



The Journal of the Institute of Chemistry of Ireland



Obituary and Tribute to James Philip Ryan

Award Winners: Industrial Chemistry Award 017 Prof Tom Moody - Almac
Annual Lecture Series (Eva Philbin) - Prof Donal O'Shea – RCSI



Enzyme Processes Past, Present & Future



Commemoration of first lady Professor of Chemistry at RCSI



Molecular gastronomy, as a prototype for discussing the issue of scientific strategy.

Prof Hervé This

The Second Dublin Werner - Prof Tony Werner 2011 - 2008



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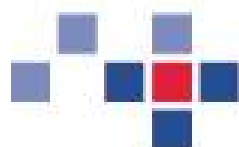
A message from the President

Dear Colleagues,

I would like to wish you a Happy new year. There are a number of exciting events happening in 2018. For Environmental Chemists, the Environmental Science Association are running a conference in CIT on March 26th- March 28th. (see <http://www.esaiweb.org/environ/>) There is a Eurachem event in Dublin on 14th - 15th May 2018, of interest to anyone interested in Quality Assurance. (see <http://eurachem2018.com/>). The 70th Irish Universities Chemistry Research Colloquium will be held in the School of Chemistry and Chemical Engineering in Queens University Belfast on 13th-15th June; an event that the ICI has been proud to support. The EUChEMS Chemistry Congress will be in Liverpool from 26th- 30th August (see <https://www.euchems2018.org/>). Furthermore we are progressing with a bid to host the Congress in Dublin in 2022. Finally I would like to wish you all a healthy and productive 2018.

John Cassidy

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Editorial

End of another year and this is the 5th Issue for the year and one short of the target of six per year for the second successive year. The fundamental is getting academic papers on time. Publication dates approach and papers do not arrive on time for editing and preparation of the mater document for checking or modifications. This is disappointing as so much high quality chemical research is taking place in our universities, colleges and research institutions. I think it is important to highlight that work and effort and communicate it to the larger chemical community in academia and industry.

Another concern is that the name of the journal may indicate that is simply a newsletter and this might discourage researchers from taking the time and effort to write papers for publications in ICN. Council are currently discussing the possibility of changing the name to better reflect the aims of the journal which is to highlight the range and quality of chemical research in Ireland and credit the researchers.

It has been a very active year for the Institute with many awards, a Congress and promotions of chemistry events. These are reported on in the following pages.

It is with great sadness that we have the obituary of our Honorary Secretary, James Philip Ryan or Philip as we knew him, a most remarkable and modest person with many achievements to his name. Most of the material has been provided by his sister Sheila Ryan with some editorial additions and a few comments from long serving Council members.

Notices of impending events coming up early in 2018 namely the Irish Lab Awards and the Industry & Business set of four parallel conferences at City West on January 31st.

Our Industrial Chemistry Award Winner Prof Tom Moody who let a team from Almac has provided a paper based on his lecture in RCSI in early December.

There follows a Tribute to the First Lady Professor of Chemistry at RCSI. Professor Ethna Gaffney.

Congress this year was on food chemistry at DIT, Kevin Street and Prof Hervé This, (Institut National de la Recherche Agronomique), France has provided an interesting paper on synthetic food from statgels to dynagels.

For this Issue a second paper has been provided by Prof Brian McMurry on “The Second Dublin Werner” Tony Werner, the son of Professor EA Werner previously written about in Issue 3.

The final sections cover announcements by the IDA, Enterprise Ireland and reports by our supporter Industry & Business.

We are preparing to bid for the EuCheMS Congress 2022 for Dublin at the 2018 Congress in Liverpool. We are working with Dr Noel Mitchell, Keynote PCO who won **The CCD Outstanding Contribution to Business Award 2017** for bringing 12,000 delegates and €20 million worth of conference business to the Dublin Convention Centre, which itself has won **‘World’s Leading Meetings & Conference Centre 2017’ at the World Travel Awards**. I appeal to PIs and Heard of Chemistry Schools to get your teams ready to attend the EUChemS Chemistry congress in Liverpool in 2018 and show support for our bid.

I also appeal to readers and researchers to encourage your colleagues to join the Institute and engage in promoting chemistry and if you are not a member to join. Membership forms are available on our website.

www.chemistryireland.org

Responses can be sent to:-

info@instituteofchemistry.org

Patrick Hobbs MSc, FICI, CChem, CSci, MRSC.
Editor
30/12/2017



7th EuCheMS Chemistry Congress

Molecular frontiers & global challenges

ACC LIVERPOOL, UK
26–30 August 2018

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About the congress

With a theme of ‘Molecular frontiers and global challenges’, the 7th EuCheMS Chemistry Congress features five days of scientific and technical sessions, plenary lectures, oral and poster communications, keynote speakers and roundtable discussions, as well as exceptional networking opportunities, an exhibition and a unique social programme.

The EuCheMS Chemistry Congresses reflect the outstanding research being done in Europe and around the world by bringing together chemists from different countries and professional backgrounds to exchange ideas, advance knowledge and discuss key issues for chemistry and society. As such, the 7th EuCheMS Chemistry Congress offers you exceptional opportunities to network with chemists from across Europe and beyond.

Registration will open in late 2017, and will be via an online system; full payment is required to guarantee your booking.

<http://www.rsc.org/events/euchems2018#>

Update: There will be seven plenary speakers and six have now been confirmed. These are:

Paul Alivisatos, University of California, Berkeley, USA

Frances Arnold, California Institute of Technology (Caltech), USA

Stefanie Dehnen, Philipps-Universität Marburg, Germany

Christopher Dobson, University of Cambridge, UK

Ben Feringa, University of Groningen, The Netherlands

Jin-Quan Yu, The Scripps Research Institute, USA

The seventh and final plenary speaker will be the winner of the European Chemistry Gold Medal which will be announced next year.

In addition, the themes and conveners for the congress have all been agreed and confirmed:

Theme A: Catalysis – Graham Hutchings (UK)	
A1: Catalysis at the homo/hetero/bio interface	Christophe Copéret (M) Switzerland
A2: Heterogeneous catalysis	Annette Trunschke (F) Germany
A3: Homogeneous catalysis	Carmen Claver (F) Spain
A4: Biological catalysis	Dick Janssen (M) Netherlands
Theme B: Chemistry in the Life Sciences – Sara Linse (Sweden)	
B1: Biomolecular assembly processes	Tuomas Knowles (M) UK
B2: Bioimaging, analysis and diagnostics	Andrew de Mello (M) Switzerland
B3: Synthetic biology	Greg Challis (M) UK
B4: Chemical biology and drug discovery	Alessio Ciulli (M) UK
Theme C: Energy, Environment & Sustainability – Ib Chorkendorff (Denmark)	
C1: New approaches to clean fuels	Beatriz Roldan (F) Germany
C2: Fuel cells and batteries	Ifan Stephens (M) UK
C3: Solar photovoltaics	Annamaria Petrozza (F) Italy
C4: Sustainable use of resources and green chemistry	Eleni Heracleous (F) Greece
C5: Clean water and air	Ester Heath (F) Slovenia
Theme D: Inorganic Chemistry Advances – Maria José Calhorda (Portugal)	
D1: Inorganic reaction mechanisms	Yann Garcia (M) Belgium
D2: Bioinorganic chemistry	Ricardo Louro (M) Portugal
D3: Main group chemistry	Jean-François Halet (M) France
D4: Transition metal chemistry	Grace Morgan (F) Ireland
Theme E: Materials, Interfaces & Devices – Barbara Albert (Germany)	
E1: Materials governed by scale and dimensionality	Joao Rocha (M) Portugal
E2: Un-conventional syntheses of inorganic solids	Natalia Dubrovinskaia (F) Germany
E3: Functional materials and their electronic, magnetic and optical properties	Amparo Fuertes (F) Spain
E4: Biomaterials	Peter Behrens (M) Germany
E5: Soft control: macromolecules and smart polymers	Klaus Müllen (M) Germany
Theme F: Organic Chemistry Advances – Josef Michl (Czech Republic)	
F1: Supramolecular and self-assembled materials	Paolo Samorì (M) France
F2: Molecular machines and designed materials	Alberto Credi (M) Italy
F3: Organic synthesis and methodology	Christina Moberg (F) Sweden
F4: Organic reaction mechanisms	Jana Roithova (F) Czech Republic
Theme G: Physical and Analytical Chemistry Advances Piero Baglioni (Italy)	
G1: Photochemistry / photophysics / electrochemistry	David Birch (M) UK
G2: Advances in physical chemistry	Marie Paule Pileni (F) France
G3: Advances in analytical chemistry and methods	Jiri Homola (M) Czech Republic
G4: Computational and theoretical chemistry	Chantal Daniel (F) France

OBITUARY AND TRIBUTE TO JAMES PHILIP RYAN
BSc, PhD, CBiol, MIBiol, EurProBiol, FIScT, CChem, MRSC, FICI, EurChem
Honory Secretary of the Institute of Chemistry of Ireland 1982 – 2017



James Philip (better known as Philip) was born in Drogheda on 5th May 1944, the only son of Dan and Grete Ryan. He was educated in St Joseph's Christian Brothers School, Drogheda, and Franciscan College, Gormanstown, Philip had two careers in mind when he left secondary school, one was to become a scientist and other a cook, and chose to go down the scientific road.

Philip as he was popularly known graduated with an honours degree in Biochemistry from UCD in 1967. While working for his PhD 1967 – 1970, he studied under Dr Hubert Ryan who is a son of the late Professor Hugh Ryan, the founder of the Chemical Association of Ireland. He received his Ph.D Degree for research on Cellular Control Mechanisms in 1970. In 1977, he completed a postgraduate BSc in Pharmacology at UCD.

Philip spent over 30 years on research and teaching attached to various departments in UCD. He had good reason to remember the year he spent lecturing in Biochemistry in the Royal College of Surgeons in Ireland, 1970-1971 during which time he met his wife. He married his wife, Fidelma, a Ph.D in Pharmacology, on 31st December 1974.

From 1971 to 1974, he held a post-doctoral fellowship in the Department of Zoology, UCD. During the Seventies he carried out a theoretical study of biological information systems which was published in the form of several definitive papers. In all, since 1969, Dr Ryan has published 250 scientific papers in many areas of research including, Analytical Biochemistry, Cell Physiology, Biochemical Pharmacology, Enzymology, Theoretical Biology, Ruminant Fermentation and Clinical Biochemistry. From 1997 he was actively involved in research on ruminant digestion, metabolism and glycosidase enzymes in the Department of Physiology and Biochemistry, Veterinary College at UCD.

He was both a Chartered Chemist and a Chartered Biologist, and was registered European Chemist in 1993.

In his younger days, Philip had many poems published and he wrote a book on Teilhardian Hyperphysics. This was a theory first put forward by the French Jesuit theologian Pierre Teilhard de Chardin in an attempt to reconcile evolution, science and religion and form an understanding with scientists.

He also studied the Connemara Dialect of the Irish language at this time.

Philip became a member of the Institute of Chemistry of Ireland in 1970 after completing his PhD and, like his father, also a Fellow. He was elected honorary secretary in 1982, archives secretary in 1985 and company secretary in 1986. Amongst many tasks, he was involved in compiling and editing Newsletters. He was renowned for his loyalty and professionalism throughout his long service of over 35 years and attended some meetings even when he became ill.

The Council of the Institute of Chemistry were honoured in the winter of 2000, when they were invited to meet and have tea with President Mary McAleese at Aras an Uachtarain. Philip presented her with a copy of his book on the History of the Institute. In fact he has written two books on the two organisations that were the forerunners of our present Institute:

1. The Chemical Association of Ireland 1922 - 1936
2. The Irish Chemical Association 1936 - 1950

The Marquis Who's Who Publications Board certified that Philip was a subject of biographical record in "Who's Who in the World" Twenty-first edition 2004. The inclusion is limited to those individuals who have

demonstrated outstanding achievement in their own fields of endeavour and who have, thereby, contributed significantly to the betterment of contemporary society because of the reference value of those achievements. Who's Who in the World provides accurate and current biographies of the day's most influential and accomplished people from around the world. Marquis Who's Who has established itself as the premier biographical resource for libraries, corporations, researchers, associations, government and media.

He received a Diploma in Psychology at Maynooth College in August 1999 and a Diploma in Theology at The Milltown Institute of Theology and Philosophy in June 1999. Philip also received Diplomas in Counselling and French Cuisine.

He worked voluntarily as Secretary for his local church, the Church of St Thérèse in Mount Merrion, for a few years quite recently and was a dab hand at their Newsletters.

Philip wrote his first Book on the History of The Chemical Association of Ireland 1922 - 1936, covering the period 1922 to 1936, in September 1997. He thanked Fidelma and said he could never have sustained the venture without her constant support and unfailing encouragement, and dedicated the book to Dan and Grete.

He wrote his second Book on the History of the Irish Chemical Association 1936 - 1950, covering the period 1936 to 1950, in June 2000. He dedicated the book to Fidelma and said he could never have completed the book without her patience and support.

Under the penname of Philip Fortune, he wrote a Childs play in 2007.

Under the penname **Richard Rydon**, Philip was an award-winning science fiction novelist, and won awards for both fiction and non-fiction work. He was a prolific writer and published over 300 papers, articles, and poems, in scientific journals, international magazines and local papers.

He wrote a Trilogy of novels on Science Fiction in 2007, 2008 and 2011 respectively, which were given excellent reviews and published by Lulu Publishing.

Philip's second novel "The Omega Wave" was selected as one of the finalists in the Science Fiction Category of the Reader Views Literary Awards and was awarded an Honorary Mention in the Reviewers Choice Awards in 2009.

In the Feathered Quill Book Awards 2014, he won the Bronze/3rd Place in the Romance Category for his third novel "The Palomar Paradox".

Philip also published an anthology of his poetry, containing 100 poems, in 2011.

He wrote a book on exploring metaphysical reality "**Matter Energy and Mentality**" in 2012.

Philip wrote a Trilogy of books on "Profiles of the Nutrients" in November 2016, December 2016 and February 2017 respectively.

Philip loved reading, both fiction and non-fiction. He was particularly interested in English poetry and ancient Irish archaeology and mythology, as well as science, nature and cookery, amongst other topics.

Throughout his life he had a great interest in photography. He was "The Photographer" at many of the Institute's Awards, Congresses and events and hence rarely appeared on photographs himself in keeping with his modest nature. In his young days, he used to develop his own photographs in an outhouse converted to a dark room. He had a "do not disturb" sign on the door when he was developing as any light would affect the quality of the prints. In later days he was really adept at enhancing and enlarging photos via his computer. He was very interested in art, especially modern art, portrait and landscape. He was an excellent painter in his own right, and produced many lovely paintings in gouache, oils and watercolour. He specialised mainly in modern art and landscape work.

He loved most kinds of music, but especially classical, opera, gospel and traditional Irish. Among his favourite popular artists were Imelda May, Bonnie Tyler, Celine Dion, Bette Midler, Leonard Cohen, Roy Orbison and Cat Stephens, to name but a few.

He was really good cook and would spend lots of time putting delicious meals and snacks together. He had some specialities and made the best prawn cocktail ever.

He was a great chess player and used to play regularly with some friends in a Stillorgan Hotel up to a few years ago.

Philip loved walking and did as much as he could, and found it to be relaxing and quite therapeutic. He enjoyed the simple things in life, like a quiet stroll to the shops and relaxing in his garden.

He also loved to relax watching TV. He was interested in the news and factual programmes, particularly nature, as well as good dramas. For lighter viewing, he particularly loved to watch “Fair City”, “Judge Judy” and some comedy.

Philip loved working on his computer; he had a great interest and was very competent using photoshop. He was ever so good at identifying errors and typos in working drafts of Irish Chemical News.

He always had a great interest in gardening and looked after his own fairly large garden until recent years, when he employed a gardener. He took pride in his garden and had some interesting and unusual plants.

When his wife Fidelma became frail in later, Philip cared for her very well. Fidelma’s sister Deirdre and her children, especially Clodagh and Rory, were always there to help out and were marvellous especially when Philip himself became unwell.

Philip truly was a lovely man, loved and respected by those close to him and those privileged to have to have touched his life. He accepted life and just got on with it, good or bad, without question and with great dignity.

He was a man of faith, integrity and wisdom. He was very loyal to his family, friends and colleagues. He was a gentle soul, kind, caring, thoughtful and understanding. He was friendly, cheerful, easy going and contented. He was witty too and loved a laugh and to crack jokes. He was also quite a private person, fairly quiet, unassuming and very understated.

Philip was extremely generous to his family and friends and would always help out if he could without hesitation.

Philip showed great courage and patience throughout his treatment for and battle with oesophageal cancer and heart failure. He never complained or bothered people unless he really had to do so and was a very good patient. He was brave and dignified throughout this difficult and sad time.

Ray Leonard – Council Member and other long serving members commented “We have had the good fortune to serve on the Council of the Institute of Chemistry of Ireland for some of the many years that Philip served as Honorary Secretary.

Our recollections of Philip are that first and foremost he was a consummate gentleman. He had an encyclopedic knowledge of the rules and regulations of the Institute as framed by its constitution. He took his duties very responsibly and was a very diligent and conscientious Hon. Secretary but always carried out his duties in a very patient, courteous and good humoured manner. It was readily apparent that it was a labour of love for him.

We now realise that the Philip we knew was merely the” tip of the iceberg” and that his unassuming manner cloaked the many attainments and achievements that bear testament to his life outside the Institute.”



Young Chemist Prize 2017

Closing Date Friday 12th January 2018

Each year the Physical, Chemical and Mathematical Sciences Committee selects a winner of the Royal Irish Academy Young Chemist Prize.

A prize is given for the most outstanding Irish PhD thesis in the general area of the chemical sciences, as described in a 1,000 word essay (maximum, but figures are permitted). The prize is the successor to the Royal Irish Academy Prize for Young Chemists established in 2000 and the award is administered by a group from the RIA's Physical, Chemical and Mathematical Sciences Committee.

The winner will be nominated by the Physical, Chemical and Mathematical Sciences Committee of the Royal Irish Academy to go forward for the prestigious International Union of Pure and Applied Chemistry young chemist prize sponsored by IUPAC.

Young Chemist Prize 2017

A prize will be given for the most outstanding Irish PhD thesis in the general area of the chemical sciences. The prize, kindly sponsored by Henkel Ireland Operations & Research, includes an award of €2,500. The winner will be nominated by the Physical, Chemical and Mathematical Sciences Committee of the Royal Irish Academy to go forward for the International Prize for Young Chemists sponsored by IUPAC.

Applicants must:

- Submit a 1,000 word essay (maximum, but figures are permitted) describing the thesis work and placing it in perspective relative to current research in the chemical sciences.
- Have received their PhD degree or completed all PhD requirements from a University or Institute of Technology in the Republic of Ireland or Northern Ireland, including a successful defence of the doctoral thesis during the calendar year 2017.
- Supply a listing of all published material arising from the PhD research performed.
- Provide two supporting letters (sent by e-mail), one from the thesis adviser and one additional faculty member. These letters should comment on the qualifications, contribution to publications and accomplishments of the applicant and the significance of the thesis work.

All documentation (in PDF format) should be e-mailed to: youngchemistprize@ria.ie by Friday 12 January 2018 at noon.

www.ria.ie





Irish Laboratory Awards 2018 – deadline for submission for our members, 26th of January 2018.

We are delighted to once again support the Irish Laboratory Awards.

Our members have an extended deadline to **26th of January 2018**. The awards seek entries from firms and individuals who have provided the highest quality of service and who can demonstrate they have added significant value and competitive advantage to their client organisations. The organisers have an entries support line for members to call where they can receive advice on entry strategy and category suitability for potential submissions.

To talk to the team and organise a free entries consultation, please contact Sophie, on 906 0684, or email sophie@labawards.ie or visit <http://www.labawards.ie/>.

Irish Laboratory Awards 2018 categories include:

- Commercial Laboratory of the Year
- Academic or Research Laboratory of the Year
- Laboratory Scientist of the Year
- Laboratory Team of the Year
- Laboratory Staff Member of the Year
- Young Leader of the Year
- Pharmaceutical Laboratory of the Year
- Healthcare Laboratory of the Year
- Chemical Laboratory of the Year
- Bio Science Laboratory of the Year
- Medical Laboratory of the Year
- Food Laboratory of the Year
- Agricultural Laboratory of the Year
- Engineering Laboratory of the Year
- Veterinary Laboratory of the Year
- Calibration or Testing Laboratory of the Year
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- Start-up Laboratory of the Year
- Laboratory Supplier of the Year
- Innovation of the Year Award
- Collaboration Achievement

*The closing date for our members is **26th of January 2018**. There is **no charge to enter** the awards. Please click [here](#) Irish Laboratory Awards Entry Guide to download the entry guide or call 906 0684.*



The Institute of Chemistry of Ireland Industrial Chemistry Award 2017 Sponsored by Henkel Ireland Ltd

Winner of the Industrial Chemistry Award 2017:-



<https://www.almacgroup.com>

A multidisciplinary team lead by Prof Tom Moody from Almac is this year's winner of the Institute's Industry Chemistry Award

Name	Title	Company
Prof. Tom Moody (lead)	VP Technology Development & Commercialisation	Almac Sciences & Arran Chemical Company
Dr. Scott Wharry	Senior Team Leader	Almac Sciences
Dr. Stefan Pohle	Senior Molecular Biologist	Almac Sciences
Dr. Jane Mueller	Senior Biologist	Almac Sciences
Dr. Megan Smyth	Chemist	Almac Sciences
Dr. Stephanie Paul	Molecular Biologist	Almac Sciences
Dr. Gonzalo Bi Dart	Research Biologist	Almac Sciences
Dr. Peter Cairns	Technical Manager	Arran Chemical Company
Dr. Mark Austin	Chemist	Arran Chemical Company
Mr. Eugene Forde	Pilot plant supervisor	Arran Chemical Company
Mr. Andrew McGuinness	Quality Manager	Arran Chemical Company

&

Annual Lecture Series Award (Eva Philbin) 2017 Winner



Professor Donal O'Shea

RCSI December 4th

The Institute of Chemistry of Ireland Industrial Chemistry Award & Annual Lecture Series Awards 2017 At RCSI Albert Lecture Theatre December 4th



Prof John Cassidy (President) Introduces the Awards



Dr David Condon (Henkel) announces the Industrial Award Winner



Prof Tom Moody giving his lecture “Enzyme “Feeds” Rapid Development and Commercialisation”



David Condon presenting the Award to Tom Moody



Tom with his colleagues from Almac



Scott Wharry, Stephanie Paul, Stefan Pohle, David Condrón, Patrick Hobbs, John Cassidy, Tom Moody, Megan Smyth.



Prof Donal O'Shea and Prof Celine Marmion (RCSI) join the group on right



Donal presenting his lecture “*Learning how to turn the (molecular) lights on - Targeted and Responsive Agents for Fluorescence Guided Precision Surgery*”



Prof John Cassidy (President) presents the Award to Donal O'Shea



Prof Donal O'Shea with Prof Kevin Nolan



Dr David Condon with Dr Brian Murray (ITT)

Reception following the Lectures and Awards





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- Chemical & bioprocess development
- *in silico* enzyme engineering & development
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Enzyme Processes Past, Present & Future

Prof. Tom Moody, VP Technology Development & Commercialisation at Almac & Arran Chemical Company

Almac, Department of Biocatalysis and Isotope Chemistry, 20 Seagoe Industrial Estate, Craigavon BT63 5QD, Northern Ireland United Kingdom; Arran Chemical Company Limited, Unit 1 Monksland Industrial Estate, Athlone, Co. Roscommon, Ireland

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Contributors to this article include: Scott Wharry, Megan Smyth, Stephanie Paul, Stefan Pohle, Peter Cairns, Eugene Forde, Mark Austin & Gonzalo BiDart

Introduction

In the pharmaceutical and fine chemical industry, there is a need for greener and more economic alternatives to current production methods due to pressures on cost and environmental legislation. Biological systems and in particular isolated or immobilised enzymes (Biocatalysis) offer a sustainable and greener alternative to traditional catalysts in for advanced chemical manufacture. Biocatalysis has risen to become a prominent and mainstream technology in pharmaceutical chemistry.^{1,2,3,4,5,6,7,8,9} A number of reasons have been responsible for this including the ability of enzymes to deliver shorter more expedient synthetic routes to sophisticated molecules, with considerably lower environmental burden than traditional chemical approaches. Furthermore, it is often the case now that in addition to lowering toxic solvent and reagent inventories, introduction of enzyme catalysis can provide cost competitive alternatives to chemical synthesis alone with resultant lower final product cost. A summary of the advantages is shown in Figure 1.

