies get energy from glucose is *the same* as for the combustion of wood. This is something many of us are familiar with: the concept that we breathe in to get oxygen into our body, and breathe out to rid our bodies of the carbon dioxide that is formed. There is, however, a good reason we don't eat wood as a source of energy. Humans lack the required molecular machinery to break the wood down into individual glucose molecules.

Since everything is made up of chemicals, I'm sure there are many other examples of chemistry to find in the image. I hope to encourage everyone to marvel in the wonder of our world, and to share this joy with the younger generation. I've said before that kids are natural born scientists and investigators – what better way to nurture these traits than to inspire a fascination in understanding how things work.



**Jeremy Just MRACI** is a Hobart-based PhD candidate in organic chemistry and a passionate science communicator, specialising in chemistry shows and demonstrations. Jeremy writes these columns for members to share with or demonstrate to friends and family without formal chemistry knowledge.



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## Environmental change could be damaging some of the world's most precious archaeology

Star Carr in North Yorkshire is perhaps the most important archaeological site in the UK relating to the Mesolithic period from the end of the last ice age.

Archaeologists have discovered unique organic artefacts at Star Carr that are over 10 000 years old. These include carved red deer antler headdresses, thought to be part of the earliest shamanic costume, and expanses of worked wood that display the earliest evidence of carpentry in Northern Europe.

But recent excavations at Star Carr have produced bone that was completely demineralised and wood that was severely compressed, representing the loss of valuable archaeological evidence. The problem was caused by environmental changes in the waterlogged soil that once preserved the evidence. And thanks to environmental changes related to things such as land modification and climate change, other important archaeology around the world could be at risk from similar destruction.

Wetlands like Star Carr and other waterlogged environments can preserve organic materials that are rarely found elsewhere. This is because the lack of oxygen in the environment prevents biological decay. This can provide unique evidence for how people lived and interacted with the natural environment, from

the remains of prehistoric buildings to delicate ecological evidence such as plant and insect remains that tell us what past environments were like.

But wetlands across the globe are increasingly at risk from environmental changes including drainage, land development and climate change. Wetland loss can contribute to flooding, drought, coastal erosion and species destruction. But we also need to make sure the effects of this environmental change on the unique archaeological information found in many wetlands aren't overlooked.

The evidence shows that the alarming deterioration of artefacts at Star Carr was the result of geochemical changes at the site. But the exact cause and timescale of these changes was until now unknown, making it hard to make decisions about how to mitigate or manage the problem.

In our most recent research, we recreated the environment of Star Carr in a lab by burying modern and archaeological bone and wood in peat taken from the site for a period of 12 months. We then used a number of chemical analysis techniques to measure how much the bone and wood had decayed and compared it to decay on artefacts excavated from the site itself.

Professor Nicky Milner from the University of York during excavations at Star Carr, uncovering Mesolithic timber.  
University of York/Lorne Campbell (Guzellian)







Valuable artefacts have been discovered in many wetlands.

iStockphoto/Paul\_Cooper

Alarmingly, we found that within only 12 months the structure of the bone had completely transformed, visibly altering its appearance. This would make it much harder to work out things like its age and what kind of bone it was. We also found chemical changes in the wood, although decay was slower. In comparison, similar material buried in sand or garden compost for the same time period showed almost no change.

### Rapid decay

The main reason for the rapid decay of evidence from Star Carr is the increased acidity in the ground caused by a recent drop in water levels. Field drains inserted near the site around the year 2000 reduced the water table – the level where the ground is permanently saturated – to below the archaeological horizons. This exposed sulfur compounds in the soil to oxygen, producing sulfuric acid. The loss of water in the ground also compressed the soil and the wooden artefacts within it, as well as creating more potential for biological decay.

Our experiments have also shown that the conditions at the site are causing the loss of organic archaeological material at an incredibly fast rate. This raises serious concerns for the continued survival of evidence buried there, and at other sites with similar conditions.

This decay causes an irreplaceable loss of our cultural heritage. The speed at which we now know it can happen means we need to take urgent action when other sites are similarly

**Our experiments have also shown that the conditions at the site are causing the loss of organic archaeological material at an incredibly fast rate. This raises serious concerns for the continued survival of evidence buried there, and at other sites with similar conditions.**

threatened. As many wetland archaeological sites are typically left unexcavated, we need to start working out the risk to the evidence they contain. If we don't improve our understanding and monitoring of wetland conditions – and come up with strategies to manage them – then we stand to lose some of the world's most valuable cultural assets.

