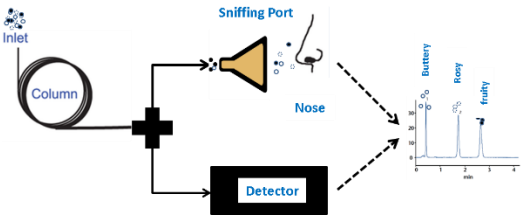
Irish Chemical News

The Journal of the Institute of Chemistry of Ireland

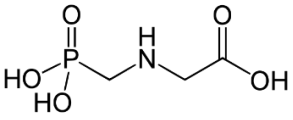
Feature Articles

New Elements

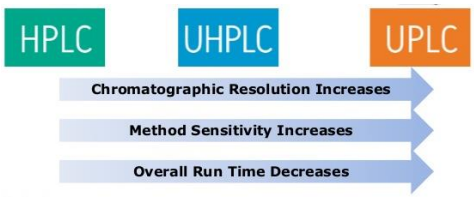
Food Flavours



Glyphosate



UPLC



Irish Chemical News

Originated 1922
Incorporated 1950

The Institute of Chemistry of Ireland

**PO Box 9322, Ravensdale Delivery Unit,
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Web: www.instituteofchemistry.org

Email: info@instituteofchemistry.org

The Professional Body for Chemists in Ireland

Contents:-

Note:

Opinions expressed in this Journal are those of the authors and not necessarily those of the Institute.

Again we thank our Sponsors:-

Sponsors of the Institute of Chemistry of Ireland Annual Dairy

School of Chemical and Pharmaceutical Sciences

A message from the President

Since the start of the last academic year and imminent start of the next, there have been a number of events that the Institute have supported over the last year: the Congress on the Topic of Food Chemistry (DIT), the 69th Irish Universities Chemistry Colloquium (DCU), along with presentations by Dr Imelda Shanahan winner of the 2016 Industrial Chemistry Award and Prof. John Sodeau winner of the Annual Chemistry Lecture Series Award (Eva Philbin) 2016. The Institute also sponsored Inorganic Ireland Symposium 2017 at RCSI in May.

In addition there has been a presentation by Prof. Henry Curren (NUIG), on receipt of the Boyle Higgins Gold Medal Award 2017 and we can look forward to this year's Annual Lecture Series (Eva Philbin) Award lecture by Prof Donal O'Shea from the RCSI this autumn. The 70th Irish Universities Chemistry Research Colloquium will be held in Queens University, Belfast in 2018. In addition the Eurachem General Assembly 2018 will take place in Dublin for the first time since 1997. To mark the occasion Eurachem Ireland in conjunction with the Eurachem Education and Training Working Group and the State Laboratory will hold an International Scientific Workshop on the topic of Data - Quality, Analysis and Integrity, in Dublin Castle on 14th -15th May. of interest to anyone interested in Quality Assurance. See Advances notice in this Issue.

I am looking forward to attending the EuCheMS meeting in Rome at the end of September where I will be lobbying for the EuCheMS Congress to be held in Dublin in 2022. I would like to wish everyone associated with the Institute the best in the coming academic year. Finally I wish to pay tribute to Pat Hobbs for his dedication in bring this edition of Irish Chemical News to Press.

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LENNOX

Editorial

Summer is over and this Issue of Irish Chemical News comes late. I had intended publishing it in late June but sufficient academic articles and papers were not available to publish it at that time. My objective is to accumulate a reserve of academic papers so I can announce a definite publication date for each Issue and avoid missing a publication date if a blip occurs. I have been working towards this objective throughout the year at the numerous chemistry events and especially during the Summer.

On the positive side this issue is very large, maybe too large. I aim for a smaller more frequent publication. In the last few months it has been demonstrated that the chemistry community in Ireland is very active. The Institute has hosted, sponsored and supported a great number of them. I start with our Congress on Food Chemistry, which covered a wide range of topics mentioned in the report and was a very stimulating and interesting. Inorganic Ireland 2017 was a very successful day with great representation from all over Ireland including a strong delegation from Queens University Belfast. Queen's will host next year's 70th Irish University Chemistry Research Colloquium. In June this year's Colloquium was hosted at DCU in its new format which was deemed a huge success.

From the industry side the big event was Irish Lab Awards 2017. I was honoured to be invited to be a judge for these awards and the standard of applicants was extremely high. These submissions really highlighted the dedicated work and high standards of scientists across the Irish science industry and research institutions. Many chemists were there competing amongst the best. I have covered the most chemistry relevant presentations in a report but there were other deserving winners as well. Not everyone could win in a category but that does not mean their standard was less, but judges have to make the call. I was also called on to present some of the winners with their plaques. The winners were announced at the gala awards luncheon on the afternoon of Thursday, May 25th at The Ballsbridge Hotel, Dublin, with hundreds of industry figures in attendance. This was a splendid affair with great lighting and sound effects. The event was hosted by BioPharmaChemical Ireland and Event Strategies who put on a great show.

From academia we have a paper from Prof Sean Corish on the new elements announced by IUPAC. Trinity Chemistry department has a new head. There is a paper on flavours in food and beverages from Teagasc Food Research Centre, Moorepark and Member of Sensory Food Network Ireland.

There is a good paper from a young undergraduategraduate chemist from AIT on UPLC: Validation for Assay a sensitive and accurate method of trace analysis. Next there is a set of articles originally published in EuCheMS Newsletter on Glyphosate. This is a controversial topic and here we have an informed European perspective. There is a short article on the Royal Irish Academy Young Chemist Prize winner, who went on to win the prestigious International Union of Pure and Applied Chemistry-Solvay International Award for Young Chemists, a second time for an Irish chemist.

The later sections cover an Enterprise report on Ireland champions of EU Research, a report by Carbon Trust on the US withdrawal from the Paris Agreement. Finally there are reports from Industry and Business magazine on various chemistry relevant topics.

Great work is being undertaken by chemists in Ireland, whether it is in industry, academia, services, and research institutions and I urge individual chemists to get involved with the Institute and consider writing a paper for ICN. Publicity for early career chemists through writing papers for ICN can only enhance your reputation amongst your peers.

Finally the closing date is approaching fast at the end of September for nominations for the Institute's Industrial Chemistry Award. From judging for the Irish Lab Awards I know there is the deserving talent out there so get your nominations in. See the conditions published in this Issue. **And** don't forget EuCheMS Chemistry Congress happens in Liverpool next August so plan to participate and highlight your good work.

Patrick Hobbs

Editor 31/8/2017

Congress 2017 Sponsors

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7th EuCheMS Chemistry Congress | LIVERPOOL UK 26–30 August 2018

7th EuCheMS Chemistry Congress

Molecular frontiers & global challenges

ACC LIVERPOOL, UK
26–30 August 2018

REGISTER YOUR INTEREST

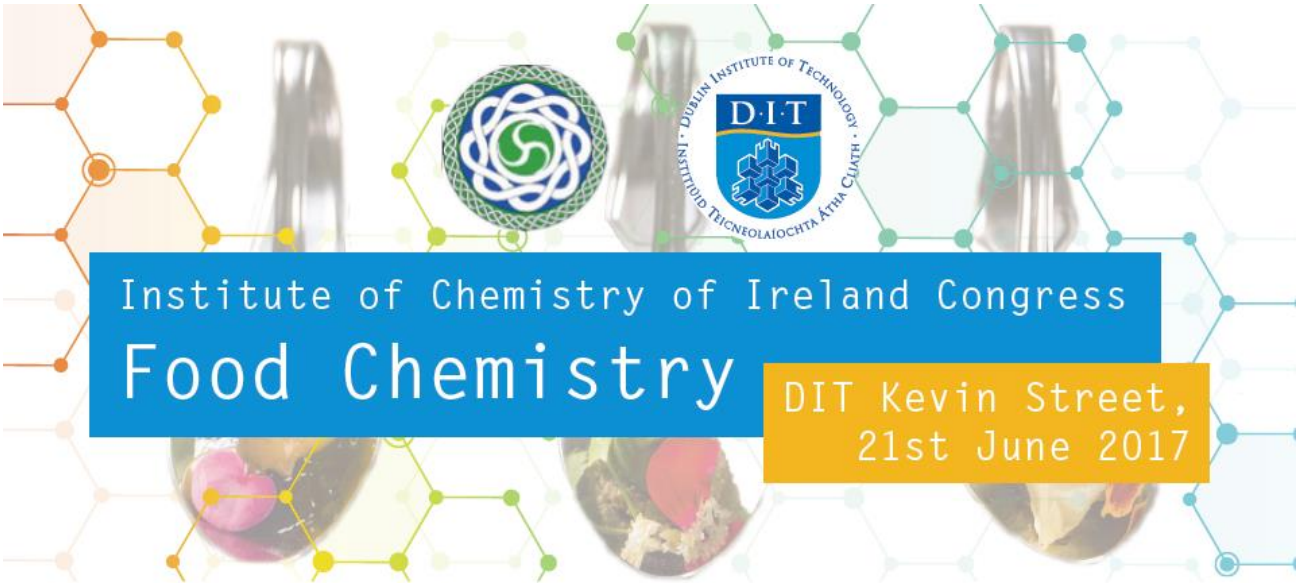
About the congress

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#



On June 21st we had a very interesting day on food chemistry covering many aspects of food chemistry. Prof John Cassidy DIT, Institute President opened the proceedings and Prof Declan McCormack welcomed delegates and did the introduction.

Speakers:-

Dr. John Keegan (Public Analyst's Laboratory, Dublin)
Dr. Amy Nagle (State Laboratory)
Prof. Vitaly Buckin(UCD)
Dr Jesus Frias (DIT)
Prof. Jean-Christophe Jacquier (UCD)
Prof. Herve This (Institut National de la Recherche Agronomique). Plenary Lecture
Prof. Seamus O'Mahony (UCC)
Mr. Tony McGorisk (Kerry Group)
Dr. Maria Hayes (TEAGASC)

The topics were wide ranging: The role of the Public Analyst Laboratories in food safety, detection of prohibited growth promotors in food producing animals, applications of ultrasonic spectroscopy in monitoring microstructural changes in food, kinetics in food, use of milk proteins to encapsulate food ingredients. An entering Plenary lecture from Prof Herve This on future synthetic food, from statgels to dynagels. Following on were lectures on controlling protein-protein interactions in development of next generation dairy ingredients. Next from the Kerry Group was functional ingredients with a focus on Wellmune® and why consumers are embracing functional food products. Finally in keeping with the Institutes interest in Green Chemistry and Sustainability a presentation from Teagasc on food chemistry for high value ingredient generation from waste food.

Posters

Y Dixit,,Maria P Casado, P Cama-Moncunill, Maria Markiewicz-Keszycka, P Cruise, Franklin Jacoby, P J Cullen, Carl Sullivan, Alan Doyle, Cormac K McElhinney, Rebecca Coughlan, Alex Lloyd, Steve meany, Catherine Barry-Ryan, A rettore, S O'Dea, R. Burke and C.barry-Ryan

Many thanks to the organising committee:-

Organising Committee: Prof. John Cassidy, Dr. Jesus Frias (DIT), Dr. Catherine Barry Ryan (DIT), Dr. Eoghan McGarrigle (UCD), Dr. Paula Bourke (DIT) and Dr. Julie Dunne (DIT) and DIT for hosting the Congress in Gleeson Hall..

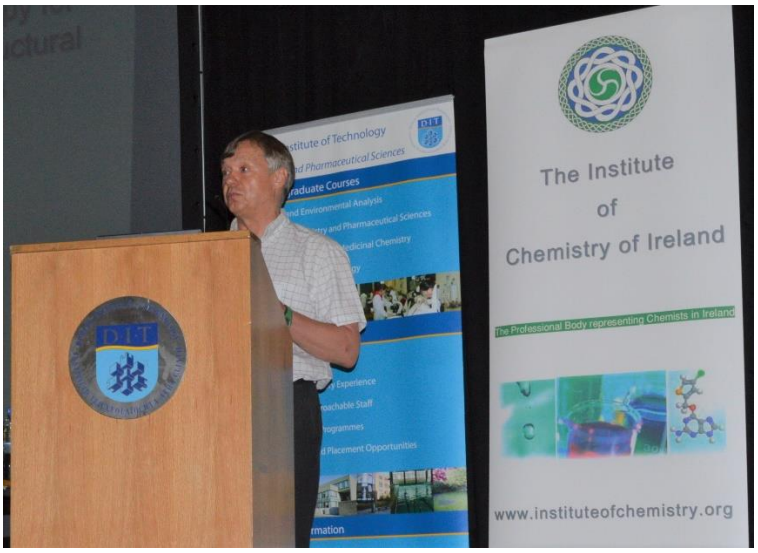
Congress 2017 Speakers

Prof John Cassidy, DIT, President Institute of Chemistry of Ireland Opens the Congress

Prof Declan McCormack, DIT, Head of Chemical & Pharmaceutical Sciences welcomed delegates

Dr John Keegan, Public Analyst's Lab, Treasurer ICI

Dr Amy Nagle, State Lab



Prof Vitally Buckin, UCD

Dr Jesus Frias UCD

Prof Jean-Christophe Jacquier

Prof Heve This, Institute National de la Recherche Argonomique

Prof Seamus O'Mahony

Mr Tony McGorisk, Kerry Group

Dr Maria Hayes, Teagasc

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Sinead Coleman Account Manager. Joe Walsh Chemistry Sales Manager

Poster Prizes

John Colleran, Secretary ROI Loal Section RSC to Rebecca Coughlan (left) and Chaitanya Sarangapani a Postgraduate researcher from DIT Cathal Brugha Street (right)

Some delegates during lunch break

EuCheMS European Chemical Sciences

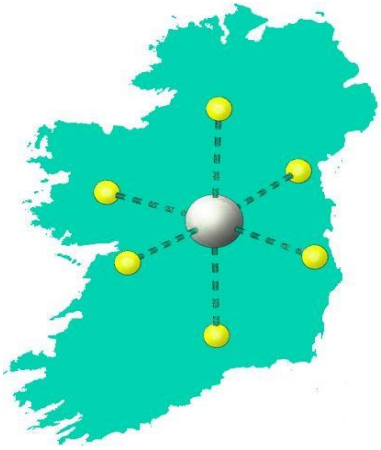
Dear chemists, dear all interested in impact of chemistry on our daily life,

You are kindly invited to read about recent chemistry and related news in the second 2017 issue of the Chemistry in Europe Newsletter at

http://www.euchems.eu/newsletters/chemistry-in-europe-2017-2/

Best Regards,
CiE Editorial Board

Inorganic Ireland Symposium 2017



Tuesday May 16 10:00-18:00

Albert Theatre in the

Royal College of Surgeons

Summary Report

The Institute of Chemistry of Ireland were delighted to co-sponsor the recent ***Inorganic Ireland*** symposium held on May 16, 2017 in the Albert Theatre at the Royal College of Surgeons in Ireland. The meeting is a biannual event designed to bring together all chemists in Ireland north and south who are working in the inorganic domain. Around 100 inorganic chemists from all corners of the island gathered in Dublin in May to enjoy plenary talks sponsored by the ICI and the RSC, together with a wealth of other speakers and poster presenters who showcased the breadth and complexity of current inorganic activity in Ireland. The meeting also served as the platform for the launch of the newly-formed Irish Biological Inorganic Chemistry Society (ICBICS).

Dr Malachy McCann opened the event with the **ICI David Brown Plenary Lecture** detailing his work on the use of phenanthroline complexes to combat different types of infection. This was followed by six lectures and three flash presentations which continued along the theme of Medicinal Inorganic Chemistry with topics ranging from copper and silver anti-bacterial agents to mechanistic studies of anti-cancer metallodrugs.

The meeting then moved to concentrate on Energy and Catalysis with seven diverse talks on topics such as heterogeneous and homogeneous catalytic routes in sustainable processes, production of solar fuels and use of ionic liquids in removing mercury from natural oil and gas.

In a final session on Materials the participants were treated to nine talks and three flash presentations on magnetic materials, ionic liquids and continuous flow methods in synthesis before the closing plenary talk on New Breakthroughs in Layered Double Hydroxide Chemistry, delivered by Professor Dermot O'Hare from the University of Oxford who gave the **RSC Tilden Award Lecture**.

The meeting was augmented by a lively poster session over the lunchbreak where 48 early stage researchers from across the island showcased their work and competed for the four poster prizes which went to Adriana Magherusan (TCD), Tadgh McGivern (RSCI), Rana Sanii (UL) and Ryan O'Gara (UCD).

A highlight of the meeting was the lively discussion enjoyed by all during the refreshment breaks, the poster session and the reception. It was agreed that the next meeting in this very successful series would take place in the last quarter of 2018.

Dr Grace Morgan
UCD

Welcome delivered by Professor Celine Marmion

We are delighted to welcome you to the Inorganic Ireland Symposium 2017.

This Symposium is a continuation of a long tradition, started as the so-called "Greystones" weekend meetings instigated by Prof. David Brown after the ICCC meeting which he organised in Dublin in 1974. The Greystones series was hosted by Prof. Malachy McCann in Maynooth University every three years until 2005, before being re-launched as a one-day event to be held approximately every two years. Recent meetings have been held in Trinity College Dublin (2008), Queen's University Belfast (2010), NUI Galway (2012) and RCSI (2014). In 2014 we introduced the David Brown Award Lecture as part of the series and this year the Award is sponsored by the Institute of Chemistry in Ireland. We are delighted that Prof. McCann is the 2017 recipient, in recognition of his many contributions to Inorganic Chemistry in Ireland over his career, not least to this meeting series.

This year the Symposium will constitute one of the Royal Society of Chemistry Dalton Regional meetings for the first time and we gratefully acknowledge the support of the RSC, both Dalton Division and the ROI Local Section. We are pleased to welcome Prof. Dermot O'Hare, RSC Tilden Award winner to give his Plenary Lecture as part of the Dalton Regional Meeting.

We are very grateful to all our sponsors, RSC, ICI, Scientific Instruments Ireland (SII), RCSI and UCD, without their support this event could not take place.

We thank you all for your support of this meeting and for the many interesting and diverse abstracts which have been submitted. We hope you will enjoy sampling current themes in inorganic chemistry in Ireland through the many oral and poster presentations, and ensuing discussions.

The organising committee

Celine Marmion
Grace Morgan
Aidan McDonald
Mark Muldoon

Sponsors

Below is the programme which illustrates nicely the depth and breadth of inorganic chemistry being conducted across the island of Ireland.