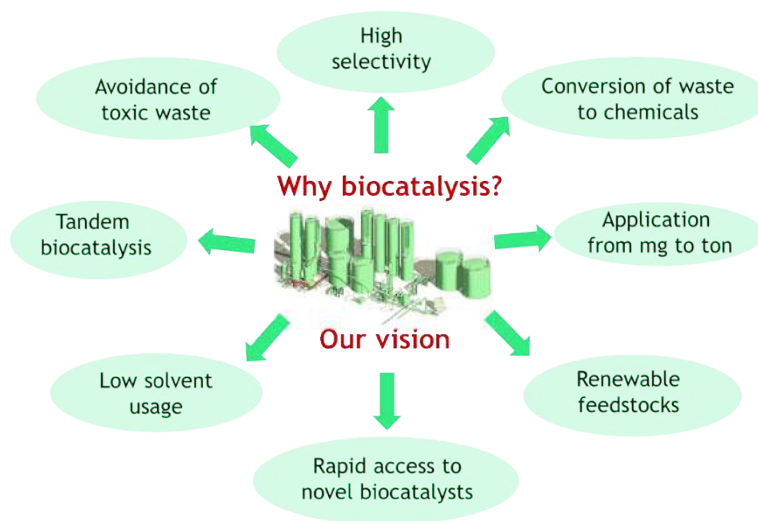


Figure 1. Summary of why to use biocatalysis

¹ D. J. Pollard and J. M. Woodley, *Trends Biotechnol.*, 2007, **25**, 66–73.

² R. N. Patel, *Biomolecules*, 2013, **3**, 741–777.

³ A. Wells and H. P. Meyer, *ChemCatChem*, 2014, **6**, 918–920.

⁴ G. W. Huisman and S. J. Collier, *Curr. Opin. Chem. Biol.*, 2013, **17**, 284–92.

⁵ A. M. Bezborodov, and N. A. Zagustina, *Appl. Biochem. Microbiol.*, 2016, **52**, 237–249.

⁶ M. S. Malik, E. –S. Park, and J. –S. Shin, *Appl. Microbiol. Biotechnol.*, 2012, **94**, 1163–1171.

⁷ T. S. Moody, S. Mix, G. Brown, D. Beecher, *Science of Synthesis, Biocatalysis in Organic Synthesis*, 2015, **2**, 421–458.

⁸ A. McMordie and T. S. Moody, *Manufacturing Chemist Pharma*, 2013, 51–53.

⁹ A. S. Wells, J. W. Wong, P. C. Michels, D. A. Entwistle, K. Fandrick, G. L. Finch, A. Goswami, H. Lee, S. Mix, T. S. Moody, *Org. Process Res. Dev.*, 2016, **20**(3), 594–601.

A number of requirements can be identified for enzymes to achieve industrial application. Firstly, a suitable collection of enzymes needs to be readily available so that a screening process can be conducted to identify candidate enzymes to be carried forward for development. Such enzymes need to be available at the required scale and at a suitable cost. Process intensity for biotransformations need to be comparable to chemical processes, with an achievable product concentration in the range of 50-100 g/L and a biocatalyst loading with respect to substrate input that enables a reasonable enzyme cost contribution to the process. Finally, processes and enzymes need to be unencumbered by intellectual property constraints and demands. A summary of key characteristics for an enzyme is shown in Figure 2.

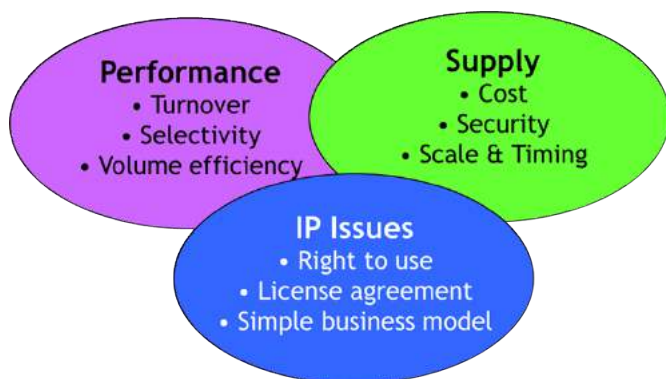


Figure 2. Summary of key enzyme characteristics

Biocatalysis predates synthetic organic chemistry, with some of the oldest chemical transformations, namely brewing fermentations, being commonplace before recorded history. The application of enzymes and whole cells to the food and drink business has been industrially important for many centuries. The use of biocatalysts in organic synthesis has a shorter history. Lactic acid was probably the first optically active compound to be produced industrially using fermentation in 1880¹⁰. In 1921 Neuberg and Hirsch discovered that the condensation of benzaldehyde with acetaldehyde in the presence of yeast forms optically active 1-hydroxy-1-phenyl-2-propanone¹¹ and nine years later the conversion of this compound into L-(-)-ephedrine was patented by Knoll AG, Ludwigshafen¹².

The application of biocatalysis to organic synthesis has grown rapidly in recent years. A Scifinder search of the terms “biocatalysis” or “biocatalyst” gave 854 references to articles published in 2002, growing to 2932 references in the same period 10 years later. A summary of the results is shown in Figure 3.

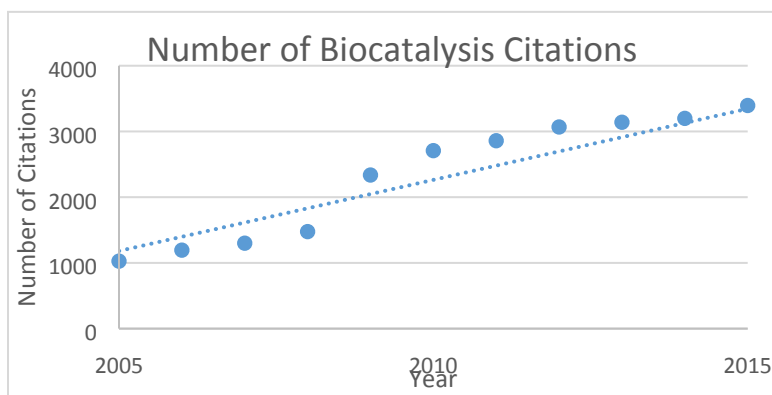


Figure 3. Number of “biocatalysis” citations from 2005 to 2017

¹⁰ Sheldon, R. A. 1993, *Chirotechnolgy*, Marcel Dekker, New York, p105.

¹¹ Neuberg, C. and Hirsch, J. *Biochem. Z.*, **1921**, 115, 282-310.

¹² Hildebrandt, G. and Klavehn, W. *Ger. Pat. 548 459* (1930).

Once the preserve of specialists, working with in-house collections of enzymes and cultures, the development of large and diverse collections at Almac and other companies is leading to biocatalysis becoming a widely and generally applied technology. In part, this increase is due to the wide range of chemical transformations that may now be achieved biocatalytically. The synthetic power of enzymes is their unequalled selectivity for the chemical reactions they catalyse. This is illustrated in Figure 4 using a hypothetical molecule.

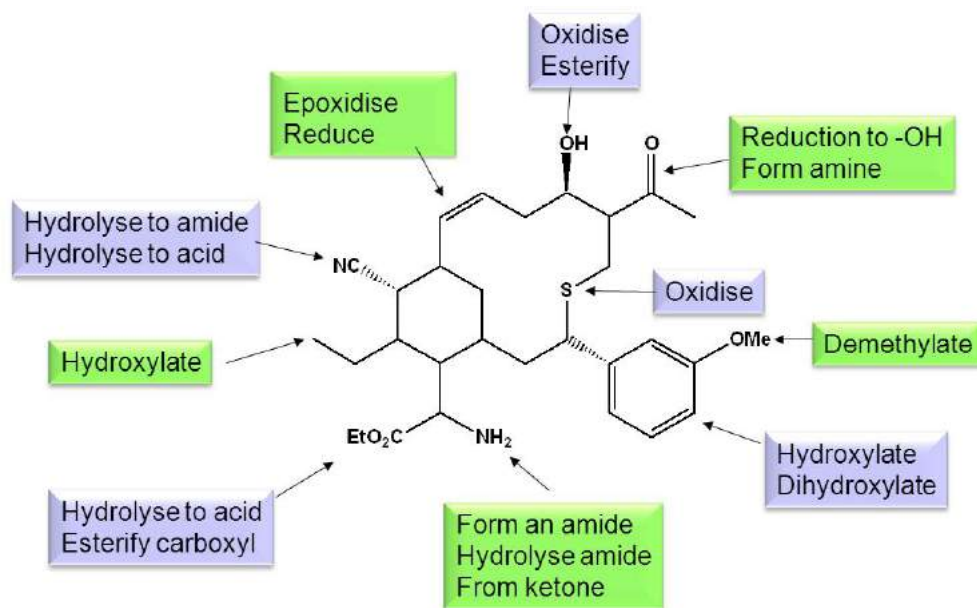


Figure 4 – selected range of possible biotransformations

The phrase ‘paradigm shift’ has been used out of turn in many technological advances in recent years, but this is certainly not the case when related to biocatalysis. The paradigm shift for the acceptance of biocatalysis is persistent and at the forefront of research within the fine chemicals and pharmaceuticals industries.

This shift in acceptance has resulted in biocatalysis becoming the work-horse of the chemists’ tool-box for chiral chemistry. Enzyme processes are now at the epicentre of key drivers in process design, scale-up and economics, including:

Route scouting:

Identification and prioritisation of routes to be investigated

Determination of key cost contributors

Key reaction optimisation methodology and DoE

Investigation into waste stream management

The reason for the surge in the application of this green technology, in our view, is simply that success breeds success. Unlike ten years ago, we now have all the supporting technologies that can really make a difference in enzyme development, such as bioinformatics, enzyme evolution and high throughput screening. Advancements in biocatalysis include:

- Improvement of Enzyme properties
 - Directed Evolution
 - Protein Engineering

- High throughput screening
- Metagenome analysis
 - Speed of analysis
 - Cost is lower
- Physical Stabilization
 - Immobilization
 - CLEAS/application of surfactants
- Enzyme Environment Engineering
 - Solvents/emulsion technology
 - Supercritical fluids

Another key advantage of running these processes is the timeline required for implementation. From selection of a catalyst to actual manufacture of product, timelines are similar to those of conventional chemistry optimisation and scale-up. A typical development programme is summarised in Figure 5.

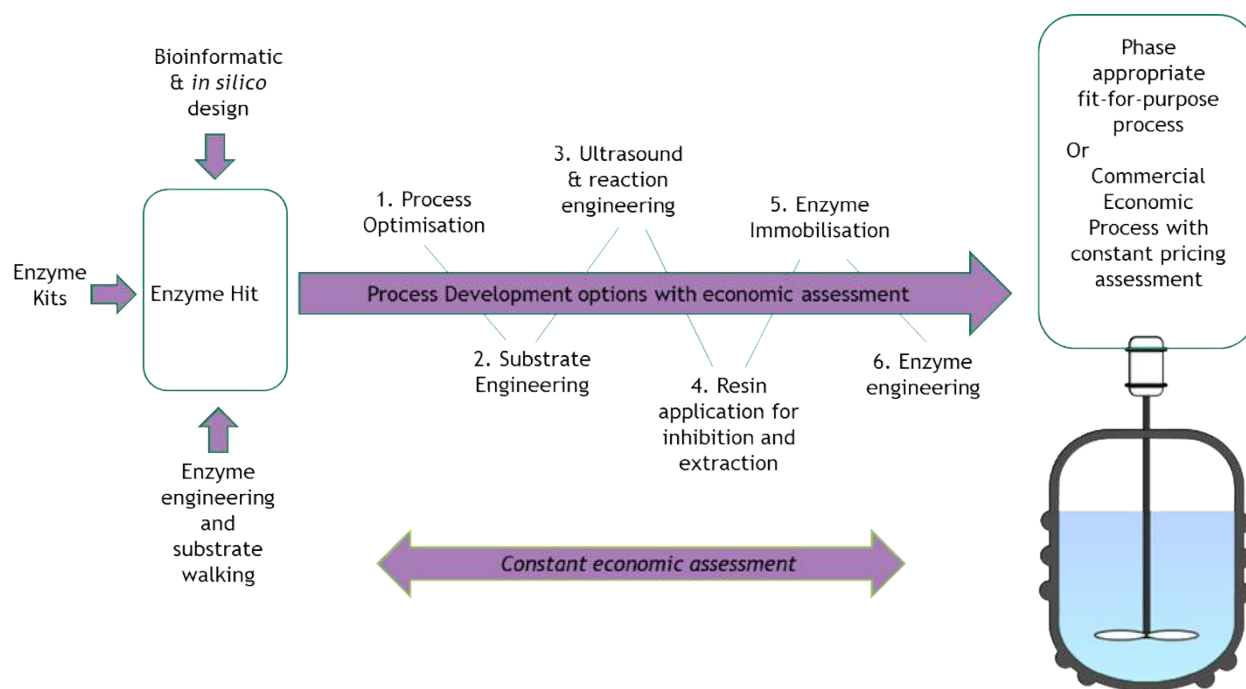


Figure 5. Process development options to a “fit-for-purpose” biocatalysis process

Biocatalysis and discovery chemistry

a. Carbonyl Reductases (CREds)

The stereoselective reduction of prochiral ketones using enzymes has moved from an academic curiosity to a mainstream technology offering in the modern era. There is a plethora of bioreduction examples, both in the research literature and in patents, spanning across different chemical motifs. The technology has proven to be a robust and reliable alternative to other asymmetric chemical methods resulting in green, economic and scalable processes for the chemical industry.

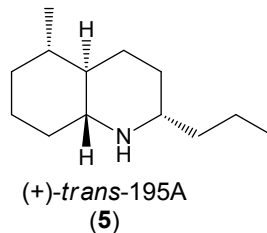
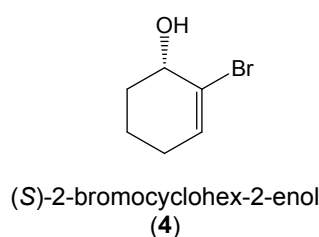
The discovery of an ever increasing number of CREDs has opened many opportunities with regard to substrate tolerance and diversity and scientists are increasingly taking advantage of this first choice technology for asymmetric reductions of prochiral ketones. As the methodology continues to improve further, it becomes even easier to use and reduces timelines to scale. Moody and co-workers showed that by simply having a small, focussed library of CREDs, seven sets of ketones could be reduced to the corresponding R and S alcohols as summarised in Table 1.¹³

Table 1. Structural motifs of the substrate classes involved in the Almac CRED study. High-performing Almac CREDs associated with each class are given underneath in blue.

Set 1 (methyl aryl-ketones)	Set 2 (α -halo aryl-ketones)	Set 3 (fused bicyclics)	Set 4 (β -cyano aryl-ketones)	Set 5 (pyrrolidinone analogues)	Set 6 (α -branched alkyl aryl-ketones)	Set 7 (α -trifluoromethyl aryl-ketones)
A131 (Prelog) A161 (Anti-Prelog) A601 (Anti-Prelog)	A131 A161 A231 (Anti-Prelog) A601	A131 A161 A231 A281 (Prelog)	A131 A161 A231 A281	A131 A161 A201 (Anti-Prelog)	A131 A161 A231 A601	A131 A161 A231 A601

To take maximum advantage of biocatalytic ketone reductions, it is essential to introduce the strategy into the process design early so that as the product progresses through the clinical pipeline, the enzyme will be there from the start.

In the timely delivery of batches of API to support clinical trials, options to simplify or shorten the synthetic route are always welcome. (S)-2-bromocyclohex-2-enol (4) is frequently encountered as the starting point in a number of natural product syntheses, including (+)-*trans*-195A (5), the name assigned to a decahydroquinoline alkaloid isolated from the skin of dendrobatid frogs¹⁴.



Blechert and coworkers prepared 4 on a 0.5g scale in 95% yield and 99% e.e. using a CBS reduction followed by chromatographic purification. Almac had a requirement to synthesise 100g quantities of 4 for a novel therapeutic agent currently under development and wanted to evaluate the use of a CRED enzyme for this. Screening of the selectAZyme™ CRED kit identified an enzyme that exhibited high conversion and high enantioselectivity, albeit using a glucose / glucose dehydrogenase coupled system¹⁵. There are a number of reaction parameters to consider when developing a CRED reduction, including temperature, pH, cofactor regeneration and % substrate loading. Systematic evaluation of these parameters identified good reaction progress at 30°C (lower temperatures gave slower reaction progress; higher temperatures also gave slower reaction progress, presumably due to denaturation of the enzyme), pH 6-6.5 (pH 8 gave significantly slower

¹³ Andrew S. Rowan, Thomas S. Moody, Roger M. Howard, Toby J. Underwood, Iain R. Miskelly, Yanan He and Bo Wang, *Tetrahedron: Asymmetry*, (2013), 24 (21-22), 1369-1381.

¹⁴ Holub, N., Neidhofer, J. and Blechert, S., *Org. Lett.*, **2005**, 7, 1227

¹⁵ Calvin, S.J., Mangan, D., Miskelly, I., Moody, T.S. and Stevenson, P.J., *OPRD*, **2012**, 16, 82-86.

progress) and 20 volumes of solvent. IPA (20% v/v wrt substrate) was shown to be effective at regenerating the cofactor. Lower (sub-stoichiometric) concentrations of IPA gave incomplete reaction while higher concentrations also produced a detrimental effect. Convenient as IPA is to use for cofactor regeneration, it does lead to an equilibrium that doesn't favour complete substrate reduction. This problem was overcome by applying a partial vacuum to the reaction mixture to remove acetone (by-product of the reaction), while sparging in IPA to maintain a sufficient concentration in the reaction mixture. Application of these conditions on 100g input substrate scale, using the CRED as a cell paste, generated the desired product as a colourless oil in 88% yield with an enantiomeric excess of 99.8%. Significantly, the product was of sufficiently high purity to use directly in the subsequent step without any further purification. A typical IPA/acetone sparge set up is shown in Figure 6.

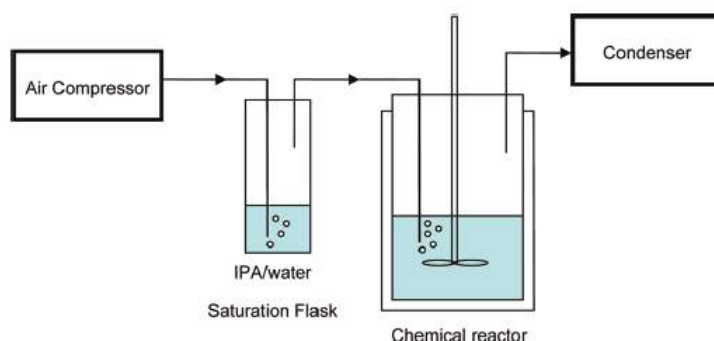
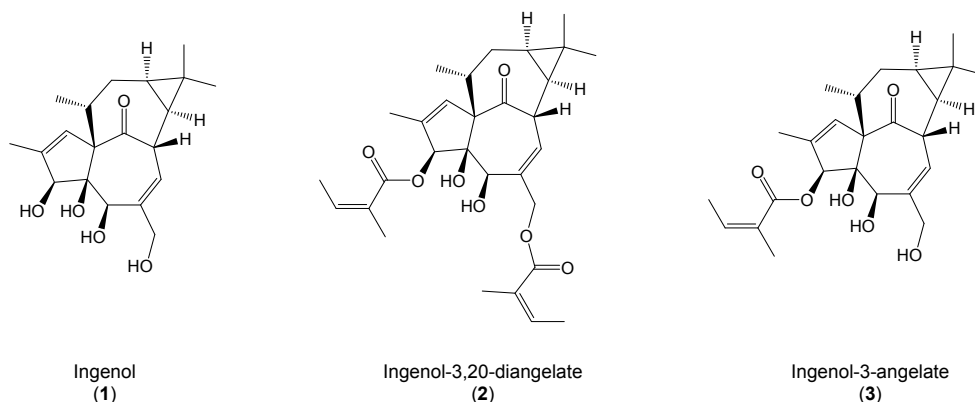


Figure 6. IPA/acetone sparge set up for driving CRED reactions to completion.

b. Hydrolases (lipase, protease, esterase)

Biocatalysis can also be employed to provide a scaleable access to natural products that are only present in nature in low levels. Ingenol-3-angelate (3) is present in relatively small amounts in plants of the *Euphorbia* plant family. It has been reported as being useful in treating a number of disorders, particularly actinic keratosis. The related compound ingenol (1), however, can be isolated from natural sources in high quantities and is an attractive entry point to supplies of its 3-angelate ester. Bearing one primary, two secondary and one tertiary alcohol, selective 3-esterification of ingenol is an obvious challenge. Reaction of ingenol with angelic anhydride yields ingenol-3,20-diangelate (2) in 48% yield after chromatography. Highly selective hydrolase mediated cleavage of the ester of the primary alcohol has been reported, yielding the desired ingenol-3-angelate in 91% yield¹⁶.



¹⁶ Liang, X., Högberg, T., Grue-Sørensen, G., Moody, T.S. and Rowan, A. S., WO 2013/110753

For many projects, biocatalysis can be purposely employed from the outset. However, biocatalysis is also a highly valuable technique when problems are encountered with a process. One example of this is shown in Figure 7.

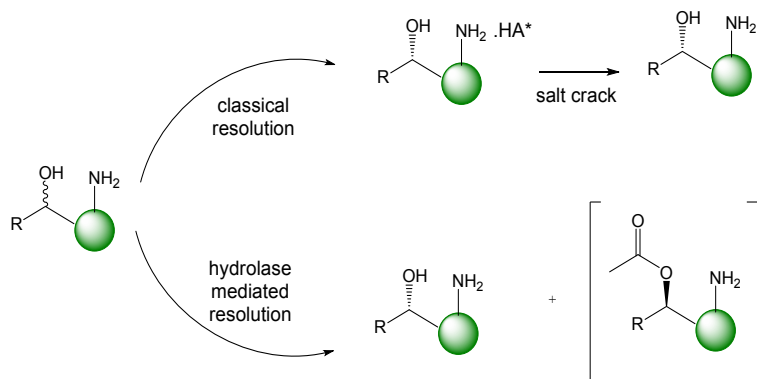


Figure 7 – resolution of an amino alcohol using classical technology and subsequent employment of biocatalysis

Delivery of this project required access to a chiral amino alcohol of high enantiomeric purity. On lab scale this had been readily achieved by a traditional diastereomeric resolution. However, as this chemistry was developed for scale up it quickly became apparent that this resolution wasn't working as required, with low yields and challenging filtration issues being observed. To ensure that the committed delivery date for the API was met, work started on an enzymatic resolution approach, while continuing to work on improving the crystallisation. Following a selectAZyme™ hydrolase enzyme screen, a lipase was identified that converted the undesired enantiomer to an acetate ester, simply by running the reaction in ethyl acetate (both as acyl donor and solvent). The two product components (desired enantiopure alcohol and undesired ester) were readily separated and, following some focussed development work, the lipase approach was successfully applied on scale, leading to on-time delivery of API of the required purity.

c. Ene reductases (EREDs)

The synthesis of substituted naphthols by an efficient enzymatic method from the corresponding tetralones has been reported using ERED technology.¹⁷ The authors in the paper utilise the ability of the ene-reductases of the Old Yellow Enzyme family to work in reverse. Screening of Almac's selectAZyme panel of EREDs resulted in over 60 % of the enzymes yielding 2-naphthol when 2-tetralone was used as the substrate. Moderate to excellent conversions (up to > 99 %) were reported for the selected ERED's for the production of a set of substituted naphthols (8). The robustness of the process was demonstrated with a 2 g scale reaction which gave a 91 % isolated yield.

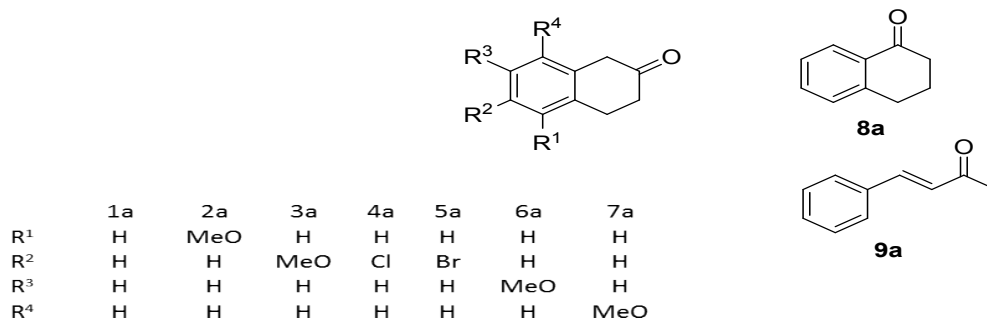


Figure 8: Range of tetralones tested for the production of naphthols using EREDs.