**Kirsty High** is a research fellow and **Kirsty Penkman** is senior lecturer in chemistry at the University of York. First published at [www.theconversation.com](http://www.theconversation.com).



iStockphoto/Simon Dannhauer

## Post-harvest vineyard activity

After the grape harvest each year, winemakers move their focus from the vineyard to the successful completion of fermentations as well as preparing wine for ageing or bottling. For the viticulturist, management of the vines continues for some time post-harvest at least until leaf fall or senescence. One of the critical issues in this post-harvest period is the build-up of reserves in the vines for the next growing season.

When I first went to the National Wine and Grape Industry Centre (NWGIC) in Wagga Wagga, I was intrigued to see how long the leaves remained green after harvest, indicating that photosynthesis was occurring. Coming from Melbourne and observing vine growth in the cooler areas, I was accustomed to leaves dropping within a few weeks after harvest, rather than 2–4 months in the warmer areas around Wagga Wagga. This difference in green leaf behaviour is even more apparent in the Côte d'Or region of Burgundy. Here, it is common for the leaves to be brown even at harvest; in some areas, leaf fall may have occurred before the grapes are picked. Obviously, there is no photosynthesis occurring in these Burgundian situations. All this becomes significant in managing the crop load for the next harvest.

When new growth occurs in the following spring, vine reserves are called on to drive this growth. The demand on vine reserves reaches a maximum around the 8–10 leaf stage and then declines as the growing leaves become sufficiently active for photosynthesis to meet the vine's demands. The vine reserves of most importance are carbohydrates and nutrients. Carbohydrates consist of starch as well as glucose, fructose and sucrose (the 'free' sugars) while nitrogen and phosphorus are the major, or macro, nutrients.

After harvest, it becomes part of the viticulturist's role to manage the vines to ensure that there are sufficient reserves for the next season. As a simple rule, it can be assumed that the higher the grape harvest yield, the greater the need to replenish the reserves. Thus, higher crop loads can be tolerated in a warmer

region as there is a longer period of active photosynthesis after harvest while lower crop loads are needed in the cool to cold regions. In some years, monitoring the water status of the vineyard and supplementing with water may be required. Nitrogen fertilisation may also be required post-harvest.

Until recently, decisions were made on experience of vineyard behaviour. While analyses for carbohydrates and nutrients can be performed, the traditional methods are slow and cumbersome. Starch analysis requires enzymatic hydrolysis of the vine tissue extract followed by glucose determination, while combustion analysis is the approach used for nitrogen. There are three sections of the vine that need to be sampled – root, trunk and cane – as each contributes to the new season growth at different development stages. Once sampled, the plant tissue needs to be dried and then milled to a consistent size so that the extraction process is uniform.

Dr Jason Smith and Dr Bruno Holzapfel from the NWGIC have worked extensively on vine reserves. Jason, now in Germany at the Geisenheim Wine Research Institute, examined the suitability of attenuated total reflectance Fourier transform IR (ATR-FT-IR) spectroscopy as a replacement technique for traditional strategies. Vine tissue that Jason had collected in several projects from Riesling, Semillon and Shiraz plants from both warm and cool regions in Australia as well as Geisenheim were used. Some 1880 samples were analysed by the starch and nitrogen traditional methods and by ATR-FT-IR spectroscopy. Interpretation of the data sets by chemometrics, performed by Dr Leigh Schmidte from the NWGIC, allowed predictive models to be developed that validated the ATR-FT-IR approach as an effective tool for monitoring vine reserves (see *Anal. Chim. Acta* 2012, vol. 732, pp. 16–25). Having access to a procedure for rapid assessment of reserves provides viticulturists with a more rigorous basis for decision-making.

From their studies, Jason and Bruno were able to propose some general guidelines relating harvest yield to the management of carbohydrate reserves. When crop yields are 20–30 or more tonnes per hectare (t/ha), the build-up of reserves may take 6–8 weeks for proper replenishment, while when yields are less than 10 t/ha, replenishment tends to occur in parallel with berry ripening, provided the canopy is healthy. For yields of 10–20 t/ha, post-harvest reserve management becomes increasingly important as the yield increases. More detail on this work can be found on the Wine Australia website ([bit.ly/2rrWILe](http://bit.ly/2rrWILe) (fact sheet) and [bit.ly/2rrIc6e](http://bit.ly/2rrIc6e) (industry presentation)). A detailed report on vine reserve management (CSU-05-01) is available at [bit.ly/2rrIc6e](http://bit.ly/2rrIc6e).

All of this assumes that there is adequate water and nutrients and that the vines are disease-free. More tasks for the hard-working viticulturists.