	09.50	Welcome, introductory remarks	Celine Marmion
MEDICINAL	10.00	**Malachy McCann** *David Brown Award Lecture (ICI)* Phenanthroline Complexes Carnival in Rio	Kevin Nolan John Cassidy
	10.35	**Matthias Tacke** Coinage Metal NHC Complexes as Novel Antibiotics and Anticancer Drugs	Bernie Creaven
	10.50	**Luca Ronconi** Gold: not just jewelry…	
	11.05	**Leila Tabrizi, Tadgh McGivern**	Short Talks 1-2 (5min each)
	11.15	**Celine Marmion** Innovative Metallodrug Chemotypes and their Therapeutic Potential	
	11.30	**Diego Montagner** A Cu(II) Complex Targeting the Translocator Protein: *in Vitro* and *in Vivo* Antitumor Potential and Mechanistic Insights	
	11.45	**Andrew Reddy, Louise MacLean, Muhib Ahmed**	Flashes 1–3 (2min each)
	11.55	**Launch of the Irish Biological Inorganic Chemistry Society (IBICS)**	
ENERGY AND CATALYSIS	13.00	**James Sullivan** Heterogeneous Catalysis in Biorefining Processes	Aidan McDonald
	13.15	**Max Garcia-Melchor** Rhodium Complexes Promoting C-O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species	
	13.30	**Ulla Gro Nielsen** Competitive reactions during the synthesis of layered double hydroxides	
	13.45	**Mark Muldoon** Mechanistic Elucidation of Wacker-Type Oxidations of Alkenes using Cationic Pd(II) Complexes and Hydrogen Peroxide as the Oxidant	
	14:00	**Pau Farràs** Production of Solar Fuels by Organic Assisted Water Splitting	
	14:15	**Davide Tiana** A Comprehensive Study on Engineering the Optical Response in Metal-Organic Frameworks	
	14:30	**John Holbrey** Using Ionic Liquids to Manage Mercury in the Oil and Gas Industry	
MATERIALS	15.15	**Constantina Papatriantafyllopoulou** High Nuclearity Cross-Shaped and Multiple-Decker Metal Clusters with Interesting Magnetic Properties	Bob Baker
	15.30	**Tony Keene** A Bridge Too Far: Testing the Limits of Polypyridyl Ligands in Bridging Solution-stable Subunits of a Coordination Polymer	
	15.45	**Matteo Lusi, Deborah Crawford**	Short Talks 3-4 (5min each)
	15.55	**Peter Dunne** Continuous-Flow Hydrothermal Synthesis of Inorganic Nanomaterials	
	16.10	**Peter Nockemann** Synthesis of Polynuclear Metal Clusters in Carboxylate Ionic Liquids	
	16.25	**Chris Hawes, Min Ying**	Short Talks 5-6 (5min each)
	16.35	**Małgorzata Swadźba-Kwaśny** Ionic Liquids with Tricoordinate Borenium Cations: Lewis Superacids	
	16.50	**Rachel Whiteside, Olan Cleary, Colm Healy**	Flashes 4-6 (2min each)
	16:55	Short Break	
	17:00	**Dermot O'Hare RSC Tilden Award Lecture** New Breakthroughs in Layered Double Hydroxide Chemistry	Grace Morgan

Dr Malachy McCann receives the David Brown Prize from ICI President Prof John Cassidy, DIT

Prof Dermot O¹Hare, University of Oxford, UK - RSC Tilden Award Lecture 'New Breakthroughs in Layered Double Hydroxide Chemistry' shown here to the right with Dr Malachy McCann (recipient of the ICI David Brown Award Lecture)

Aidan McDonald (TCD), Celine Marmion (RCSI), Grace Morgan (UCD), Mark Muldoon (QUB)

Prof Kevin Nolan (RCSI) introducing the ICI David Brown Award Lecture

Dr Bernie Creaven (ITT)

Adriana Magherusan TCD, Tadgh McGivern RCSI, Rana Sanii UL, Dr Robert Baker TCD, Dr Mark Muldoon QUB and Dr Aidan McDonald TCD

Dr Malgorzata Swadzba-Kwasny (QUB)

Dr Tony Keene (UCD)

Delegates in the Albert Theatre

Refreshments at Reception after the lectures

Networking & socialising after the lectures

Dalton Division Council
of the Royal Society of Chemistry
The RSC Republic of Ireland
Local Section

Institute of Chemistry of Ireland

Scientific Instruments Ireland

The Royal College of Surgeons in Ireland

University College Dublin

Eurachem Ireland A Focus for Analytical Chemistry in Europe

Eurachem Ireland is an organisation for people working in chemistry in Ireland, with a focus on analytical chemistry. Chemistry students are welcome too. Eurachem Ireland promotes the objectives of Eurachem (www.eurachem.org) in Ireland including good quality practices. To learn more about Eurachem's current activities, please click here Eurachem Activities. Other objectives of Eurachem Ireland include, but are not limited to:

- **Facilitate networking among Irish analytical chemistry laboratories from the public sector, private sector and education sector;**
- **Provide a forum for the discussion of common issues;**
- **Encourage Irish participation in Eurachem working groups;**
- **Increase awareness of opportunities for organisations to participate in research;**
- **Contribute to the development of chemistry students to meet the needs of Irish employers.**
-

Autumn Event

Eurachem Ireland are hosting a one-day workshop entitled "Hyphenated Analytical Techniques - Fundamentals, Applications and Challenges". The workshop will have a particular emphasis on LC-MS, ICP-MS and GC-Ms and will be delivered by experts working in the relevant areas in Ireland. It takes place Thursday 19th October 2017 in the Backweston Laboratory Campus, Celbridge, Co. Kildare.

Check back here for updates at www.statelab.ie/eurachem.html

You can become involved in Eurachem Ireland by:

1. **Joining the mailing list to stay informed of the activities of Eurachem Ireland. Email eurachem@statelab.ie to request to join the mailing list. Information will also be available on www.statelab.ie/eurachem.html.**
2. **Joining the Linkedin group 'Eurachem Ireland' to stay informed of Eurachem and Eurachem Ireland activities.**
3. **Emailing your suggestions for Eurachem Ireland activities to a member of the Eurachem Ireland Committee.**

Eurachem's technical activity is carried out by its various Working Groups. Working groups activities typically involve:

- **Producing Technical guidance**
- **Initiating or contributing to international workshops and other events**

Irish members of Eurachem Working Groups:
Please click here for reports of working group meetings attended by Irish Representatives.

69th Irish Universities Chemistry Research Colloquium 2017

The School of Chemical Sciences hosted the **69th Irish Universities Chemistry Research Colloquium** on the 21st and 22nd June this year. This annual conference is run under the auspices of the Institute of Chemistry of Ireland, ICI, and brings together postgraduate researchers in chemistry from across the island of Ireland. The format of the meeting was changed from previous years in order to try to foster a stronger community spirit amongst our national chemistry postgraduate students.

There were over 180 registered delegates at this meeting and it was deemed a huge success. Exceptionally high quality presentations were given with representation from all around the country. There were 19 oral presentations and 11 flash presentations from postgraduate students, as well as 49 poster presentations.

Exciting plenary sessions were given by Prof Nicholas Farrell (University of Virginia), Prof. Henry Curran (NUIG), Prof. Fiona Regan (DCU) and Prof. Patrick Guiry (UCD). These talks served to open up sessions related to bioinorganic chemistry, energy, organic chemistry and environmental and analytical science.

Prizes for oral presentations were awarded to Eolann Kitteringham, RCSI (Eli Lilly presentation award), Aoife Lucid, TCD (Eli Lilly runner-up presentation award), Mark Kelada, NUIM, (Eli Lilly flash presentation award) and Killian Stokes (UL) (Microscopy Society of Ireland award).

Three poster prizes were sponsored by Evonik, in association with the European Young Chemist Network, EYCN, and these were awarded to Vuslat Buk (UCC), Aisling Dunne (DCU) and Daria Firsova (NUIG).

Following a very interactive poster session, sponsored by BOC Gases, on the first evening, there was the *Biotage AB and Life Scientific BBQ* in a local watering hole (The Whitworth) to encourage the continuation of the great scientific conversations, and to unwind and socialise. Other sponsors included Fluorochem, Advion, Labquip and Merck Life Science.

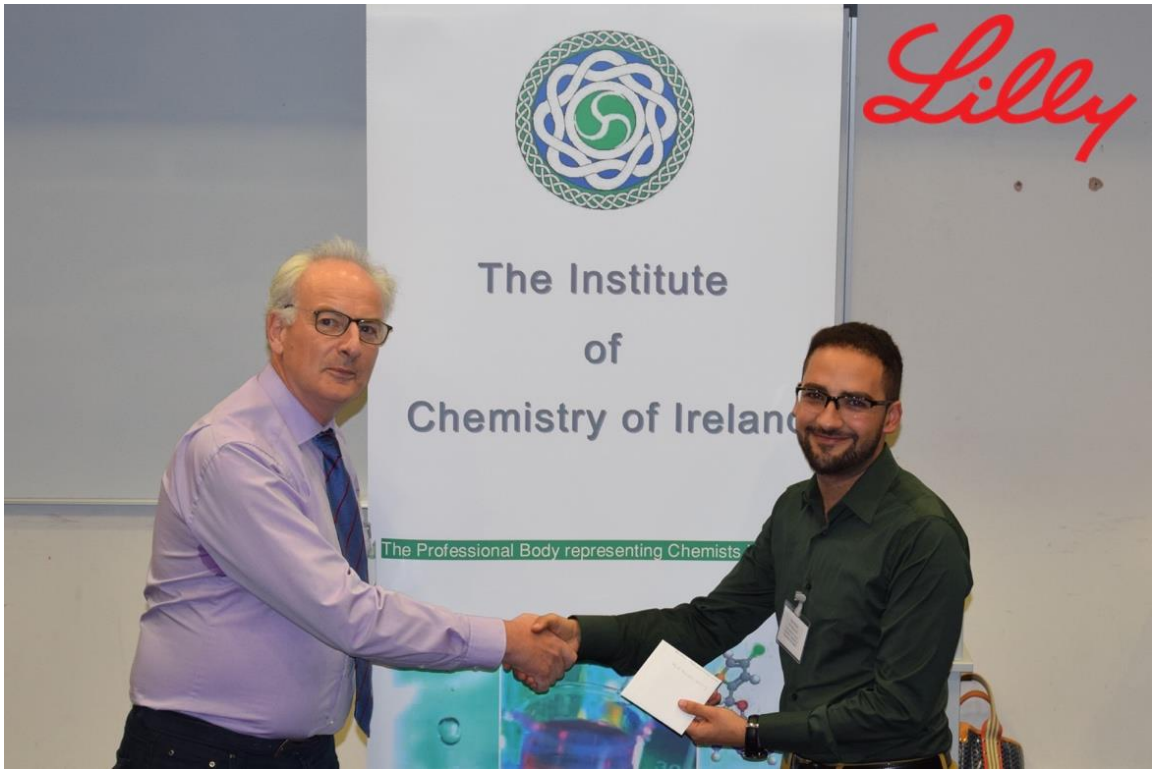
Certainly a memorable Colloquium. Best of luck to Queens University who are hosting the 70th meeting in this series next year.

Report compiled by

Aoife Morrin
School of Chemical Sciences

National Centre for Sensor Research
Dublin City University

Images from the Prize Giving Ceremony:



Mark Kelada, recipient of the Eli Lilly Award for Best Flash Presentation

Presented by Dr Brian Murray, IT Tallaght, former President ICI and Council Member

Eolann Kitteringham, RCSI, recipient of the Eli Lilly Award for Best Presentation, and Aoife Morrin, DCU

Aisling Dunne (DCU), Vuslat Buk (UCC), recipients of Evonik Poster Prize, and Mark Kelada (NUIM)

Killian Stokes (UL), recipient of the Microscopy Society of Ireland Award, with Sarah Martyn

PHARMA INDUSTRY AWARDS 2017

in association with

KUEHNE+NAGEL

The Pharma Industry Awards 2017 will take place on the

5th of October 2017 in the Clayton Hotel, Burlington Road, Dublin

Closing date for entries is 20 July 2017
Check out our website for easy to follow entry details: www.pharmaawards.ie

Since launching in 2014, the Pharma Industry Awards has established itself as the benchmark for excellence for those operating in Ireland's pharma industry. The Awards recognise and celebrate the most original and innovative individuals and companies demonstrating excellence in the Irish pharma industry over the past 12 months.

Business River

We wish all entrants
the best of luck with their entries

The Irish Laboratory Awards 2017

The Irish Laboratory Gala Luncheon Awards 2017 took place on the 25th of May 2017 in the Ballsbridge Hotel,

WELCOME
The Institute of Chemistry Ireland
As Trade Media Partners

Congratulations to The Irish Laboratory Awards 2017 winners!

The winners were announced at the gala awards luncheon on the afternoon of Thursday, May 25th at The Ballsbridge Hotel, Dublin, with hundreds of industry figures in attendance.

21 trophies were awarded to very worthy winners of the Irish Laboratory Awards 2017 at the gala awards luncheon on May 25th at The Ballsbridge Hotel, Dublin.

Conor O'Brien, President of the Irish Science Teachers Association presents the Chemical Laboratory of the Year award to Prof. Gavin Walker, Bernal Process Engineering Lab - Bernal Institute, University of Limerick.

Matt Moran, Director, BioPharmaChem Ireland presents the Bio Science Laboratory of the Year award to the Macular Pigment Research Group – WIT Team.

Patrick Hobbs, Editor of Irish Chemical News and Former President at Institute of Chemistry of Ireland presents the Calibration or Testing Laboratory of the Year award to the Anecto Team.

Dr Julie Naughton, Irish Research Staff Association presents the Research Laboratory of the Year award to the Tissue Engineering Research Group - RCSI Team.

Patrick Hobbs, Editor of Irish Chemical News and Former President at Institute of Chemistry of Ireland presents the Laboratory Supplier of the Year award to Bryan Tobin, Susan Phelan and Laura Daly, Roche Diagnostics Ireland.

Irene Regan, President, Academy of Clinical Science & Laboratory Medicine presents the Innovation of the Year Award to Dr. Shourjya Sanyal, Think Biosolution.

Virginia Walls, Communications & Admin Officer, Molecular Medicine Ireland presents the Laboratory Team of the Year award to the Jazz Pharmaceuticals Team.

Irene Regan, President, Academy of Clinical Science & Laboratory Medicine presents the Laboratory Scientist of the Year award to Prof. Catherine Stanton, Moorepark Food Research Centre, Teagasc Fermoy.

Virginia Walls, Communications & Admin Officer, Molecular Medicine Ireland, presents the Laboratory Staff Member of the Year award to Ollie Burns, Nokia Bell Labs.

Dr. Joe McPartlin, Director of Trinity Biobank presents the Pharmaceutical Laboratory of the Year award to Prof. Gavin Walker, Bernal Process Engineering Lab - Bernal Institute, University of Limerick.

Conor O'Brien, President of the Irish Science Teachers Association presents the Healthcare Laboratory of the Year award to the Diet & Microbes at the Extremes of Life, Research Laboratory Team.

Matt Moran, Director, BioPharmaChem Ireland presents the Commercial Laboratory of the Year award to the Vision I Food Research Laboratory - Teagasc Fermoy Team.

Matt Moran, Director, BioPharmaChem Ireland presents the Food Laboratory of the Year to Dr. Grace O'Callaghan, Vision I Food Research Laboratory - Teagasc Fermoy.

The New Elements - are we nearly there yet?

John Corish

School of Chemistry, Trinity College, University of Dublin, Dublin 2, Ireland.

John Corish studied in University College Dublin and taught at the University of Western Ontario and at UCD before moving to Trinity College Dublin in 1983. He is a Fellow Emeritus and former Professor of Physical Chemistry at Trinity. He has been Head of its School of Chemistry, Dean of the Faculty of Science, Bursar of the College and was the College's first Dean of Research. His research interests are in theoretical and experimental aspects of matter transport in the solid state and he was co-inventor of the world's first commercial nicotine transdermal patch. He is a member of the Royal Irish Academy since 1986 and has served as Vice-President, International Secretary and was Treasurer of the Academy from 2008 to 2013. He has been Chairman of the Commission for High Temperatures and Refractory Materials in IUPAC, President of the IUPAC Inorganic Chemistry Division, Treasurer of the Union from 2008 to 2015 and currently chairs its Finance Committee. He has been Treasurer of the Institute of Chemistry of Ireland, its President in 1990 -1992 and received its Boyle Higgins Gold Medal in 2009.

Making new elements

Very exceptionally four new elements were formally inaugurated this year by the President of IUPAC, Professor Natalia Tarasova, and added to the periodic table at ceremonies held in Moscow and Tokyo. In the beautiful and ornate Hall of Science of the Russian Academy of Sciences in Moscow on March 2nd the elements with Atomic numbers 115, 117 and 118 were named as moscovium (Mc), tenessine (Ts) and oganesson (Og), respectively, while the ceremony in Tokyo on March 14th naming the element with atomic number 113 as nihonium (Nh) was honoured by the attendance of the crown prince of Japan. These names had been first announced by IUPAC on November 28th 2016. As is evident from the IUPAC periodic table (Fig. 1 below), the first seven periods have now been completed, one hundred and eighteen elements in all, and this has naturally given rise to questions as to whether any more superheavy elements are likely to be made by the chemists and physicists who work in the facilities around the world dedicated to this field of endeavour. Plotting the total number of the known elements as a function of their time of discovery expressed in calendar years shows that elements have been added to the list in an approximately linear progression at an average rate of one element per 2.55years [1] though not always, of course, in sequence.

New superheavy elements are now made in special facilities with the principle of the method followed in producing them being quite easy to understand [2]. The atoms of two elements with a total number of protons equal to the atomic number of the new element required, or perhaps equal to the number of protons which following a radioactive decay might equal that number, are caused to collide together in the hope that they will fuse and result in the formation of the new nucleus. For two nuclei to fuse in such a collision the need to overcome the electrostatic repulsion between the positive charges in the nuclei obviously requires the use of very high energies. Carrying out such a process in practice is therefore difficult and requires powerful linear accelerators or cyclotrons to accelerate and energise the projectiles. In the very great majority of cases the colliding atoms do not fuse or coalesce because the strong repulsive forces between the protons dominate the attractive forces that bind a nucleus and the atoms simply fly apart again rather than combining as was the objective of the experiment. And on the rare occasions when a new nucleus is formed the next problem is to separate the single atom that has been produced from all the unreacted atoms and

other unwanted products that can emerge and direct it to a suitable detector. The new nucleus will disintegrate into a cascade of lighter elements which makes it possible to prove what it is that has been produced by detecting and recording the chain of decays that it emits and comparing this with known chains. Finally, these processes occur extremely quickly with new nuclei typically having half-lives of the order of milli- or even micro-seconds. All of this means that the production and detection of new elements is a very difficult technical problem requiring expensive major dedicated facilities both for the syntheses and for the prior production of feedstocks of projectiles and targets used in the experiments.

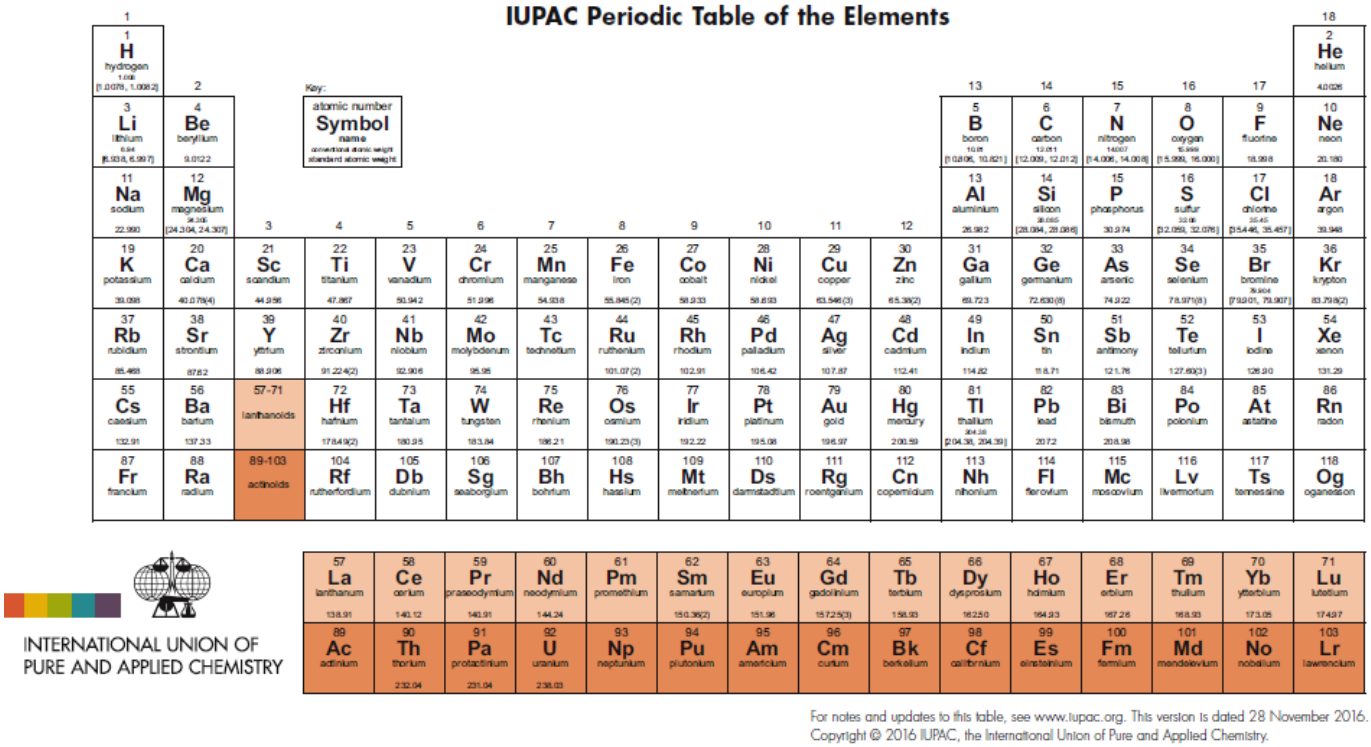


Fig. 1 IUPAC Copyright © 2016 Periodic Table of the elements reproduced with permission.