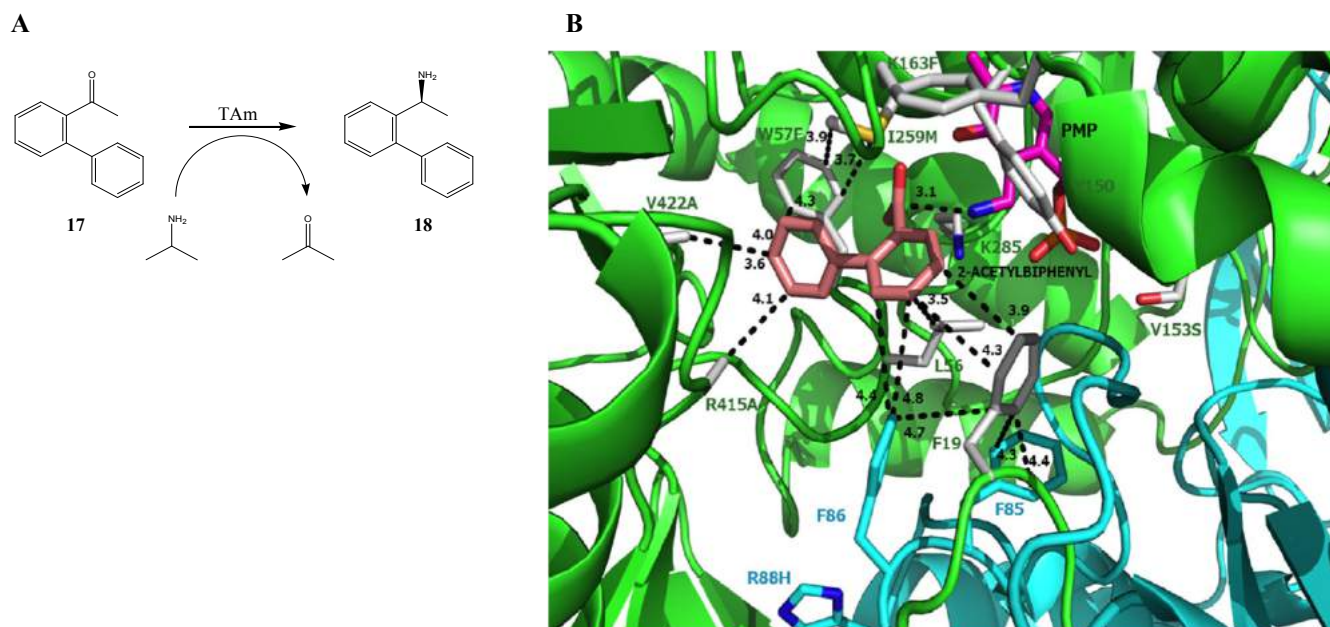
¹⁷ P. P. Kelly, D. Lipscomb, D. J. Quinn, K. Lemon, J. Caswell, J. Spratt, B. Kosjek, M. Truppo and T. S. Moody, *Adv. Synth. Catal.*, 2016, **358**, 731-736.

Whilst the application of ene reductases as oxidative catalysts is very much embryonic, there is good potential for reaction and enzyme engineering to advance this mode of application towards routine viability. The main challenges to be addressed include broadening the range of substrates amenable to oxidation, dealing with limited oxygen solubility at higher temperature and increasing enzyme stability, turnover and selectivity.

d. Transaminases (TAm)

Work by the Moody group¹⁸ demonstrated the applicability of rational protein engineering to an industrially relevant (S)-selective TAm from *V. fluvialis* (*Vf*- ω -TAm). The wild type enzyme showed no catalytic activity towards the bulky ketone 2-acetylbiphenyl. Using a combination of computational modelling and rational mutagenesis, *Vf*- ω -TAm was engineered to convert the ketone to its corresponding amine with excellent conversion (>99% *ee*), representing >1716-fold increase in activity (Figure 9). By modelling the enzyme in the presence of the PMP intermediate and focusing on enlarging the large binding pocket, in total only 7 mutations were required to bring about these improvements. As well as being larger than the substrates studied in previous research, no activity had previously been shown towards ketone by the well-characterized *Vf*- ω -TA. Critically, this work shows that initial weak promiscuous activity towards a substrate is not always necessary for enzyme evolution. Instead, selecting functionally relevant mutations and combining these with multistep rational mutagenesis can provide a more efficient pathway for protein engineering. As well as providing an excellent example of expanding substrate scope in a currently scarce list of successes, this study could have a significant influence on the approach adopted for enzyme engineering for the biocatalysis industry going forward.

Figure 9. TAm engineering to access chiral amine



Schematic showing (S)-selective TAm-catalyzed reaction converting 2-acetylbiphenyl to (1S)-1-(1,1'-biphenyl-2-yl)ethanamine employing IPAM as amine donor. **B.** MD reference structure of ketone docked to *V. fluvialis* TAm with mutations W57F/R88H/V153S/K163F/I259M/V422A/R415A in the presence of PMP. The active center residues are represented by sticks with the carbons of Chain A (green ribbon) coloured in gray and the carbons of Chain B (cyan ribbon) coloured in cyan. Relevant distances are shown (in units of Å). The MD reference structure corresponds to the structure with lowest root-mean-square deviation (RMSD) (α -C atoms), relative to the average structure of the simulation. No significant changes were observed in the MD replicas⁶⁸.

¹⁸ Dourado, Daniel ; Pohle, Stefan; Carvalho, Alexandra; Dheeman , Dharmendra; Caswell , Jill ; Skvortsov, Timofey ; Miskelly, Iain; Brown, Rodney; Quinn, Derek; Allen, Christopher; Kulakov , Leonid ; Huang, Meilan; Moody, Thomas S., ACS Catalysis (2016), 6(11), 7749-7759..

e. Dioxygenases (DOs)

The enzyme benzoate dioxygenase (BZDO) from *Ralstonia eutropha* B9 is able to dihydroxylate benzoic acids in a dearomative process that proceeds with a different regioselectivity than other known dioxygenase enzymes. In a recent paper by Moody et al. 4-fluorobenzoic acid is oxidised by BZDO to give an enantiopure diol that can be rapidly elaborated to highly oxygenated homochiral building blocks with quaternary centres.¹⁹ Notably, the diol produced in this biotransformation displays reactivity which is distinct from that of the more extensively studied non-fluorinated analogue.

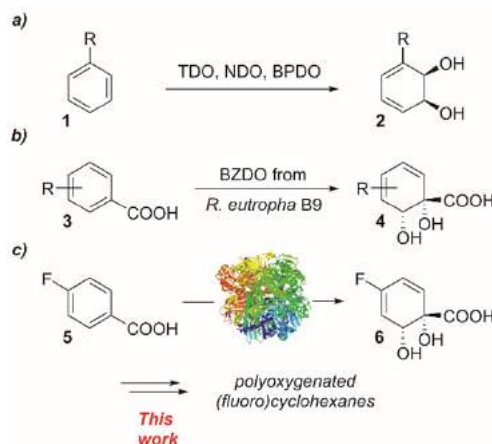


Figure 10. Application of DO enzymes for dearomatising dihydroxylation of aromatic compounds with arene dioxygenase enzymes.

f. Enzyme immobilisation

In the pursuit of robust and reusable biocatalysts for industrial synthetic chemistry, nanobiotechnology is currently taking a significant part. Recently, enzymes have been immobilized on different nanoscaffold supports. Carbon coated metallic nanoparticles were found to be a practically useful support for enzyme immobilization due to their large surface area, high magnetic saturation, and manipulatable surface chemistry. In a recent study by Moody et al. carbon coated cobalt nanoparticles were chemically functionalized (diazonium chemistry), activated for bioconjugation (N,N-disuccinimidyl carbonate), and subsequently used in enzyme immobilization.²⁰ Three enzymes, β -glucosidase, α -chymotrypsin, and lipase B were successfully covalently immobilized on the magnetic nonsupport. The enzyme-particle conjugates formed retained their activity and stability after immobilization and were efficiently recycled from milliliter to liter scales in short recycle times. A summary of the process recycle is shown in Figure 11.

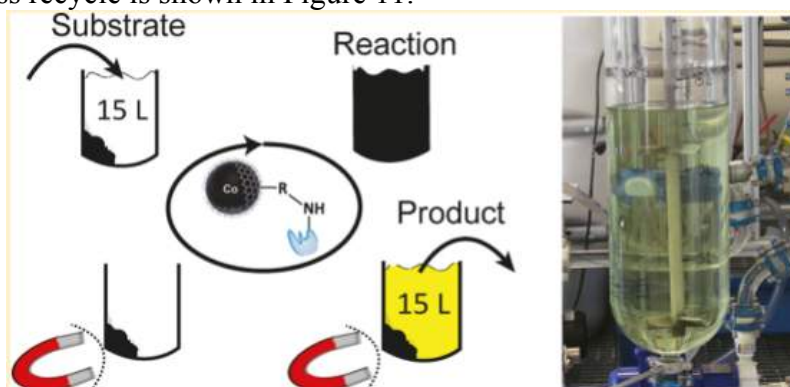


Figure 11. Application of magnetic immobilised enzymes.

¹⁹ Toby J. Nash, Scott Wharry, Thomas S. Moody, Simon E. Lewis, *Chimica Oggi - Chemistry Today* - vol. 35(5), 90-94, September/October (2017).

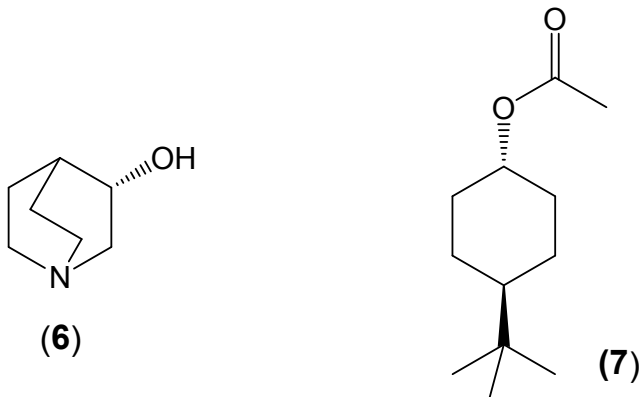
²⁰ Vladimir Zlateski, Roland Fuhrer, Fabian M. Koehler, Scott Wharry, Martin Zeltner, Wendelin J. Stark, Thomas S. Moody, and Robert N. Grass, *Bioconjugate Chem.*, (2014), 25 (4), pp 677–684.

Perceived barriers

Although the positive impact of biocatalysis is now generally widely accepted, there remain a number of perceived barriers to its use, which have now been proven to be incorrect. They include for example:

1. *“Biotransformations are always too dilute to be useful on scale”.*

While it is certainly true that some biotransformations run better at high dilution, it is commonplace to run biocatalytic reactions at high concentration. For example, the chiral building block 3S-quinuclidinol (6) has been prepared using the enzyme subtilisin at a concentration of 300g substrate / L reaction mixture²¹. The fragrance agent woody acetate (7) has been prepared (0.5kg) using a selectAZyme™ CRED at a concentration of 500g substrate / L reaction mixture, followed by acetylation with acetic anhydride²².



2. *“The supply chain for larger quantities of a selected enzyme is too slow”*

The key difference between biocatalysis today, compared with 10 years ago, is the availability of supporting technologies such as bioinformatics, enzyme evolution and high throughput screening, which make a real difference in enzyme development. Processes can now commence within weeks and enzymes evolved in months.

3. *“The biocatalyst provider will want to have IP on my molecule”*

Many enzyme companies now offer a straightforward price / kg of enzyme with all project related IP belonging to the customer.

4. *“There will be residual protein in the product and this won’t be acceptable to our regulator”*

There are a number of reliable techniques for ensuring that there is no residual protein in the manufactured product and many regulatory approvals have now been made for commercial processes that employ biocatalysts.

5. *“Use of an enzyme requires specialist knowledge”*

Some knowledge is required to get started but this information is readily available and most enzyme supply companies will be happy to help you get started.

Quality

The absence of clear regulatory guidance, especially coupled with a shortage of clear precedents and experience, can inhibit the uptake and use of new manufacturing technologies. The application of enzymes (biocatalysis) in the manufacture of intermediates and active pharmaceutical ingredients (API) is a good example. To help address a perceived lack in regulatory clarity for this rapidly advancing field, a paper by

²¹ Brossat, M., Moody, T.S., Taylor, S.J.C. and Wiffen, J.W., *Tetrahedron: Asymmetry*, **2009**, 20, 2112-2116

²² Brown, G., Mangan, D., Miskelly, I. and Moody, T.S., *OPRD*, **2011**, 15(5), 1036-1039

Moody et al. proposed a science and risk based approach to ensure patient safety and drug quality when using biocatalysts was adopted. The goal of the publication is to provide a clear path and knowledge base to enable a robust and sound science and risk-based philosophy for utilizing biocatalysis whenever appropriate for the manufacture of small molecule pharmaceuticals.²³

Conclusion

The proven ability of biocatalytic technology to produce hard cost savings for pre-existing processes or to provide novel routes to access NCEs is at the forefront of Almac's key technologies and investments. The key difference between biocatalysis today and ten years ago is that we now have excellent supporting technologies that greatly simplify enzyme identification, development and preparation of easy-to-use catalysts.

Future development of enzyme reaction systems could investigate and integrate the use of technologies that are known to speed up catalysis in other systems. One such approach may be to utilize ultrasonication, which has been shown to greatly increase the rate of some enzyme reactions, sometimes by an order of magnitude. Ultrasound can induce physical phenomena such as cavitation and acoustic streaming, and these lead to extreme conditions of liquid turbulence that can benefit mass transfer, but also influence behaviour at the molecular level such as protein conformation and secondary structure, and lower catalytic activation energies. If applied carefully, beneficial effects such as increased reaction rates outweigh any negative damaging effects to the cells or enzymes.

Biocatalysis is truly a 21st century technology readily available to all chemists. It brings many benefits, including new route options, process simplification, increased speed of delivery, no heavy metals to control and the potential to generate some new IP to protect your invention. It's time to give it a go!



Prof. Tom Moody is the Vice President of Technology Development and Commercialization at Almac and Arran Chemicals and is responsible for driving new technology processes from conception to commercial scale-up across multi-disciplinary research including biocatalysis, flow chemistry, radiochemistry, custom synthesis and commercial production. He graduated from The Queen's University of Belfast with a 1st Class BSc(Hons) in chemistry in June 1998 before returning to gain a Ph.D. in Physical Organic chemistry in December 2001. He has also completed a Masters in Business graduating with distinction in July 2007 specializing in business strategy. His work has earned him numerous accolades and is co-author and author of >60 publications and patents.

He is a strategic leader and technical expert in chiral chemistry and biocatalysis with >18 years of extensive academic and industry experience. A leader in the field of hydrolase, oxidoreductase and transferase enzymes in >90 projects completed in the past 3 years for the synthesis of chiral molecules, metabolites and labelled compounds. Tom is responsible for managing a multi-disciplinary team of both chemists and biologists to obtain commercially useful biocatalysts and their intended applications at multi-tonne scale. Biocatalytic processes have been developed from mg to tonne manufacture including development of

²³ Wells, Andrew S.; Wong, John W.; Michels, Peter C.; Entwistle, David A.; Fandrick, Keith; Finch, Gregory L.; Goswami, Animesh; Lee, Heewon; Mix, Stefan; Moody, Thomas S., Organic Process Research & Development (2016), 20(3), 594-601.

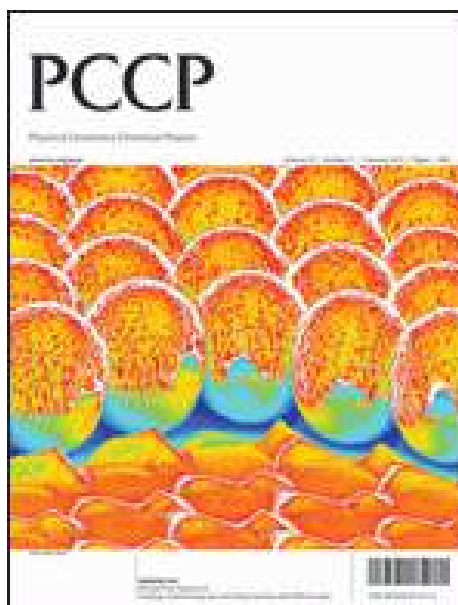
fermentation processes to yield the desired biocatalyst. He has extensive publication record, budgetary and executive committee experience and leadership of multi-discipline research departments. He is also an honorary Professor at Queen's University of Belfast since 2013 in the area of biocatalysis. Tom may be contacted at tom.moody@almacgroup.com.

About Almac Group

The Almac Group is an established contract development and manufacturing organisation that provides an extensive range of integrated services to the pharmaceutical and biotech sectors globally. The services range from R&D, biomarker discovery development and commercialisation, API manufacture, formulation development, clinical trial supply, IXRS® technology (IVRS/IWRS) through to commercial-scale manufacture.

The international company is a privately owned organisation that has organically grown over almost 50 years and now employs close to 5,000 highly skilled personnel. Almac is headquartered in Craigavon, Northern Ireland with operations in the UK, Ireland, across the US (Pennsylvania, North Carolina and California) and in Asia (Singapore and Tokyo).

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Report on EuCheMS General Assembly Meeting

26-27 September 2017,

University of Rome 'La Sapienza'

Background

EuCheMS, the European Association for Chemical and Molecular Sciences, aims to nurture a platform for scientific discussion and to provide a single, unbiased European voice on key policy issues in chemistry and related fields.

EuCheMS has been active since 1970, initially under the name of FECS (Federation of European Chemical Sciences). FECS was established on 3 July 1970 in Prague by 17 Member Societies from both east and west Europe. On 14 October 2004 in its General Assembly in Bucharest, FECS decided to adopt the EuCheMS designation, with its headquarters in Belgium, and to prepare a new constitution, which was published in the Belgian Gazette on 28 April 2006.

Representing more than 160,000 chemists from more than 40 Member Societies and other chemistry related organisations, EuCheMS relies on a unique network of active researchers involved in all the fields of chemistry. Through this network, EuCheMS organises several specialised academic conferences as well as the biannual EuCheMS Chemistry Congress, the European congress of chemical sciences. EuCheMS also promotes the role and image of the chemical sciences among the general public and policy-makers through social media, newsletters and through the organisation of conferences and workshops open to the society.

Through the promotion of chemistry and by providing expert and scientific advice, EuCheMS aims to take part in the solution to today's major societal challenges.

At the moment there are 41 separate national chemistry organisations (including the ICI & RSC) as members of EuCheMS. The present chair is David Cole-Hamilton and his tenure lasts to December 2017 and P Goya will take up the chair at that stage.

Topics Covered at the General Assembly

1. There were six nominations for four positions on the Executive board. And each candidate presented on why they were aiming to be on the executive board. The candidate elected by votes were

Mr Nicola Armaroli (Italy, interests in Energy)

Mr.Kenneth Ruud (Norway, theoretical Chemist)

Ms Livia Simon Sarlkadi (Hungarian chemist)

Ms Saskia van der Vies (Belgium)

It was pointed out that there was no industrial member of the Executive and efforts should be made in the future to appoint one.

2. It was agreed that the name of EuCheMS be changed to 'European Chemistry Society' with the slightly altered logo of (EuChemS)
3. There are a number of divisions (about 10) by discipline in EuCheMS , such as physical chemistry, chemical education etc. Each are required to have a minimum number of members (20). Before becoming a division, they start off as a professional network and if this grows in number it can be a division. Divisions are self funded through running conferences.

A new professional network was proposed in 'Formulation' by Alain Durand and accepted. In addition a professional network for senior chemists was also proposed by Pavel Drasar and accepted.

4. The department of chemical sciences and materials technology (supported by the national research council of Italy) was adopted as a supporting member of EuChemS.
5. The budget was discussed. There are 2.5-3 administrators in EuChemS presided by Nineta and much of the total funding of 300,000 euro is from the RSC (over 100,000 euro). Ireland contributes 1440 (which next year will increase to 1550 since the CPL (which is an indication of how the national economy in general is performing) has raised a little. The CPL is taken from 2 years ago and so it is from 2015. Most of the funding supports renting the office and paying the administrators, along with publication and IT costs.
6. Reports were given for the divisions, who in each case were responsible for running conferences and workshops. For example the analytical division ran the EUROANALYSIS XIX recently in Stockholm and the young chemists division had a variety of activities. Most of the divisions are self funding and each has a chair, secretary and treasurer. It was proposed that in future 20% of any 'profit' made by a division would go toward central funds. In addition, any losses would be supported by central funds.
7. In conclusion, the future of EuChemS will depend on how the divisions flourish and how they report to the central administration. There was no great discussion of Brexit. The point was made that chemistry education sections of various Universities were being closed down and transferred to Pedagogical departments.
8. The next Congress will be in Liverpool on 26-30 August 2018. Submission for the 2022 congress will be sought in the next few months, followed by a formal offer to apply. Next a presentation to the executive board will be required in June 2018 and the decision will be made shortly after. A draft cooperation agreement will be drawn up.

Prof John Cassidy,

President Institute of Chemistry of Ireland

September 28th 2017

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Report on the 7th Eurovariety in University Chemistry Teaching held at the University of Belgrade, Belgrade, Serbia 28-30th July 2017

<http://chem.bg.ac.rs/eurovariety>

Peter E. Childs

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The conference building, University of Belgrade

The Eurovariety conferences are sponsored by the EuCheMS Division of Chemical Education and alternate with the ECRICE conferences. The Eurovariety conferences (EViCE) started in 2005 and were a spin-off from the successful Variety in Chemistry Education (ViCE) conferences held in the UK and aimed at university chemistry lecturers. The emphasis is on both research and practice with the aim of improving the teaching and learning of chemistry at tertiary (university) level, including the training of chemistry teachers. An Irish version, IViCE, was held in DIT in April this year for academics based in Irish institutions. The challenge is to get university academics to attend such conferences as they are not about chemistry research and teaching is often seen as a peripheral activity. Often only 1 or 2 people in a Department are interested in chemical education unless they are involved in training chemistry teachers and in many European countries this takes place within the chemistry departments, rather than in an education department. However, the increased emphasis on teaching quality in UK universities is evidenced by the greater emphasis on chemical education within UK chemistry departments. It was notable at this year's Eurovariety that both the University of Reading and University of Keele were strongly represented and each has a group of academics focused on chemical education. Reading has two professors of Chemical Education.

Around 60 people attended this conference and there were 2 plenary lectures, 4 keynotes, 40 oral papers, 3 workshops and 18 posters.



Michael Seery giving his plenary lecture

The first plenary lecture was given by Michael Seery, formerly of DIT, and now a Reader in Chemical Education at the University of Edinburgh, which has a strong focus on chemical education in order to improve its undergraduate teaching. Michael presented an interesting range of ideas being tried out in Edinburgh to improve the undergraduate practical experience, by improving their practical skills, integrating theory and practice better and developing scientific process skills. One idea to improve practical techniques was to get students working in pairs, videoing each other's performance using smart phones, with commentary, and uploading these for evaluation. (<http://bit.ly/skillstitrating>). Another interesting idea was to award digital badges of competence, using the Open Badge idea (openbadges.org), so that students build up a portfolio of lab skills that they have mastered. (See badginglabskills.wordpress.com for more details).

The second plenary lecture was given by Silvija Markic, now at the University of Ludwigsberg, Germany and formerly at the University of Bremen, dealing with the challenges of heterogeneity in classes. She stressed the importance of cooperation between teachers, science education researchers and language teachers, for dealing with the special needs of second language learners.

Natasha Brouwer from Holland reported on an interesting project from ECTN to produce an online course to help university lecturers develop best practice in running undergraduate practical classes. This will be offered in six modules over 6 weeks and involve 2 hours study per week.

Matthew Almond from Reading talked about ideas being developed in Reading to improve students' transferable skills, for example through a course Chemical Concepts in Context in year 1 and in year 2 a collaborative case study, the Titan Project. Also from Reading, Philippa Cranwell described a first year course to develop inquiry skills, often lacking in school leavers, but using a series of guided investigations to develop independent investigatory skills. The course has had a positive effect on students' understanding and generic skills.



Odilla Finlayson (DCU) giving her talk

Unusually Ireland was not well represented this year, with only Odilla Finlayson (DCU) and Peter Childs (UL) in attendance, if we don't count Michael Seery (ex DIT).



The poster session

The three workshops were useful in involving participants in the topics: team teaching redesigning first year labs using student inputs, and careers in chemistry.



The River Danube from the castle

Belgrade was an excellent city to hold the conference and the conference hotel was only 5 minutes walk from the conference venue, though the 35 degrees plus temperature was a challenge. The conference was well organised, except for no time was allowed to move between sessions. However, all the rooms were conveniently located within one building. It was a pity that more chemistry academics don't take the opportunity to attend such conferences, or those at a national level, in order to share experience and ideas and use evidence from research to improve the teaching and learning experience of students. The RSC open access journal *Chemistry Education Research and Practice* provides a platform for such research and is now the highest ranked journal in chemical education. An increasing amount of research from third level institutions is being published in this journal, as well as papers on second level chemical education. CERP was a spin-off from an ECRICE conference held in Ioannina, Greece in 1998.



The Tesla Museum, Belgrade

Serbia is the birthplace of the inventor Nicolas Tesla and the Tesla Museum (above) in Belgrade is a key tourist attraction. Tesla invented the induction motor amongst many other significant inventions.

Report on EuCheMS Division of Chemical Education Council Meeting 30/7/16 Belgrade



Peter E. Childs (Delegate for Republic of Ireland)

Election of officers

Iwona Majieowska (Poland) was confirmed for a second three-year term as Chair. A new post of Treasurer was created as Divisions are now allowed to have an account, and Antonella Rossi from Italy agreed to serve. The joint secretaries are Rachel Mamlok-Naaman and Ron Blonder from Israel. The co-vice-chairs for Western Europe are Karolina Broman (Sweden) and Ilka Parchmann (Germany) and for Eastern Europe Dragica Trivic (Serbia).

Division website: <http://www.euchems.eu/divisions/chemical-education-2/>

Finance

EuCheMS is to give each Division €3,000 seed money. It is also intended that any surplus from EuCheMS conferences should be divided in future: 80% to the national chemical society, 10% to the sponsoring Division and 10% to EuCheMS. In the case of a loss the national chemical society is responsible.