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## Dr Findlay, the phase rule and its admirers

I have previously written about Alexander Findlay (1874–1966), including his books *Chemistry in the service of man* and *Introduction to physical chemistry* (see June issue, p. 41, and July issue, p. 41). Another of Findlay's books, *The phase rule and its applications* (1904), is so prized by chemists that it is available online today. It was revised from time to time, latterly with co-authors for the ninth edition in 1951. While firmly based in chemical theory, Findlay's book also has an eye to industry, with an extensive treatment of iron–carbon alloys, and the characteristics of steel, with carbon content in the order of 1%. The phase diagram, in which cementite,  $\text{Fe}_3\text{C}$ , features strongly, is a complex one. Findlay's book was one of the first in a series published by Longman Green and Co. Included in the book by way of introduction was a philosophical essay by the series editor Sir William Ramsay on the differences between physics and chemistry. It rambled on for about 20 pages without ever reaching a conclusion.

Not everyone was a great fan of Findlay's book, however, as I discovered when I consulted A.C.D. Rivett's *The phase rule and the study of heterogeneous equilibria. An introductory study* (1923). Rivett's interest in the phase rule is said to derive from his experience in Britain during World War 1 where he was in charge of a factory producing ammonium nitrate. He comments that it is based on his lectures at the University of Melbourne, where he eventually succeeded Masson, only to decamp after a few years to the fledgling CSIR. Rivett wrote that Findlay's book 'covers considerable ground, especially in one- and two-component systems, though the omission of references to typical space diagrams showing the relations between all the variables in these respective cases make it difficult for beginning students. It was not clear to me whether Rivett was referring to a lack of citations – there were hardly any in his book – or to the lack of diagrams with the specific characteristics. Probably the latter, since his diagrams were more complex than the 134 figures in Findlay's text.

As did Findlay, Rivett drew attention to the work of Ostwald, who had included 'a great deal that is fundamental' in his *Lehrbuch der allgemeinen Chemie* (1885). Findlay was a student of Ostwald's and included him with Roozeboom and Bancroft as influences on his thinking, while retaining Josiah Willard Gibbs (1839–1903) as the father of the phase rule.

While Findlay's *Phase rule* was evidently of interest to chemists, it also attracted the attention of the American historian Henry Brooks Adams (1838–1918). Adams was a member of a political dynasty that started with John Adams (1735–1806), who served two terms as Vice-President to George Washington before becoming America's second President (1797–1801). He was succeeded by Thomas Jefferson (1801–9). John Adams' son, John Quincy Adams (1767–1848), was the sixth American President, serving from 1825 to 1829. His son, Charles Francis Adams was President Lincoln's ambassador to Britain, and his grandson was the aforesaid historian.

Henry Adams took a 'scientific' view of history and made a rather tenuous connection between phases of historical development and the phases of matter that were being carefully defined by 19th-century scientists. It's not clear to me that he understood what the phase rule was all about, but in the early years of the 20th century he would not have been alone in that. In 1908, he wrote a long essay entitled *The rule of phase applied to history* in which he commented on the work of Yale Professor Willard Gibbs. '(H)is Rule of Phases defies translation into literary language', Adams wrote, possibly because '(T)he mathematical formulas in which he hid it were with difficulty intelligible to chemists themselves, and are quite unintelligible to an unmathematical public'.

**Henry Adams took a 'scientific' view of history and made a rather tenuous connection between phases of historical development and the phases of matter that were being carefully defined by 19th-century scientists.**

This was no passing fancy of Adams'. It is clear that he was familiar with Gibbs' memoir on equilibrium of heterogeneous substances and 'on the existent phases of matter', published in the 1870s in the *Transactions of the Connecticut Academy*. And it is known that he possessed a copy of Findlay's *The phase rule and its applications*. He wrote about ice, water and steam, and understood that the phases were in equilibrium. He speculated about how rapidly an equilibrium could be established, and that led him to attempt reconciliation of the evolutionary theory of history and the laws of thermodynamics.

Drawing on the work of other historians, he labelled the years before 1600 as the Religious Phase that changed, as ice did to water, into the period 1600–1900 that he described as the Mechanical Phase, and was followed by the Electric Phase. He questioned how long humans could go on developing new phases, and noted that the process of phase-change seemed to be accelerating and could be described by a 'law of squares'.

Adams felt that Gibbs got most help from a book called the *Grammar of science* by Karl Pearson, but since this book was published only in 1892 I have my doubts about that assertion.