Priority and Naming of New Elements

Because of the great general interest in new elements and the considerable international kudos that the discovery of an element generates coupled with the accompanying right to propose a name for it there has been keen competition between the laboratories that have the facilities to undertake the procedures required. Prior to 1992 laboratories sometimes named a new element that they claimed to have discovered without reference to the international scientific community. This led to existence of considerable confusion and uncertainty that is sometimes referred to as the ‘transfermium wars’. For example, elements 104 and 105 were kurchatovium and neilsbohrium to the Russians but rutherfordium and hahnium to the Americans. This situation was resolved only in 1997 [3] when the names rutherfordium and dubnium were assigned by IUPAC to these two elements, respectively, together with names for seven other elements; in all numbers 101 to 109. Also about this time new standard procedures for assigning priority for its discovery and subsequently naming a new element were accepted and put in place. The criteria for discovery used had been developed by the 1991-1993 IUPAC/IUPAP Transfermium Working Group [4-6] and the complete procedure used to assign priority and name new elements has been recently described in detail [7]. Briefly the priority for discovery is assigned by a joint IUPAC/IUPAP working group (JWG) that collects and

examines all the documentation that has been published in support of the discovery claims. The Technical Report of the JWG is published in Pure and Applied Chemistry after rigorous refereeing and must be also approved by the Unions. The laboratory or laboratories to which priority has been assigned is then invited to propose a name and symbol to the IUPAC Division of Inorganic Chemistry, Division II. The name should comply with guidelines as laid down in 2002 [8] and recently revised and extended [9]. If the name and symbol are deemed suitable and approved by Division II they are published as a IUPAC Recommendation [10]. As such, the Recommendation must undergo extensive expert refereeing and, in addition, is subject to a five-month period of public review before the Recommendation can be formally approved by the IUPAC Council. The four elements formally inaugurated this year went through these procedures and all the names comply with the traditional guidelines.

Element 113

The discovery of element 113 was assigned to the RIKEN Nishina Centre for Accelerator-Based Science in Japan [11]. It is the first element to be discovered in Asia and the name **nihonium** with symbol **Nh**, one of the two ways to say 'Japan' in Japanese was chosen to make a connection to the nation where it was discovered.

Elements 115 & 117

The JWG assigned the discovery of elements 115 and 117 to a collaboration organised by Professor Yuri T. Oganessian between the Joint Institute for Nuclear Research (JINR) Dubna (Russia), Oak Ridge National Laboratory (USA) and Lawrence Livermore National Laboratory (USA) and the discovery of element 118 to a collaboration between Dubna and Livermore [12]. The name **moscovium** (symbol **Mc**) was proposed for element **115** to recognise the Moscow region and the ancient Russian land in which the JINR is located. The elements to make these elements were carried out with the heavy ion accelerator facilities at the Flerov Laboratory of Nuclear Reactions and the Dubna Gas-Filled Recoil Separator both at JINR. The name **Tennessine** (symbol **Ts**) for element **117** recognises the contribution of Oak Ridge National Laboratory, Vanderbilt University and the University of Knoxville, all in the state of Tennessee, to superheavy element research. Unique actinoid materials from Oakridge, produced and separated in Tessessee, have been used in the discovery and/or confirmation of nine superheavy elements.

Element 118

The name **oganesson** (symbol **Og**) was proposed by the collaborating teams for element **118** to honour Yuri T. Oganessian, born 1933, for his lifelong contributions to trans-actinoid elements research. It is only the second element ever to be named after a living scientist: in 1997 element 106 was named after Glenn T. Seaborg [3]. Included in Professor Oganessian's many achievements are the discovery of superheavy elements together with a range of notable valuable advances in the understanding of the nuclear physics of superheavy elements particularly in the experimental evidence for the concept of the 'island of stability'. The island of stability in this part of the periodic table has been recently discussed by Greiner [13].

On a personal level Oganessian possesses a remarkable ability to persuade scientists from around the world to work constructively together as is witnessed by the different locations of the laboratories credited with recent discoveries of new elements. In fact, despite its highly competitive aspect research collaboration in this area provides a wonderful example of the international nature and power of science and has been maintained very effectively even through the most difficult periods of the cold war. The technical difficulties of the work and the expense of producing the specialised isotopes necessary for the syntheses

have meant that the successes achieved to date would not have been possible without international collaboration and good will.

Prospects for the Future

The completion of the seventh period of the periodic table naturally raises the question as to whether the chemists and physicists working in the field are now likely to synthesise any further new elements? On the day following the inauguration of three of the four newest elements in Moscow Professor Oganessian chaired a symposium at JINR at Dubna. This was dedicated to remaining problems in the field of superheavy elements and was attended by experts from all the laboratories in the world engaged in this type of research. The many contributions and animated discussions during the sessions clearly signalled that the subject is very much alive and well. Professor Paul J. Karol, who has chaired the recent JWGs that assigned priorities for discoveries, has earlier this year listed six attempts [1] that have already been made, two at Dubna and four at GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt in Germany, to synthesise elements in period eight of the periodic table. None of these have been able to report success at a level that would satisfy the criteria for discovery of a new element. But the work goes on at many centres and the search is destined to be intensified in the years to come. In terms of facilities, in addition to those already referred to there are currently accelerators at the University of Jyväskylä, Finland, the K-130, and at Caen in France, the Grand Accélérateur National d'Ions Lourds (GANIL) where new facilities will open in the near future. GSI is also scheduled to be capable soon of producing substantially increased beam intensities. A major facility to produce rare isotope beams using a linear accelerator is under construction at Michigan State University in the United States and will become operational in 2022. At Dubna a new Superheavy Element Factory is already partly constructed with the magnet of the cyclotron now in place. It is designed to produce a beam that will be ten times more intense than that of the current U400 cyclotron at the site. This will be coupled with a new separator which is anticipated to be twice as efficient as that currently in use and the hope is that elements 119 and 120 may be synthesised within the next two to four years. The improvements in the facilities are considered sufficient to compensate for the lessening of the rate of production of new nuclei that will occur due to the necessity to replace the beam composed of calcium-48 that has been used for the recent syntheses with one of titanium-50. The facility at RIKEN has also been upgraded and the team there will in future utilise a five-fold increase in beam intensity and a new gas-filled separator. The very substantial investments evident in all these advances clearly indicate the importance attached by the responsible governments and funding agencies to achieving progress in our understanding of the fundamental principles governing the formation and stabilities of new nuclei. They also signal confidence that the efforts will be successful and signal challenging but exciting times ahead for those working in the field.

Another question that naturally arises as the exploration of new elements moves into the next period of the Table is whether new 'islands of stability', analogous to the island that has been vindicated in the discoveries of the more recent elements, which exhibit increased lifetimes although these do remain brief, can be expected to be encountered? If they do exist for the atoms of higher atomic numbers is it possible to predict where they may occur? First it is necessary to consider the stability of the nucleus as even further protons and neutrons are added. The early classical liquid drop model of the nucleus, which predicted a maximum cut-off atomic number of 110, has of course long been discarded. The protons and neutrons in nuclei are now thought to occupy 'shells', analogous to the orbiting electrons, with additional stabilities being realised when shells close thereby introducing the possibility of double 'magic' numbers. This stability can be sufficient to prevent the very high probabilities of fission and alpha decay endemic in large nuclei and give stable nuclei. Attempting to extrapolate to any large extent beyond the current island of stability is, however, obviously asking a great deal particularly because there are suggestions that changes in

nuclear shape and size can have very major effects on the expectations. Notwithstanding these uncertainties, a predicted island of stability stands at a distant Z = 164. Turning now to the electrons, relativistic considerations become increasingly important and are to be seen in several different ways in attempts that have been made to predict the appearance of an extended Periodic Table. The most straightforward of these, the Mendeleev-Seabourg construction [14] follows on in a regular fashion with the 8s, 5g, 6f, 7d and 8p blocks completing the 8^{th} row at Z = 168. Alternative predictions with different ordering of the electron orbital energies have been made by Frick et al. [15], Fricke and Soff [16] and Pyykkö [17]. This ordering is rendered a very difficult task because of its sensitivity to the introduction of relativistic considerations which are not yet clearly defined.

A separate but related and very intriguing question about the behaviour of electrons in these heavy atoms and one to which answers have already being sought for some of the more recently discovered elements at the JINR concerns whether their chemical properties continue to follow the classical periodicity. A collaborative group from the Paul Scherrer Institute, Villigen, Switzerland working with colleagues at Dubna has used the beam there to produce superheavy elements in sufficiently large amounts and with sufficiently long half-lives to investigate some of their chemical properties. The questions being asked in the experiments are whether copernicium is a homologue of mercury which is directly above it in group 12 and similarly for flerovium and lead in group 14. Relativistic effects become more important as the charge of the nucleus is increased and Oganessian proposes that if relativistic effects are sufficiently pronounced heavier elements may no longer follow the trends of their period. For example, is oganesson, element 118 at the end of period 7, a noble gas or not? If it is found to be reactive rather than inert then we will have already seen the end of periodicity. The results to hand for copernicium and flerovium show that relativistic effects are indeed having the anticipated influence. The improved facilities at Dubna should make it possible to produce element 118 in sufficient quantities in the near future to allow its reactivity to be tested experimentally and if it is found not to be inert, as is indicated by current trends, then this will signal that the superheavy elements do not fit the pattern of periodicity so beloved of chemists through the years.

Despite the attainment of the completed seventh period in the Mendeleev periodic table the investment in and commitment to the search for new elements remains as international and as strong as ever. It is also noteworthy that the Presidents of IUPAC and IUPAP late last year set terms of reference for and put in place an expert Joint Working Party to examine the criteria used to assign priority for the discovery of new elements. Twenty-five years had elapsed since the criteria currently used were agreed and the announcements of November last provided a natural opportunity to review these criteria to take account of experimental and theoretical advances made during those years. The Joint Working Party will report soon and the scientific community will then be set up to process new claims that will certainly emerge for the continued growth in the number of elements in this small exclusive group of unique substances.

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IUPAC Periodic Table of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H hydrogen [1.0078, 1.0082]																	2 He helium 4.0026
3 Li lithium [6.938, 6.997]	4 Be beryllium 9.0122											5 B boron [10.806, 10.821]	6 C carbon [12.009, 12.012]	7 N nitrogen [14.006, 14.008]	8 O oxygen [15.999, 16.000]	9 F fluorine 18.998	10 Ne neon 20.180
11 Na sodium 22.990	12 Mg magnesium [24.304, 24.307]											13 Al aluminium 26.982	14 Si silicon [28.084, 28.086]	15 P phosphorus 30.974	16 S sulfur [32.059, 32.076]	17 Cl chlorine [35.446, 35.457]	18 Ar argon 39.948
19 K potassium 39.098	20 Ca calcium 40.078(4)	21 Sc scandium 44.956	22 Ti titanium 47.867	23 V vanadium 50.942	24 Cr chromium 51.996	25 Mn manganese 54.938	26 Fe iron 55.845(2)	27 Co cobalt 58.933	28 Ni nickel 58.693	29 Cu copper 63.546(3)	30 Zn zinc 65.38(2)	31 Ga gallium 69.723	32 Ge germanium 72.630(8)	33 As arsenic 74.922	34 Se selenium 78.971(8)	35 Br bromine [79.901, 79.907]	36 Kr krypton 83.798(2)
37 Rb rubidium 85.468	38 Sr strontium 87.62	39 Y yttrium 88.906	40 Zr zirconium 91.224(2)	41 Nb niobium 92.906	42 Mo molybdenum 95.95	43 Tc technetium	44 Ru ruthenium 101.07(2)	45 Rh rhodium 102.91	46 Pd palladium 106.42	47 Ag silver 107.87	48 Cd cadmium 112.41	49 In indium 114.82	50 Sn tin 118.71	51 Sb antimony 121.76	52 Te tellurium 127.60(3)	53 I iodine 126.90	54 Xe xenon 131.29
55 Cs caesium 132.91	56 Ba barium 137.33	57-71 lanthanoids	72 Hf hafnium 178.49(2)	73 Ta tantalum 180.95	74 W tungsten 183.84	75 Re rhenium 186.21	76 Os osmium 190.23(3)	77 Ir iridium 192.22	78 Pt platinum 195.08	79 Au gold 196.97	80 Hg mercury 200.59	81 Tl thallium [204.38, 204.39]	82 Pb lead 207.2	83 Bi bismuth 208.98	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Key: atomic number **Symbol** name (conventional atomic weight / standard atomic weight)

57 La lanthanum 138.91	58 Ce cerium 140.12	59 Pr praseodymium 140.91	60 Nd neodymium 144.24	61 Pm promethium	62 Sm samarium 150.36(2)	63 Eu europium 151.96	64 Gd gadolinium 157.25(3)	65 Tb terbium 158.93	66 Dy dysprosium 162.50	67 Ho holmium 164.93	68 Er erbium 167.26	69 Tm thulium 168.93	70 Yb ytterbium 173.05	71 Lu lutetium 174.97
89 Ac actinium	90 Th thorium 232.04	91 Pa protactinium 231.04	92 U uranium 238.03	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

For notes and updates to this table, see www.iupac.org. This version is dated 28 November 2016.

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

School of Chemistry
Faculty of Engineering, Mathematics and Science

Professor Mike Lyons, New Head of School of Chemistry, Trinity College Dublin.

Mike Lyons is Professor in Physical Chemistry and SFI Principal Investigator in the School of Chemistry, Principal Investigator in the CRANN Research Institute, and an Investigator in the AMBER National Research Centre, Trinity College Dublin, Ireland. Professor Lyons is Head of the School of Chemistry TCD (first term: 2017-2020).

Born in Cork city (1956) he was educated in CBC Cork and is a graduate of University College Cork (1979) where he read Chemistry and Mathematical Physics. He obtained his Ph.D degree from the same University in 1983 under the supervision of the late Prof. Declan Burke in metal oxide electrochemistry. He worked with the late Prof. John Albery FRS and Prof. Brian Steele at Imperial College London on metal oxide electrocatalysis before being appointed to a lectureship in Physical Chemistry at Trinity College Dublin in 1984. Mike was elected to Fellowship, Trinity College Dublin in 1992 on the basis of publication and research. His research interests encompass Physical & Analytical Electrochemistry and in a publication output of 2 books and more than 130 peer reviewed papers he has made significant contributions to electrode kinetics, metal oxide electrocatalysis, electrochemical water splitting, electroactive polymer electrochemistry, electrochemical sensors and the mathematical modelling of electrochemical systems.

His H-index is 36 and current research interests include the development of metal oxide nanomaterials for the catalysis of electrochemical water splitting and as electrodes in electrochemical fuel cells. He also leads the TCD activity in Raw Materials within the EIT Raw Materials KIC, a multinational EU funded initiative involving industry, research institutes and academia. In this capacity he currently coordinates a major industry focused up scaling project and is Academic Director of the NEAT Materials PhD Programme. Mike has lectured extensively in UK, Europe, US, Latin America, Pakistan, India, Australia and New Zealand.

Mike Lyons has served both on the University Academic Council and the Governing Body (Board) of Trinity College, and has been Director of Undergraduate Teaching & Learning and Head of Physical Materials & Computational Chemistry within the School of Chemistry. He was Director of Science of Materials for some years. Prof. Lyons is a member of the International Editorial Board of the Journal of Solid State Electrochemistry and Current Opinion in Electrochemistry and co- editor of the International Journal of Electrochemical Science. He served as Project co-ordinator for the EU/LA ALFA Project Materials Engineering for the Design of Intelligent Sensors (Project MEDIS) with partners located in Universities in Belgium, France, Brazil, Argentina and Uruguay. He was the Conference Chair of the very successful Electrochem 2012 meeting which was held in TCD 2-4th September 2012 and co-edited a special issue of the journal Physical Chemistry Chemical Physics arising from the Electrochem Conference. He was guest editor for a special issue of the journal Sensors dealing with Ultramicroelectrodes: Fundamentals & Applications. He also hosted the first IFOSTER (The Irish Forum for Sustainable Trade, Treatment, Exploitation & Exploration of Raw Materials) conference entitled ‘Sustainable raw materials for a high quality future’.

In his spare time Mike follows Irish & Munster Rugby (although he will on occasion cheer on Leinster) and Cork Hurling. He enjoys classical music and escapist movies, and is an avid reader of history and popular science books.

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Agriculture and Food Development Authority

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Research Review

Searching for volatiles that characterise the flavour of foods and beverages.

By Dr Kieran Kilcawley

Principal Research Officer, Food Quality and Sensory Science, Teagasc Food Research Centre, Moorepark and Member of Sensory Food Network Ireland.

Sensory analysis is the ultimate measure of product quality and success and comprises a variety of powerful and sensitive tools (affective, effective and descriptive) to measure human responses to products. Sensory analysis has been defined as a scientific procedure used to evoke, measure, analyse and interpret responses to products as perceived by sight, smell, touch, taste and hearing. Incorporation of flavour chemistry into sensory science provides a mechanism in which a compound or compounds directly responsible for products sensory characteristics can be determined. Such information is invaluable in product development, product quality, brand identity, but also in finding the source of taints, off-flavours and for shelf life studies. Flavour chemistry often acquires large data sets as the volatile profiles of various products are complex and therefore in order to maximise data interpretation multivariate statistical analysis such as chemometrics are required.

The flavour chemistry facility at Teagasc Food Research Centre, Moorepark was established 10 years ago to aid our understanding of the volatile and non-volatile compounds that influence the flavour of food and beverages and to offer support to industry; particularly with respect to product matching, volatile profiling, identification of taints of off-flavours, and shelf life stability amongst others. The non-volatile components investigated mainly include acids and carbohydrates however the main focus of the flavour chemistry facility involves the extraction, concentration, identification and quantification of a wide range of volatiles (acids, ketones, aldehydes, esters, thiols, lactones, hydrocarbons, terpenes, phenols, sulphur compounds, etc.). The flavour chemistry facility is an integral component of Sensory Food Network Ireland which was established to bring all the sensory expertise on the island of Ireland under one umbrella to promote sensory science, enhance existing expertise and capability, garner funding and to support industry and to provide a platform to support and train future sensory scientists. The network comprises 10 leading institutions from Ireland with expertise in sensory science. These partners include Agri-Food and Biosciences Institute; University College Dublin; Teagasc; Dublin Institute of Technology; College of Agriculture, Food and Rural Enterprise; St Angela's College, Sligo; Galway-Mayo Institute of Technology; University of Ulster and Limerick Institute of Technology.

Sensory Food Network Ireland also supports the food and beverage industry in the areas of new product development and enhancing understanding of consumer behaviour within specific market segments.

Membership of Sensory Food Network Ireland is open to any company or organisation with an interest in sensory science. Find out more at www.sensoryfoodnetworkireland.ie

The research group at Moorepark, have worked primarily on dairy products (milk, cheese, whey, butter, yoghurts & various dairy powders), but as part of wider internal and external research collaborations have also been involved investigating the flavour of chocolate, beef (raw and cooked), lamb, salami, vegetables, fruit, cereals, kefir, fish, whiskey and are developing databases of compounds for each product type. Our aim is to continually expand our capability and expertise and a major part of this is to ensure that we are up to date with latest developments and have state of the art equipment. We already have an array of advanced gas chromatographic mass spectrometry systems, which mainly consist of single and triple quadrupole mass spectrometers and these provide the backbone of most of our research on volatile compounds. Each of these systems is set up differently in terms of automated extraction/concentration systems and column polarity. Recently I won a Science Foundation Ireland (SFI) infrastructure grant for a gas chromatography by gas chromatography time of flight mass spectrometer (GCxGC TOF-MS), which enables us to separate individual components in two dimensions, and enhances acquisition rates. This instruments enhances sensitivity of detection, but also the increases resolving powder which makes it easier to identify individual components from complex mixtures which is a common problem in foods.