National reports

Delegates produce an annual national report on chemical activities in their countries, which go on the Division website. It was suggested that these reports also be sent to the IUPAC Committee of Chemical Education and the national chemical societies (as is already done by Ireland).

International Year of the Periodic Table

An International Year of the Periodic Table (PT) has been proposed to UNESCO by IUPAC in 2019 to mark 150 years of the Periodic Table. It was suggested that countries could try and get Mendeleev and the PT on a stamp in that year and have a focus on the PT in conferences.

Decisions on future conferences

These must be sponsored by the national chemical society and are hosted by a university in that country.

ECRICE – the next ECRICE was due to be in Greece in 2018 but the offer to host it has been withdrawn. Three offers were on the table: Warsaw and Lodz in Poland and Antalya in Turkey, The Council agreed to accept the bid from Warsaw, with the exact dates in 2018 to be confirmed.

Offers were received for 2020 from Germany and Israel and for 2022 from Sweden. The Council is to liaise with the IUPAC Committee of Chemical Education (CCE) to see whether the 2022 ECRICE could be a joint meeting with ICCE (as in the successful 2012 Rome conference).

Eurovariety: a proposal was received from Professor Tina Overton, Monash University, Australia to hold a joint European-Australian Eurovariety in 2019 at Monash's campus in Italy. This was agreed in principle subject to agreement from the Italian Chemical Society to support and co-host the conference. No proposal has been received for 2021.

There was some discussion of how to promote attendance at Eurovariety conferences, with its more limited target audience, compared to ECRICE conferences, which cover all levels of chemical education. It was suggested to promote the idea nationally first, to encourage university academics to start thinking about improving teaching and learning, as a feeder into the European conference. This is already done in the UK and Ireland. There is an increased interest in chemical education in UK chemistry departments (e.g. Reading and Keele) and several professors of chemical education now exist. Lecturers who are convinced of the value of chemical education research should promote good ideas at faculty meetings and bring staff members' attention to relevant articles in journals like CERP. Another suggestion was to run Eurovariety alongside a national chemistry conference. However, the experience of the education section at the European Chemistry Congresses sponsored by EuCheMS has not been very positive in reaching out to the wider chemical community. There would seem to be more interest and involvement in chemistry education research at third level in Anglophone countries than in most European countries.

The next meeting will be held in conjunction with ECRICE 2018 in Warsaw, Poland. The meeting was followed by a dinner hosted by the Serbian Chemical Society.

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The machine offers good sensitivity and the high resolution allows spectra to be measured quickly. The data can be processed directly (even while wearing safety gloves) through the built-in resistive touchscreen without connecting an external computer.

Contact Information:

GPE Scientific Ltd, Unit 5, Greaves Way Industrial Estate, Stanbridge Road, Leighton Buzzard, Bedfordshire, LU7 4UB. UK.

Phone: +44(0)1525 382277

E-mail: info@gpescientific.co.uk

Website: <http://www.gpescientific.co.uk/products/chemistry/nanalysis-nmready-benchtop-spectrometer>

Company Information:

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First circular



Scientific Workshop in connection with Eurachem General Assembly 2018

Data - Quality, Analysis and Integrity

DUBLIN, IRELAND
Dublin Castle - 14th & 15th May 2018



Local organising committee

Vicki Barwick (UK), Blanaid White (Ireland), Patrice Behan (Ireland), Ted McGowan (Ireland), Rosemary Hayden (Ireland), Helen Cantwell (Ireland), Hugh Fay (Ireland), Barbara O'Leary (Ireland), Sean Hyland (Ireland), Colman O'Riordain (Ireland), Sean McGowan (Ireland).

Scientific committee

Vicki Barwick (UK), Perihan Yolci Omeroglu (Turkey), Brian Murphy (Ireland), Lorens Sibbesen (Denmark), Alessandra Rachetti (Austria), Michael Koch (Germany), Kyriacos Tsimillis (Cyprus), Elizabeth Prichard (UK), Oktay Cankur (Turkey), Eugenia Eftimie Totu (Romania), Wolfhard Wegscheider (Austria), David Milde (Czech Republic), Alex Williams (UK), Blanaid White (Ireland), Patrice Behan (Ireland), Ted McGowan (Ireland), Rosemary Hayden (Ireland), Helen Cantwell (Ireland), Hugh Fay (Ireland), Barbara O'Leary (Ireland), Michelle O'Connor (Ireland).

Registration

Registration is open from 1st OCTOBER 2017 at

www.eurachem2018.com

You are advised to register early, as places are limited.

**Please refer to the workshop website for
information regarding hotels close to
Dublin Castle**

Location

Dublin is...

a compact, authentic city where the past and present co-exist in perfect balance. Walking through the city is like travelling through time: you turn the corner and just like that, you go from the fourteenth century to the twenty-first.

With a great transport infrastructure, Dublin is easy to get around, meaning nothing is ever too far away!

Why visit Ireland?

Right now, Ireland has it all. From the haunting beauty of the pure, unspoiled landscapes and the drama of the coastline, to the urban buzz of the country's dynamic cities mixed with the magic of thousands of years' worth of culture and history, Ireland is a country that never fails to surprise.

Wild and beautiful, inspiring and exciting, Ireland's energy and romance will win you over in an instant. And with some of the friendliest people in the world, this perfectly sized and surprisingly diverse island will keep you coming back for more. 4 out of every 5 people asked say that Ireland is in their list of top 5 places to visit.





This workshop will be directly relevant to everyone involved in state, semi-state, pharmaceutical, analytical, medical, environmental and academic sectors.

Aims

- Understand the importance of scientific data integrity and how to achieve it
- Understand risks and opportunities related to data
- Discuss future challenges in data quality, analysis, integrity and compliance
- Discuss the impact of new developments on data quality, analysis, integrity and security

Topics covered during the workshop will include:

Current Practices

- International guidance
- Extent of validation/verification studies
- Analysis of validation data
- Examples of best practices in different fields
- Analysis of meta-data
- Data management systems
- Operation of advanced instrumentation
- Accreditation requirements

Future Challenges

- Future developments - Accreditation Body viewpoint
- Compliance assessment
- Risk based approaches to quality
- Validation of multiparameter methods
- Implementing principles of Quality by Design (QbD)
- Human errors
- Machine learning algorithms, including artificial neural networks

In addition to the presentations, participants will be given ample opportunity to discuss these subjects in detail and exchange experiences in a number of working group sessions.

Eurachem is a network of organisations in Europe having the objective of establishing a system for the international traceability of chemical measurements and the promotion of good quality practices.

Workshop Programme

Monday 14th May 2018

- Welcome address and workshop opening
- Presentations exploring current best practices
- Plenary, keynote and flash presentations
- Round table discussions
- Poster session and wine reception
- Workshop dinner

Tuesday 15th May 2018

- Presentations of risks and emerging challenges
- Plenary, keynote and flash presentations
- Round table discussions
- Closing lectures
- Closing the workshop

For more details on the workshop
and to register visit
www.eurachem2018.com

Invited contributions

The Scientific Committee invites participants to present posters on subjects related to the theme of this workshop.

Poster abstracts presented according to the format available from the website should be submitted before **January 19th 2018**.

Early career scientists submitting a poster abstract will be given the opportunity to have their abstract considered for an **oral presentation**.

Proposed abstracts will be subject to approval by the Scientific Committee.

Participants will be notified of acceptance on **February 28th 2018**.

Early bird registration rate closes:
March 31st 2018

Exhibition

Products and services related to the workshop topics can be presented in the exhibition area for the 2 days of the workshop.

Requests should be sent to the workshop organisers, jayne@happeningconferences.com by **1st February 2018**.

Supporting organisations



Eurachem Analytical Measurement Competition 2017

DIT hosts national competition for top chemistry students

Fifty chemistry students from third-level institutions across Ireland competed in the 18th National Eurachem Analytical Measurement Competition (EAMC) hosted in the Environmental Sustainability and Health Institute, DIT Grangegoman on Friday 7 April.

The team from Sligo Institute of Technology, Samera McGrath and Kris O'Dowd, were the overall winners.



Dr Ray Leonard, Samera McGrath, Kris O'Dowd and Dr Ted McGowan (Lecturer Sligo IT)

The runners up spot went to two teams: Lisa Kelly and Vlasta Chyzna from Athlone Institute of Technology.



Runner-up prize winners for AIT, Vlasta Chyzna and Lisa Kelly with Dr. Sean Reidy (Chemistry lecturer, AIT), Margaret Franklin (President ICI) and Dr. Ann O'Malley (Chemistry lecturer, AIT)

and to Lucy Prendeville and Seán Kavanagh from Trinity College Dublin.



Seán Kavanagh, Lucy Prendeville, Dr Noelle Scully (TCD)

The EAMC Competition is open to teams of two full-time third-level students studying in their second year of laboratory sciences in Universities or Institutes of Technology anywhere in Ireland. The students, nominated by their institution, are some of the top chemistry students in the country.

Each team carried out experiments in the laboratory, including a back titration and a spectrophotometric determination using supplied Standard Operating Procedures. Competitors were expected to report and quantify all possible sources of error.

A panel of three esteemed judges observed the students: Dr Darragh Cunningham, Scientific Officer from the Environmental Protection Agency, Dr Tom Hannigan, Director of Chemical Sciences at the Forensic Science Laboratory, Dr Ray Leonard Henkel Ireland Ltd ex-Directorate Analytical Services.



Dr Patrice Behan, Lecturer, School of Chemical and Pharmaceutical Sciences, DIT and organiser of the Competition commented that *'The competition is designed to promote critical, analytical and observational skills, and raises awareness among chemistry students about the importance of reporting accurate and precise measurements.'*

Guest Speaker, Vicki Barwick from the Laboratory of Government Chemist in the UK and Chair of the European Education and Training Working Group for analytical chemistry, gave a talk on the importance of valid measurements.

Eurachem is an association of Professional European Analysts with close links to bodies charged with promoting excellence and reliability in analytical measurement worldwide.

Many thanks to the sponsors of this year's competition: Agilent Technologies, Analytical Chemistry Trust Fund, BioPharmaChem Ireland, Dublin Institute of Technology, Eurachem Ireland, Henkel Ireland Ltd, The Institute of Chemistry of Ireland and The Royal Society of Chemistry- Ireland Local Section Committee.

Notes: The competition is hosted by the School of Chemical and Pharmaceutical Sciences at DIT.

The 23 participating teams were from Athlone Institute of Technology (AIT), Dublin Institute of Technology (DIT), Galway-Mayo Institute of Technology (GMIT), Limerick Institute of Technology (LIT), IT-Sligo, Institute of Technology Tallaght (IT-Tallaght), Institute of Technology Tralee (IT-Tralee), Waterford Institute of Technology (WIT), Dublin City University (DCU), National University of Ireland Galway (NUIG), University College Dublin (UCD) and Trinity College Dublin (TCD).

For Further Information Contact: Dr Patrice Behan, School of Chemical and Pharmaceutical Sciences, DIT. patrice.behan@dit.ie, Ph: 01 402 4664

Young Chemists' Group of the ICI

July 2016 – December 2017

This is a report of all the work done by the Young Chemists' Group of the Institute of Chemistry of Ireland (ICI) and its convenor, Mr Mark Kelada. The Young Chemists' Group was re-established in July 2016 by the appointment of Mark Kelada. Since then, more young chemists joined the ICI, the Facebook page has been more active, representatives from each Irish institution have been appointed, as well as participation with the EYCN, and raising awareness of the ICI and the Young Chemists' Group. This is a short summary of all the work carried out to date.



July 2016: Mark Kelada was appointed as the convenor of the Young Chemists' Group. Mark is a current fourth year PhD Student at Maynooth University, under the supervision of Dr John Stephens. He works on a project that aims to synthesise novel small molecules that could potentially act as antidiabetic agents. Mark got in contact with Dr Aurora Walsh who was the previous convenor of the Young Chemists' Group (2011 – 2012). Aurora gave Mark advice on what to do in his new role and how she found her experience. She encouraged him to participate and attend the EYCN.

□ **E-mails:** Since his appointment, Mark has been staying in contact with all the young chemists of the ICI via E-mail. With the help of past president, Dr Margaret Franklin, they compiled together a list of all the E-mail addresses of all the current young chemists. Mark sends them regular E-mails including the Irish Chemical News Newsletter, the monthly EYCN newsletter, and any updates on the ICI, events or job prospects. When a new young chemist joins the ICI, they are immediately added to the mailing list of the young chemists.

□ **Facebook:** Mark was also appointed as the main administrator for the Institute of Chemistry of Ireland's Facebook page. This page had not been active for a long time since its previous administrator, Ms Lisa Phelan, got a new job. It has since been active with a new post almost every 2 months. There have been a lot more views and likes over the last few months. Regular posts include ICI and EYCN news and competitions, as well as invites to several events organised by the ICI throughout the year.



EYCN: As convenor of the Young Chemists Group, Mark was invited to attend the European Young Chemists' Network (EYCN) Delegates' Assembly, held in Crete in May 2017. The ICI sponsored Mark to act as the Irish Delegate in this three-day meeting. The EYCN is a network that brings together all the young chemists of Europe aged 18 – 35 years old. The delegates from each country meet in a different country every year and make decisions concerning various projects, teams, and elections. Mark made a small presentation about the ICI and the Young Chemists' Group. He participated in the meetings and joined the Membership team.



Membership Team: As part of the membership team of the EYCN, Mark has been in contact several times with the Team Leader, Ms Jelena Lazic, to discuss different tasks. These include various ways to increase membership to the EYCN and the ICI, raising awareness on social media, editing the EYCN website, and carrying out a survey for EYCN statistics. Mark regularly informed Jelena and other European Delegates of the Irish Young Chemists' Group news and events, in order to maintain an Irish presence on a European Level.



Colloquium DCU: In June 2017, Mark attended the 69th Irish Chemistry Colloquium, which was held in DCU. During this event, he got over 25 membership forms signed from young chemists from all over Ireland. He also made a presentation about the ICI and the Young Chemists' Group, which helped raise awareness and gain more memberships.



Representatives: During the Colloquium, Mark spoke to all the different groups present from all third level institutions in Ireland. He assigned a representative from each third level institution to help him raise awareness of the ICI, plan various events, and stay in contact with the young chemists from their respective institutions. Mark had two meetings with all the representatives during the Colloquium and they shared ideas of what events they would like to do.

□ **Future Plans:** The Young Chemists' Group of the ICI plans to have another meeting in 2018, possibly during the Colloquium. They plan to have a Young Chemists' Conference (pending approval by ICI) in order to showcase the outstanding research carried out by postgraduates, postdoctoral researchers, and young academics in third level institutions. Mark might go to represent the ICI and the Young Chemists' Group during the EYCN meeting in 2018, which will be held in Turin, Italy.



Senior Science Quiz National Final 2017

The National Finals of the annual ISTA Senior Science Quiz took place in the **Tercentenary Hall in Trinity Biomedical Sciences Institute** on **Saturday 25th November**. It was full to capacity with **50 teams** of Leaving Certificate science students representing **22 counties** from all around Ireland and their teachers. Almost 1100 Leaving Certificate students took part in the Regional Finals held during Science Week and the top **150 LC students** were invited to the **BioPharmaChemical Ireland** sponsored **National Final**.

The charity associated with the quiz this year was the **Irish Kidney Association** highlighting organ donation. Thanks to Colin White IKA National Projects Manager for attending the quiz and accepting a small donation. Thanks also to **Enda Dempsey** who represented **BioPharmaChemical Ireland**.



John Daly ISTA Dublin Branch (Head Judge), Dr. Conor O'Brien (Honorary President of ISTA), Dr. Jennifer Cleary (Guest Quizmaster), Enda Dempsey (BioPharmaChemical Ireland, main sponsor) Ms. Mary Mullaghy (ISTA Quiz Coordinator) & Colin White (National Projects Manager - Irish Kidney Association)

Thanks to all the local coordinators and their teams in the **14 Branches** who facilitated the Regionals Rounds during Science Week. (**Sarah Brusey, Maura Conneally, Brendan Duane, Yvonne Higgins, Michelle Lyons, Mary McDonagh, Siobhán Mc Cormack, Triona Mulcahy, Catherine Murphy, Sam Pearson, Seamus O'Donghaile, Aodhagan O'Suilleabhain, Seán Reidy, Maria Sheehan & Brian Smyth**). Thanks also to the **Dublin Branch of ISTA** who organised the Final. A special thanks to **Prof Luke O'Neill** who welcomed us to Trinity College, **Dr. Conor O'Brien**, current Honorary President of ISTA, **Dr. Jennifer Cleary** who acted as guest quizmaster, BioPharmaChemical **Ireland** main sponsor, Trinity **College** who provided the venue. Also thanks to **CJ Fallon, Folens, ICI, IoP Ireland, RSC, SEAI & StudyClix** who provided **spot prizes** and last but not least the students and their teachers who attended.

Congratulations and well done to **ALL** who participated.

- **Colaiste Críost Rí, Capwell Road, Cork**
- **Crescent College Comprehensive, Dooradoyle, Limerick**
- **St Gerard's Bray, Co Wicklow**
- **St. Michael's, Listowel, Co. Kerry**
- **Coláiste Pádraig, Lucan, Co. Dublin**
- **Ashton School, Blackrock Road, Cork**
- **The High School, Zion Road, Rathgar, Dublin**
- **St Mary's CBS, Portlaoise, Co. Laois**
- **Calasactius College, Oranmore, Co Galway**
- **Davis College, Mallow, Co Cork**



Colaiste Críost Rí, Capwell Road, Cork overall winners for 2017.

Dr. Jennifer Cleary (Quizmaster), Dr. Conor O'Brien (Honorary President of ISTA), Luke Quigley, Michal Polak Szarkowicz, Maxim Chopivskyy, Ms Susan O'Connell (Teacher), Mr. Enda Dempsey (BPCI) & Ms. Mary Mullaghy (National Quiz Coordinator)

Commemoration of first lady Professor of Chemistry at RCSI

RCSI recently marked the anniversaries of pioneering RCSI women in both Biomedical Science and Clinical Science with the unveiling of two portraits; one in recognition of Professor Gaffney who achieved her Chair in Chemistry in 1962 – 55 years ago last year (2017) and another, in recognition of Prof Moorhouse who received her Chair in Microbiology in 1968 – 50 years ago this year (2018). On 9/11/2017 in the Board Room at RCSI, on Stephens Green, Dublin RCSI celebrated the career of Professor Ethna Gaffney by unveiling her portrait.



Phyllis, Daughter of Prof Gaffney, Prof Kevin Nolan, and Prof Celine Marmion



A Tribute to the First Lady Professor of Chemistry at RCSI. Professor Ethna Gaffney (*née* O'Malley) (1920–2011)

RCSI

Ethna Elizabeth O'Malley was born in Galway in May 1920 and educated at the Dominican Convent, Galway and Loreto Abbey, Rathfarnham, in Co. Dublin. After taking a BSc (1940) at University College Galway, she moved to University College Dublin for postgraduate study in Biochemistry, where she worked under Professor E. J. Conway.



She earned an MSc (1941) for work on elaborating micro-diffusion biochemical techniques for the determination of ammonia. She obtained a research scholarship (1941–44) from the Medical Research Council of Ireland to work on the development of a microdiffusion technique for the determination of blood glucose; her PhD (1945) was awarded for a thesis on the interchange of electrolytes across the yeast cell membrane during fermentation.

In September 1944, on the inauguration of the Dietetics Course in St Mary's College of Domestic Science, Cathal Brugha Street, she was appointed to design and deliver the science programme, lecturing in Chemistry, Biochemistry, Bacteriology, Physiology and Nutrition in Health.

Subsequent to her marriage (August 1947) she resigned from this position in March 1948.

Suddenly widowed in January 1952 following a plane crash, she was obliged to return to work. In September of that year she was awarded a 3-year Lasdon Research Fellowship in Bacteriology, where she worked with Dr Vincent Barry, Director of the Medical Research Council of Ireland laboratories, Trinity College Dublin, on the chemotherapy of tuberculosis. In addition, she lectured on Dietetics to 2nd-year Social Science students at Trinity.

Her official association with the Royal College of Surgeons began in the academic year 1952–53, when she was appointed External Examiner in Chemistry and Physics to the College. In the spring of 1954 she lectured in Chemistry while Professor Rae was on sick leave, and finally joined the staff as Lecturer in Chemistry and Physics in September 1954.

She was appointed Professor of Chemistry and Physics and Director of the Department of Chemistry and Physics in 1962, and remained at Surgeons until her retirement in 1987.

She died in Dublin in September 2011.

Professor Gaffney's career as a woman academic

Professor Gaffney's career is both typical and atypical of the professional profile of married women academics in mid- to late twentieth-century Ireland. Given the social and cultural pressures on wives not to work outside the home, there is frequently a hiatus when women left work to look after children. Once married, Ethna Gaffney resigned from her first lectureship. Suddenly widowed less than five years later, she managed successfully to combine childrearing with the world of work — a particularly male world. She was very proud of being the first woman to be promoted professor in Surgeons, and used to recall formal dinners and honorary conferrings where she was the only woman present in a room full of men. This would not have intimidated her, as her older brother, Eoin O'Malley, was a surgeon, later to serve as President of the RCSI.

In mid-twentieth-century Ireland, it was rare for a woman to have done a PhD, and still rarer a PhD in Science. Nothing in her early education had pointed Ethna O'Malley in the direction she took; she had not studied Science at school. She used to say that she opted for a BSc degree because the queue was the shortest at registration. Perhaps her family background played a role too: her father was Professor of Surgery in Galway and had three medical brothers; a maternal aunt had done an MSc in Chemistry and was a public analyst.

And Ethna proved to have some aptitude. After a promising start to her career (NUI entrance scholarship, brilliant undergraduate results, a completed doctorate at the age of 24), her research output is heavily weighted to the early years. Accounts of her investigations for and with Prof EJ Conway and Dr Vincent Barry appeared, some co-authored, in *Nature*, *The Biochemical Journal*, *The Lancet* and *The Irish Journal of Medical Science*.

However, there is no record of further research publications. This discontinuity in research profile may have been typical of the age, and can be partly ascribed to the lack of incentives for full-time teaching academics to carry out research. Ethna Gaffney's teaching commitments were confined to the pre-Medical year. Perhaps even

more pertinently, her particular domestic circumstances vitiated any research projects she might have entertained. Plunged into widowhood as a young mother of 31 with three children under the age of 3, she faced a heavy workload involving daily lectures and labs and meeting the needs of large classes of students from a wider range of cultures than would have been found in other Irish institutions of higher learning. Combining such pressures with lone parenting was not easy in Ireland of the 1950s and 1960s and holiday time with her children was precious (all the more so, it should be added, because her eldest, a 3-year-old, had died accidentally three months before his father's death). For a number of personal and professional reasons, then, Ethna's teaching and administration duties were inevitably prioritised over research activities. These gender-related constraints and discontinuities, still relevant, are only now being fully recognised and addressed.

Taken as a whole, her career trajectory also illustrates the way wives can often become involved, unseen, in behind-the-scenes work to assist their husbands. In Ethna Gaffney's case, it was behind-the-scenes work that gave her link with the Royal College of Surgeons a valued continuity. She had in fact been unofficially associated with the College, as a married woman, for several years before she sought full-time employment there as a widow. She told the tale of how she came to assist the RCSI external examiner in Chemistry and Physics, her husband, Jim Gaffney, who was a pathologist lecturing in Trinity. A couple of months before they were married, Professor Alan O'Meara suggested to the engaged couple that Ethna could "work extramurally" for Jim. O'Meara, as RCSI's outgoing extern in Chemistry and Physics, wanted to propose Jim for the job. In his view, they would make an ideal husband and wife team: Jim was a fellow of the Royal College of Physicians, the essential qualification, but his wife would be able to correct the scripts in Chemistry and Physics at home, as well as coach him for the orals in Physics. And so it happened. Jim was external examiner at Surgeons from 1948 until he was killed in a plane crash in January 1952. The work was onerous (for Ethna), but (to quote her) "it paid very well, and Jim did enjoy attending the Charter Day dinners ...". After Jim's death, Professor O'Meara proposed her name as extern and, despite not being a fellow of the Royal College of Physicians, she was appointed. In her own words, "since the Medical Research Council paid me only £600 a year, and examining brought in over £300, the appointment meant a great deal to me."

That association with the RCSI — both unofficial and official — was perhaps a key factor tipping the balance in favour of the College of Surgeons when, in 1954, she was faced with a choice between returning to UCD's Biochemistry Department (as Prof Conway was urging her to do) and taking up the offer of a lectureship at the RCSI. In the long run she had no regrets.

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Molecular gastronomy, as a prototype for discussing the issue of scientific strategy.

Professor Hervé This



Hervé This, physical chemist at INRA and professor at AgroParisTech, is the Director of the AgroParisTech-INRA International Centre for Molecular Gastronomy, in Paris. As early as 1980, Hervé This created the scientific discipline called Molecular and Physical Gastronomy with Nicholas Kurti (1908-1998), and he also proposed a modernization of culinary activities ("Molecular Cooking").