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**Fundamentals of Process Safety**

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[www.icheme.org/shop/events/courses/2017/aus%202017/fundamentals%20of%20process%20safety%20-%20nz.aspx](http://www.icheme.org/shop/events/courses/2017/aus%202017/fundamentals%20of%20process%20safety%20-%20nz.aspx)

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[www.icheme.org/sitecore/content/ICHEME/icheme\\_home/Shop/Events/Courses/2017/Aus%202017/energy-cost-reduction](http://www.icheme.org/sitecore/content/ICHEME/icheme_home/Shop/Events/Courses/2017/Aus%202017/energy-cost-reduction)

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**2nd International Conference on Pharmaceutical Chemistry**

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**ChemComm Symposia on Energy Science and Materials – Beijing**

9 October 2017, Beijing, China  
[www.rsc.org/events/detail/26254/chemcomm-symposia-on-energy-science-and-materials-beijing](http://www.rsc.org/events/detail/26254/chemcomm-symposia-on-energy-science-and-materials-beijing)

**6th Modern Solid Phase Peptide Synthesis and its Applications Symposium**

12–14 October 2017, Fraser Island, Qld  
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**International Conference and Exhibition on Pharmaceutical Nanotechnology**

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**2nd International Conference on Applied Chemistry**

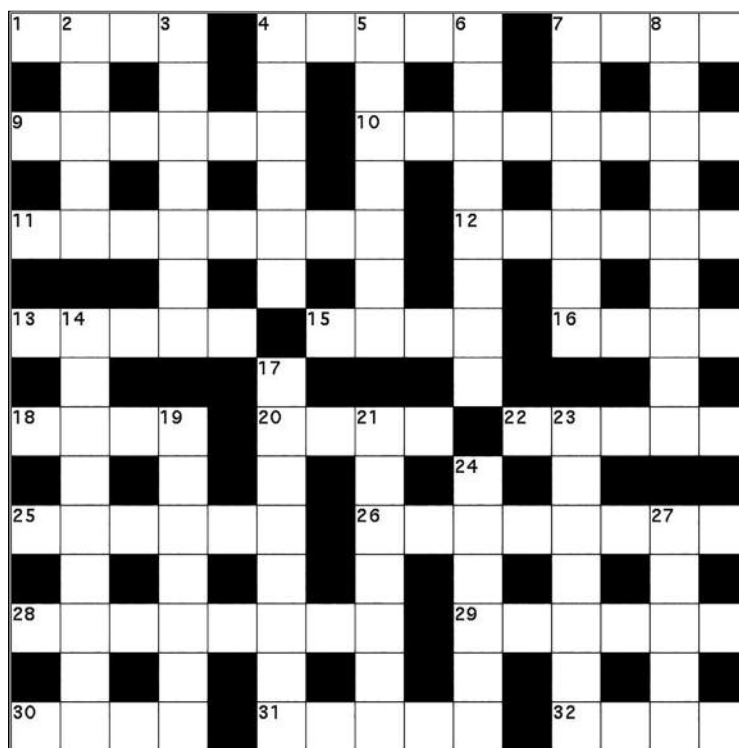
30 October – 1 November 2017, Chicago, Illinois, USA  
<http://appliedchemistry.conferenceseries.com>

**Emerging Polymer Technologies Summit**

22–24 November 2017, RMIT University, Melbourne, Vic.  
<http://epts17.org/index.html>

**QACS 2017 – Qld Annual Chemistry Symposium**

27 November 2017, Queensland University of Technology, Brisbane, Qld

**Across**

- 1 Two elements of a lawsuit. (4)  
 4 Absence of colour brought about by boron deficiency. (5)  
 7 Ceremonial staff 5 Down for self defence. (4)  
 9 Character creation. (6)  
 10 Rubbish! A bell sound is coming about. (8)  
 11 Employs tulip size change taking out fifteen. (8)  
 12 Heat over neon compound. (6)  
 13 Telly Tubbies come over with a radical . . . (5)  
 15 . . . and three elements. (4)  
 16 Aforementioned four elements. (4)  
 18 Compete with tungsten opinion. (4)  
 20 Red stone composed of three elements. (4)  
 22 Complete tungsten void. (5)  
 25 Chooks' levels. (6)  
 26 Boron and phosphorus behind letting only some frequencies through. (4-4)  
 28 Hamlet on new compound. (8)  
 29 Iridium holds some with a different arrangement. (6)  
 30 Way with argon plasma sphere. (4)  
 31 Found sooner than expected in extranuclear lysine studies. (5)  
 32 Even teams may recognise good television. (4)

**Down**

- 2 Isolated a component. (5)  
 3 50:50 partner pursues start of estimated quarterly usage. (7)  
 4 Wind easy. (6)  
 5 Gives a spray for a looser arrangement. (7)  
 6 Tautomerism displayed by ethyl acetoacetate, for example, makes likely doctoral commentary monopolising centres. (4-4)  
 7 Tests for fire lighting. (7)  
 8 Can changes in coal be accepted? (9)  
 14 Sodium, for example, is such via tunnel reaction. (9)  
 17 Ghost occupancy. (8)  
 19 Hydrogen with  $R_1OR_2$  on tungsten suggests possibilities. (7)  
 21 Blubber used to exclude air from a reaction. (7)  
 23 A monosaccharide fed to sheep. (7)  
 24 Object to its 9 Across. (6)  
 27 Hot water cooked meats. (5)

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



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