A key part of volatile research is to extract and concentrate volatiles as despite huge advances in mass spectrometry technology the human nose remains more sensitive. Numerous automated techniques exist to do this but all have inherent bias mainly due to the materials used to trap, absorb or adsorb the volatiles, the surface area available, and the time and temperature of the extraction. Therefore we spend a significant part of our research efforts investigating and optimising extraction and concentration methods for individual products. We mainly utilise four different extraction techniques; solid phase micro extraction (SPME), In tube extraction (ITEX), thermal desorption (TD) and sorptive extraction (SE). By far the most widely used technique internationally is SPME which can be performed by direct immersion or as a headspace technique. The popularity of this technique is due its automation, reproducibility and the considerable choice of different trapping materials available. However, it has limitations due to a low interfacial surface area (although this has recently been addressed by the new SPME Arrow technology), passive volatile adsorption/absorption and fibre swelling when used as a direct immersion technique. In Tube Extraction (ITEX) is effectively a dynamic version of SPME but designed as a more automated version of an earlier technique called purge and trap. In theory it has a much greater concentration capacity than SPME but is more difficult to optimise as the number of factors influencing the extraction are greater. To date ITEX has been used in the wine industry and is likely to garner more interest in other foods and beverages as it easily automated but the range of trapping materials currently available is limited. Another technique widely used in Moorepark is thermal desorption. This is also a dynamic technique with the widest range of trapping materials available. This is the technique of choice for air monitoring but has found increased use in the food industry as it has a much greater trapping capacity and can provide much greater control of the extraction and concentration process than most techniques. Although it has limitations in terms of moisture control, and works much better in products with low moisture it is especially useful in the analysis of powders. SE is a relatively new technique and can be used as direct immersion technique or as a headspace technique. An advantage of SE is its high adsorption capacity and the minimal risk of thermal degradation of volatiles because the extraction does not require high temperatures; however there are currently limited trapping materials available with polydimethylsiloxane (PDMS) the main choice. Currently SE is only partially automated which reduces the number of samples than be analysed in comparison to other extraction systems.

We also use gas chromatography-olfactometry (GC-O) to directly identify the most odour active compounds in products but also to try and identify the key impact volatiles most influencing sensory perception. As stated earlier the human nose remains the most sensitive detector and in GC-O trained panellists are used identify and provide odour activity values to individual or co-eluted compounds (peaks) in a chromatogram from volatiles extracted from the product. This approach can be used in association with or as a replacement for descriptive sensory analysis. Various methodologies exist in GC-O but currently in Moorepark we utilise a detection frequency approach as it's relatively less time consuming and requires less training than some other methods. We also utilise gas chromatography flame ionization detection (GC FID). FID is the most commonly used detector in GC analysis mainly because of its relative low-cost, long-term reliability and

universal applicability for compounds with carbon-hydrogen bonds in their chemical structure. It remains the technique of choice for fatty acid analysis, but is still widely used in the quantification of volatile flavour compounds. Another very useful detector for flavour research is the pulsed flame photometric detector (PFPD) which is more selective and sensitive for sulphur compounds, and is low-cost and easy-to-use. Even though at high concentrations sulphur compounds are often perceived as off-flavours, they remain very important volatile compounds contributing to the flavour of many food products at low concentrations.

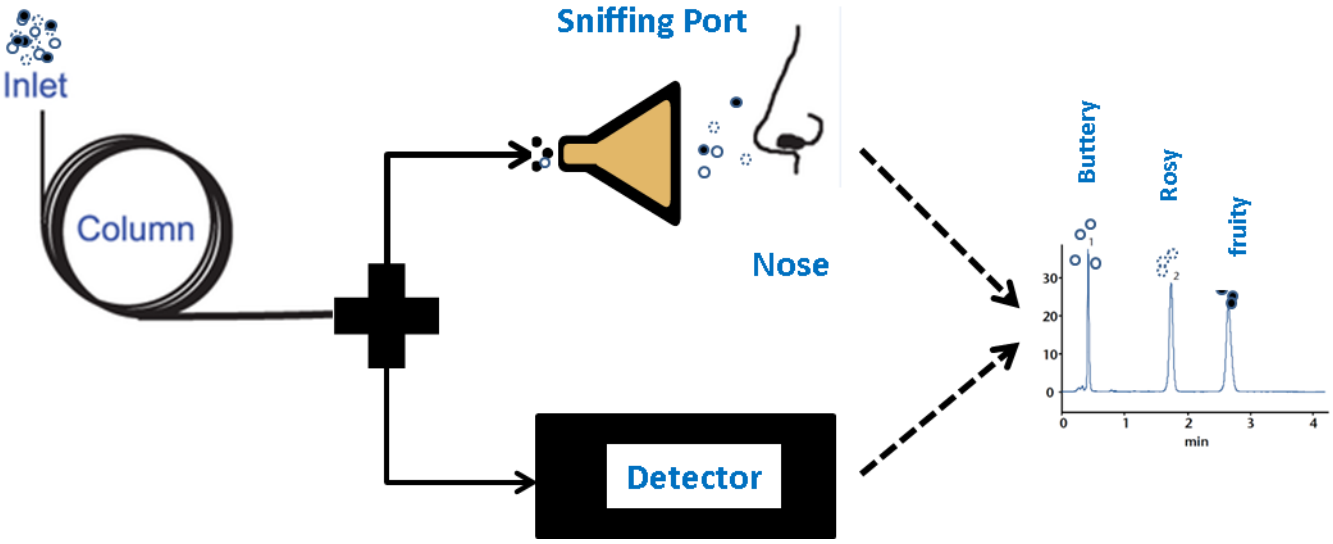

Figure One: Gas Chromatography Olfactormetry

Another integral part of our work is data processing. In relation to mass spectral analysis our approach is atypical in that we are not in general doing targeted analysis but rather untargeted analysis where we are scanning all compounds within the volatile range. Thus we often end up with in excess of 200 volatiles in a total ion chromatogram. It is important to correctly identify each component or as many as possible, and this can be difficult as we often have multiple co-elution of components. In many cases individual standards do not exist for every component, but even if they did it would it would be too time consuming to each run every standard. We utilise a number of different techniques to aid identification and to process data as quickly as possible. Mass spectral libraries are very important, some are generic and others are vendor specific or specific for flavour chemistry analysis. As we also utilise deconvolution software which removes interfering ions and attempts to clean up spectra aiding spectral library matches, however experience is required so that useful information is not inadvertently lost. We also utilise linear retention indices (LRI), which are related to sets of specific standards (usually alkanes) that elute uniformly under controlled GC conditions related to specific column types. These can be used in addition to mass spectral matching to aid compound identification. In some situations we also run external standards to aid identification if required. We also utilise an internal standard mixes to monitor method performance and compare results from different extraction methods. Recently we have started to utilise metabolomic software to rapidly process large data sets using individual libraries developed in-house and simultaneously carry out multivariate statistical analysis. Data analysis and speed of processing remains an important aspect of flavour chemistry as sensitivity of detection increases.

We also collaborate with other national and international groups involved in flavour chemistry to evaluate different extraction techniques and to validate methods for specific applications. We are also actively involved in cross cultural sensory projects where we are trying to understand chemical factors that maybe

influencing cultural differences in sensory perception of the same products. We have also been involved in authentication and traceability projects in relation to identifying specific biomarkers that connect foods to unique aspects of production or specific geographical areas of production. Recently we identified compounds that can potentially be used to identify dairy products produced from grass based feeding systems, some of which were directly impacting on sensory perception. We are now applying this same approach to other products that can be used to extenuate a products uniqueness to enhance a point of difference for marketing purposes. We also work closely with genetic groups investing the potential of bacteria and yeasts to produce specific flavours through biochemical pathways. Initially microbes are screened using advanced genomic techniques to determine if they have the genetic capability to produce these volatile flavour compounds, then we determine if they are expressing this capability in optimised model systems. The flavour compounds are quantified and interesting strains can be subsequently evaluated at pilot scale to see if they have potential for specific applications in the foods industry.

Overall the role of a flavour chemist is ever expanding in line with developments in relation to sensitivity of detection, advances in data processing, sensory science and through involvement with other scientific disciplines.

About the Author

Dr Kieran Kilcawley holds a PhD in Food and Nutritional Sciences from University College Cork and a BSc in Biotechnology from the University of Westminster. Dr Kilcawley's research interests lie in the exploitation of enzymes that influence flavour development. His main focus is on dairy flavours, but also works with any food or beverage. This research requires expertise in fermentation, biochemistry, flavour chemistry and sensory science.

Dr Kilcawely represents Teagasc Moorepark as one of the partner organisations making up Sensory Food Network Ireland.

About Sensory Food Network Ireland

Sensory Food Network Ireland is a national network of excellence, promoting integration and ensuring sustainability for all sensory science activities on the island of Ireland.

Sensory Food Network Ireland is a non-profit organisation committed to delivering a comprehensive and excellent sensory science service to the food and beverage industry on the island of Ireland and abroad.

Membership is open to any company or organisation with an interest in sensory science.

For more information visit: www.sensoryfoodnetworkireland.ie

UPLC® method development and validation for the assay of the photolabile drug nifedipine and its trace level degradation products

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Introduction

Quality assurance regulations require that pharmaceutical drugs are highly pure. This is in order to ensure the safety and efficacy of medicines for patients, two fundamental issues of importance in treatment. The safety of a drug is determined by both its pharmacological and toxicological profile as well as impurities present in its dosage form. Impurities may have pharmacological and toxicological effects that outweigh any benefit from the dosage form administration. While the use of a drug to treat a patient is a balance of risk and benefit, impurities in pharmaceuticals provide only risk.

Therefore, pharmaceutical companies must characterise what molecules may be present and be able to identify them at low levels or as low as reasonably practicable (ALARP). This involves reducing risk to an acceptable level without disproportionate resource expenditure. Molecule characterisation involves the identification, structural elucidation and quantitative determination of impurities and degradation products. Impurity analysis is therefore a very important field in pharmaceutical characterisation as it allows assurance that a drug is safe and of sufficient quality (Görög, 2000).

Due to newer analysis methods becoming available and the need to detect impurities at ever lower levels, ongoing method development and transfer of newer techniques to the quality control laboratory is a reasonable regulatory expectation. However pharmaceutical companies can be innately conservative, with change and adaptation to new techniques that can require significant resource investment. Although current techniques may appear adequate, when dealing with impurities that can impact patient safety, in particular genotoxic impurities, this resource allocation is prudent.

Impurities present in drug products are classified as organic, inorganic and residual solvents by the United States Food and Drug Administration (FDA) (FDA, 2008A). The source of impurities can be from the manufacturing process and/or during storage including contact with packaging. Possible impurities include: starting materials, by-products, intermediates, degradation products, reagents, ligands and catalysts (The International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH)). Potential impurities may be known or unknown, volatile or non-volatile. Additionally, there may be impurities from products of incomplete or over reaction, enantiomeric impurities, impurities in materials used for synthesis and impurities in excipients (Nageswara Rao and Nagaraju, 2003).

Genotoxic impurities are a special case of impurities defined by the ICH as “a broad term that refers to any deleterious change in the genetic material regardless of the mechanism by which the change is induced.” (ICH, 2011). Genotoxic impurities, even at low concentrations pose significant health risks as they can potentially be mutagenic and thus damage DNA. Therefore, they pose a cancer development risk for patients (Jacobsonkram and McGovern, 2007). Due to the potential for adverse safety posed by these types of impurities the European Medicines Agency and FDA have given emphasis on tackling this issue by introducing a threshold of toxicological concern of 1.5 µg/day for genotoxic impurities in new commercial drugs (FDA, 2008B) (EMA, 2006). The International Council for Harmonisation provides a more detailed complementary document for guidance on genotoxic impurities titled ICH M7 (ICH,2015). Increasingly, the analyst must relate to this new paradigm and augment historical units for determination of impurities.

The object of this work was to provide a valid method capable of separating nifedipine and its by-products (Figure 1) in an efficient manner using UPLC coupled with diode array detection.

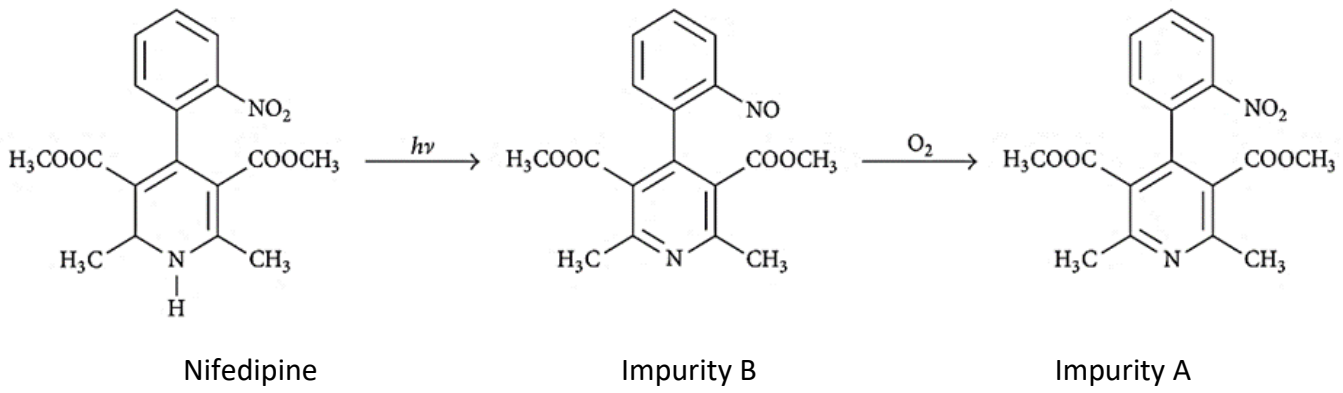

Figure 1: Nifedipine photolysis followed by oxidation producing major breakdown products (Ahmad et al., 2016).

Nifedipine is photolabile and undergoes photodehydrogenation by intra-molecular mechanisms to nitro- and nitroso-pyridine analogues (Handa, Singh and Singh, 2014). These analogues are not known genotoxins but it is prudent to monitor the reduction of a nitro group to its nitroso analogue. Due to the unpredictability of photolytic degradation these products have historically had different thresholds for their presence in lots passing through the supply chain as an active pharmaceutical ingredient or finished product.

No UPLC method existed in the literature for the analysis of photo-degradants in nifedipine. The aim was to make available a *pharmacopeial* assay method validated using the ICH Q2(R1) *Validation of Analytical Procedures* document, using the isocratic mode to maximise baseline stability and enabling identification of photo-induced degradation products of nifedipine. Q2(R1) is a tripartite harmonised ICH Guideline that informs on the required validation parameters for a validated method.

ICH limits for impurities in new drug products are shown in Table 1 (ICH, 2006). Identification below limits may be necessary for unusually potent or toxic impurities. Impurities should be reduced to the lowest level reasonably possible but it is acknowledged that impurities cannot be reduced to zero thus specifications are used.

The maximum daily dose of nifedipine is 90 mg. The approach outlined by the ICH in the document Q3B(R2) is an identification threshold of 0.2% or 2 mg total daily intake of impurity (TDI) (whichever is lower) for 10-2000 mg (ICH, 2006). Therefore, for a 100 µg/mL (ppm) solution of drug in the laboratory, impurity levels above 0.2 ppm must be detectable.

Table 1: Q3B(R2) Impurities in new drug product's limits.

Maximum Daily Dose		**Threshold**
	Reporting thresholds	
≤ 1 g > 1 g		0.1% 0.05%
	Identification thresholds	
< 1 mg 1 mg - 10 mg >10 mg - 2 g > 2 g		1.0% or 5 µg TDI, whichever is lower 0.5% or 20 µg TDI, whichever is lower 0.2% or 2 mg TDI, whichever is lower 0.10%
	Qualification thresholds	
< 10 mg 10 mg - 100 mg >100 mg - 2 g > 2 g		1.0% or 50 µg TDI, whichever is lower 0.5% or 200 µg TDI, whichever is lower 0.2% or 3 mg TDI, whichever is lower 0.15%

The increases in analytical technology in the last 30 plus years have allowed development of newer, superior methods to determine purity of medicines. High performance liquid chromatography (HPLC) is now the method of choice for impurity analysis as it can replace all non-specific assay methods with a highly specific and precise one. For the last 20 years HPLC has been used for nearly all organic impurity determinations (Nageswara Rao and Nagaraju, 2003).

Validated HPLC methods are especially required due to their powerful precision, specificity and accuracy. However, adequate system suitability testing must be employed to ensure optimal set up.

Recent developments have seen a shift towards newer liquid chromatography systems called ultra-performance or UPLC. Waters released the first such instrument equipped with the capability to function at higher operating pressures in 2004. It was designed to exploit the performance advantages of a sub 2 µm stationary phase. Smaller particle sizes of UPLC cause the Van Deemter curve to flatten allowing a more usable range of flow rates with subsequent faster analysis times. Van Deemeter plots of efficiency *vs* flow rate for UPLC columns show none or little deterioration with these increased flow rates due to the smaller particles having shorter diffusion path lengths with the analyte not spending long inside the particle where diffusion could happen (Figure 2).

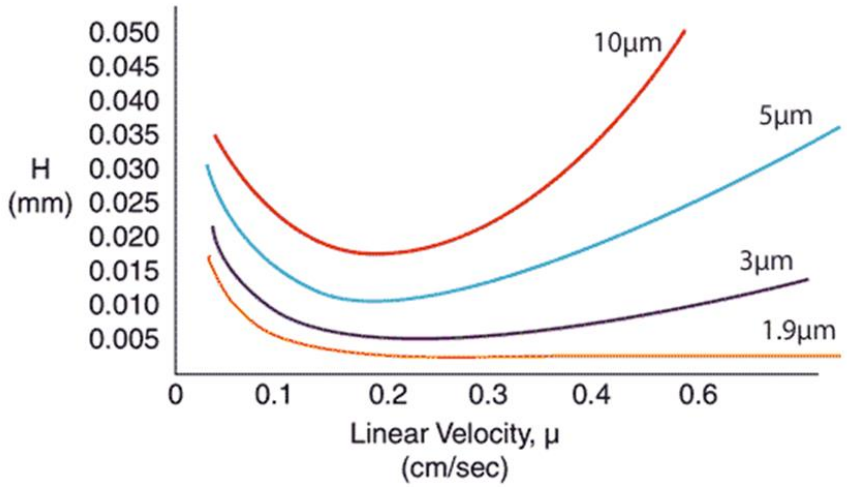

Figure 2: Van Deemter plot of various particle size columns (Restek.com, 2017).

Reducing particle size in columns to increase separation efficiency had reached a limit due to instrument band spreading and a limited pressure range. Higher pressures were required to be tolerable as smaller particles result in a higher density, increasing resistance to flow. By providing access to higher pressures of 15,000 psi these limitations were overcome. Waters approach has since been replicated by competitors, resulting in the more widespread use of such systems. UPLC has advantages of improved analysis speed, thereby increasing sample throughput, resolution and sensitivity (Waters.com, 2016). Therefore, it is fast becoming the analytical technique of choice.

It is critical new analytical methods are validated in order to ensure accurate data sets and regulatory compliance. Failure to validate can lead to issuance of FDA form 483 or similar, which indicates excellence is not being achieved and beyond the laboratory can have negative reputational consequences.

ICH Q2(R1) document outlines the parameters that must be investigated and recorded as well as recommended methods for examining each. These include robustness, linearity and range, limit of detection (LOD), and limit of quantitation (LOQ). Chromatographic specific parameters that are of daily importance for the resultant validated method include those system suitability aspects which examine separation efficiency (N), capacity factor (K), selectivity (α) and resolution (R).

Separation efficiency (N) is a measure of the sharpness of peaks. It reflects column performance and expresses the number of theoretical plates in a column. A perfect peak would be like a pencil line however due to dispersion effects this is not the case in practice. A plate is a distance where the sample components achieve one equilibration between the mobile phase and stationary phase in the column. More theoretical plates equate to a more efficient separation, therefore knowledge of N is a key component in evaluating a method.

Capacity factor (k) is the ratio of analyte retention time to an unretained molecule's retention time. The unretained molecule has no affinity for the stationary phase and elutes with the solvent front. It is generally independent of the equipment, being instead a function of mobile phase and column choice. This makes it a useful point of reference when comparing the retention of peaks that were obtained using a different chromatographic system.

Selectivity (α) is a measure of the chromatographic system's ability to separate two components. It is a measure of the ratio of capacity factors of each, therefore a function of their distance. Selectivity is dependent on the analyte, column and mobile phase with alterations to each affecting its value.

Resolution (R) is perhaps the most crucial factor to consider when evaluating a chromatogram with the main goal being to have the best resolution possible in the shortest time. It is determined by the difference between retention times of each peak divided by the average width of both peaks at the baseline. Resolution is influenced by N, K and α.

Chemicals and Reagents

Nifedipine (1,4-Dihydro-2,6-dimethyl-4-(2-nitrophenyl)-3,5-pyridinedicarboxylic acid dimethyl ester), impurity A (2,6-Dimethyl-4-(2´-nitrophenyl)-3,5-pyridinecarboxylic acid dimethyl ester) and impurity B (Dimethyl 2,6-dimethyl-4-(2-nitrosophenyl)-3,5-pyridinedicarboxylate) were sourced from Sigma-Aldrich. Formic acid was supplied by Waters. HPLC grade 99.8% acetonitrile sourced from Macron Fine Chemicals was used as was Elga deionised 18 megohm water.