He is also the Scientific Director of the Fondation Science & Culture Alimentaire, the president of the Human Food Section of the Académie d'Agriculture de France, the president of the Educational Committee of the Hautes Etudes du Goût. He is also a member of the Academy of sciences, letters and art of Alsace, and of the Royal Academy of Belgium, among others.

In 1994, he proposed Note by Note cooking, a new way of cooking that he is promoting all over the world, along as developing laboratories of molecular gastronomy.

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Abstract:

In order to make discoveries, scientists need strategies. But which one? Some proposals are illustrated by results in the particular field of molecular gastronomy, the science that looks for the mechanisms of phenomena occurring during food preparation. Also the relationship between science and technology is discussed, in particular in view of recent results about "dynagels", i.e. dynamic gels.

Molecular Gastronomy

Molecular gastronomy, molecular cooking, and molecular cuisine: in many circles, these three expressions are confused, for reasons that we have to analyze. But before that, we have to say what each describes really. First molecular gastronomy was introduced in 1988 under the longer name "molecular and physical gastronomy" (This, 1995a). The expression is based on the word "gastronomy", that does not mean haute cuisine, but rather "knowledge about food and man's nourishment" (Brillat-Savarin, 1825). Indeed, it was this last meaning that was used when we defined molecular and physical gastronomy, with the late Nicholas Kurti

(Budapest, 1908-Oxford, 1998), in 1988 (This, 1999). The word “molecular” was added with the same meaning as in the expression “molecular biology” (This, 2009a). A concise definition of molecular gastronomy is “the scientific discipline that looks for the mechanisms of phenomena that occur during food preparation” (Burke et al., 2016).

At the same time as the first molecular gastronomy results were published (This and Kurti, 1995a), it was proposed to use the scientific knowledge to find ways for improving culinary techniques (This, 1995b). In particular, we proposed to use chemistry hardware for food preparation, and this is what was called “molecular cooking” in 1999 (Inicon, 2003). Later, when a new culinary style was introduced by chefs, we proposed to distinguish molecular cooking (the modern technical way of preparing food) and molecular cuisine, as the new style based on the new techniques.

Why the confusion between molecular gastronomy and molecular cuisine? Perhaps because some confuse gastronomy with cooking, but perhaps also because we invited chefs to participate to our “Molecular and Physical Gastronomy Workshops”, in the Ettore Majorana Centre for Scientific Culture, in Erice, Sicily (AgroParisTech, 2017). Indeed, we wanted the chefs to be present because, in the first times of molecular gastronomy, we felt that we had to study well defined techniques, as chef know. As a result of our invitation, the large media coverage confused the presence of chefs and our scientific activity. Worst, some chefs who were probably happy to be associated with scientists told them “molecular gastronomists” for some time, when molecular gastronomy became popular.

In all these discussions, there was a main confusion between technique, technology and sciences (of nature). Indeed this confusion is frequent, not only in the field of molecular gastronomy but also in the field of chemistry, and more generally about sciences of nature. For chemistry, for example, what does it mean (This, 2009b)? Indeed, this question should be answered remembering that technique is the production of goods (and physicians are technicians, as was well demonstrated by the French physiologist Claude Bernard (1813-1878), because they cure technically) (Bernard, 1865), technology is the study of technique in view of improving it, and sciences of nature are the activities that looks for the mechanisms of phenomena. Chemistry, in this regard? When chemistry became slowly separated from alchemy, in the 17th century (Joly, 2013), it was clear that chemistry was a science, as is shown in the title *The Sceptical Chymist*, by Robert Boyle (Boyle, 1661), or by the various articles of the Encyclopédie, edited by Denis Diderot and Jean Le Rond d'Alembert (Encyclopedie, 1751). Later, when the “chemical industry” developed, some confusion was created, but we insist that the same name cannot be given to two different activities, and we propose to keep “chemistry” for the scientific activity that looks for the mechanisms of phenomena occurring during atomic rearrangements.

What it is, how it is linked to chemistry and physics

For molecular gastronomy, it was initially conceived as a scientific activity, rather a technology, and we propose to keep this idea (This, 2002). How is it possible, knowing that culinary processes are concerned? Of course, molecular gastronomy can have applications, but we devised it as a scientific discipline because we had the idea that cooking, involving many transformations of physical or chemical nature, could be investigated in view of discovering physical or chemical mechanisms. And it is a fact that in the history of sciences, many culinary activities were the starting point of scientific discoveries, such as convection (Rumford, 1797) or Maillard reactions, for example (This, 2016a).

Indeed it is fair to recognize that historically speaking molecular gastronomy was also introduced at a time when food sciences were focused on technology (the food technology used in the industry) and on the analysis of food ingredients, i.e. primarily plant and animal tissues. It is interesting to observe that even in the 1999 edition of the famous textbook initially published by Belitz and Grosch under the title Food Chemistry (Belitz and Grosch, 1999), there was nothing about meat cooking, except for sausage making, and wine was never discussed under the perspective of cooking, in spite of the fact that about 48 % of all French classical sauces include wine that is cooked (Académie des gastronomes and Académie culinaire de France, 1991).

On the other hand, it is not always known that the French chemist Antoine Laurent de Lavoisier (1743 - 1794) recognized well the difference between science and technology, when he published his article on “meat stock” (producing aqueous solutions by thermal processing of muscular tissues in water) (This et al., 2006). Incidentally, in his article, and in the article that he quotes as a scientific example, the question of mechanisms is not discussed.

All this led us to propose that it should be taught to students in science and technology that sciences of nature are based on the following steps:

- (1) identification of a phenomenon
- (2) quantitative characterization of this phenomenon;
- (3) synthesizing the data in “laws”, i.e. equations
- (4) looking for mechanisms and models quantitatively compatible with the laws
- (5) looking for theoretical consequences of the models
- (6) testing experimentally the theoretical predictions (This, 2009)

Scientific strategy with illustrations

The goal and method of sciences of nature being clear, the question of reaching it can be discussed. In this section we recall some results obtained in the INRA Group of Molecular Gastronomy at AgroParisTech, Paris, France, in relationship with questions of scientific strategy.

Indeed, most scientists would admit that their goal is to make “discoveries”, but the ways to reach it remain vague. Let's compare discoveries with “mountains”. When one looks at the past, it's easy to recognize “summits” such as aromaticity, isomerism, entropy, Le Chatellier's principle, fullerenes, quantum description of the chemical bond, supramolecular chemistry... However scientists are not historians, and they have to look forward, when nothing is clear. In which direction should they go? Indeed, for molecular gastronomy, open questions are many. For example, why are apricot tarts so “sour”, even when they are made from very ripe and sweet apricots (it was checked that the pH does not change during cooking)? Or how are proteins released from animal tissues when such tissues are thermally processed in an aqueous solution, in view of making a “stock”? Or is there an influence of the microstructure of dairy gels (“yogurts”) on the sensation of freshness they convey?

Such questions can lead to discoveries, but which one is the most fruitful, assuming that this last question is meaningful? Indeed we miss a “way”, or a “strategy”, either for choosing the promising questions or to explore them efficiently. For years, discussions with colleagues (including Pierre-Gilles de Gennes, Pierre Potier and Jean-Marie Lehn) and reading of texts on the history of science (Jacques, 1991; Partington, 1998; Ihde, 1984 among many others) led to the identification of some methods for scientific strategy; we propose to the scientific community to answer this important question “which others are missing?” (This, 2016b).

Today the list that we propose for discussion is:

- (1) Transforming adjectives and adverbs into quantitative parameters (introduction of new concepts);
- (2) Looking for the mechanisms of phenomena;
- (3) Focusing on oddities, contradictions, discrepancies... and “symptoms”;
- (4) Designing new observational tools;
- (5) Making science from a technical question;
- (6) Refuting a theory;
- (7) Solving a problem;
- (8) Assuming that any fact, result, observation, phenomenon... should be considered as a particular example of general categories that we have to invent;
- (9) Looking behind the “ordinary”: this means not accepting what was accepted;

- (10) Making the contrary of what was proposed before;
- (11) Looking deeply enough to what an experiment can reveal, and work deep enough to see the impact.

As this can seem abstract, we show the application of these ideas to various questions that arose in molecular gastronomy.

(1) *Transforming adjectives and adverbs into quantitative parameters (introduction of new concepts)*: This idea is certainly useful while preparing scientific manuscripts, but it can be used before works. For molecular gastronomy, it was implemented in a study of the “robustness” of recipes, and it holds for any process. Initially there was the observation that many culinary tips, old wives’ tales, proverbs, sayings (what we proposed to call “culinary precisions”) are wrong, and there was this question: why was wrong technical information transmitted? The analysis of mayonnaise sauce led to a proposal. Indeed the oldest recipe of a sauce of the kind of mayonnaise was published in a French culinary book in 1674 (LSR, 1674): almond oils was dispersed in a stock. Then in 1742, an emulsion more like our modern mayonnaise was published under the name “beurre de Provence” (butter of Provence) (Marin, 1742). The name “mayonnaise” (or mahonnaise, or also magnonnaise) appeared later (Höfler, 1996), and the sauce made of egg yolk, vinegar and oil (from olives) became popular. With time, tips, sayings, old wives’ tales, proverbs, and all technical information that we proposed to name “culinary precisions”, but why? Indeed the sauce can “fail” (phase separation), so that it can be assumed that cooks of the past tried to guess why. As they did not have molecular clues as we have today, and because they did not know about the microscopic structure of emulsions, they proposed various ideas: for example, mayonnaise would have failed if the temperature of the various ingredients was not the same, or if the vessel containing the sauce was not put on ice cubes (Carême, 1847), or if the room was too hot, (Dubois, 1875), or if women having their periods were present, or if the direction of moving the whisk was not constant (Olliver, 1858; Anonymous, 1920).

Many culinary precisions about mayonnaise were experimentally tested (This, 1998), and obviously many were wrong... but some were right: for example, it was written that the oil addition should be “slow” at the beginning, and this is true (Saint-Ange, 1925), otherwise a water into oil emulsion is promoted instead of the oil into water, metastable, emulsion (Anton and Gandemer, 1997).

Why so many culinary precisions about mayonnaise, and so few about roasting meat, for example? It was assumed that culinary precisions appear when recipes can fail, because they are “fragile”. In order to test this assumption, a mathematical description of the “fragility” of recipes was proposed: in 2004, a parameter of “robustness of processes” was introduced (This, 2005) assuming that dishes are obtained as the application of a function of many variables (proportions of ingredients, parameters of processes...). A recipe is said “successful” when the product obtained by the application of the transformation to the ingredients is included in a certain hypervolume, and it fails otherwise. Moreover, a recipe is “robust” when a cook can easily reach the target hypervolume, i.e. when the precision is better than the maximum width of the way starting to the beginning of the recipe and leading to the target hypervolume. In practice it was proposed to define the robustness by comparing the precision of the particular process being used and the possibilities of variation.

For example, when mayonnaise is prepared, the rate of oil addition is important at the beginning of the process: if one litre of oil were added to one egg yolk (about 15 g of water), the whipping would not lead to an oil into water emulsion, and the sauce would fail. On the contrary, adding the oil by small amounts (compared to the volume of water in the egg yolk) at the beginning of the process is leading to a metastable emulsion. The precision with which oil is added is most important: if one could not add the oil by amounts less than a certain maximum quantity, the sauce would fail generally. In other words, the robustness relative to the addition of oil can be defined as the ratio of the maximum oil quantity that can be added (15 g) to the precision on this addition. If the precision is 1 g, the robustness is equal to $15/1 = 15$; on the other hand, if the precision of oil addition is 30 g, the robustness falls to $15/30 = 0.5$.

As said above, the analysis of the tens of thousands of French culinary precisions collected since 1980 had led to the assumption of an invert relationship between the number of culinary precisions for a recipe and

robustness. This assumption was quantitatively tested for some recipes such as hard boiled eggs, soft eggs, mayonnaise, carrot salad, custard, etc., and a law in $1/n^{1.12}$ (where n is the number of culinary precisions) was indeed found... but only when culinary precisions about meat stocks are excluded, because stock making was so important in the past that it attracted a huge number of culinary precisions (This, 2004).

(2) *Looking for the mechanisms of phenomena:* One could obviously say that looking for the mechanisms of phenomena is science itself, or similar to making models, but the following example of the study of the coagulation of egg albumen will show that it can be indeed different.

In the 1980's, we wanted to know if it was true that “chicken eggs thermally processed at 100 °C for more than about 10 minutes become rubbery (Oliver, 1958). As egg albumen is a 10 % (w/w) solution of about 12 main proteins in solution in water (Belitz and Grosch, 1999), the question was first reduced to: which chemical forces can be responsible for egg albumen coagulation? The answer was based on a ranking of forces by increasing energy, from van der Waals weak forces up to electrostatic attractions between charged species.

Clearly, van der Waals, hydrophobic and hydrogen forces are active between adjacent proteins in solution in water, but the question was to know whether the strongest bonds were disulfides bonds or covalent bonds (the latter being unlikely, in view of the chemical constitution of proteins). The possibility that disulfide bridges were responsible for the making of the gel obtained by thermal processing of egg albumen was tested using a reducing agent, i.e. sodium borohydride (NaBH_4), and it was observed that coagulated egg albumen could be transformed back into a solution (This, 1996). Indeed, the assumption tested in this experiment was that egg proteins denature with heat, exposing their thiol groups from cysteine residues. An oxidation would then form disulfide bridges. Using sodium borohydride, it is easy to “uncook” a cooked egg, showing that this mechanisms is indeed responsible for the gel formation. Fortunately, this discovery that was not recognized recently (Improbable Research, 2015) allowed us to avoid the IgNobel prize.

However the issue of the long processing times remained, and we assumed that heating eggs in boiling water would progressively denature more and more proteins, leading to a jellified system with many different networks being formed progressively, when the temperature inside eggs increased by conduction. In order to test this mechanism, eggs were heated for more than 2 hours (in order to reach the thermal equilibrium in all the egg) at 65°C, a temperature chosen to be able to denature only ovotransferrin. It was observed, as predicted, that a very soft gel was made (Figure 1).



Figure 1. An egg thermally processed in hot air at 65°C for 2 hrs.

Then, heating at more than 70 °C, a more robust gel was obtained. And other results can be obtained at different temperatures, corroborating the proposed mechanism. By the way, all these different eggs were proposed to cooks as part as “molecular cuisine” under the name of “eggs at 6X °C”, the letter X standing for the various possible figures (indeed, this name is wrong as one could also cook at 7X °C, or 8X °C, for example) (This,

2007).

(3) *Focusing on oddities, contradictions, discrepancies... and "symptoms"*: Focusing on oddities seems to be an obvious scientific strategy, as oddities can probably be defined as observations, or facts that don't fit well with our theories, allowing their refutation, and, hence, scientific advance. Indeed, they play a similar role as the refutation of consequences of theories (step 6 of the method of science).

In the history of our group, one of the most typical work in this line was the observation of different colors for two solutions ("stocks") prepared exactly in the same way from the same plant tissue (This et al., 2008). More precisely, one root of *Daucus carota* L. had been prepared as discussed in Cazor et al. (Cazor et al., 2006), cut longitudinally, and the two halves had been heated separately in water for the same time at the same temperature of 100 °C, but it was once observed that one solution was "orange", while the other was "brown". How was it possible?

Finally it was analyzed that one stock was made using an oil bath, and the other was prepared using a heating mantle, so that different quantities of light could reach the solution (Figure 2).



Figure 2. The experimental setup used for the discovery of the impact of light on aqueous solutions produced by thermally processing carrot (*Daucus carota* L.) roots in water.

Indeed it was discovered that this was the cause of the different colors, as the reproduction of the experiment with the same heating systems, but with or without light (aluminum foil around the equipment versus controlled light) could reproduce the different colors. This confirmation led to a theory for the explanation of the spirals that was previously observed without explanation in the (a^* , b^*) colorimetric plane.

Indeed, when the initial observation was reproduced rigorously, the colour of aqueous solutions being prepared in the $L^*a^*b^*$ colorimetric system was quantitatively determined. Because the L^* variation was not the main discriminant factor, a curve was shown in the (a^* , b^*) plane, with a first evolution toward the negative values of a^* and the positive value of b^* , before the curves moved to the right in order to reach the first quadrant (of course with differences depending on the quantity of light being received by the experimental system) (Figure 3). Why this spiral shape?

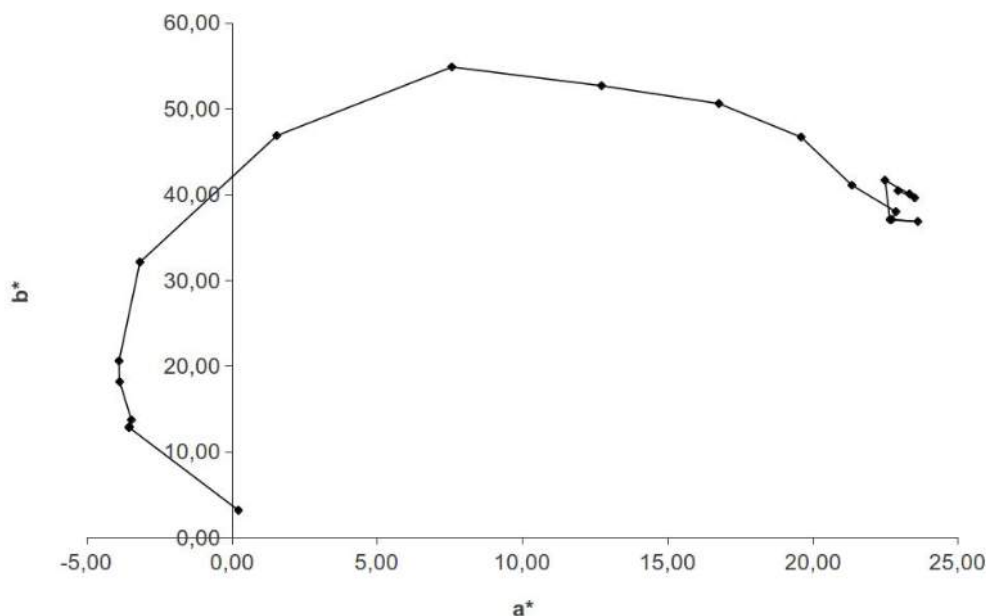


Figure 3. The color curve for carrot stocks in the (a^* , b^*) plane.

There are many possibilities that can be described by simple sets of differential equations. For example, if one colored compound moved first out of the plant tissue, the accumulation of this compound in the solution would change its color from the origin of the (a^* , b^*) plane toward a point corresponding to the saturated color due to this compound; then a chemical modification of this compound would move the color point toward the color of the products formed after reaction of the first extracted compound. Another possibility, corresponding to another group of equations would be that first a particular compound would first move out of the plant tissue, shifting the color in a defined direction of the (a^* , b^*) plane, before another compound having a different colour would be released, changing the color of the solution toward the direction of this second compound in the (a^* , b^*) plane (Figure 4).

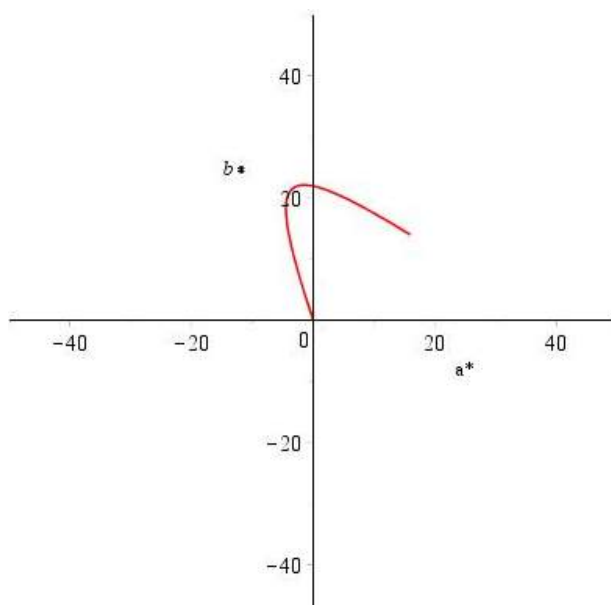


Figure 4. Modelling the color evolution of carrot stocks with two compounds released from plant tissues.

Of course, this needs to be analyzed chemically. But the colorimetric determination of solutions of galacturonic acid being thermally processed in the same conditions as carrot tissues showed a similar color evolution as

carrot stocks. This work could usefully go on identifying the various products formed during this degradation of galacturonic acid, and measuring their light absorption.

(4) *Designing new observational tools*: Creating such tools is obviously a good way to make discoveries, as if some objects that were invisible to the previous observational methods become visible, they are really “discovered”. Here, we deal with the technique that we called *in situ* quantitative nuclear magnetic resonance spectroscopy (*is q NMR*), because there are two “lessons” behind the introduction of this technique, and also because many open scientific questions remain about it.

Quantitative NMR has been used in our group since the 90's, because, contrary to an idea that was popular in chemistry laboratories, it was not impossible to analyze complex liquid systems such as carrot stocks using high field (frequency domain) NMR. The initial doubts were about the big number of signals in spectra acquired from such samples: weren't they too many and would interpretation be possible? Our first studies were based on the assumption that NMR signals, as well as quantities of solutes, can be ranked by decreasing order of magnitudes, so that the analysis would be easier: first only large (first order of magnitude) signals are analyzed, then second order signals, and so on. Indeed, our studies of carrot stocks showed that the quantitative analysis of complex systems can be done readily using NMR spectroscopy (Cazor et al., 2006).

When we began using this technique, the samples were lyophilized twice, with redissolution in deuterated water, and the variation coefficient on the measured concentrations of solutes in initial samples was about 10 %. However the second improvement of the technique made it possible to improve greatly the results. Indeed, this second step was to analyze directly the solutions as well as “gels”, without any preparation of the samples (This et al., 2010). Of course, there is a large signal corresponding to the protons of water (~ 4.7 ppm, depending on the pH), but 90 % of this signal falls within a 0.02 ppm interval, so that there is no difficulty analyzing all signals outside this interval; and even within this signal, decomposition methods can give access to smaller signals making shoulders for example (Bauchard and This, 2015).

Applying this new “*in situ* quantitative NMR spectroscopy” to sample of carrots roots, it was shown that it was possible to analyze rapidly (about the time of some hundreds of scans, i.e. some tens of minutes), without extraction and without using solvents, all saccharides from samples as small as 100 mm³ with an average variation coefficient of 0.038 (with a standard deviation of 0.047). And because the samples can be small, we could get information on stripes of plant tissue cut at different distances from the axis of the carrot root.

(5) *Making science from a technical question*: The first example, about soufflé expansion, was studied in the 80's (This et Kurti, 1995b), at a time when the main culinary books were explaining that soufflés expanded because of the dilatation of air bubbles (Larousse, 1984).

Soufflés are preparations made of a viscous suspension (custard, fruit purée...) mixed with a foam such as whipped egg whites; they are cooked in an oven at temperature around 180 °C and they are considered successful when they expand (sometimes by up to 200 %). Indeed it was after years of measurements of temperature and pressure inside soufflés that finally the observation of bubbles at the surface of soufflés, in the oven, made us understand that soufflés expansion was probably due mainly to water evaporation (This, 2002). For sure, air bubble dilatation can occur, but with a maximum increase of about 30 %, as can be calculated using the ideal gas law. Moreover when the mass of a soufflé is followed, it can be observed that this 10 % decrease could produce as much as 10 L of soufflé from only 100 g of initial preparation.

Clearly, the old theory was wrong, and even if the discovery has almost no scientific importance in this case, it can be shown that the technique of soufflé making can be modified using the new ideas: indeed whipping the egg albumen is useless, as soufflés heated by below can expand as much as soufflés with whipped egg whites, as was demonstrated during public lectures. This is technology, and not science, but we can see here more clearly the relationship between the two fields.

(6) *Refuting a theory*: About the sixth strategy -refuting a theory-, we propose to consider again the question of

“carrot stock” production. In the 2000's, the question of how compounds exchange between plant tissues and aqueous solutions in which these tissues are thermally processed was poorly known. After some studies, we came to the conclusion that diffusion of compounds from the sap (minerals from raw sap in xylem; mainly saccharides, amino acids and organic acids from the elaborated sap in phloem) could explain the composition of stocks (Tardieu et al., 2009). This idea was based on the analysis of stocks in function of time, but also on microscopic studies of plant tissues soaked in solutions of colorants such as methylene blue: in some tens of minutes, the colorant appears in conductive channels of the plant tissues, indicating that the same diffusion mechanisms could be responsible for the appearance of compounds in outside water during stock making. However the presence of methylene blue around the channels, and not only in them, showed as well that this purely diffusive theory was not enough. And this is why we proposed a more complex models (Figure 5), with more than simply two exchanging compartments (the conductive tissues, the outside aqueous solution).