Experimental

Table 2: Final Chromatographic system details.

UPLC	Waters ACQUITY
Column	ACQUITY UPLC BEH C18 1.7 µm.
Column dimensions	2.1 x 50 mm
PDA Detector wavelength	237 nm (Recording in the range 210-400 nm)
UV Block filter	Below 210 nm
Injection size	5 µL
Mobile phase	Water/acetonitrile (73:27)
Flow rate	0.5 mL/min
Run time	5 mins
Sample loop	Partial loop
Injection volume of loop	20 µL
Weak wash	Water/acetonitrile (95:05)
Strong wash	Water/acetonitrile (50:50)
Sampling rate	20 pts/s
Auto sampler temperature	7°C
Column temperature	45°C

Results

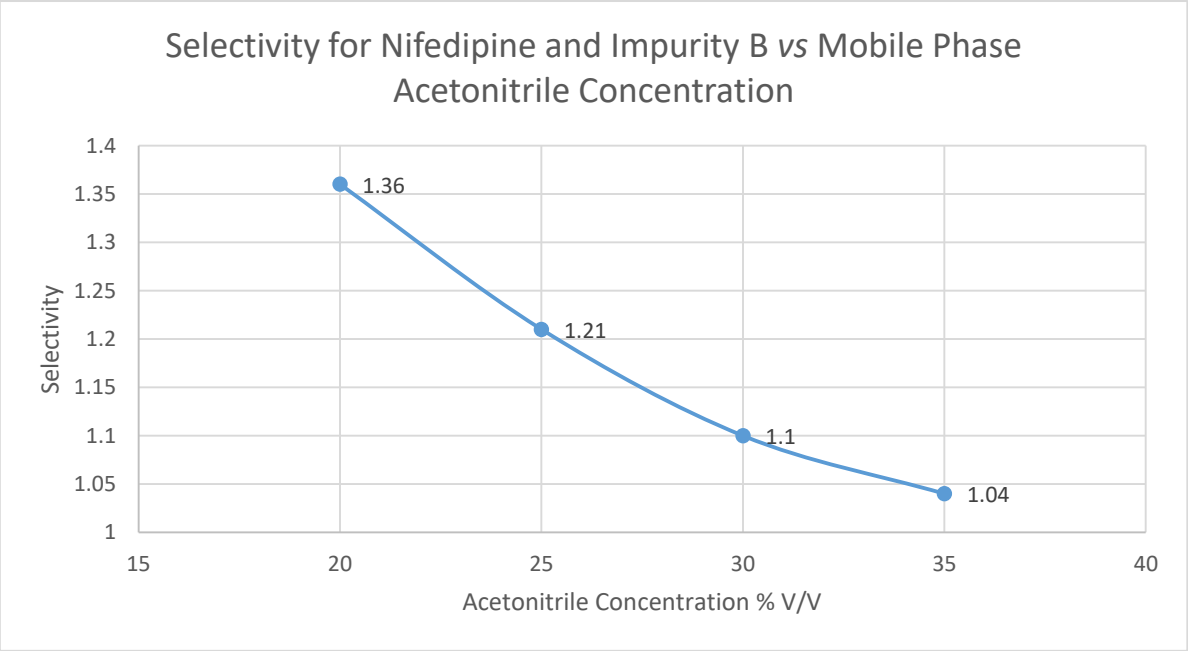

Figure 3: Graph of selectivity vs acetonitrile concentration with remainder made up of Elga deionised 18 megaohm water.

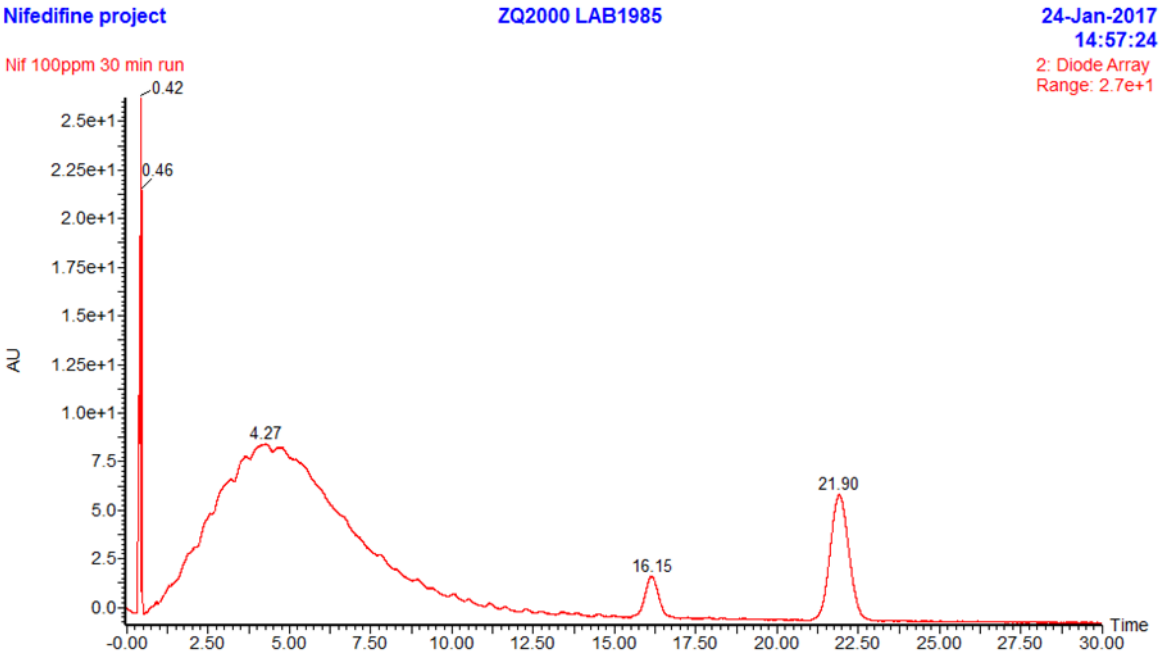

Figure 4: 100 ppm Each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (80:20) with 0.1% formic acid. Column temperature 35°C. Flow rate: 0.4 mL/min. Injection: 8 µL.

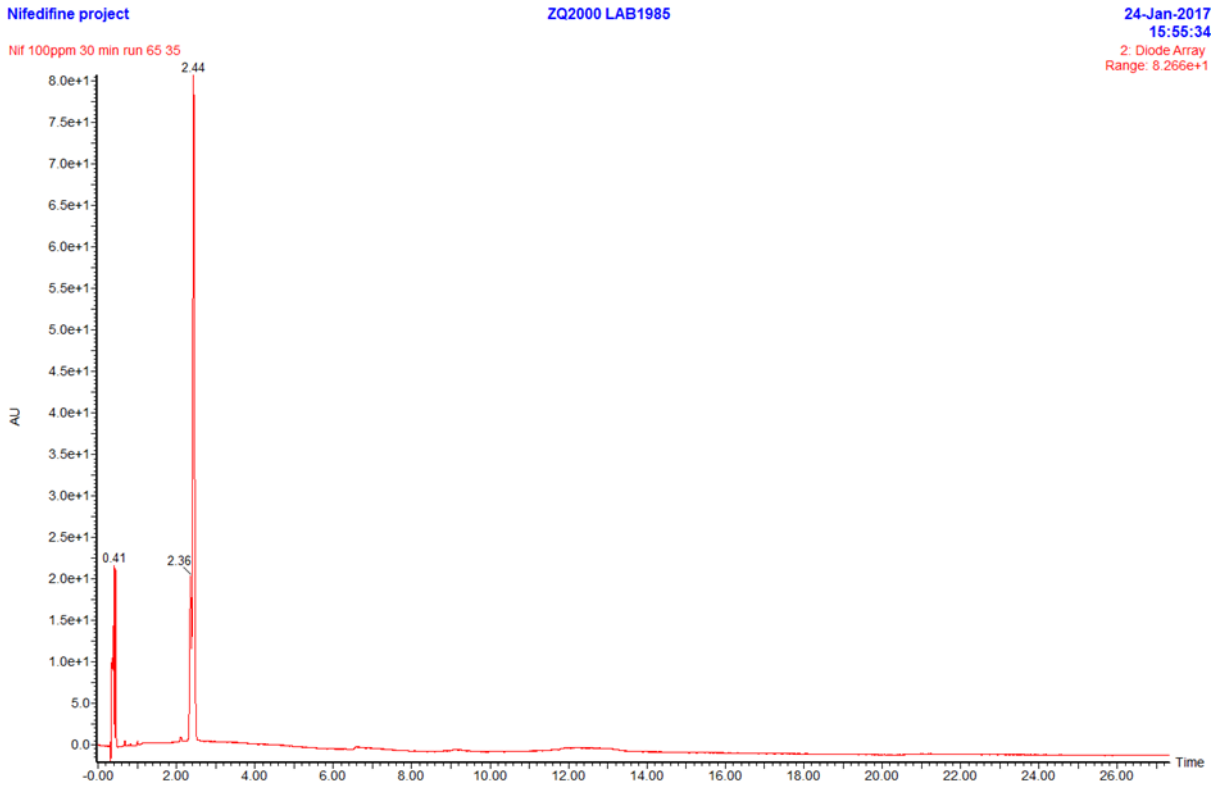

Figure 5: 100 ppm Each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (65:35) with 0.1% formic acid. Column temperature 35°C. Flow rate: 0.4 mL/min. Injection: 8 µL.

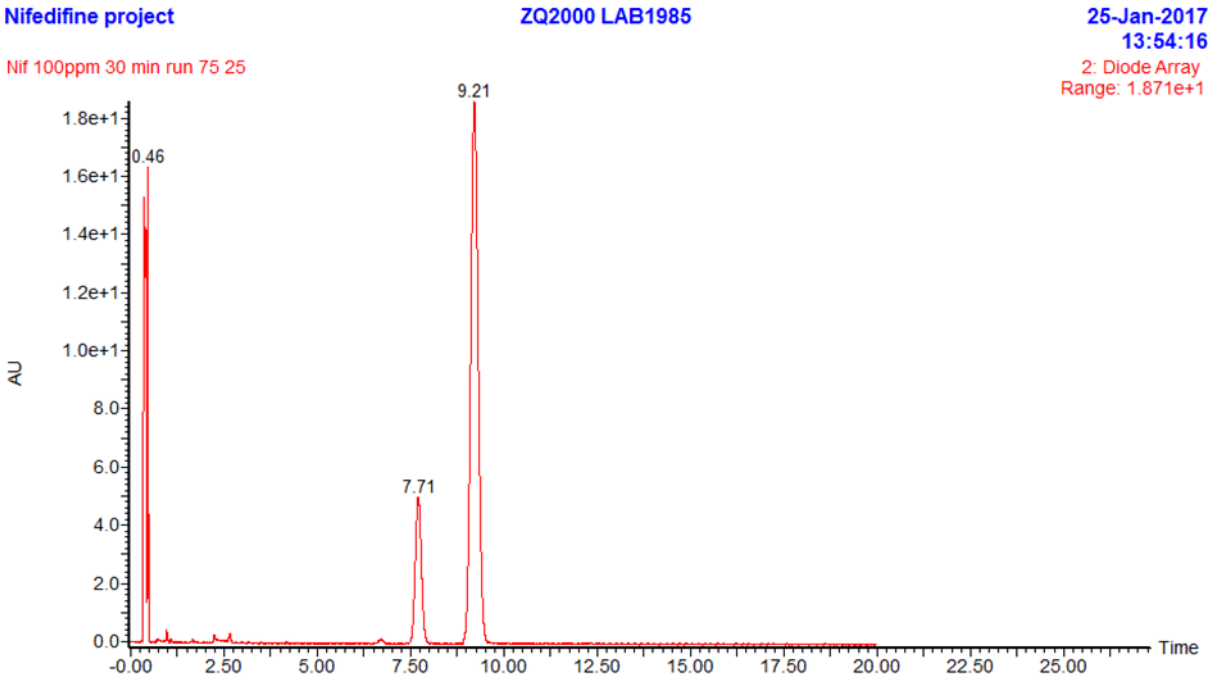

Figure 6: 100 ppm Each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (75:25) with 0.1% formic acid. Column temperature 35°C. Flow rate: 0.4 mL/min. Injection: 5 µL.

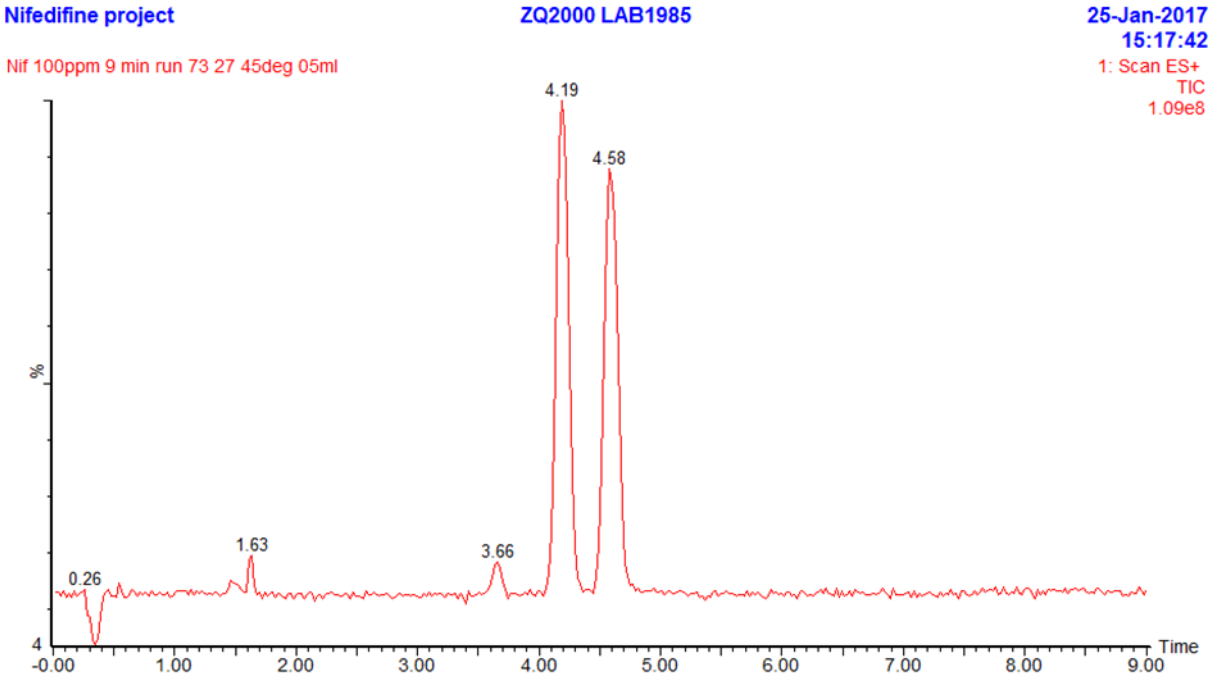

Figure 7: 100 ppm Each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (73:27) with 0.1% formic acid. Column temperature 45°C. Flow rate: 0.5 mL/min. Injection: 5 µL.

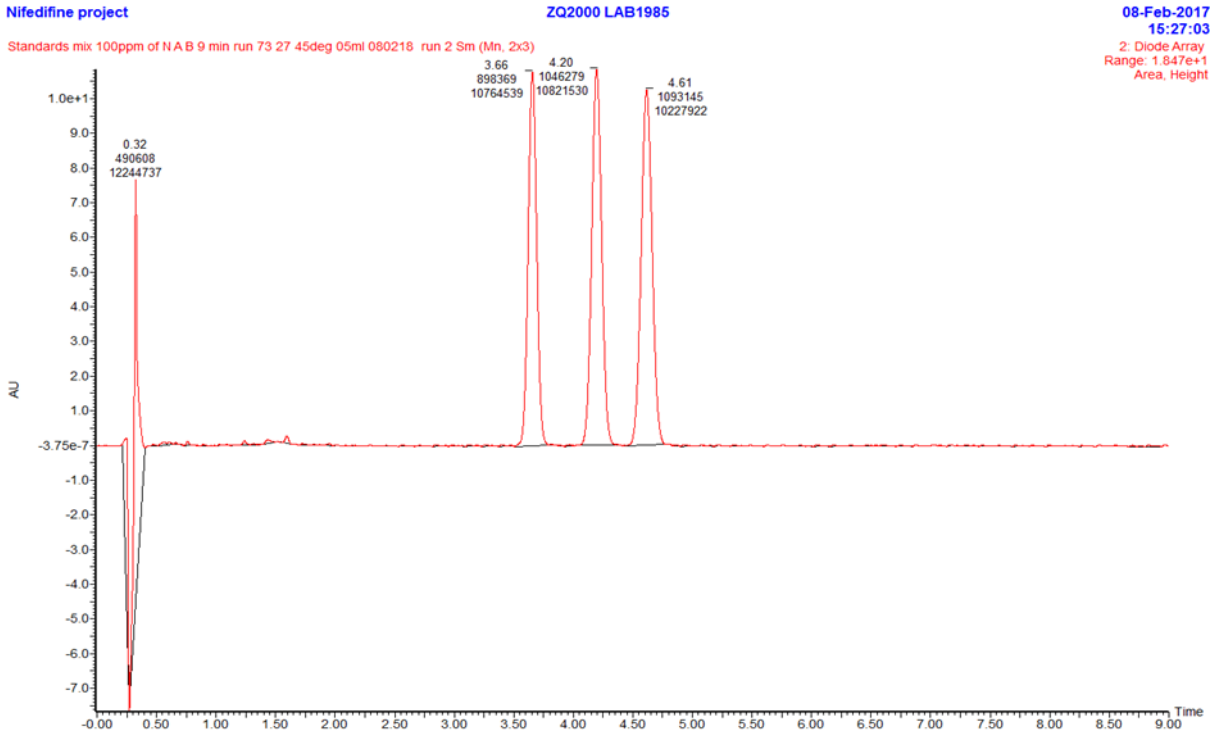

Figure 8: ***Developed method*** *with 33.3 ppm each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (73:27) with 0.1% formic acid. Column temperature 45°C. Flow rate: 0.5 mL/min. Injection: 5 µL.*

Table 3: Table of selectivity and resolution for Fig 7.

Peak	**α**	**R**
Impurity A to B	1.16	2.07
Impurity B to Nifedipine	1.10	1.5

Table 4: Table of capacity factors and theoretical number of plates for Fig 7.

Peak	**K**	**N/m**
Impurity A	10.43	195,195
Impurity B	12.13	257,042
Nifedipine	13.44	193,336

Discussion

A mixture consisting of nifedipine, impurity A and impurity B was run for the purpose of optimising the system on a qualitative basis so as to establish a functional method capable of being assessed through relevant, advantageous, system suitability criteria. This was analysed with alteration of various conditions which included mobile phase ratio, column temperature, and flow rate.

In this investigation, a balance was required of speed, resolution and elution time of the photo degradant impurities. Acetonitrile at 27% was ultimately determined after development steps to be optimal, giving the desired balance. The higher the acetonitrile concentration, the higher the affinity of the non-polar mobile phase for non-polar nifedipine reducing its retention time significantly due to less time spent bound to the non-polar stationary phase. The acetonitrile competes with the stationary phase for nifedipine; Figure 3 shows how the selectivity changes with mobile phase strength changes as acetonitrile concentration is

altered. This therefore has a significant effect on retention time requiring the aforementioned balance of speed, resolution and elution time.

Figures 4-7 inclusive show the transformative effects of quite small alterations of chromatographic conditions and informed the selection of conditions that achieved the requisite balance of chromatographic efficiency, speed and limit of detection (LOD).

In Figure 5 the mobile phase was changed from a starting ratio of water/acetonitrile (80:20) to water/acetonitrile (65:35). A dramatic effect was observed with nifedipine's retention time reducing to 2.44 minutes, an almost 20-minute reduction. This was due to the selectivity changing.

Further adjustments to the mobile phase of water/acetonitrile (75:25), gave a more acceptable chromatogram with sharp, symmetrical peaks and a good resolution of 2.93 and a drug retention time of 9.2 mins, seen in Figure 6. However, the peak for impurity A was poor and difficult to identify.

As temperature affects retention and selectivity (with improved mass transfer kinetics), it was increased. Changing the column temperature to 45°C improved impurity A's peak height, seen in Figure 7. The flow rate was also changed from 0.4 mL/min to 0.5 mL/min. This was afforded due to the reduced viscosity and subsequently reduced backpressure gained from increasing temperature.

The outcome was a further significant decrease in the retention time to 4.6 mins for nifedipine. The peaks also sharpened up with the bonus of impurity A's height increasing. However, the resolution was not optimal so the mobile phase was slightly altered again to water/acetonitrile (73:27) and shown in Figure 8. This 'spread' the peaks and still had an acceptable retention time of 4.6 mins for nifedipine which eluted last, an ideal scenario for most drug impurity analysis. When acetonitrile is increased in concentration it has a stronger binding effect on nifedipine and its degradation products which results in earlier elution (Plumley et al., 2009). This series of alterations culminated in the final chromatographic system setup (Table 2).

Table 3 shows the selectivity values. Values between 1.10 and 1.16 were obtained. A value of 1 would indicate coeluting peaks. The value on paper was a little low but the resolution obtained in Fig 7 demonstrates no issues as does the high plate count. The initial wait of 3.5 mins before elution began is responsible for this.

Table 4 shows the chosen system had a high number of theoretical plates. This indicates the high separation efficiency of the system. The small particle size of the column is a significant contributing factor to the high N value.

Resolution (R) is certainly the most crucial factor to consider when evaluating a chromatogram with the main goal being to have the best resolution possible from potential impurities in the shortest time. An R value of 1.5 is ideal as it ensures the analytes are well separated allowing accurate peak areas to be determined while doing so in the minimum time required, therefore increasing throughput. The resolution between impurity A & impurity B was 2.07 and between impurity B & nifedipine, 1.5, as shown by Figure 8. This indicates the peaks were well resolved and that when analysing a manufactured tablet or capsule for impurities, that they can be separated and accurately quantified. This is especially critical when dealing with substances that are potentially toxic and failure to resolve them can have grave consequences for product quality and patient safety. That is why the method development template and process of the type described here is critical to undertake, to ensure that the system can conduct the analysis required, especially when the analyst possesses a reference portion of the impurity.

Precision was determined over 3 runs with the coefficient of variance calculated as 0.32% for nifedipine 0.45% for impurity B and 0.93% for impurity A. The lower level of variation for an active pharmaceutical ingredient compared with an impurity is not surprising with more variability to be expected of impurities. These figures were low indicating the system benefited from the isocratic approach and produced precise data. Linearity tests were conducted over the range of 0.1-20 ppm using impurity A, impurity B and

nifedipine in a mix. Excellent linearity was observed over this range with R^2 values being between 0.9999 and 1.0000. The limits of detection and quantitation was determined through the use of signal to noise ratios using matching blank solutions (figures 9-10). The LOD was 0.2 ppm and LOQ 0.5 ppm. These values mean that the method has a high sensitivity and the ability to quantitate at low levels which can be somewhat unusual for a photo diode array (PDA) detection. In this instance degradation of photolabile nifedipine could be monitored for a drug solution concentration of 100 µg/mL. These attributes are more and more vital for impurities' analysis as pharmaceutical medicines become more potent and are dosed at lower levels.

As part of a method robustness examination, the mobile phase composition in particular, column temperature and flow rate require control due to their potential effect on retention times.

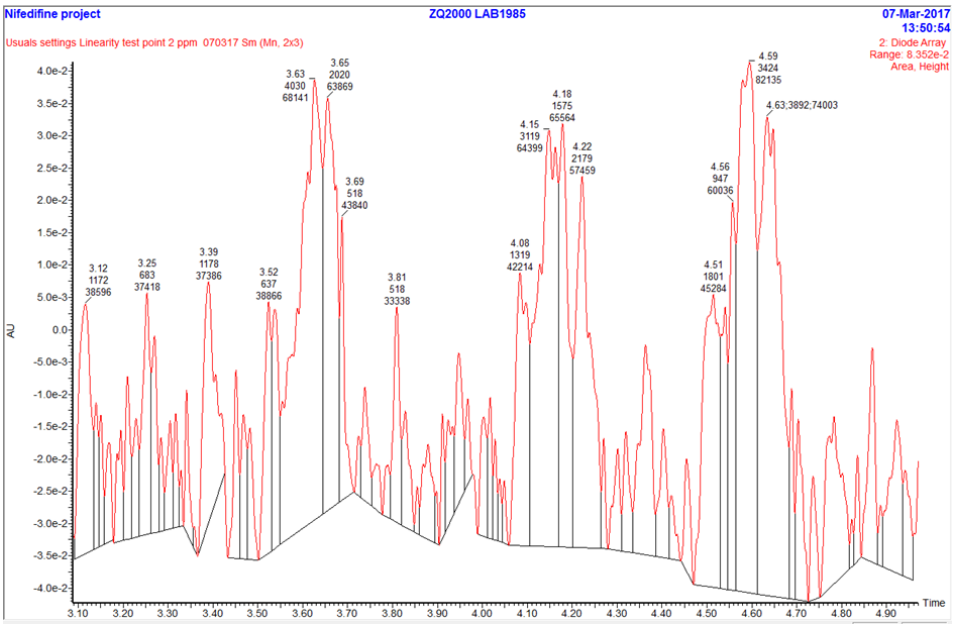

Figure 9: 0.2 ppm Each of nifedipine, impurity A and impurity B. Mobile phase: water/acetonitrile (73:27) with 0.1% formic acid. Column temperature 45°C. Flow rate: 0.5 mL/min. Injection: 5 µL.

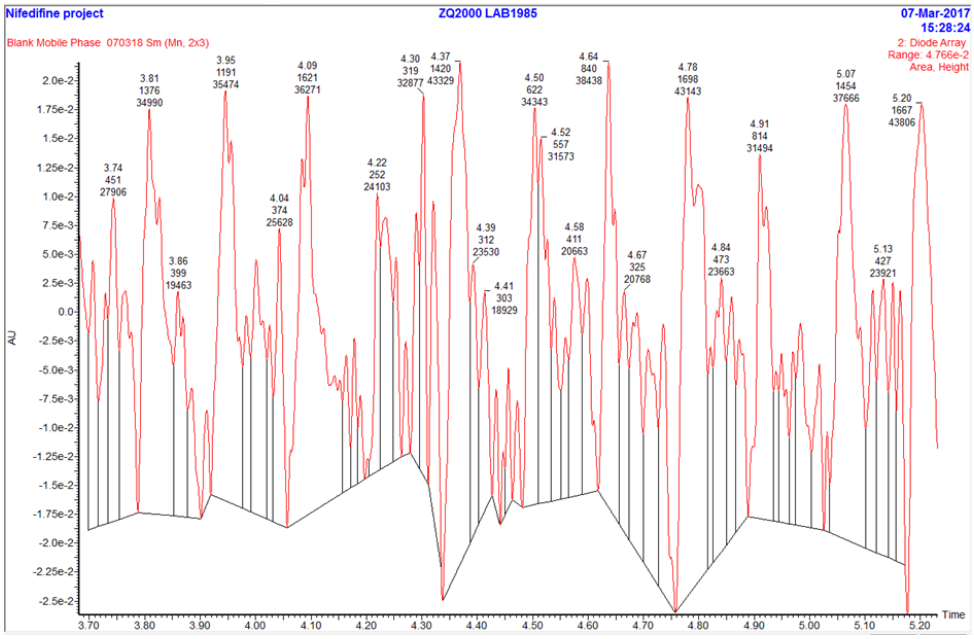

Figure 10: Blank mobile phase. Mobile phase: water/acetonitrile (73:27) with 0.1% formic acid. Column temperature 45°C. Flow rate: 0.5 mL/min. Injection: 5 µL.

As 100 ppm concentrations were analysed for method development purposes and at a 0.2 ppm detection limit this works out as 0.2% detection at this concentration. However, this is right on the limit of PDA capability and some cushion would be desirable by either increasing detection performance, increasing sample concentration administered or both. As it stands the validated system is within the permissible specifications and no impurity was noted in some nifedipine drug products sampled for challenge.

These results show the benefits of investigating the development of new methods on newer chromatographic analysis techniques as superior data sets can hope to be achieved by the analyst.

Conclusion

The developed method is able to distinguish between nifedipine and its degradation products with a low LOD of 0.2 ppm for identification, and a LOQ of 0.5 ppm allowing quantitation to be performed with low sample amounts. This method gave excellent peaks with little tailing, flat baselines and very good resolution all within a short retention time of 5 minutes. ICH method validation was performed satisfactorily demonstrating the suitability of this method for use in nifedipine impurity analysis.

About the authors

James Phelan has recently completed a B.Sc. (Honours) Pharmaceutical Science degree at Athlone Institute of Technology achieving first-class honours. He recently commenced working at BioClin Research Laboratories in the Bioanalysis department using LC-MS/MS.

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First circular

Eurachem Dublin 2018

Scientific Workshop in connection with Eurachem General Assembly 2018

Data - Quality, Analysis and Integrity

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

The State Laboratory
An tSaotharlann Stáit

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

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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.

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Eurachem Dublin 2018

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 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

DCU

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Schools News Letter 2016 - 2017

Leaving Cert Chemistry Winner 2016

Prof John Cassidy presents prize to Hannah Fitzpatrick winner of the

Schools Chemistry Newsletter Competition 2016/17 during Congress 2017

Leaving Cert Chemistry Runner Up 2016

The runner-up prizes in the 2016-2017 Schools Newsletter competition, on the topic of 'The Chemistry of Climate Change', was presented to Euan McDonnell, at Moate Community School by Immediate Past President Margaret Franklin on Monday 15th May 2017.

His Chemistry teacher, Mairead Cusack, took this photo of the presentation.

Immediate Past President Margaret Franklin presents Euan McDonnell

CHEMISTRY in Europe
Newsletter for European Chemistry, published by EuCheMS

http://www.euchems.eu/newsletters/chemistry-in-europe-2017-3/

EDITORIAL

MEP Pavel Poc on Glyphosate

The debate on glyphosate reauthorisation in the European Union (EU) has recently culminated under the shade of the so-called Monsanto papers scandal. The European Parliament (EP) played an important role in the postponement of the authorisation in the beginning of 2016 and will probably have to act again regarding how the EU legislation on pesticide authorisation is executed by the agencies and the European Commission (EC).

Despite a clear position voiced in the EP Resolution from 13 April 2016 on renewal of the approval of the active substance glyphosate, there is still a lot of confusion about the EP's position about the reauthorisation of the world's best-selling herbicide.

EP urged EC to acknowledge a majority of two decisive political groups and to mirror the outcome of the vote in their proposal, but despite the EC's claims about respecting this, only a very limited part of the EP resolution was eventually reflected in the EC draft proposal. As a consequence, the Member States refused to back the Commission proposal with a qualified majority, effectively leaving the whole situation without a decision.

Let us look closer at the EP's Resolution adopted in 2016 to clarify some of the recent developments. The objection to the re-approval of glyphosate as adopted in the Committee for Environment, Public Health and Food Safety (ENVI) was modified into a 7-year re-approval in the plenary of the EP. The 7-year option got a majority of only sixteen votes and many MEPs wanted a stricter time frame. In addition, crucial restrictions were adopted leaving only few uses for re-approval. Parliament agreed on no approval of non-professional use; close to public areas; where integrated pest management systems are sufficient for weed control; and on limited pre-harvest applications (for weed control and to enhance crop ripening). This means, that the EP did not call for a complete rejection of the approval as adopted in the ENVI committee but for a realistic option with many restrictions. The EC previously stated that if the two political groups reached an agreement (and they did), the EC would respect it, but that was not the case. EP criticized the EC draft implementing act for

failing to ensure a high level of protection of human and animal health and the environment. MEPs also called for an independent review of overall toxicity of glyphosate and asked the EC and the European Food Safety Authority (EFSA) to immediately disclose all scientific evidence for the positive classification of glyphosate. EP also wanted the EC to start testing and monitoring glyphosate residues in foods and drinks produced in the EU as well as in imported products. There was also criticism of the EC for accepting an incomplete dossier with regard to endocrine disruption and a call to provide reference to further evidence of adverse effects of glyphosate. The resolution as a whole was adopted by majority.

The addition of key specific restrictions, most of which were supported by a large majority, provided an excellent basis for further discussion with the Member States against the EC proposal. As a rapporteur of the resolution, I am strongly convinced that we achieved a good result that was however not reflected in the EC's actions. I think this was a missed opportunity to accommodate the different positions and to effectively address the problem of glyphosate re-authorisation before the situation is clear with concerns about its carcinogenicity and genotoxicity or potentially devastating effects on cellular metabolism due to suppression of CYP 450 enzymes.

Pavel Poc
Member of European Parliament

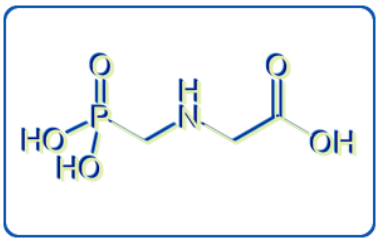
POLICY

Sadly, I was not able to attend the European Parliamentary Workshop on glyphosate organised by Pavel Poc, Member of the European Parliament, EuCheMS and ECTN on 1 0th May, 201 7, but I have watched the video and was impressed by the very high level of scientific debate with most, but sadly not all, approaching the discussion with an open mind. I t was appropriate that this debate focussed mainly on the science but it got me thinking about the whole issue of hazard/risk and risk versus benefit. More generally, can it ever be justifiable to use a hazardous chemical? Of course, if the risk can be contained to an acceptably low level. Petrol (gasoline) is a very hazardous material because it forms highly explosive mixtures with air, which is why it works as a fuel . Yet, al l of us are happy to drive around with many litres of it in the back of our cars. I t is contained in such a way that the risk of an uncontrolled explosion is very slight, but it is not zero (...) You can read the entire article at https://wp.me/P7iPLy-LA

David Cole-Hamilton

EuCheMS President

Can the Benefits of Using Agricultural Chemicals Outweigh the Risks?



Sadly, I was not able to attend the European Parliamentary Workshop on glyphosate organised by Pavel Poc, Member of the European Parliament, EuCheMS and ECTN on 10th May, 2017, but I have watched the video and was impressed by the very high level of scientific debate with most, but sadly not all, approaching the discussion with an open mind. It was appropriate that this debate focussed mainly on the science but it got me thinking about the whole issue of hazard/risk and risk *versus* benefit.

More generally, can it ever be justifiable to use a hazardous chemical? Of course, if the risk can be contained to an acceptably low level. Petrol (gasoline) is a very hazardous material because it forms highly

explosive mixtures with air, which is why it works as a fuel. Yet, all of us are happy to drive around with many litres of it in the back of our cars. It is contained in such a way that the risk of an uncontrolled explosion is very slight, but it is not zero. Sometimes, there are accidents and massive explosions that take lives. In this case, the hazard can be controlled and the risk minimised to such an extent that we accept that the benefits far outweigh the risks.

Similarly with glyphosate. If, and the jury is still out, there is a higher risk of contracting lymphomas amongst those who apply glyphosate, and this risk can be controlled by the use of suitable protective clothing, then the benefits in terms of food yield, cost, quality and nutrient use may very much outweigh the risks. If, and again evidence is not there for humans, very low levels of glyphosate lead, for example, to very much increased incidences of non-alcohol based liver damage, the situation is quite different.

There are some people who would argue that the use of all manmade chemicals in agriculture should be banned. Currently, we produce about as much food as we need to feed the 7 billion people in the world.[1] In some places, we eat too much and waste food in others there is too little. It is estimated that crop yields are increased by around 25 – 40 % by using agricultural chemicals.[2] So, if we ban them, 1/5 of the world's population will starve. Do we really want that to happen? Organic farming cannot solve this problem without human sewage being recycled onto the earth. Unless this is done, there is a one-way stream of nutrients (mainly phosphorus and nitrogen, but also trace elements) from the soil through plants, animals and humans into the sea or sewage deposits, thus depleting the soil. Nitrogen can be replaced by growing leguminous crops, but one of the few companies in Europe trying to extract and recycle phosphorus from sewage failed.

we should certainly continue to test (and sometimes withdraw) chemicals used in agriculture, reduce the amounts used to the minimum effective dose, improve application methods and protect workers

Every death by whatever cause is regrettable and should be avoided. Hence, we should certainly continue to test (and sometimes withdraw) chemicals used in agriculture, reduce the amounts used to the minimum effective dose, improve application methods and protect workers. Ideally there would be no deaths associated with the use of agricultural chemicals, but if banning them will cause the deaths of 1-2 billion people, how many people would we be prepared to see die in their manufacture, application and as a result of the ingestion of their residues if we continue to use them? When do their benefits exceed their risks?

[1] http://www.fao.org/worldfoodsituation/en/
[2] https://www.nature.com/nature/journal/v485/n7397/full/nature11069.html; https://www.scribd.com/doc/283996769/The-Yield-Gap-For-Organic-Farming; http://rspb.royalsocietypublishing.org/content/282/1799/20141396

David Cole-Hamilton
EuCheMS President

The Case of Glyphosate

The re-authorisation of a substance, herbicides, involvement of chemists, farmers, ghost-writers, courts, multinationals, NGOs, policy makers, and a lot of EU Legislation – these are the unlikely ingredients of a policy file whose outcome is unpredictable. Given the particular complexity and importance of this topic, I will be providing a wide range of sources for several points of this article.

The initial years

Glyphosate [N-(phosphonomethyl) glycine] was discovered by Dr. Henri Martin in 1950, a chemist working for a pharmaceutical company that sold this molecule to other companies as no pharmaceutical use for glyphosate could be identified. In 1970 Dr. John Franz, a scientist working for the company Monsanto, discovered the herbicidal properties of glyphosate and in 1974 the commercialisation of glyphosate-based

herbicides started. A commercial success, glyphosate is the world´s most used herbicide (sold under many different formulations, including Roundup), and it is estimated that 8.6 billion kilograms of glyphosate active principle have been used globally between 1974 and 2016.[1]

The approval system

Throughout the 70s and until 2002, glyphosate, as well as other chemicals, was assessed and approved for commercialisation by each country´s national authorities. This situation changed when in July 2002 glyphosate was deemed safe and approved for commercialisation at the EU level for the first time,[2] in accordance with EU law.[3] This authorisation extended for a period until the end of 2015, the date by when the substance should have been reassessed. So how does the assessment of chemicals work at the EU level?

First, we should take into consideration that glyphosate is an herbicide, thus falling under the EU plant protection products (PPP) Regulation. According to the PPP Regulation, the European Food Safety Authority (EFSA) is responsible for performing the risk assessment of active substances, while the European Commission will be the risk manager and take the final decision. For each substance, an application is submitted by the industry to an EU Rapporteur Member State (RMS), this RMS verifies the validity of the application, prepares a risk-assessment report (draft assessment report (DAR) or renewal assessment report (RAR)) and shares it with EFSA, Member States, and the European Commission. Next, EFSA peer-reviews the RMS report together with experts designated by Member States and with the applicants, and organises a public consultation for collecting views from stakeholders. Additional information might be requested if needed from the RMS/applicant and EFSA drafts a report ("Conclusion") on the active substance and informs the Commission. The Commission, through the Standing Committee on Plants, Animals, Food and Feed (PAFF) where Member States are represented, votes on approval or non-approval. Based on the voting of the Standing Committee, the Commission adopts a decision which is later published in the EU official Journal. The whole process should take around 3 years. As for the authorisation periods, first authorisations can go up to 10 years while re-authorisations can go up to 15 years.

You should bear in mind that this approval system only concerns the approval or non-approval of the active substances. After a substance is approved at the EU level, it is up to each Member State to allow the commercialisation of specific products containing this substance.

EFSA and IARC

So how did this process go with glyphosate? In May 2012 the RMS, in this case Germany, received the dossier for the possible authorisation of glyphosate. In December 2013, Germany sent the Renewal Assessment Report to EFSA. In January 2014, the peer-review began, in March 2014 a public consultation was launched, lasting 60 days. In July 2014 EFSA evaluated all comments, and in August 2014, additional information was requested from the applicants. In February/March 2015, EFSA organised expert consultations in the areas of mammalian toxicology, residues, environmental fate, and ecotoxicology. In parallel to the EFSA approval system, on 20 March 2015, the International Agency for Research on Cancer (IARC) of the World Health Organisation classified glyphosate as "probably carcinogenic to humans" .[4] In view of IARC´s conclusions, the European Commission also mandated EFSA to assess the potential carcinogenicity of glyphosate or glyphosate-containing plant protection products in the on-going peer review of the active substance. In July 2015, a Member State consultation was launched on the conclusions arising from peer review. In August 2015, Germany, the RMS, prepared the assessment of the monograph, which was circulated to Member States for comments. Following receipt of comments, EFSA organised a second expert consultation on carcinogenicity and mammalian toxicology in September. In October, Glyphosate authorisation was provisionally extended until June 2016. The peer review was updated and published in November 2015. In it, EFSA states that EFSA *"*concluded that glyphosate is unlikely to pose a carcinogenic hazard to humans and the evidence does not support classification with regard to its carcinogenic potential" .[5] At this point, many scientists[6] and environmental non-governmental organisations (NGOs) raised their voice against EFSA´s conclusions, questioning the transparency of EFSA´s analysis and pointing

out that EFSA used not only open academic, peer-reviewed sources but also industry sponsored unpublished studies and data (to which EFSA was granted access), as is actually allowed by EU law. NGOs state that only IARC´s conclusions are acceptable as IARC strictly used open academic, peer-reviewed studies in their analysis.[7]

The standing committee.