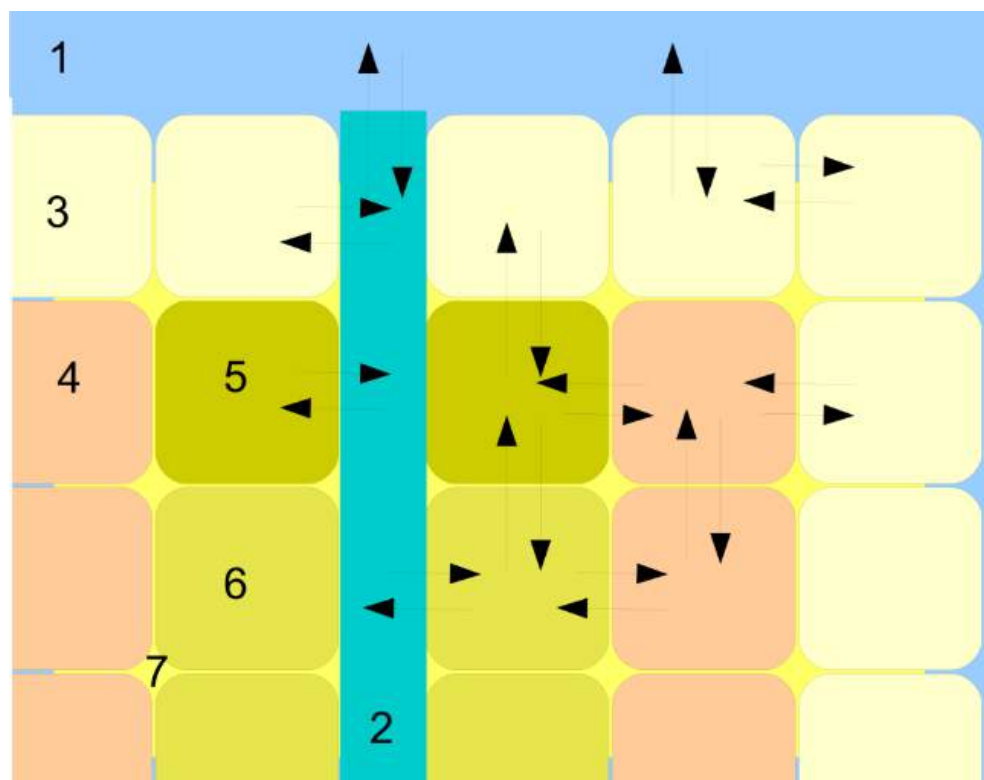


Figure 5. A model for the exchange of matter between a plant tissue and an aqueous environment.

Using this new model, fitting the kinetic variations of aqueous solution composition lead to showing that it is necessary to include more than simple diffusion in the theory. Parameters were introduced in this model, and current work is trying to determine them. (Tardieu et al., 2011).

(7) *Solving a problem*: Part of the activity of our group is described in this way by Jean-Marie Lehn, and we interpret it as for students solving problems, or answering questions in exercises. One example of such a strategy was the study of the crystallization of fats in yogurts (Bouteille et al., 2013).

The question was based on the traditional view of crystallization of a liquid phase upon cooling that generally occurs on “seeds crystals”, so that it can be promoted by impurities in the liquid phase. Dairy gels, such as yoghurts, contain both solid and liquid fats when consumed, as their temperature is between 10 °C and 24 °C after 5 s in the mouth when they are put initially at 4 °C. The mass ratio between solid and liquid fats, which depends on the temperature, impacts organoleptic properties of dairy gels.

How does fat crystallize when yogurts are cooled? Do the surfactants at the surface of the dispersed fat droplets promote crystallization from the outside toward the inside? Do they change the crystallization behavior? As the

usual methods to determine the liquid/solid fat ratio requires fat extraction, they prevent the study of the potential impact of the colloidal structure on milk fat fusion behavior. We used *in situ* ^1H NMR in order to follow this behavior directly in dairy gels: at temperatures between 20.0 °C and 70.0 °C, the liquid fat content and the composition of triacylglycerols of the liquid phase (in terms of length of alkyl chains) were determined; spectra of isolated milk fat also enable the quantification of the double bonds of triacylglycerols. Statistical tests showed no significant difference between isolated milk fat and milk fat inside a dairy gel in terms of melting behavior: the fat globule membrane does not seem to have a significant influence on the fat melting behavior. It remains to understand why.

(8) *Assuming that any fact, result, observation, phenomenon... should be considered as a particular example of general categories that we have to invent:* Traditionnally “gels” are defined by IUPAC (IUPAC, 1972) as particular “colloids”, i.e. systems in which the molecules or polymolecular particles dispersed in a medium have at least in one direction a dimension roughly between 1 nm and 1 μm , or that in a system discontinuities are found at distances of that order of length; it is not necessary for all three dimensions to be in the colloidal range: fibers in which only two dimensions are in the 1 nm / 1 μm range, and thin films, in which one dimension is in this range, may also be classified as colloidal. Nor is it necessary for the units of a colloidal system to be discrete: continuous network structures, the basic units of which are of colloidal dimensions, also fall in this class (e.g. porous solids, gels and foams). In gels, there are two phases: one liquid and one solid. In order to envision all kinds of “simple” gels (i.e. gels including only one liquid phase and one solid phase), it is not difficult to write some lines of computer program producing systematically all formulas in a formal language called “disperse systems formalism” (DSF) (This, 2002). Programs for such purpose have to include the three possible phases O, S, W (alphabetic order), the three operators “/”, “x”, “@” (they correspond respectively to random dispersion, intermixing of two continuous phases and inclusion), and the four possibilities for the dimensions of objects D_0 , D_1 , D_2 , D_3 (respectively for objects of dimension zero, one, two and three); the solid continuous network has necessarily three dimensions, and it has to be used as the last term of the formula, in spite of DSF using preferably the alphabetic order.

The list of all simple possibilities is then: $D_0(\text{O})/D_3(\text{S})$, $D_0(\text{W})/D_3(\text{S})$, $D_1(\text{O})/D_3(\text{S})$, $D_1(\text{W})/D_3(\text{S})$, $D_2(\text{O})/D_3(\text{S})$, $D_2(\text{W})/D_3(\text{S})$, $D_1(\text{O})\times D_3(\text{S})$, $D_1(\text{W})\times D_3(\text{S})$, $D_2(\text{O})\times D_3(\text{S})$, $D_2(\text{W})\times D_3(\text{S})$, $D_3(\text{O})\times D_3(\text{S})$, $D_3(\text{W})\times D_3(\text{S})$, $D_3(\text{O})@D_3(\text{S})$, $D_1(\text{W})@D_3(\text{S})$, $D_2(\text{O})@D_3(\text{S})$, $D_2(\text{W})@D_3(\text{S})$ (This, 2016a).

What do these formula mean? Envisioning all of them one after the other would be tedious, but the first of the list ($D_0(\text{O})/D_3(\text{S})$), for example, corresponds to a random dispersion of oil droplets in a continuous solid, and this can be made by freezing, at a temperature below 0°C, an oil in water (O/W) emulsion, for which the “oil” is a compound that would not be miscible with water and would solidify at temperature below 0°C (for example carbon disulfide, for which the freezing point is – 111.5 °C). Another interesting example is obtained using the formula $D_3(\text{O})\times D_3(\text{S})$: when one first makes a O/W emulsion, with cystein residue-containing proteins dissolved in the liquid phase, the heating of the system leads to protein coagulation ($D_3(\text{O})/[D_3(\text{W})\times D_3(\text{S})]$); drying the gelled emulsion (called a “gibbs”) (This, 2009) can lead to the desired gel (called a “graham”). “Natural” systems already exist having this formula, such as chocolate, as a liquid continuous “oil” phase is dispersed in a continuous solid network (Loisel et al., 1997).

This list of simple gels being made, it can be observed that more than one phase (“water” or “oil”) can be dispersed in the three dimensional, continuous, solid phase. This leads to envision connected or non-connected gels with a disperse phase which is either simple (water, oil), or an emulsion, or a suspension, etc. When only one phase is dispersed, the gels are said to be of “class 1”, and the systems are of “class k ” (k being an integer) when k phases are dispersed in the continuous solid network.

The whole list of all possible gels is infinite, including, for example: connected gels with sponge water-oil phase, non-connected gels with sponge water-oil phase (Wadsten et al., 2006), connected gels of aqueous channels, non-connected gels of aqueous channels, connected or non-connected gels with liquid channels, connected or non-connected gels with oil channels... Sometimes very long names such as “non-connected gel of liquid suspensions in oil sheets” are needed.

However, whereas these names in natural language can be used, they are cumbersome. The DSF makes it easier to envision possible gels: again a small program based on it can produce all possibilities for the successive classes of gels. For two phases and more than two dimensions, the program examines systematically phases, dimensions, taking care of parentheses and imposing that the end of the formula is " $D_3(S)$ ".

For example, the complex name given above ("non-connected gel of liquid suspensions in oil sheets") corresponds to the formula $[D_0(S)/D_2(O)]/D_3(S)$. The most simple program does not reject impossible formulas (such as $D_0(S) \times D_3(W)$, with a phase of zero dimension that would extend in all three dimensional space), but it is easy to filter manually the possible solutions.

After such simplification, by increasing order of classes, the list can be used to envision complex gels, which can be identified in natural objects: for example, a sample of plant tissue (e.g. a part of the root of *Daucus carota* L.) is made of parenchymatous tissue and of connective tissue (xylem, phloem), so that the system has the formula $[[D_0(W_1)]+[D_1(W_2)x]]D_3(S)$. In this formula, both " $D_0(W_1)$ " and " $D_1(W_2)x$ " operate on the same $D_3(S)$. It is assumed that the cytosol is a liquid (W_1), but if it is more realistically preferred that it is itself a gel, then W_1/S' could be used instead of W_1 (Cazor et al., 2006).

Moreover new gels can be produced using the formulas as guides: for example, the gel $D_1(W)/[D_3(W) \times D_3(S)]$ can be made by dispersing cylinders of an aqueous gelatin gel in an agar-agar gel where protease enzymes (EC 3.4) are dissolved: after gelling of agar-agar, enzymes diffuse toward the gelatin gel, and they destroy the solid network, leaving liquid channels in the agar-agar gel. Another example is the use of "chaotic mixers" (Tabeling et al., 2004) where two solutions would be injected: one aqueous solution, and one solution of a gelling agent; after dispersion and gelling, the result is a multisheets gels. Of course, each particular gel has specific bioactive properties.

Indeed making new gels is only a first step. It is also interesting to characterize them chemically, physically, biologically. It was proposed to use a general description called "bioactivity", along with the definition of a "matrix effect" (This, 2012). Gels are often used in technology, in particular for formulation activities, because compounds dissolved in the liquid phase can diffuse toward the environment and vice versa. When released compounds interact with biological receptors, they have been called "bioactive" (bc). In some cases, a physical binding is needed to trigger physiological effects (olfaction, sapiction, trigeminal effects, calcium perception, perception of unsaturated fatty acids) (Martin et al., 2011; Tordoff, 2012), but for vision the effect is indirect, and for receptors inside tissues, a transfer into the blood system is needed, sometimes after modifications during digestion. Here let us remark that even compounds that would be trapped by the swallowed bits of food are encompassed by the given definition, such as tasty ions adhering surfaces, complexed salivary proteins on some compounds in food.

Theoretical and experimental determination of bioactivities have to be analyzed specifically. For example, supramolecular interactions (van der Waals forces, hydrophobic pseudo forces, hydrogen bonds, disulfide bridges...) between the solvent and the solid network of gels can reduce the self-diffusion coefficient of the solvent molecules or of the dissolved bc, so that the release would be delayed (Matsukawa et Ando, 1996). Also various compartments can release differently bc, such as plant tissues (modeled as $D_1(W) \times D_3(S) + D_0(W)/D_3(S)$ systems), for which it was shown that the release of solutes in the sap is fastest than from parenchyma cells (This, 2012).

(9) *Looking behind the "ordinary"*: this means not accepting what was accepted before, and we propose to consider here the case of "dynagels", that were introduced after dynamers were discussed by Jean-Marie Lehn (Lehn, 2005).

In all the previous section, we considered only "static" gels, where solutes and solvent could diffuse in liquid compartments (diffusion in the solid parts would be much slower) inside a fixed solid network. They do not take into account the fact that another analytical frame can introduce new phenomena, and different

mechanisms. Indeed the analysis of "culinary systems" shows that there are "physical gels", with a solid network made from the reversible assembly of constituent molecules (for example, gelatin gels), and "chemical gels", with a fixed structure (This, 1996). The examination of the diffusion of bc in a fixed gel is like the Born-Oppenheimer assumption for the calculation of molecular orbitals (McQuarrie, 2007), but one can also have a more dynamical approach, in particular when the thermal energy is of the same order of magnitude as the binding energy of the "monomers" (subunits) which can make the solid, "polymeric" network.

Here the words "monomer" and "polymer" call for a discussion on dynamers, i.e. dynamic polymers which can reorganize, because their subunits are linked by supramolecular forces (Lehn, 2010). Dynamers are defined as constitutional dynamic polymers, i.e. polymeric entities whose monomeric components are linked through reversible connections and have therefore the capacity to modify their constitution by exchange and reshuffling of their components. They may be either of supramolecular or molecular nature depending on whether the connections are non-covalent interactions or reversible covalent bonds (Lehn 2010).

For gels, also, "dynagels" and "statgels" can be considered. As for dynamers, dynagels can be defined as constitutional dynamic gels, i.e. gels whose subunits of the solid network are linked through reversible connections and have therefore the capacity to modify their constitution by exchange and reshuffling of their components. They may be either of supramolecular or molecular nature depending on whether the connections are non-covalent interactions or reversible covalent bonds. Dynamers can be chemically dynamic, involving a reversible chemical reaction, and physically dynamic, based on physical non covalent interactions; the same idea holds for dynagels, as their solid network is often a polymer. However, in this case, the description is made more complex as the solvent, and possible solutes, can interact with the solid network.

One example of dynagels is gelatin gels at a temperature close to the critical melting point (Djabourov et al., 1988). Of course, gelling of gelatin depends on the particular chemical composition of the aqueous solvent in which gelatin is dissolved (Bellini et al., 2015), but a simple thermodynamical description can be made. Let us assume, for example, that the continuous solid network is obtained by the linking of a certain number n of subunits at each "node" (for gelatin gels; $n = 3$) with a constant binding energy E for each subunit. In the assumption of the Boltzmann distribution, the proportion $p(b,f)$ of subunits being bound (b) on one end and free (f) at the other at a certain absolute temperature T would be $p(b,f) = K e^{-E/kT}$, k being the Boltzmann constant, and K a normalization constant. If the binding or release of a particular end of a subunit does not depend on the bound of free state of the other end, then the probability for a subunit to be entirely free (f,f) is simply proportional to $e^{-2E/kT}$. The sharp exponential variation of this proportion in function of temperature explains why gelatin gel can be dynamic only within a narrow range of temperatures. For example, when the temperature is equal to $2E/0.693k$, half the subunits would be free, which means that the mechanical properties of the gel are changed. Of course, this simple view can be improved by considering a distribution of energy for the different nodes, but it can be shown that the shape of the curve of the free subunits does not change much with this modification.

The bioactivity of statgels and dynagels having the same DSF formula (i.e. the same physical organization) can be very different, even with constant binding energy between the solutes or the solvent, on one hand, and the solid network, on the other hand, because of a new component of diffusion of monomers (with their surrounding of solute and solvent molecules) in the constantly reorganizing system.

As for dynamers, dynagels can exist by nature or by intent. In order to explore dynagels by intent, one could first focus on the non-connected gels, so that diffusion of solutes of the solvent could (by slow diffusion) progressively interact with monomers and influence gelling. In this way, we would have adaptive materials. In this way, not only fixed systems having a particular DSF formula have to be considered, but also equilibrium between "limit DSF formula" must be studied, making new diffusion issues for dynagels. About dynamic bioactivity, how the knowledge of the bioactivities of limit formula can allow the calculation of the dynamic bioactivity of the dynagel? Other questions are also asked, such as how the dynamic reorganization of such colloidal systems change the self diffusion coefficient of solutes or solvent?

Conversely, one can also ask how the presence of solutes that have specific chemical affinities for the monomers would change the equilibrium of monomer association-dissociation? If solutes indeed change such equilibria, one can envision new ways of controlling the formation of dynagels, as effectors can change the equilibrium of dynamers (Lehn, 2005).

Dynagels are particular cases of dynamic materials (“dynamats”) (Lehn, 1999a), these systems being defined as material whose constituents are linked through reversible connections (non-covalent or covalent) and are able to continuously reorganize through assembly/disassembly processes and exchange of components in a given set of conditions, usually under thermodynamic control (Lehn, 1999b), but eventually involving kinetic bottlenecks or traps.

As dynamers, dynagels are adaptable and self assembling systems (Lehn, 1995; Atwood et al., 1996; Lehn, 2002; Philp and Stoddart, 1996) capable to select in principle their components in response to external stimuli or to environmental factors, so that they behave as adaptive materials (Lehn, 1999a; Lehn, 1999b; Lehn, 2002). As supramolecular dynamers, supramolecular dynagels are defined as the entities whose solid network is generated by the polyassociation of molecular monomers bearing complementary binding groups capable of connecting through the usual non-covalent interactions implemented in supramolecular chemistry: electrostatic, hydrogen bonding, donor–acceptor, van der Waals as well as metal ion coordination. Of course, the building of the solid network of dynagels is imposing some particular characteristics to supramonomers, as for dynamers, and in particular the presence of more than two binding sites (otherwise, the suprapolymer would be linear). Molecular dynagels, as molecular dynamers, are reversible covalent systems which open a range of perspectives to polymer chemistry.

Finally, as for double dynamic polymers, one can envision double dynagels, combining monomers that bear complementary non-covalent interaction units as well as complementary reversible functional groups. This allows the generation of polygels presenting double dynamic behavior, gels that are dynamic on both molecular and supramolecular levels.

In conclusion, the operation of the various new kinds of gels in chemistry, and more generally in materials science, confers to the gel entities new physical and chemical characteristics. In particular, dynagels can have many of the properties of dynamers, including the ability to respond to external stimuli and to environmental conditions, i.e. adaptability, a major tenet of constitutional dynamic chemistry, which enables the development of adaptive chemistry (Lehn, 2002). The further exploration of these features may be expected to open wide perspectives for basic research in colloidal science as well as to give access to a range of novel properties and applications in colloid technology.

(10) Making the contrary of what was proposed before: This proposal is from Jean-Marie Lehn, and the example behind the idea is the initial proposal of supramolecular chemistry, when it was attempted to make “unstable molecules”, whereas it was always considered that molecules had to be stable atomic groupings. Until now, this idea was not implemented by our group.

(11) Looking deeply enough to what an experiment can reveal, and work deep enough to see the impact: Indeed this strategy was used when we analyzed the results of experiments that we performed in order to analyze the time course evolution of “tomato and onion sauces”, i.e. solid-liquid extraction, as for “carrot stocks” previously studied (Tardieu et al., 2009).

As carrots roots, onions (*Allium cepa* L.) bulbs are widely consumed vegetables, being important ingredients in many dishes and sauces. Consequently, their chemical composition is of interest, as a source of both nutrients and flavor molecules. During carrot stock making as during the thermal processing of onion bulbs in the aqueous environment that makes up sauces, water soluble compounds can be transferred from the onion tissue into the aqueous environment of the sauce. Little is known about the processes by which such transfer occurs, yet they can have an impact on the ultimate food product. Taste, an important part of flavor, is due to these aqueous soluble molecules, including nonstructural saccharides, amino acids, organic acids, and phenolics. These compounds migrate from the food to saliva, where they can contribute to taste by binding to taste receptors. Furthermore,

upon storage of prepared foods, such compounds might continue to be transferred from the plant tissue into the surroundings and ultimately cause changes to the taste.

The identification and quantification of the water soluble compounds in onions have been the subject of numerous studies. While the exact composition of plant tissues can vary with cultivars, growing conditions, time of harvest, and storage subsequent to harvest, there is general agreement that the main non-structural aqueous soluble saccharides in onions are glucose (Glc), fructose (Fru), sucrose (Suc), and fructooligosaccharides (FOS) of up to 12 units. Using q NMR, we followed the time course evolution of water soluble compounds, and we identified the main compounds extracted from onion tissue into aqueous solution as Suc, Glc, Fru, 17 amino acids, and 5 organic acids.

Then we focused on the release of saccharides into aqueous solution because (1) the mechanisms for the extraction of saccharides from plant tissue could be the same as those for the extraction of other water soluble compounds, (2) the nutritional interest of saccharides in the diet, and (3) their impact on the development of flavor. In addition, saccharides are the main component of dry matter (DM); the onion bulb is a storage organ, and nonstructural saccharides have been shown to account for as much as 64-80 % of the dry weight.

As said before, the major mechanism of extraction appears to be diffusion in the conductive channels, but it is not the only one. In one study, we decided to use the time course evolution of concentration in saccharides in the aqueous medium, considering that the compounds of interest could come from one of the two “compartments”, i.e. the parenchyma or the “channels” (xylem plus phloem). We considered a larger amount of solutes located either in channels or in parenchyma cells, in order to explain the time course extraction features. Short and long time of extraction were studied.

General scheme of the different phenomena that could occur during extraction of water soluble compounds from plant tissues. Two main limit profiles for metabolites can be considered:

- (1) quantity in parenchyma tissue >> quantity in channels,
- (2) quantity in channels >> quantity in parenchyma tissue.

For each case, there are 2 possibilities: (i) kinetic in the parenchyma tissue >> kinetic in the channel, (ii) kinetic in the channel >> kinetic in the parenchyma tissue. Another case (3) could be: quantity in parenchyma tissue ~ quantity in channels, with two kinetics equal or different.

Fitting the extraction profiles with these possibilities, it was observed that Case 3 does not seem to be relevant. If molecular diffusion occurs, data seem to be in favor of Case 2.ii. This assumption remains to be mathematically quantified. We also modelled diffusion from channels using the *Femlab* software in the particular case of a non turbulent system. Using such model, the calculated diffusion coefficient for Case 2.ii are close to data from literature. Further studies shall now be carried out in a turbulent system in order to take into account the influence of convection and other phenomena that could play a role in such extraction.

Conclusion

Finally it is hoped that this text appears clearly as a plea in favor of the constitution of a bank of strategic ideas that would be transmitted to young scientists (and to ourselves). We invite colleagues to submit their ideas, along with examples, to the International Journal of Molecular Gastronomy, even if their ideas concern other fields of science.

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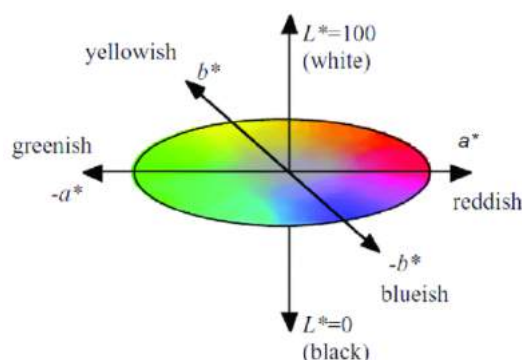
Editors Note:

From experience I am aware that confusion often arises when discussing colour. This is not helped by there being several systems of expressing colour values. The most common are Hunter and CIE systems. The following web pages are helpful.

<https://support.hunterlab.com/hc/en-us/articles/204137825-Measuring-Color-using-Hunter-L-a-b-versus-CIE-1976-L-a-b-AN-1005b>

<https://support.hunterlab.com/hc/en-us/categories/201319586-Color-Theory>

Colour Space



Hunter L, a, b and CIE L, a*, b* systems

These systems can be mathematically interconverted.

L, a, b Color Scales



There are two popular L,a,b color scales in use today: **Hunter L,a,b** and **CIE L*,a*,b***.



While similar in organization, a color will have different numerical values in these two color spaces.

L, a, b Color Scales



Hunter L, a, b and CIE L*,a*,b* scales are both mathematically derived from CIE X, Y, Z values.



Neither scale is visually uniform. Hunter L, a, b is over expanded in the blue region of color space and CIE L*,a*,b* is over expanded in the yellow region.



The current CIE recommendation is to use L*,a*,b*.

CIE: 'Commission Internationale de l'Eclairage'



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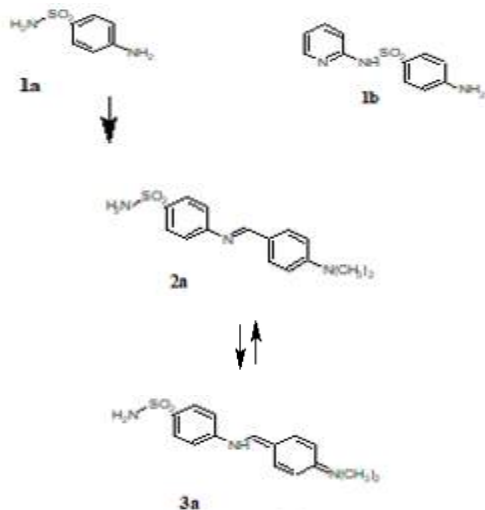
The Second Dublin Werner

Prof Brian McMurry

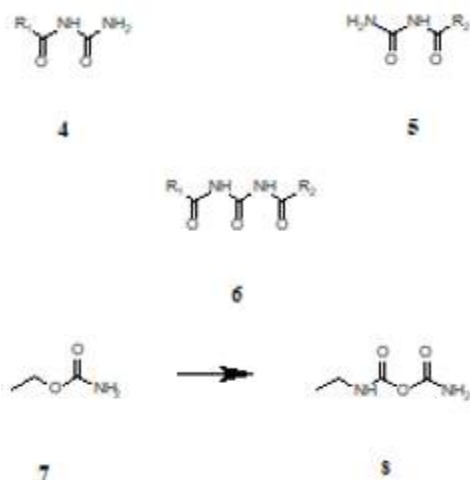


Brian McMurry graduated with 1st Class honors and Gold Medal in Experimental Science in 1953 (specialising in Chemistry) from Dublin University, and received his PhD in 1956. He joined the staff of the Chemistry Department in Trinity College in 1955, and was elected a Fellow of the College and a Member of the Royal Irish Academy in 1959. He went to Harvard for the year 1961-1962 where he worked with RB Woodward at the start of the synthesis of Vitamin B12. In 1964 he went to the University of Lagos, Nigeria as the first Professor of Chemistry as part of an exchange programme between the two Universities. Unfortunately a tribal conflict arose in the University, it closed, five of the six deans were sacked and there were mass resignations. Back in Trinity, he served as Dean of Graduate Studies and later Registrar, on the Board of the College as a Senior Fellow, and a Treasurer and Trustee of the Trinity Association and Trust. He served as Treasurer of the Royal Irish Academy, and on the Executive Committee of the Irish Council for International Students. He started as a natural product chemist, went over to organic photochemistry, and finished up as a medicinal chemist, when he was one of the leaders of a group that developed a drug that got into Phase-2 Trials against Melanoma. It proved too toxic at this level and was dropped. He retired in 2001.