As discussions surrounding glyphosate entered the public debate in many EU countries, this hot dossier finally went into the hands of the risk manager, the European Commission and the Standing Committee on Plants, Animals, Food and Feed (PAFF) where all EU Member States have a seat. This and other standing committees are used by the European Commission when approving "delegated acts" and "implementing acts", two types of legal act which derive from the higher level legislation, "regulations" and "directives". In the case of glyphosate, an herbicide, re-authorisation is provided via an "implementing act" and under a procedure called "examination procedure"[8] which is activated given the importance of this dossier to the environment and to public health. Under this committee, if a qualified majority[9] of Member States approves or non-approves a Commission´s proposal, the Commission must follow the vote. If no qualified majority is achieved, the Commission may proceed with its initial proposal, or submit a new one for voting. An Appeal Committee (also composed by Member States) is convened when there is no qualified majority and the Commission decides to advance on its own. If the appeal committee rules against the Commission's proposed action, the Commission must abide by this decision

In March 2016, the PAFF Standing Committee did not reach a qualified majority on the re-authorisation of glyphosate.[10] The Commission presented two revised proposals which did not gather a qualified majority decision and eventually withdrew its proposal.[11]

European Parliament takes political action

As a major actor in the public debate on glyphosate, the European Parliament entered the discussion and on 22 March 2016, the European Parliament´s Committee on Environment, Public Health and Food Safety (ENVI) presented a motion for a resolution calling for the non-renewal of glyphosate and for the Commission and EFSA to "immediately disclose all the scientific evidence that has been a basis for the positive classification of glyphosate and the proposed re-authorisation, given the overriding public interest in disclosure" .[12] This motion was put to plenary debate and vote and finally, on 13 April 2016, the Members of the European Parliament passed a resolution asking for a seven-year authorisation of glyphosate and to limit its commercialisation for professional uses only, among many other restrictions. This resolution has certainly had an impact on the above-mentioned PAFF Standing Committee "non-decision".

Entropy increases – New assessment, Citizens´ Initiative, Monsanto Papers

In May 2016, a Joint Meeting of the Food and Agriculture Organization of the United Nations (FAO) Panel of Experts on Pesticide Residues in Food and the Environment and the World Health Organization (WHO) Core Assessment Group on Pesticide Residues (JMPR) published a report stating that glyphosate was "unlikely to pose a carcinogenic risk to humans from exposure through the diet."[13] This report uses not only IARC source studies but also unpublished papers.[14] That same month, accusations of conflict of interest of members of this panel appeared, as well as questions regarding the apparently different conclusions of this panel and IARC´s and the comment that "WHO officials maintain there is no contradiction between the two papers, noting that IARC was identifying a potential hazard, whereas the JMPR was quantifying the associated risk."[15]

Taking into consideration the fact that the extension of authorisation period given to glyphosate was June 2016 (and note that the initial authorisation period was to end in December 2015) and not having an EU decision regarding its renewal, nor an agreement with Member States regarding the extension of the authorisation period, the European Commission decided to unilaterally extend (as defined by EU law) the

authorisation period of glyphosate.[16] This extension should allow for the European Chemicals Agency (ECHA) to access the possible hazardous character of glyphosate, as a dossier had been submitted in March 2016 for ECHA to give its opinion in accordance with Article 37(4) of Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.[17] The extension is therefore of 6 months from the date of receipt of the opinion of ECHA or 31 December 2017, whichever is the earlier. By doing this, the Commission also expects that the opinion of ECHA might enable a decision by Member States at the PAFF Standing Committee.

In November 2016, as an outcome of a case opposing NGOs and the Commission where NGOs requested access to confidential environmental information from industry, the Court of Justice of the European Union decided that "when a person requests access to environmental documents, the concept of ' information on emissions into the environment ' covers, inter alia , information concerning the nature and effects of the release of a pesticide into air, water or soil , or onto plants The confidentiality of commercial and industrial information may not be invoked to preclude the disclosure of such information".[18] In the upcoming weeks, EFSA would share redacted documents from the glyphosate review with a restricted number of members of the European Parliament[19] who later requested a full disclosure of these documents.[20] As stated by the European Commissioner for Health and Food Safety, Vytenis Andriukaitis, "the Commission and Member States are currently assessing the consequences of this judgement."[21]

In January 2017, the Commission registered a European Citizens´ Initiative (ECI) named "ban glyphosate" .[22] This initiative invites the Commission "to propose to Member States a ban on glyphosate, to reform the pesticide/herbicide approval procedure, and to set EU-wide mandatory reduction targets for pesticide use". If this initiative gathers sufficient validated signatures before January 2018, the Commission will have to decide whether or not it would act, and explain the reasons for that choice.[23]

Following rumours that the German multinational Bayer wants to buy Monsanto, and the resulting concerns arising among NGOs and Members of the European Parliament,[24] a news report came out, on 14 March 2017, stating that a court from the United States of America had disclosed correspondence from Monsanto which suggested that the company had ghost-written papers which would have been used in the EFSA´s assessment of glyphosate.[25]

Exactly one day after the revelations regarding the "Monsanto papers", ECHA published its conclusion on glyphosate, saying that the available scientific evidence did not meet the criteria to classify glyphosate as a carcinogen, as a mutagen or as toxic for reproduction, thus not classifying it as a carcinogen.[26] As in EFSA´s review, ECHA used both published scientific studies and undisclosed industry studies in its review.

In May 2017, the European Commission questioned EFSA regarding possible implications of the "Monsanto Papers" in EFSA´s scientific review. EFSA clarified that the two papers mentioned in the "Monsanto Papers" and used in EFSA´s review have a minor impact in the overall evaluation and that EFSA mainly used the papers´ raw data to produce its own conclusions.[27]

The Commission will be presenting a new proposal on glyphosate later on this year, which will again have to pass in the standing committee. In the meantime some Members of the European Parliament are calling for an Inquiry Committee to investigate the Monsanto Papers and their implications on glyphosate´s assessment

What´s Next?

As I finish writing this article, there are still many unknowns regarding the future of glyphosate. The Commission will be presenting a new proposal on glyphosate later on this year, which will again have to pass in the standing committee. In the meantime some Members of the European Parliament are calling for an Inquiry Committee to investigate the Monsanto Papers and their implications on glyphosate´s assessment.[28] EuCheMS is also getting involved in the debate and has recently published a series of conclusions from a workshop on glyphosate co-organised with Pavel Poc, Member of European Parliament, and ECTN, where among other measures EuCheMS calls for more transparency in the assessment of

substances by using Horizon 2020 to publicly fund and publicly make available the studies submitted by industry when preparing an application. Whatever is the outcome for this particular substance, it is crucial to support chemists and their research in developing new substances, assessing substances, designing new analytical methods, to keep on the scientific debate and to provide the best available science to policy-makers and to society.

[1] https://enveurope.springeropen.com/articles/10.1186/s12302-016-0070-0
[2] http://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/public/?event=activesubstance.detail&language=EN&selectedID=1438
[3] Directive 91/414/EEC concerning the placing of plant protection products on the market http://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX:31991L0414. This Directive (a EU law that must be transposed into each EU Member State´s national law) was later substituted by Regulation No 1107/2009 concerning the placing of plant protection products on the market (http://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX:32009R1107) (a Regulation is a EU law that is automatically transposed as EU Member State´s national law).
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Bruno Vilela
EuCheMS Public Affairs Officer

Young Chemist Prize

Winner of Ireland's Young Chemist Prize to be awarded prestigious international award at the World Chemistry Congress

The Prize

Every year the Royal Irish Academy awards a prize for the most outstanding Irish PhD thesis in the general area of the chemical sciences. In 2016 the Academy selected Dr Fergus Poynton and his name was put forward for the prestigious International Union of Pure and Applied Chemistry-Solvay International Award for Young Chemists.

International success

The Academy is delighted to announce that Dr Poynton has been selected as one of five winners of the International Award for Young Chemists. The award was presented to Fergus at the World Chemistry Congress in Sao Paulo, Brazil in July. Dr Poynton's thesis was entitled "Spectroscopic investigations into the excited state processes and reactivity of Ruthenium(II) polypyridyl complexes". His novel research explored the (photophysical) properties of a Ru metal ion based complex which can act as an ultrafast light switch in the presence of DNA. It is also possible to determine the nature of the interaction of such complex molecules with DNA to improve our understanding as to how light-activated drug molecules may operate within living cells for phototherapeutic applications. The award winning essay described the thesis work and placed it in perspective to current research in the chemical sciences. A number of publications have also arisen from this research including a feature on the December 2015 issue of Nature Chemistry.

In 2008 the Irish prize winner, Dr Emilie Banide, also won one of the five international awards. In the history of the awards there have only ever been two winners from Ireland.

The Irish Young Chemist Prize was presented to Dr Poynton on 21 June in Academy House.

Professor Pat Guiry, MRIA, Science Secretary, with Dr Fergus Poynton. Image: Johnny Bambury

Following the award of the Royal Irish Academy Young Chemist Prize in June 2017, Dr Fergus Poynton was nominated by the Academy for the prestigious International Union of Pure and Applied Chemistry-Solvay International Award for Young Chemists. Fergus one of five winners of the International Award for Young Chemists and was presented with his award at the World Chemistry Congress in Sao Paulo, Brazil in July.

Dr Poynton presented with his $1,000 prize by Prof Natalia Tarasova, President IUPAC

Prof John Kelly, MRIA, Dr Susan Quinn, Fergus, Prof Clive Williams, MRIA, Prof Thorri Gunnlaugsson, MRIA

Professor Pat Guiry, MRIA, Fergus and Prof Declan McCormack, Vice President, Physical, Chemical & Mathematical Committee

Call for applications for 2017

The call for applications for 2017 Young Chemist Prize will **open** in **November**. For more information please contact the Academy on **youngchemistprize@ria.ie**

PHYSICAL, CHEMICAL AND MATHEMATICAL SCIENCES COMMITTEEGRANTS AND AWARDS

Institiúid Ceimice na hÉireann
Institute of Chemistry of Ireland

Henkel Excellence is our Passion

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

This award has been instituted to recognise the achievement of an individual chemist, or team of chemists, for making a significant contribution to the chemical or pharmaceutical industry in Ireland

1) **Eligibility (Membership):** FICI, MICI (applicant who is not a member can apply for membership at same time, but membership process including entry fee and payment for first year must be completed by closing date for award).

2) **Eligibility (Industry Award):**

a) Employees, a group or principals of the ***chemical, pharmaceutical industry, and related sectors on the island of Ireland, involving work substantially chemical in nature (consideration will be given to self-employed and service sector entries)*** that can clearly show support of industrial chemistry functions.

b) A **Group** or **Team** may be nominated provided at least one member of which is a Member or Fellow of the Institute or whose company/employer/organisation is a member of the Institute and who has played a principal role in the team. This Chemist will be nominated by the team to accept the award on behalf of the group.

c) Current members of Council are not eligible.

d) For former Council members to be eligible, a period of 3 years must have elapsed since the end of their term on Council.

e) Employees of Henkel Ireland and its subsidiaries are not eligible (while Henkel Ireland is sponsor).

3) **Application** must include:

a) 2-page general CV. Candidates may self-nominate or be nominated by their company or organisation.

b) List of publications (3 most significant to be at the top *i.e.* ones the applicant considers best supports their case for award or list of up to 5 significant contributions of the applicant(s) to his/her/their industry based in Ireland accompanied by confirmatory evidence. Such evidence might include technical documents, patents, journal articles, contribution to formulation of industrial standards etc.

c) Brief summary of research/investigational work/developmental work and its particular value (*i.e.* why applicant considers themselves worthy of award).

d) Brief summary (400 words) of article for ICN should applicant be successful (for consideration, *inter alia*, by editor of ICN).

e) Names of 2 referees prepared to support application (and their connection with/knowledge of applicant, including length of time they have known applicant), one of whom (at least) should be FICI/MICI or Fellow/Member of an EuCheMS chemical society (these referees should write a statement of support of 250-400 words to be submitted by the same deadline as applicant).

4) Confidentiality: Applicant should make clear any issues of confidentiality concerning their application, but are advised that any independent adjudicators will only be considering the material for the purpose of award adjudication, and such adjudicators will not be connected with the applicant's employer/organisation.

5) Adjudication: possible shortlisting by ICI sub-committee (depending on the number of applicants, with proviso that sub-committee members initially declare any conflict of interest with respect to applicants) … then an independent panel (2-4 persons) and should include a Council Member, an FICI with an industrial background and a senior representative of the sponsoring organisation. Each to be checked for conflict of interest with respect to group they are adjudicating on *i.e.* in respect of all applicants, or in respect of shortlist, as relevant; panel to carry out their work via correspondence, with tele- or video-conference if necessary.

6) Prize: **a) Award Certificate + b) Memorial Trophy + c) €1000**. The candidate will be required to give a Public Lecture and contribute an Article to ICN. The award will not be arranged until prospective Awardee has agreed date for the lecture and supplied the article for ICN. The Lecture would coincide with date for the formal ceremony for Award.

Awardee's organisation to get free company membership for 1 year (if not already a company member).

7) Publicity: Awardee to provide reasonable assistance to advance publicity for award ceremony, and publicity arising from it; sponsor to be consulted on format/timing and venue of Public Lecture & Award.

Closing Date for Nominations Friday 29th September 2017

Inquiries can be E-mailed to: - info@instituteofchemistry.org

Check website: - www.chemistryireland.org

ENTERPRISE IRELAND
where innovation means business

Recognising the achievements of Ireland's Champions of EU Research

Dublin, Ireland 28th June, 2017.

Pictured above (left to right): Dr. Imelda Lambkin, Director National support network for Horizon 2020 in Ireland, Minister Halligan and Julie Sinnamon, CEO Enterprise Ireland with Des O'Leary, ONCOMARK LTD recipient of a special Horizon 2020 Champion of EU Research Award

Researchers winning equivalent of €2.7 million in Horizon 2020 funding per week

John Halligan T.D., Minister of State for Training, Skills, Innovation, Research and Development with Julie Sinnamon, CEO of Enterprise Ireland will present outstanding achievement awards to academic researchers, companies and research organisations that have reached the pinnacle of European research at 'Ireland's Champions of EU Research' event taking place in the Royal Hospital Kilmainham, Dublin today (Wednesday 28th June, 2017).

Sixteen individuals will receive Horizon 2020 achievement awards for their projects which exhibited outstanding leadership in their respective programme areas.

The aim of the event is to recognise the immense contribution of the award winners and all project leaders from Ireland to our national success in the €75 billion Horizon 2020 EU Framework Programme for research and innovation. Enterprise Ireland is hosting the event on behalf of Ireland's National Support Network for Horizon 2020.

Speaking ahead of the presentation of awards the Minister said "I am delighted to be here today among this impressive and diverse representation of the Irish research community. The breadth of projects nominated for awards today inspires confidence in the continued excellence and dedication to research and innovation in Irish society. I was particularly impressed to note the variety of Universities, Higher Education Institutes, agencies and companies that are competing at the highest levels of European research."

Julie Sinnamon, CEO of Enterprise Ireland added "Today's event celebrates the achievements of collaboration between academic research and industry. Horizon 2020 is an important source of funding for research and innovation and provides a mechanism for researchers and Irish enterprise to network and collaborate with the best researchers and leading companies across Europe. These benefits are particularly important for a small, open economy like ours. The award winners here today are a source of inspiration for others and I'd like to wish them every success with their current projects and in their future endeavours."

A panel discussion at the event will focus on Ireland's success in Horizon 2020 to date, how to maximise participation in the final period 2018-2020 (launching later this year with a budget of €30 billion), and how to capitalise on the opportunities presented by the successor programme which will commence in 2021.

Dr Imelda Lambkin, National Director for Horizon 2020 reiterated that "today is about recognising what has worked well for Ireland's researchers to date and applying that knowledge to position Ireland to make best use of the available funding from Horizon 2020 and FP9. We call on our EU Champions to lead this initiative as role models and mentors".

ENDS

NOTES FOR EDITORS

Horizon 2020 is the EU Framework Programme for research and innovation. It runs over the period 2014-2020 and has a total budget of €75 billion. Ireland's national target of securing €1.25 billion in EU funding is equivalent to 1.67% of the overall Horizon 2020 budget. To date, Ireland has secured funding of €424 million, representing 1.66% of the total EU budget committed.

Enterprise Ireland leads the national support network for Horizon 2020, working to increase participation by Irish companies and academic institutions in the EU's main instrument for funding research in Europe. Led by Enterprise Ireland, the national support network for Horizon 2020 has 9 member organisations; the Department of Agriculture, Food & the Marine, Enterprise Ireland, the Environmental Protection Agency, the Health Research Board, the Irish Research Council, the Irish Universities Association, the Marine Institute, the Sustainable Energy Authority of Ireland and Science Foundation Ireland.

For more information visit www.horizon2020.ie

Download full list of Ireland's Champions of EU Research award recipients

List of winners

1. **European Research Council (ERC) awardees**

Professor Suzanne Kingston, UNIVERSITY COLLEGE DUBLIN for her ERC Starting Grant. Suzanne's project focuses on Legal Architectures: The Influence of New Environmental Governance Rules on Environmental Compliance – it achieved the highest ranking for an Irish applicant for this grant type.

Professor Anna Davies, TRINITY COLLEGE DUBLIN for her ERC Consolidator Grant. Anna's project is SHARECITY: Assessing the practice and sustainability potential of city-based food sharing economies – also ranked highest.

Professor Poul Holm, TRINITY COLLEGE DUBLIN for his ERC Advanced Grant. Poul's project is NorFish North Atlantic Fisheries: An Environmental History, 1400-1700 – also ranked highest.

2. **Recognising the career development of our next generation researchers**

Dr Conor O'Byrne, NATIONAL UNIVERSITY OF IRELAND, GALWAY and Dr Fiona Doohan, UNIVERSITY COLLEGE DUBLIN for leadership of their Marie Skłodowska-Curie Innovative Training Networks in the areas of Understanding and Exploiting Mechanisms of Sensory Perception in Bacteria and training in innovative and integrated control of cereal diseases - both ranked first in their respective calls.

Dr Brian Cahill, INSTITUTE OF BIOPROCESSING AND ANALYTICAL MEASUREMENT TECHNIQUES, HEILBAD HEILIGENSTADT and MARIE CURIE ALUMNI ASSOCIATION on behalf of all of Ireland's Marie Skłodowska-Curie Individual Fellows. Individual Fellowships support the mobility of researchers within and beyond Europe - as well as helping to attract the best foreign researchers to work in the EU.

Professor Jane Ohlmeyer, Chair of the IRISH RESEARCH COUNCIL for leadership of the CAROLINE programme for Collaborative Research Fellowships for a Responsive and Innovative Europe. The CAROLINE Fellowship Programme provides a unique opportunity for 50 researchers to develop their skills, competencies and experience through collaboration with NGOs and International Organisations under the overarching theme of global sustainable development as set out under the United Nations 2030 Agenda.

Professor Linda Doyle, Director of CONNECT, TRINITY COLLEGE DUBLIN for leadership of the EDGE training and development programme for postdoctoral researchers that offers a unique combination of disciplines and industry engagement to the 71 fellows it will recruit. Leveraging the strengths and assets of three Irish National Research Centres, AMBER, CONNECT and ADAPT, headquartered in TCD, EDGE will form the next generation of thought leaders in ICT.

3. **Northern Ireland and North-South successes**

Ms Julie-Ann Walkden, BUSINESS SERVICES ORGANISATION, HEALTH AND SOCIAL CARE NORTHERN IRELAND for leadership of the Northern Ireland-led project, 'Mobile Assistance for Groups and Individuals in the Community' (MAGIC). The MAGIC project is designed to discover innovative approaches to post-stroke care with a view to improving the independence of stroke survivors. This Pre-commercial Procurement project is the only one of its kind on the Island of Ireland, focusing on engaging with industry providers that will compete through several phases of solution development, testing and deployment in live healthcare environments in both Northern Ireland and Italy.