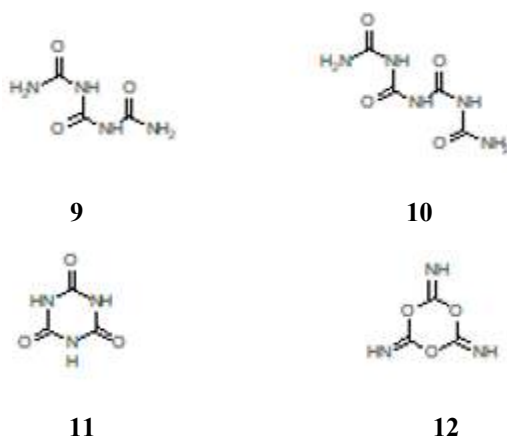
Tony Werner was born on 18th June, 1911, the son of Professor EA Werner¹, at that time Professor of Applied Chemistry in Trinity College. He was educated in St Gerard's School outside Bray – a private Catholic school, and entered the College in 1929. He graduated with a 1st Class Moderatorship in Experimental Science in 1934 and completed an MSc degree the following year. He received an Alexander von Humboldt scholarship from the German Government, which allowed him to study in the University of Freiburg in Breisgau where he received a PhD in 1937. He was appointed a Lecturer in the Department in Trinity College in the same year. Material from his PhD studies involving measurement of the K_M of cellulose acetate appeared in a paper in *Chemische Berichte* in 1938² and there was a steady stream of papers thereafter. His interest in analytical methods was reflected in their subject matter. One appeared in the first ever issue of the *Lancet*³, where he an analytical method for determining the concentration of sulfapyridine (1a) in biological fluids⁴. This involved the formation of an anil between the amino-group of the sulfonamide with *p*-dimethylaminobenzaldehyde (2a). The product is pale yellow at neutral pH's, but in acid it affords a bright orange salt (3a); the concentration of sulfonamide could be estimated colorimetrically. He returns to the area later, when he applies his method to sulfanilamide (1b)^{4,5}. He used selenious acid as an oxidising agent to provide a method for the quantitative analysis of thiourea; elemental selenium precipitated out. The method did not work for other sulfur compounds as the selenium was contaminated with sulfur⁶.



Many of them were published in the *Scientific Proceedings of the Royal Dublin Society*. In these he describes aspects of urea chemistry. In one he shows that the two acyl groups in diacylureas are located on the nitrogens⁷; his experiments showed that the two monoacylureas (4) and (5) had the acyl group attached to nitrogen and he subjected them to the alternative acylating agent; the two reactions gave the same product (6). With his father, he studied the conversion of ethyl urethane (carbamate) (7) to ethyl allophanate (8)⁸. Their mechanism was questioned by others, and, with Gray, he returned to print with a vigorous defence of their theory⁹.



He studied the chemistry of triuret (9), and dismissed the existence of tetrauret (10)¹⁰; here he gives the correct structure of urea, one that his father did not believe in¹. He studied the polymerization of cyanic acid¹¹; it had been reported that cyclisation yielded two products, cyanuric acid (11) and cyamilide, assigned the structure (12)¹¹. In a careful study, Tony was able to show that neat cyanic acid polymerises at low temperatures, but that more cyanuric acid appeared in the mixture the higher the temperature. This suggests that cyamilide is the kinetic product of the cyclisation, while cyanuric acid is the thermodynamical product. He agreed that Hollwach's acid, the subject of some debate was in fact cyanourea¹².



He had become a member of the Common Room Committee, so he was well integrated into the College academic community; the Common Room was the academic Staff Club. He was appointed Reader in Organic Chemistry in 1945. His father had retired in that year as the University Professor of Chemistry. I suspect that Tony had been told by the Registrar and Professor of Physical Chemistry, KC Bailey, that the College would be looking for someone from outside to replace his father. The Readership was College's compensation. It was not enough. Wesley Cocker arrived in 1946; he was a new broom and immediately completely revised the chemistry syllabus. Tony would have very uncomfortable in the new regime, and he chose to leave, moving to the National Gallery in London in 1948 as a research chemist. Curiously, had he stayed in Trinity, he would have provided a skill in analytical methods that was not in the department when he left. Much of the

information about his later career comes from the obituaries in the (*London*) *Independent* written by Alfred Odding¹⁴ and in the *London Times*¹⁵.

Move to London

In the National Gallery, he developed a wax polish for use on wood and other surfaces which is still used; a soluble nylon to strengthen fragile objects has not survived. It was also in this period that he played a small part in the unmasking of the Piltdown Man; he and Joyce Plesters showed that the stain on its teeth was of more recent origin. With JS Mills, he investigated the structures of the triterpenoid constituents of Dammar Resin¹⁶, used to protect oil paintings; the determination of triterpene structures was an area of great interest at the time.

British Museum

He moved to the British Museum in 1954 as a Principal Scientific Officer. Tony's arrival helped to sort out a problem as his predecessor had fallen out with his immediate boss. His more relaxed manner smoothed out the problem. Together with A C Baynes-Cope, another Trinity graduate, he showed that the Vinland Map was a forgery^{14, 15}. Baynes-Cope was a couple of years ahead of me in College; I remember him as an analytical chemist in the making, eccentric, fastidious and meticulous in his practical work. Tony was promoted to Keeper of the Research laboratory in 1959; he was the obvious choice when his predecessor retired. He became widely respected in the world of antique artefact restoration. He personally recovered the paten and ring from the grave of Archbishop de Gray, a medieval Archbishop of York in the Cathedral crypt, and brought them back to the Museum for attention. He was in charge when the artefacts from the Sutton Hoo Hoard were brought in and restored in the Laboratory¹⁵. The number of chemical and physical methods available for the examination of archaeological and artistic objects was multiplying. Werner, with his chemical training, was ideally placed to make use of them, and he became a powerful advocate for their use. He was recognised as an authority and was a much sought after lecturer by UNESCO and the British Council, both of which sent him abroad to many countries, both in Europe, Asia and Australasia^{14, 15}. He greatly enjoyed travelling, but his absence from his desk was noticed¹⁴! He was a joint author with his boss in the second edition of HJ Plenderleith's *The conservation of antiquities and works of art*¹⁶. He had been thanked by Plenderleith in the first edition for his comments, but the second has been considerably rewritten.

In Ireland he had been elected a Member of the Royal Irish Academy in 1963, and received an Honorary Doctorate of Science (ScD) from his old University in 1971¹⁷. He provided encouragement and help when the Trinity College Library was setting up its Conservation Laboratory¹⁸. He continued to take an interest in the Laboratory and entered into correspondence with Tony Cains, the Director. Cains recommended Tony Werner to a correspondent who had sought the Laboratory's help; he could not help himself but thought that Tony Werner would be interested¹⁹. Though he was not directly responsible, it was his Laboratory in London that was responsible for the cleaning and restoration of the Ardagh Chalice and the Tara Brooch¹⁵. Every time he was in Dublin he looked into the Trinity chemistry department at coffee time; he was particularly friendly with Professor David Pepper, who had been in the department before Tony had left. Even when David retired, he still came in and he was delightful to entertain.

He had been elected a Fellow of the Society of Antiquaries of London in 1958. He played an influential part in the International Institute for Conservation of Historic and Artistic Works. He became a Fellow while in the National Gallery, and subsequently served, initially on its Council, as Hon Treasurer and then as President^{6,7}. He was prominent in the Museum's Association, becoming a Fellow in 1958 and President in 1967. While he was President he had a new boss; Sir John Wolfenden was appointed Director of the British Museum. This appointment disturbed the 'Museum world' and the Association passed a resolution critical of the appointment. As President, Tony signed a Press Release which objected to the appointment of his new boss. There is no evidence that relations between the two men suffered as a result!

Hawaii

In 1974, Tony was asked to provide a plan for the future conservation of material from the Pacific area. He suggested that a conservation laboratory be set up in Hawaii to deal with artefacts from the Pacific islands; he drew up a job description for its Head, and indicated that he might be interested himself. He was appointed Director in 1975 and took early retirement from the British Museum. However he did not relish the continual effort to obtain funding for the project. He retired in 1982. With one daughter in the UK and the other in Tasmania he was able to have two summers every year. He died on 21 January, 2008.

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The 2018 National Sustainability Summit will be held on the 31st January in the Citywest Hotel, Dublin. Firstly, thanks to everyone that made last year's event such a success. Over 1000 delegate gathered to hear from 80 speakers and network with over 50 exhibitors offering cutting edge technology and services.

This year we plan to expand the scope over the event with over 120 speakers. The speaker line up is drawn from senior management from the largest and most influential Irish and international companies who have delivered quantifiable eco results. Speakers come from areas such as pharmaceutical, food, aviation, retail, hospitality, food, construction, manufacturing, IT, logistics and supply chain and energy sectors will deliver compelling case studies that will help you create a sustainable business of your own or adapt your current business model.

Get ahead of your peers, and participate in the National Sustainability Summit for an engaging and thought-provoking event, which will stimulate debate and help you to make the correct decisions to improve sustainability and profitability.

Key topics will include:

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The day consists of a main stage with senior quality, environment and health and safety directors from Irelands largest companies in sectors such as construction, food, manufacturing, tech, transport etc. Furthermore an All-day seminar on ISO 9001, ISO 14001 & OHSAS 18001/ISO 45001 will also occur , giving you all the information required to comply with the new standards and how to get certification.

Key Topics on the day include

Education, Contamination Management, ISO, Quality Assurance, Compliance, Recall and Crisis Plans, , Traceability, audit and certification, Safety culture, cleaning and hygiene, legislation, product inspection, Enterprise Risk Management, Chemical Safety, Sustainability, environmental monitoring, health and safety, Energy reduction, waste reduction, rapid analysis, Risk Assessment and Management, Occupational hygiene, data management and analysis, Laboratory technology, protecting brand integrity, Managing supplier quality, Health Risk Assessment, Cleaning and Decontamination, Testing & Monitoring, , Standards, rapid analysis,

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The purpose of the event has a singular focus — Bring together 1000+ senior management from sectors such as Manufacturing, Food, IT, Retail, Hospitality and tourism, Utilities and energy, banking and Finance, Aviation, healthcare etc that have an interest in improving their business performance, productivity and cost performance.

Key delegates will include:

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The aim is to facilitate knowledge sharing, networking and the demonstration of lean, productivity and continuous improvement trends, technology and innovations.

The speaker line up is drawn from senior management from leading Irish and multinational companies that are leading the way in making their business more efficient and productive.

Key topics will include:

Business transformation, Waste reduction, change management. lean sigma, leadership and culture, continuous improvement, reducing downtime, Data/ IT, decreasing workplace footprint ,business excellence, production optimisation, sustainability, yield management, employee efficiency, process efficiency, quality management, skills and training, cost reduction, OEE, ERP, competitiveness, business intelligence, consumption reduction, inventory optimisation, manufacturing intelligence and much more

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Lake Region Manufacturing, Roche Ireland, Sanofi Aventis Ireland, Pinewood Laboratories, Clonmare Healthcare, Schwartz Pharma, Merit Medical and many more....

New approaches and technology have been introduced in recent years that have created significant organisational and process improvements. The aim of the conference is to showcase such innovative approaches and to disseminate the cutting edge research that underpins them.

The conference will be of interest to senior management, established practicing engineers and researchers together with those that are much earlier in their careers.

Delegates have registered from leading food, pharmaceutical, medical, chemical, electronics and engineering manufacturing sectors.

Manufacturing on this island of Ireland has some of the best people, products, brands and innovation. We deserve nothing less than the best business environment to chart a new economic course to growth. But government needs to set the climate and conditions to allow this to happen.

Manufacturers small and large from across the country will gather to challenge political decision makers to deliver a business environment which manufacturing deserves. Delegates attending the conference will:

- gain industry insights to help their business plan ahead
- share good practice and learn from each other's experience
- connected with senior business leaders to find new business opportunities
- meet with key technology providers in the dedicated exhibition area

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Almac Acquires BioClin Laboratories

Significant global expansion of existing analytical services

Almac Group, the global contract development and manufacturing organization, has acquired BioClin Laboratories, an independent and privately owned organization based in Athlone, Ireland.

Established in 2002 and located in Garrycastle, just two hours away from Almac Group's headquarters in Northern Ireland, BioClin is internationally recognized for providing expert analytical services including cGMP pharmaceutical and biopharmaceutical analysis, GMP microbiology testing and GLP bioanalysis. The company also boasts Ireland's leading GLP certified (INAB), cGMP certified (HPRA) and FDA registered contract laboratory.

BioClin's bespoke 14,000 square foot modern facility significantly increases Almac's analytical capacity and complements its existing business enabling strategic expansion and greater ability to serve clients' needs globally. The acquisition will see BioClin's analytical experts join Almac Sciences' network of almost 600 employees across multiple sites in Europe and North America.

Almac also recently completed significant expansion of its existing analytical facilities at its global headquarter site in Northern Ireland with the creation of a new, bespoke, MHRA approved laboratory.

News of this acquisition comes just days after announcing a multi-million pound expansion of Almac-owned, Arran Chemical Company, also based in Athlone, which substantially increased Almac's manufacturing capacity for fine chemicals, pharmaceutical intermediates and advanced building blocks.

"We are delighted to announce this acquisition demonstrating further commitment to strategic growth and development of our global business," said Stephen Barr, managing director, Almac Sciences. "Adding BioClin's highly complementary analytical capacity and technical expertise to our existing capabilities, we are able to broaden our service offerings and address our global clients' growing demands for a high quality, integrated, efficient service. We look forward to working with the BioClin team and plan to invest significantly in this facility."

Mary Burke, managing director, BioClin Laboratories, said, "We are very pleased to join Almac. With our shared values for outstanding quality, expertise and innovation we see this as an excellent strategic fit for BioClin enabling us to expand and deliver an enhanced range of analytical solutions to an international client market."

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Beckman Coulter Expands County Clare Facility; Creates 70 Jobs

December 19, 2017 (Lismeehan, County Clare) Beckman Coulter, which develops, manufactures and markets products that simplify, automate and innovate complex biomedical testing, is expanding the company's development and manufacturing facility at Lismeehan, County Clare, creating 70 jobs over the next two to three years.

The project is supported by the Irish Government through IDA Ireland.

The company's 9,700 sq. metre site at Lismeehan in County Clare is a strategic site for the global Beckman Coulter Diagnostics business, with 330 people working there. Development, manufacture and support of reagents (mixtures for use in chemical analysis) for clinical chemistry, immunochemistry and haematology product lines are currently carried out at the site.

The expansion will provide capacity for two new product streams at the Clare site, and will also provide for the ongoing growth of the current product streams.

The new expansion will add an additional 6,700 Sq. meters to the facility.

Planning permission has been granted for the new facilities by Clare County Council and construction is expected to commence in the first quarter of 2018.

Welcoming today's announcement, Minister of State for Employment and Small Business Pat Breen TD said: "Beckman Coulter's expansion is a great win for County Clare, the Irish Government and the IDA. As Minister for Employment I warmly welcome the creation of 70 additional jobs over the next two to three years. This is a great boost for Clare and the Mid West Region. This expansion now places Beckman Coulter to the forefront of the biomedical testing industry and the investment made by the company also allows for ongoing growth of current product streams."

Piers Devereux, VP of Operations for Beckman Coulter, said, "We are excited to build out our site here in County Clare. The caliber of the local workforce and the excellent support we receive from the community really sets this site apart. Our Ireland presence is essential for Beckman Coulter to achieve our vision of advancing healthcare for every person.

IDA CEO Martin Shanahan said: "This is very welcome news. Regional investment is a top priority for IDA Ireland. Supporting established companies to grow and add jobs is a key focus for us and this expansion, adding significant additional capacity to the Lismeehan site, will be of great benefit to County Clare the Mid West Region. It will also act as a strong reference seller for this regional location. It demonstrates substantial commitment by Beckman Coulter to the County Clare site. I wish the company every success with this new phase of development."

Recruitment for the new positions will commence immediately. Roles include scientist, engineering quality, manufacturing and other support functions. Interested applicants can apply via the Careers page on the Beckman Coulter website found at: <https://www.beckmancoulter.com/wsrportal/wsr/company/careers/overview/index.htm>

Beckman Coulter is an equal opportunity employer. We evaluate qualified applicants without regard to race, colour, national origin, religion, gender, age, marital status, disability, veteran status, sexual orientation, gender identity, or any other characteristic protected by law.

About Beckman Coulter

Beckman Coulter Diagnostics helps healthcare and laboratory professionals provide better patient care by delivering the accurate diagnostic information they need, when they need it. For over 80 years, Beckman Coulter has been the partner of choice for healthcare organizations. Our scalable instruments, comprehensive diagnostic tests and business management services are trusted by hospitals, laboratories and other critical care settings around the world. We share in our customers' mission toward continuous improvement and quality patient care because we believe when efficiency and clinical outcomes are improved, patients benefit and we can move healthcare forward for every person.

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€1.5m fund created for 20 academia-industry SFI research projects



The programme places academic researchers in companies and industry researchers in Irish Higher Education Institutes (HEIs).

This round of funding has seen applicants from various sectors, including aquaculture and medical care.

The 20 projects announced involve major multinationals and small Irish companies, in areas such as medicine and pharmaceuticals, materials science, data management, agriculture and aquaculture. Companies participating include AbbVie, Cellix Ltd, Genentech, Intel Ireland Ltd, Marine Harvest, Merck Millipore, Perkin Elmer, Pilot Photonics Ltd, Second Genome, Sigmoid Pharma and Tullow Oil.

One example of a projects that will see academia partnering with industry will be the team-up of Dr Eugene Mahon from University College Dublin (UCD) and Sigmoid Pharma to advance state-of-the-art oral drug delivery.

Meanwhile, Dr Nicola Piana Agostinetti from the Dublin Institute of Advanced Studies (DIAS) will partner with Tullow Oil on shallow crustal exploration using passive seismics, to bridge the gap between academic research and industrial-scale applications.

Speaking of the programme's success to-date, director general of the SFI said: "The SFI Industry Fellowship programme is of value to all companies, both large and small, and is key for strengthening the research ecosystem and encouraging the movement of talented people between academia and industry. I am delighted that we have funded 20 SFI industry Fellowships across diverse companies, and encourage more applications to the current call."

Colm Gorey

This article was originally published on www.siliconrepublic.com and can be found at:

<https://www.siliconrepublic.com/innovation/2015/06/18/fund-created-20-sfi-research-projects>

Wasdell Group to establish Pharmaceutical Packaging & Distribution Facility in Dundalk, creating 300 jobs over five years



November 27th 2017 – Dundalk

Minister of State for Employment and Small Business, Pat Breen TD today announced that UK speciality pharmaceutical services company Wasdell Group is to establish a pharmaceutical packaging, testing and distribution facility in Dundalk, creating 300 jobs over five years.

The project is supported by the Irish Government through IDA Ireland.

The privately owned British company's capability includes clinical trials packing, primary and secondary packaging and distribution of biopharmaceutical products. The company also offers contract manufacturing services with FDA and MHRA approved analytical and microbiology laboratories.

The new Dundalk facility will be the company's EU hub for qualified persons in (QP) release, analytical testing, primary and secondary pharmaceutical packaging and distribution.

Wasdell is to build a 70,000 sq. ft. greenfield facility on a c.2.88 hectare site at IDA's site in Mullagharlin, Dundalk, representing an investment of €30M.

Speaking at today's announcement, **Minister of State for Employment and Small Business, Pat Breen TD** said "Wasdell's decision to locate this new operation in Dundalk bringing 300 new jobs to the town is a great vote of confidence in what Ireland has to offer, especially in a regional location. The Government has been driving job creation in locations which are away from the bigger cities, and this new operation in Dundalk is a great vindication of that policy. It will provide additional facilities and services for our thriving pharmaceutical sector. This project builds on the tremendous success we have had, in bringing new foreign project to Dundalk which has helped transform the economic standing of the town over a relatively short period."

Martin Tedham, Wadell Group MD stated: “Due to the rate of growth we are experiencing and the ongoing requirement to maintain capacity, a site in Ireland will be a means to facilitate this as well as an exciting opportunity for the group and specifically the Wadell Packaging division. We have always had a strong customer base in Ireland and we are certain that this trend will continue with the impending Brexit situation as companies typically from the UK and USA look to securing a base to service their European markets.”

He also stated: “We have always been a business that changes to accommodate the needs of the market and its customer base. Having a facility in Ireland and the European market makes sense and we are very excited about this new opportunity as well as extending our geographical footprint.”

CEO of IDA Ireland, Martin Shanahan said: “Wadell’s decision to establish operations in Dundalk is great for the town, for County Louth and Ireland. The Border Region is a key target regional location for investment for us. The company will add to the growing cluster of life sciences companies in Ireland. The availability of this range of clinical and pharmaceutical services will increase the attractiveness of Ireland as an international base for early stage specialty Biopharma companies. It also an ideal example of the type of Brexit linked opportunity IDA is working hard to secure.”

Roles in Wadell’s new manufacturing plant in Dundalk will include: general management, QA/QC including QPs, production manager and supervisors, laboratory, engineering and maintenance, production operatives, warehouse, finance and administration, health & safety and human resources.

For more information on the new roles please email Jobs@wasdell.eu

About the company

Wadell Group is a privately owned speciality pharmaceutical services company headquartered in Swindon, England. It employs 800 staff in Swindon and in its operations in Burnley and Newcastle.

Established in 1971, the company is now one of the largest and most experienced contract primary and secondary packaging suppliers to the pharmaceutical and healthcare industry in Europe.

The company provides clinical trials packing, primary and secondary packaging and distribution of biopharmaceutical products. It also offers contract manufacturing services with FDA and MHRA approved analytical and microbiology laboratories.

NUI Galway to lead €5m project to turn waste into fuel



Image: Chokniti Khongchum/Shutterstock

With Ireland's target of 16pc renewable energy generation by 2020 in mind, newly appointed Prof Piet Lens and his team from NUI Galway are looking to microbial life to help make up the difference.

As part of a new €5m project funded by Science Foundation Ireland's (SFI) Research Professorship Programme, Lens will be looking to develop novel bioreactor concepts that will recover energy from waste and wastewater.

This will potentially add new biofuels to the Irish energy sector, particularly in the agricultural industry, where methane emissions from livestock are significant.

Right now, technology is being developed that can take waste products such as methane and use them to produce fuel and other valuable products, while reducing pathogen levels and greenhouse gas emissions.

In countries such as Germany and France, methane has already become an important energy source.

Contribute to green Irish economy

As part of his research, Lens will focus on finding new marine bacteria for potential energy generation, developing mathematical models for bioenergy production, creating new bioreactor configurations and then turning these ideas into a working product.

Lens will collaborate nationally with research teams in NUI Galway, the MaREI and Beacon research centres, and the Energy and Dairy Processing Technology Centres.

"Prof Lens is a world-leading researcher dedicated to developing novel bioprocesses for the recovery of resources such as energy, metals and nutrients from waste," said Prof Mark Ferguson, director general of the SFI.

"His work will contribute to the greening of our economy and Ireland's energy sector, and will support the implementation of a circular economy in Ireland through the invention and application of new technologies."

Lens said that he is "committed to contributing to further developments in this area, and to supporting a strong national and international network of academic and industrial partners linked to this university".

Colm Gorey

This article originally appeared on www.siliconrepublic.com and can be found at:
<https://www.siliconrepublic.com/machines/nui-galway-biofuels-research>

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7 Irish start-ups with science at their core. One of these is Nuritas

by Gordon Hunt



Dr Nora Khaldi, founder of Nuritas, speaking about being a scientist and entrepreneur at Inspirefest 2016.

Image: Conor McCabe Photography

Nuritas

Nuritas was founded by mathematician and bioinformatics expert Dr Nora Khaldi in 2014. Nuritas uses big-data techniques to sift through large amounts of data to discover peptides from food and food by-products, which provide unique solutions for the maintenance of health and wellness.

These benefits include: anti-inflammatory activity, antimicrobial activity, muscle recovery enhancement, anti-ageing solutions, and the potential management of blood sugar levels for type 2 diabetics and other glucose transportation related areas.

Nuritas uses proprietary search tools and artificial intelligence (AI) algorithms, including deep learning, to predict which novel food-derived bioactive peptides deliver specific, pre-determined effects. This cuts out many thousands of hours of trial and error.

Gordon Hunt is senior communications and context executive at NDRC. He previously worked as a journalist with Silicon Republic.

European Commission to Invest €30 Billion in Research and Innovation Over Next 3 Years

November 7th

The European Commission has announced how it will spend €30 billion of the EU research and innovation funding programme Horizon 2020 during 2018-2020, including €2.7 billion to kick-start a European Innovation Council. Horizon 2020, the EU's €77 billion research and innovation funding programme, supports scientific excellence in Europe and has contributed to high-profile scientific breakthroughs such as the discovery of [exoplanets](#) and [gravitational waves](#).

Over the next 3 years, the Commission will seek greater impact of its research funding by focusing on fewer, but critical topics such as migration, security, climate, clean energy and digital economy. Horizon 2020 will also be more geared towards boosting breakthrough, market-creating innovation.

Carlos Moedas, Commissioner for Research, Science and Innovation, said: "Artificial Intelligence, genetics, blockchain: science is at the core of today's most promising breakthrough innovations. Europe is a world leader in science and technology and will play a major role in driving innovation. The Commission is making a concerted effort – including with the European Innovation Council which takes its first steps today – to give Europe's many innovators a springboard to become world leading companies."

Supporting breakthrough, market-creating innovation

Since the beginning of its mandate, the Juncker Commission has been working hard to give Europe's many [innovative entrepreneurs](#) every opportunity to thrive. Now, the Commission is launching the first phase of the **European Innovation Council**. Between 2018 and 2020, the Commission will mobilise €2.7 billion from Horizon 2020 to support high-risk, high-gain innovation to create the markets of the future. Moreover, Horizon 2020 will make better use of its "crack the challenge" prizes to deliver breakthrough technology solutions to pressing problems faced by our citizens.

Focusing on political priorities

The 2018-2020 Work Programme will focus efforts on fewer topics with bigger budgets, directly supporting the [Commission's political priorities](#):

- **A low-carbon, climate resilient future:** €3.3 billion
- **Circular Economy:** €1 billion
- **Digitising and transforming European industry and services:** €1.7 billion
- **Security Union:** €1 billion
- **Migration:** €200 million

€2.2 billion will be earmarked for **clean energy** projects in four interrelated areas: renewables, energy efficient buildings, electro-mobility and storage solutions, including €200 million to support the [development and production in Europe of the next generation of electric batteries](#).

Boosting 'blue sky' research

At the same time, Horizon 2020 will continue to fund 'curiosity-driven science' (often referred to as 'blue sky science' or 'frontier research'). The annual [Work Programme of the European Research Council](#) for 2018, adopted in August, will enable support for excellent researchers with nearly €1.86 billion. Marie Skłodowska-Curie Actions,

which fund fellowships for researchers at all stages of their careers, receive a boost with €2.9 billion in total over three years.

Enhancing international cooperation

The new Work Programme also strengthens international cooperation in research and innovation. It will invest over €1 billion in **30 flagship initiatives** in areas of mutual benefit. Examples include working with Canada on personalised medicine, with the US, Japan, South Korea, Singapore and Australia on road transport automation, with India on water challenges and with African countries on food security and renewable energies.

Spreading excellence

Between 2018 and 2020, €460 million under Horizon 2020 will be allocated specifically to supporting Member States and associated countries that do not yet participate in the programme to their full potential. The aim is to tap into the unexploited pockets of excellence in Europe and beyond. In addition, the programme also continues to promote closer synergies with the [European Structural and Investment Funds](#).

Simplifying rules of participation further

Another novelty is the introduction of the **lump-sum pilot**, a new, simpler approach to providing financial support to participants. It will shift the focus of ex-ante controls from financial checks to the scientific-technical content of the projects.

Open Science

The programme marks a step change in promoting Open Science by shifting from publishing research results in scientific publications towards sharing knowledge sooner in the research process. €2 billion will be channelled to support Open Science, and €600 million will be dedicated to the **European Open Science Cloud**, European Data Infrastructure and High Performance Computing.

€77 Billion Budget

Horizon 2020 is the EU's biggest ever research and innovation framework programme with a budget of €77 billion over seven years (2014-2020). While most research and innovation activities are still underway or yet to start, the programme is delivering.

Horizon 2020 researchers have contributed to major discoveries like [exoplanets](#), the [Higgs boson](#) and [gravitational waves](#), and at least 19 Nobel Prize winners received EU research funding prior or after their award.

As of October 2017, Horizon 2020 has in total funded more than 15,000 grants to the tune of €26.65 billion, of which almost €3.79 billion went to SMEs. The programme has also provided companies, in particular SMEs, with access to risk finance worth over €17 million under the "InnovFin – EU finance for innovators" scheme. Furthermore, 3,143 ERC Principal Investigators in host organisations and 10,176 fellows under the Marie Skłodowska-Curie Actions have received grants worth almost €4.87 billion and €2.89 billion respectively.

Simultaneous to the adoption of the Horizon 2020 Work Programme 2018-2020, the Euratom Work Programme 2018 has been adopted, investing €32 million in research into the management and disposal of radioactive waste. It will also develop a research roadmap on safe decommissioning of nuclear power plants to reduce environmental impact and costs.

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European Investment Bank and DLL Confirm €200 Million Support For Irish Business Investment. December 6th



Pictured (from left to right) are: Fergal O'Mongain, country manager Ireland for DLL, and Andrew McDowell, EIB Vice President.

Companies across Ireland are expected to benefit from cheaper financing following a new €200 million initiative agreed by the European Investment Bank and DLL, a global vendor finance company and 100% subsidiary of Rabobank. The new scheme will strengthen leasing and financing for SMEs and mid-cap companies active in agri-business and the food industry, construction, transport and other sectors.

The scheme will be managed in Ireland by DLL Ireland DAC. It will be supported by a €100 million EIB loan with additional financing matched by DLL. This represents the largest EIB support for investment by Irish companies with a commercial financing partner for six years.

“The European Investment Bank is pleased to strengthen successful cooperation with DLL to support €200 million of new investment by Irish companies. Food, agri-business and construction companies across Ireland will be able to grasp new business opportunities and expand activity with the significant new financing being made available,” said Andrew McDowell, European Investment Bank Vice President.

“DLL is committed to financing Irish companies and has a global understanding of leasing and investment needs of smaller companies seeking to grow. Partnership with the EIB will both increase available finance and reduce the cost of leasing for DLL’s Irish customers,” said Fergal O'Mongain, Group Treasurer & Country Manager Ireland of DLL.

The new programme follows the successful roll out of DLL financing backed by €25 million, for climate impact projects, from the EIB earlier this year. The European Investment Bank is the world’s largest international public bank and last year the EIB Group provided a record €33 billion for SME financing that benefited of 300,000 companies worldwide.

New Precision Medicine Centre of Excellence Will Improve Patient Treatment



Alastair Hamilton (right), Invest NI, is pictured with (L–R) Professor Manuel Salto-Tellez and Professor James McElnay, Queen's University Belfast.

A £10 million Centre of Excellence in Precision Medicine has been launched by Invest Northern Ireland and Queen's University Belfast. The Centre of Excellence in Precision Medicine will develop an internationally accredited laboratory focusing on diagnostics which can be used to predict a cancer patients' response to treatment. This will allow potentially costly drugs to be used more effectively by being prescribed only to those that can benefit from them.

Invest NI's Chief Executive, Alastair Hamilton said: "This new Precision Medicine Centre will provide access to R&D facilities for both local and international companies. It has the potential to develop ground breaking treatments for cancer patients and will further enhance the personalised medicine and oncology research sector in Northern Ireland. While initially research will focus on cancer, this could extend into other areas of precision medicine in the future.

"Northern Ireland has a strong and internationally recognised Life & Health Sciences sector, which boasts globally renowned leaders including Almac and Randox. The Centre will contribute to the continued international recognition of Northern Ireland based research in this field.

"The Centre will also create 17 new high quality roles which will generate over £800,000 in annual salaries for the Northern Ireland economy."

The Centre will be located at the Centre of Cancer Research and Cell Biology at Queen's University. The 17 new roles will attract average salaries of £48,000.

Invest NI has offered £5.8million of support towards the £10million project.

Queen's University Belfast Acting President and Vice-Chancellor Professor James McElnay said: "Queen's University Belfast is at the forefront of Molecular Pathology, biomarker validation and test adoption in the UK. This Centre of Excellence brings a unique dimension to the bridging of academia and industry, making the fabric of our biotechnology sector in NI and the UK as a whole significantly stronger."

Climate Change Advisory Council Calls For Urgent New Measures to Reduce Carbon Emissions

December 7th

Ireland is not on track to meet its 2020 targets or to decarbonise its economy by 2050, according to the Climate Change Advisory Council's first Annual Review. "The actions in the current National Mitigation Plan do not put Ireland on a pathway to achieve our 2020 targets or our long term decarbonisation objective," said Chair of the Council, Professor John FitzGerald.

The Council's first Annual Review considered national greenhouse gas inventory data from 1990-2015. The Review states that if Ireland does not introduce major new policies and measures it will miss its 2020 targets and, on its current trajectory, will also miss the proposed 2030 EU target and the objective of reducing emissions of carbon dioxide by at least 80% by 2050. The provisional greenhouse gas emissions data released last week by the EPA show continued increases in emissions across the Irish economy in 2016.

The Council said that the pace and scale of greenhouse gas emissions reductions needed to be accelerated across all sectors of the Irish economy.

In the Annual Review, the Council is tasked with assessing Ireland's progress on the long-term low-carbon transition to 2050. While the Review found some progress had been made in the built environment and the energy sectors, Professor FitzGerald said: "Ireland is still over-reliant on fossil fuels. For example, Ireland has the third highest emissions per capita for residential energy use in the EU, reflecting high dependence on oil, coal and peat. This has significant implications for both greenhouse gas emissions and air quality, and it has significant negative impacts on health. A clear medium-term strategy to phase out fossil fuels in the electricity, transport and residential sectors is required."

"There is an urgent requirement for new policies and measures, and action beyond what is committed to in the National Mitigation Plan if Ireland is to reduce emissions by 2020 and to move onto a sustainable path to 2050 to tackle climate change," said Professor FitzGerald.

"These new measures should include a substantial increase in the carbon tax, and a phasing out of coal and peat for both residential heating and power generation. In particular, the subsidy for peat-fired electricity generation should be ended. In transport, investments in public transport fleets should avoid fossil fuel lock-in while overall capital investment should be rebalanced away from roads towards public transport," said Professor FitzGerald.

The Council said incentivising the take-up of electric vehicles over the coming decade will be vital in moving Ireland to a sustainable growth path and it recommended an assessment of the adequacy of the current electric vehicle charging network. Improved planning to minimise commuting in the future will also be crucial. The Council emphasised that the agriculture sector needed to urgently adopt and implement all cost-effective measures. The goal of carbon neutrality in the agriculture sector needs to be defined and policies put in place to achieve it.

The Council's Review of the emissions data shows that Ireland's greenhouse gas emissions increased by 3.7% in 2015, illustrating that Ireland's economy and emissions have not been decoupled, with emissions increasing across all key sectors.

The Council is an independent statutory body, established under the Climate Action and Low Carbon Development Act 2015. Its role is to review national climate policy and advise government on how Ireland can move to a low carbon, climate resilient economy and society by 2050.

The full report will be available for download at www.climatecouncil.ie.

Greater Skill Utilisation and Skilled Migration Needed to Boost Productivity in Ireland

December 8th



New research published by the ESRI finds that greater skill utilisation and skilled migration are required to support a productive and competitive economy. The research examines the difference between the skills possessed by employees and those required to do their job. The report also explores sources of future skilled labour supply, including Ireland's ability to attract high-skilled migrant workers.

Skills mismatch

- 46 per cent of full-time Irish employees report that their skills are greater than those required to do their job. This is the fourth highest rate of skill underutilisation out of 28 EU countries.
- Approximately 8 per cent of Irish employees state that their skill levels are below what is required to do their job. While this is much lower than the rate of skill underutilisation, it is still relatively high by European standards.
- Consequently, a relatively low number of Irish employees feel that their skills are matched to their job. The rate of "matched employment" in Ireland, at 46 percent, is the fourth lowest in the EU.
- By better aligning peoples' skills and their jobs, we could potentially boost economic growth.

Potential sources of future labour supply

- Ireland attracts high-skilled migrant workers. The share of highly-educated, foreign-born workers in Ireland is the third highest in the EU, at 57 per cent.
- People who are outside of the labour force – neither employed nor looking for work – are predominantly female, over 45 years of age with relatively low levels of education.
- The unemployed are predominately male and, relative to those outside the labour force, are younger and have higher levels of education.
- Only a very small proportion of those outside the labour force have some attachment to the labour market: being classified as either 'seeking work but not immediately available' or 'available for work but not seeking'. As such, the potential to increase the workforce from this group appears relatively weak. Therefore, as has been the case in recent decades, it is likely that immigration will represent an important source of skilled labour for Ireland in the future.

Paul Redmond, Research Officer, ESRI, stated: "Cultivating a skilled labour force is key to supporting a productive and competitive economy. As this analysis finds evidence of skill underutilisation in Ireland, policymakers must consider new approaches that harness the education and skills already acquired by workers."

PM Group Appoints a New Non-Executive Director December 13th



Michael McNicholas has been appointed as a Non-Executive Director of Project Management Holdings (PM Group), the Irish headquartered international project delivery specialists.



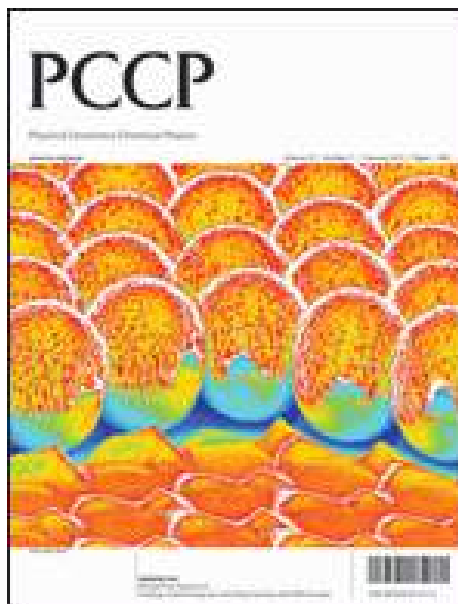
Michael McNicholas.

Michael has over 35 years' experience in senior leadership positions in the public and private sectors. He is the former CEO of Ervia, NTR plc and Managing Director of ESB International. During his career, Michael has led large complex organisations with operations in Ireland, the USA and across the world. He has significant experience in growing international businesses in the utilities, engineering and infrastructure sectors.

Announcing the appointment, PM Group Chairman, Dan Flinter said: "I am very pleased to welcome Michael to the PM Group board. Michael is a very high calibre addition to our board, bringing deep sectoral knowledge and expertise which I am confident will be invaluable in supporting the Group's future development, especially in international markets."

Michael is a Civil Engineering graduate from NUIG and holds an honorary fellowship from Engineers Ireland. He attended the Advanced Management Programme at Harvard, holds an IT qualification from Trinity College Dublin and is a recipient of the Alumni Award in Business and Engineering from the National University of Ireland, Galway. Michael is a member of the board of the Irish Management Institute (IMI) and is the Chair of the IMI Council.

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Publishing frequency: 48 per year

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Intel Goes 100% Renewable to Power 360-acre Leixlip Campus November 24th



Pictured at the Intel campus are Intel Ireland General Manager Eamonn Sinnott and ESB Chief Executive Pat O'Doherty.

Intel Ireland has announced that 100% of all electricity supplied to its Leixlip campus in 2016 was generated from indigenous renewable sources, making Intel one of the largest voluntary, private purchasers of renewable energy in the country. This action forms part of Intel Ireland's multi-faceted approach to reduce its impact on the environment and to support its commitment as a global energy sustainability champion.

Intel's 360-acre Leixlip campus is home to one of the world's most advanced manufacturing processes. Intel employs 4900 people in Ireland and has been operating here since 1989.

Since 2016, Intel Ireland has bought all of its power from its key supplier, Electric Ireland. Ireland is the first major Intel location outside of the U.S. to have bought 100% certifiable renewable electricity. Simultaneously, Intel has greened its energy supply in over a dozen major European facilities to 100%.

Speaking about the renewable energy purchase, Intel Ireland General Manager Eamonn Sinnott said: "We hope that our decision to go green will help to further stimulate the renewable energy market and encourage other businesses to follow suit. The more participation in the green power market and the more additional capacity that can come on stream will ultimately further help the environment and help to lower costs."

Electric Ireland is the retail arm of ESB, and ESB Chief Executive Pat O'Doherty was on hand today to welcome the announcement. "It is a genuine pleasure for ESB and Electric Ireland to partner with Intel – one of the world's leading companies – so that it can run its Leixlip plants entirely on renewable electricity. When ESB was founded 90 years ago, 100% of the energy we generated was renewable, harnessed from the River Shannon. As we face into the energy challenges of the coming decades, this provides us with inspiration to play a leading role in Ireland's transition to a low carbon future. The Electric Ireland agreement with Intel is an example of how we seek to place our customer at the centre of this low carbon future, powered by clean, reliable and affordable electricity."

Based on Electric Ireland data, Intel is the largest, voluntary, private purchaser of indigenous renewable energy in Ireland. Intel is also the largest voluntary green power purchaser in the United States for the past nine years, according to EPA data from the United States.

Climate Change a Key Priority For Irish Business November 23rd

Ireland's business community is forging ahead with innovations and actions in the area of climate change because it makes good business sense. Those who ignore the sustainability agenda will simply be left behind, according to Sustainable Nation Ireland the body that promotes Ireland as a hub for sustainable investment and business.

Responding to a new Climate Change Index which shows Ireland has slipped to 49th out of 56 ranked countries, Sustainable Nation CEO Stephen Nolan says that while more needs to be achieved, the Irish business community is playing a key role. "Businesses must, and will lead on climate change because quite simply it's the only direction of travel," said Nolan. "While it must be acknowledged that more needs to be done, from a business perspective, this is a key priority and the necessary changes are well underway."

He adds: "Embracing the sustainability agenda is not only good business, it's the responsible thing to do. Irish businesses – from the smallest startup, to SMEs and corporates, are heavily invested in helping to reach our climate change targets."

Sustainable Nation is a not-for-profit, working with both the public and private sectors. Its purpose is to stimulate greater investment into smart innovations, new enterprises and sustainable business practices. It is a platform for those working right across the low-carbon sector and capital markets to come together, understand each other – and ultimately do business together at a local and global level.

The body recently hosted a Dublin talk by Canadian Environment and Climate Change Minister Catherine McKenna, who is pressing for a complete phasing out of the production of fossil fuels such as coal.



Recent positive developments from an Irish business perspective include:

- Dublin's IFSC in October joined a UN-supported initiative called the 'Casablanca Declaration' which has created a cluster of green finance hubs that actively seek green investment opportunities. Over €28 billion in green financial activities including €11 billion in green bonds listed on the Irish Stock Exchange, is managed from, domiciled or listed in Ireland
- Microsoft has signed a 15-year power purchase agreement (PPA) with GE to purchase 100 percent of the wind energy from a 37-megawatt wind farm in County Kerry
- Kingspan has been named for the third year in a row on The Climate 'A List' by CDP, the international not-for-profit that measures the environmental impact of thousands of companies around the world. Kingspan is one of only two Irish companies to make the list of 112 companies, which includes Unilever, Microsoft, and Toyota
- Three Irish cleantech companies were finalists in the EU's recent marquee business competition Climatelaunchpad that promotes ideas and innovations to tackle climate change. They were SizeU, NuWardrobe and AquaRoot
- Tallaght-based HubControls was named in the global top 3 cleantech companies at a ceremony in London, organised by the Global Cleantech Cluster Association (GCCA)

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Purification by SFC or Prep-LC

Burning Solid Fuel is Biggest Threat to Good Air Quality in Ireland November 9th

The EPA's latest report on air quality shows that burning of solid fuel is the biggest threat to good air quality in Ireland, followed by emissions from vehicle exhausts. Despite monitored air quality being within EU limit values we face challenges in maintaining this position. And, at a number of locations, air quality failed to meet the World Health Organisation (WHO) guideline values for a range of pollutants including fine particulate matter, which pose risks to people's health.

The levels of particulate matter in our air is of growing concern, especially during the winter months when people's fuel choices can directly impact on our air quality and on our health, particularly in small towns and villages. The predominant source of fine particulate matter is from the burning of solid fuel. Also, in urban areas, we face potential exceedances of nitrogen dioxide limit values unless we reduce our dependence on the private motor car.

In recognition of these challenges to our air quality, the EPA has launched a new national ambient air quality monitoring programme. The programme will significantly increase the availability of localised real-time air quality information to enable the public to make informed decisions and better inform national and regional policymakers. The programme is built around three key pillars:

- A greatly expanded national monitoring network with 38 new automatic monitoring stations, providing enhanced real-time information to the public.
- Modelling and forecasting capability, to provide an ongoing air quality forecast to the public.
- Encouraging greater understanding and involvement of the public in air quality issues utilising citizen engagement and citizen science initiatives.

In launching the new programme, Laura Burke, Director General of the EPA, said: "Poor air quality is a major public health issue with approximately 1,500 premature deaths in Ireland in 2014 directly attributable to air pollution, mainly due to cardiopulmonary and respiratory health impacts from particulate matter. It has become increasingly clear that there are no safe level of pollutants and with this in mind, it is time to tackle the biggest issue impacting on air quality in Ireland – emissions from solid fuels in our small towns around the country. While the EU has introduced and implemented a range of legal instruments to improve air quality, these standards are still not in line with the tighter WHO air quality guidelines. The EPA again calls for movement towards the adoption of these stricter guidelines, especially for particulates and ozone, as legal and enforceable standards across Europe and in Ireland."

According to Patrick Kenny, EPA Air Quality Manager: "Ireland met all EU legal standards for air quality in 2016 at EPA monitoring stations but values for particulate matter (with the predominant source solid fuel burning), ozone, nitrogen dioxide and sulphur dioxide were above the WHO air quality guidelines at some of these stations. Polycyclic aromatic hydrocarbons (PAH), which originate from solid fuel and "back yard" burning were also above the European Environment Agency (EEA) reference level.

"A key part of the approach to tackling these issues is better engagement with the public on the topic of air quality. The first step in this process is improved access to air quality data and information. The National Ambient Air Quality Monitoring Programme (AAMP) will significantly improve the availability of localised real-time air quality information to enable the public to make informed decisions and better inform national and regional policymakers."

The National Ambient Air Quality Monitoring Programme 2017-2022 and the report Air Quality in Ireland 2016 – Key Indicators of Ambient Air Quality are available on the [EPA website](#).

The EPA continually monitors air quality across Ireland and provides the [air quality index for health](#) and [real-time results](#) on its website. Results are updated hourly on the website, and you can log on at any time to check whether the current air quality in your locality is good, fair or poor.

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Citizens' Assembly Issues Clarion Call For Government to Step Up Climate Action

November 7th



Following four days of presentations and deliberation, the Citizens' Assembly voted to make 13 recommendations for State action on climate change. The Stop Climate Chaos coalition described the the outcome as “a clarion call for the Government to immediately step up climate action.”

Oisín Coghlan, Director of Friends of the Earth, commented: “These common-sense, practical recommendations for climate action will not get us from laggard to leader. But they will allow us to catch up with our European neighbours. If implemented by Government they will end nearly a decade of dithering and delay.”

Niamh Garvey, Head of Policy and Advocacy at Trócaire, said: “Climate change is here, it is now, and it is everywhere. It's impacting most profoundly on those who have done least to cause it. For the communities that Trócaire works with, the impacts of climate change are already too much.”

Taken together, the 13 recommendations from the Citizens Assembly have the potential to ensure Ireland draws nearer to the European average for greenhouse gas emissions reductions.

The most striking recommendations to the Government from the Citizens' Assembly include:

- Prioritise public transport investment over new road infrastructure spending at a ratio of no less than 2-to-1. Currently the majority of state investment goes to road building which means more cars and more emissions.
- The Citizens' own willingness to pay higher taxes on carbon pollution and their recommendation that the agriculture sector should also apply the ‘polluter pays principle’ to its emissions, along with a further recommendation that the resulting revenue should be reinvested to support climate friendly agricultural practices.
- An end to State all subsidies for peat extraction on a phased basis over the next five years. That would bring peat-firing for electricity to an end a lot sooner than 2030, which is Bord Na Mona's current plan. An end to subsidies for peat extraction would cover not just the subsidies for burning peat for electricity but the subsidies for burning biomass with peat as well.
 - Establishment of an independent watchdog with clear powers to make sure the State sets and meets five-yearly targets for emissions reductions. The introduction of such targets were removed from climate legislation by the government before it passed in 2015.

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