Dr Michaela Black, ULSTER UNIVERSITY for leadership of the MIDAS project on Meaningful Integration of Data, Analytics and Services. The MIDAS consortium is a partnership involving health authorities in five EU countries and the U.S. and technical big data experts from research institutions, MNCs and SMEs. Managing big data for 'health in all' is a monumental challenge for policy makers. MIDAS is developing an integrated solution which will liberate knowledge from data silos and unify heterogeneous big data sources to provide evidence-based actionable information and transform the way care is provided. DCU and IBM Ireland are partners in the project.

Professor Chris Elliot, QUEEN'S UNIVERSITY BELFAST for leadership of the EU-China-Safe project Delivering an Effective, Resilient and Sustainable EU-China Food Safety Partnership. EU-China-Safe will mobilise resources in Europe and China to deliver a shared vision for food safety and authenticity and work towards "mutual recognition". Comprising 15 participants from the EU and 18 from China, EU-China-Safe will develop and jointly implement major advances in improving food safety and combating food fraud in the two trading blocks. Teagasc and UCD are partners in the project.

4. **SME Instruments**

Mr Des O'Leary, ONCOMARK LTD for leadership of the OncoMasTR project developing a Novel Prognostic Assay for Early Stage Breast Cancer: the highest scoring Irish project in the Horizon 2020 SME Instrument. OncoMark, a spin-out from UCD, is developing a novel, game-changing breast cancer prognostic assay which has the potential to transform patient care. OncoMasTR will help clinicians to decide which patients should receive chemotherapy for early stage breast cancer, which is a pressing clinical and economic issue worldwide. OncoMark's plans to release its innovative breast cancer diagnostic test in 2018 have been bolstered by the company's latest investment round. The company ranked first for its Health Pitch at the European Commission's Innovation Summit.

Mr Paul Collins, DP DESIGNPRO LTD for leadership of the DP Renewables project developing a range of HydroKinetic turbines that will enable users to exploit the huge potential of clean, predictable energy in the world's rivers, canals and estuaries: the second highest scoring Irish project in the Horizon 2020 SME Instrument. Europe, as well as many countries around the world, is rich in small and medium-sized rivers and straits between islands. Existing technologies require very fast flow speeds and large deployment spaces in order to make turbine outputs viable. DP DesignPro aims to commercialise a range of innovative, hydrokinetic turbines that will offer a reliable solution for generating zero-carbon energy from rivers, estuaries and canals.

5. **Collaborative Research**

Mr Gal Weiss, IBM IRELAND LTD for achievement of a Horizon 2020 collaborative project portfolio of scale; IBM Ireland is one of the European Commission's Top 50 Companies in Horizon 2020. IBM Ireland has had 18 projects approved with funding of approximately €11 million. Projects span the areas of Information and Communication Technologies with applications in Internet of Things, Health, Energy and Security.

Dr Michael Madden, NATIONAL UNIVERSITY OF IRELAND, GALWAY for leadership of the ROCSAFE Remotely Operated CBRNe Scene Assessment Forensic Examination project under the SECURITY programme – a €4.7 million 13 partner project with Irish partners REAMDA LIMITED, SCORPION NETWORKS LTD, UNIVERSITY COLLEGE CORK, DEPARTMENT OF DEFENCE and the HEALTH SERVICE EXECUTIVE. The overall goal of ROCSAFE is to fundamentally change how CBRNe events are assessed, in order to ensure the safety of crime scene investigators by reducing the need for them to enter high-risk scenes. For this, ROCSAFE will make use of cost-effective remotely-controlled robotic air and ground vehicles that are designed for use in rain, wind, and challenging ground surfaces.

Dr Peter O'BRIEN, TYNDALL NATIONAL INSTITUTE, UNIVERSITY COLLEGE CORK for leadership of the PIXAPP Photonic Integrated Circuits Assembly and Packaging Pilot Line project in the ICT programme – a €15 million 18 partner key enabling technologies project. PIXAPP will establish the world's first open access Photonic Integrated Circuit assembly and packaging Pilot Line. It combines a highly-interdisciplinary team of Europe's leading industrial and research organisations and provides Europe's SMEs with a unique one-stop-shop, enabling them to exploit the breakthrough advantages of PIC technologies. Irish company EBLANA PHOTONICS will work with UCC in the project.

For more information, please contact:

Grace Labanyi

Communications Officer

Enterprise Ireland

How should the world react to US withdrawal from the Paris Agreement? Ignore Trump and get on with the job

Posted by **Michael Rea** | 2 June 2017 | **Viewpoint**

In pursuit of his America First agenda, Donald Trump has announced that he wants America to be the first country to withdraw from the Paris Agreement, just seven months after it entered into force.

With the exception of Nicaragua and Syria, every country in the world signed the Paris Agreement. The overwhelming majority have now also ratified it. They signed it for a very good reason – the consequences of even 2 degrees of warming are severe.

Changing weather patterns and rising sea levels will cause chaos. They can destroy ecosystems and damage the economy. In turn this poses a **real risk to global stability and security**, leading to migration and provoking conflict.

We are **already experiencing** the early effects from record high temperatures and increasingly extreme weather events. The **clock is ticking** and urgent action is needed.

By pulling out of the Paris Agreement, Donald Trump will undoubtedly slow progress in some areas. One of the biggest impacts from US withdrawal is likely to be the loss of climate finance and assistance for developing countries.

Under the Paris Agreement each country pledges its own nationally-determined contributions to global emissions reductions. But many countries made both absolute and contingent pledges, where a higher level of ambition was dependent on receiving international support. Without US federal money on the table, it is likely that some countries will take the easier of the two paths at least in the short term.

However, Trump's actions are unlikely to have any effect on the direction in which the world is travelling, which is increasingly towards a low carbon economy – primarily driven by the business opportunity.

Progress to date is genuinely promising. The **growth in global emissions** has stalled, even as the economy grows. Investment in **coal is collapsing**, with **stocks falling** even in the face of US withdrawal. Renewable energy is **far cheaper than predicted** and being deployed at a faster rate. **Battery technology** is advancing far quicker than expected and the **expectations for electric vehicle sales** are going upwards in an increasingly steep curve.

In the face of US backsliding, **China and the European Union** have stepped forward as global leaders and strengthened their commitments. Other major emitters like India are **increasing their level of ambition** and taking action ahead of schedule.

This isn't being done purely out of a spirit of altruism and goodwill. These countries believe it will give them a competitive advantage, creating wealth and new jobs. This is a business opportunity that could be missed out on by a nation that has a rich history of innovation, but is refocusing its efforts on the economy of the past rather than the economy of the future.

But it is not all bad news. Even within the United States much of the current impetus for action on climate change will be unaffected. This is because the states, cities and businesses that are directly responsible for a large proportion of US carbon emissions are making their own bold commitments to action that will deliver meaningful change.

The **governors of twelve states** representing a population of over 100 million Americans and almost 40 percent of GDP wrote to Trump to affirm their commitment to US commitments under the Paris Agreement, aiming if possible to go further and faster. The newly-formed **United States Climate Alliance** is already moving this forward, with founding members California, New York and Washington.

Mayors are leading the charge locally, as they realise the hard benefits that green energy and clean transportation can deliver for their citizens, as well as understanding the risks of physical damage and disruption to services that climate change can cause. Trump's actions have been strongly opposed collectively by the **US Covenant of Mayors**, with a number of individual cities making their voices heard, such as **Nashville** and **Pittsburgh**.

And US businesses are continuing to boost their own levels of action on climate change and have been calling for continued government commitment. The Silicon Valley titans are on board – with the likes of Apple, HP, Microsoft, Intel, Google, Salesforce and Facebook taking out **full page adverts** to state their support, alongside others huge corporations including Mars and Morgan Stanley.

The CEO of ExxonMobil, America's biggest oil company, wrote personally to President Trump asking him to keep a seat at the negotiating table. And over one thousand companies and investors are signed up to the **Business Backs Low-Carbon** USA pledge, with a host of blue chip signatories including DuPont, NIKE, Kellogg Company, Hilton and Johnson & Johnson

The reason this is all happening is because the evidence is clear and the case for action is unequivocal – or at least it is unequivocal outside of the current US administration. We have finally reached a tipping point where there is a clear and affordable path emerging to achieving a zero carbon world this century. And most governments, businesses and investors have woken up to the severe risks of failure to adapt, as well as the considerable opportunities in doing things better.

When logic and common sense fail in the face of illogical and intractable opposition, there is only one thing to do, which is to ignore Trump and keep taking action on climate change. It is the right thing to do and many of the right things are already happening.

It is time to get on with the job.

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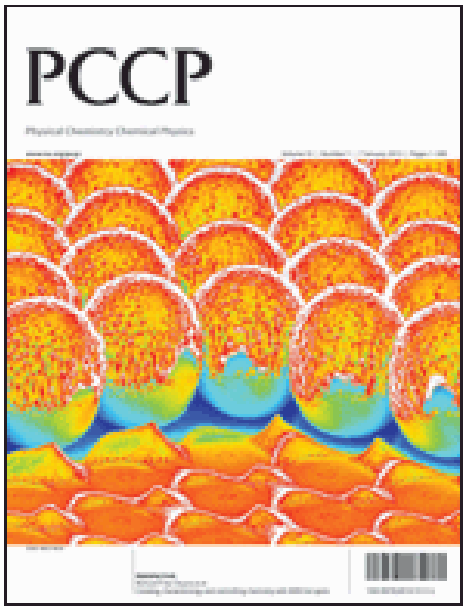

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The journal has a broad scope which includes spectroscopy, dynamics, kinetics, statistical mechanics, thermodynamics, electrochemistry, catalysis, surface science, quantum mechanics and theoretical developments play an important part in the journal. Interdisciplinary research areas such as polymers and soft matter, materials, nanoscience, surfaces/interfaces, and biophysical chemistry are especially welcomed whenever they include a physico-chemical approach.

PCCP is proud to be a Society journal and is co-owned by 19 national chemical societies. The journal is published by the Royal Society of Chemistry on a not-for-profit basis for the benefit of the whole scientific community.

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Synexa Life Sciences opens international HQ in Dublin

August 01 by Editor Denise Maguire

Synexa Life Sciences, a global leader in biomarker services, has announced the opening of its international headquarters in Dublin. The new centre will be home to Synexa's global business development activities and a new Bioinformatics Lab, and is expected to create up to 30 highly skilled jobs over the next five years.

Welcoming the decision by Synexa to open their international headquarters in Dublin, the Tánaiste and Minister for Enterprise and Innovation, Frances Fitzgerald said: "This is a great win for Ireland, bringing high quality jobs involving cutting-edge science and research for the biotechnology and pharmaceutical industry and will help drive the development of new products by the industry. The presence of Synexa here will bring considerable weight to our growing cluster of companies in a niche area of the life sciences sector and build on our existing expertise. I am confident that the company will be able to source the talent necessary, as a result of the Government's commitment to pursuing skills availability for our high technology industries".

Synexa operates biomarker research laboratories in Berlin, London and Cape Town, where the company was founded in 2003 by Irishman Paul O'Riordan (CEO) and two local scientists, Dr. Justin Devine and Prof. Patrick Bouic. Mr O'Riordan qualified as an Irish chartered accountant in 1989, is a member of the Global Irish Network and sees Ireland as the perfect base from which to manage the company's continued rapid growth.

"Ireland has a well-deserved reputation as one of the world's most open and business-friendly environments, making the decision to locate our international HQ here very straightforward. The IDA has been extremely welcoming and professional, and Dublin's rapidly growing ecosystem of high-tech companies, innovative

research institutions and skilled young people makes it a very attractive place to build a business like ours," he said.

Synexa's new facility will include the creation of a Bioinformatics Lab, in which specialised data analysts and machine learning systems will interrogate the data generated in the company's biomarker labs. Mr. O'Riordan believes "that that the richness of insight available about a drug's performance and the ability to identify biomarker-based 'signatures' of response and non-response among patients will mean that bioinformatics analysis will become an essential tool for improving the efficiency of new drug development over the next decade."

Synexa provides biomarker services to the global biotech and pharmaceutical industry. Biomarker analysis helps drug researchers to determine and predict a new drug's safety and efficacy profile, identify likely patient responders and non-responders, and better understand how the drug works. The global biomarker services industry has been growing very rapidly since 2010, as biopharma companies invest heavily in 'precision medicine' solutions – a future in which medical treatment and therapies are tailored to individual patients based on their predicted response or risk of disease.

Commenting on the announcement, Martin Shanahan, CEO of IDA Ireland said: "The decision by Synexa, to locate its International Headquarters in Dublin, marks an important win for Ireland in further developing the pharmaceutical biotechnology sector. The Synexa headquarters will be a welcome addition to the ever expanding life sciences cluster in Ireland and I look forward to working with the company as it continues to grow".

Industry and Business
Promoting Manufacturing Excellence http://www.industryandbusiness.ie

BioMarin expands facility to manufacture medicine for rare genetic diseases

July 31 by Editor Denise Maguire

Simon Coveney, Minister for Foreign Affairs and Trade, has officially opened a new expansion at BioMarin Pharmaceutical Inc. in Shanbally, Co Cork. BioMarin has recently extended its site footprint to 20 acres as the company continues to experience a rise in the global demand for its therapies to treat rare genetic diseases that mostly affect children.

Since opening its doors in 2011, the company has grown to 365 employees in Cork, with an additional 67 people based in Dublin and 2,400 employees globally. BioMarin focuses on developing first--in-class and best-in-class therapeutics that have the potential to improve clinical outcomes of patients with rare genetic diseases. The company currently has six approved products that are the only drugs available on the market today for the diseases they treat.

This expansion project began two years ago to cater for continued growth at the site and includes an expanded warehouse, new administration and utilities offices, a canteen and conference facilities. The overall project will allow the company to maximise the flexibility of the site with the expansion of the operational manufacturing capacity. The site will also see the installation of a Waste Water Treatment Plant later this year, while three new lab expansions are to be completed by Q3 2018.

Jean-Jacques Bienaimé, Chairman and Chief Executive Officer of BioMarin stated: “Ireland has proved to be an ideal location to expand our operations. The team at Shanbally has enabled us to accommodate our growing commercial portfolio and advancing clinical programs. Mostly children, our patients suffer from diseases so rare that the entire afflicted population may number as few as 1,000 worldwide. Often inherited, difficult to diagnose, and progressively debilitating, these conditions have, up until now, been largely ignored. As we continue to grow in Shanbally, we are looking to recruit the best and brightest in a variety of disciplines to help us continue our inspiring work for patients.”

Welcoming the expansion, Simon Coveney said: “Today’s announcement represents a significant investment in the local economy. Shanbally is BioMarin’s only manufacturing facility outside the US and what they have done in such a few short years is very impressive. The company is continuing to grow and I understand that there are up to 50 open positions across a variety of departments at Shanbally waiting to be filled. BioMarin is a prime example of the high--tech Life Sciences companies that this area of Cork has a reputation for.”

CEO of IDA Ireland Martin Shanahan said: “I am delighted that BioMarin continues to consolidate its commitment to its Irish operations in Shanbally. The company’s presence in Cork strengthens Ireland’s global reputation as a biopharmaceutical industry leader and brings high quality jobs to countless people across the south-west region. We look forward to working closely with the company as it further develops its operations here.”

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GSK opens new €8m state of the art biomass energy plant at Dungarvan site

June 26 by Editor Denise Maguire

GSK has announced the opening of an €8 million investment project at its manufacturing site in Dungarvan. The facility was officially opened Friday 23 June, by Site Director Brian Fox. The investment has been utilised to develop a new purpose-built biomass energy facility which is expected to reduce the site's carbon emissions by up to 33%. The facility uses locally sourced woodchips to create a carbon neutral fuel source for the site.

The development of the biomass energy facility in Dungarvan is part of GSK's global sustainability strategy which supports the company's carbon neutral policy. This policy has set challenging carbon, water and waste reduction targets for all GSK manufacturing sites across the world. Dungarvan has responded with significant reductions in energy usage across its plant, delivered by highly efficient, world class engineering and energy management systems. The biomass energy facility also utilises a sustainable fuel supply as the wood chip it burns is made from waste wood by-product and the ash produced is used in fertiliser, which grow more trees.

GSK, who this year celebrate 35 years in Dungarvan, employs over 700 employees at two sites in the area: The '*oral care'* facility produces a range of products including *'Poligrip'* – the denture care range formulated to improve the comfort and oral health of people who wear dentures or partials. The facility produces 40% of the world's supply of denture care products under the *Poligrip* and *Polident* brands. The '*over-the-counter'* medical site produces a variety of medicinal products such as Panadol. Approximately 6.5 billion Panadol tablets are produced in Dungarvan each year – that's 150 Panadol tablets per second which are then exported to 70 countries worldwide.

The announcement follows two recent investments made by GSK in the Dungarvan facility:
€8 million was invested in the implementation of a new environmentally friendly packaging line that utilises a 100% recyclable material called Polypropylene. This offers a sustainable solution for the production of

‘blister’ packaged products as it allows the entire blister pack to be manufactured from one recyclable material.

GSK also invested in a €7.2m extension to the denture care facility in 2017 to expand tablet compression and packaging capacity.

Brian Fox, Site Director at GSK Dungarvan, commented: “This investment from GSK is a significant vote of confidence in the Dungarvan facility, as well as in the capabilities of the town and people of Dungarvan to support such strategic developments. GSK is in Dungarvan 35 years this year and this investment will underpin our existing investments here and our sizeable workforce. It will also significantly enhance Dungarvan’s role in GSK’s global business and today’s investment is a strong recognition of the strong technical and scientific capability we have here.”

Kevin Meehan, Engineer Director, GSK Dungarvan added: “This substantial investment in the new biomass facility demonstrates our strong commitment to sustainability and to the local community. We also worked with local suppliers on the build and are using locally sourced woodchip to run the facility as well. GSK Dungarvan has a highly skilled engineering team across multiple disciplines that ensures the facility continually operates to world class standards. The success of the Biomass Energy facility is a testament to their skills in electrical, mechanical and automation engineering.”

About Sigma-Aldrich: Sigma-Aldrich is a leading Life Science and High Technology company whose biochemical, organic chemical products, kits and services are used in scientific research, including genomic and proteomic research, biotechnology, pharmaceutical development, the diagnosis of disease and as key components in pharmaceutical, diagnostics and high technology manufacturing.

Sigma-Aldrich customers include more than 1.3 million scientists and technologists in life science companies, university and government institutions, hospitals and industry. The Company operates in 35 countries and has nearly 9,000 employees whose objective is to provide excellent service worldwide.

Sigma-Aldrich is committed to accelerating customer success through innovation and leadership in Life Science and High Technology.

For more information about Sigma-Aldrich, please visit its website at **www.sigma-aldrich.com**

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Construction to start on GCP2 Production Facility at Takeda Ireland Ltd site

June 01 2017 by Editor Denise Maguire

Takeda Pharmaceutical Company Limited has announced that a groundbreaking ceremony has been held for its new production facility at the existing Grange Castle site in Ireland. Takeda's existing footprint at the Grange Castle site will be expanded with the construction of a new standalone, high-containment production facility dedicated to manufacturing its oncology product NINLARO for global markets. The investment will create approximately 40 new jobs over the next two years.

"Our new plant in Grange Castle, Ireland is a strategic investment for Takeda," said Thomas Wozniewski, Head of Global Manufacturing & Supply. "It will give us the crucial in-house manufacturing capacity to meet the increasing demand for our innovative product NINLARO."

The construction of the plant, which begins in June 2017, will be managed by Project Management Group with over €40 million investment in total. The plant is scheduled to be completed in Q2 FY18 and become operational to commence shipment of secondary packaged product in the second half of FY18.

The new production facility will be unique in that it will house the Drug Substance, Drug Product, Primary and Secondary Packaging and QC processes all under one roof.

NINLARO was approved in November 2015 by the U.S. Food and Drug Administration (FDA). It is the first and only once-weekly oral proteasome inhibitor launched in the U.S. for the treatment of patients with multiple myeloma who have received at least one prior therapy, enabling an all-oral proteasome inhibitor-based triplet treatment regimen for the first time. Additionally, NINLARO® was approved by the Japanese Ministry of Health, Labour and Welfare in March 2017 and launched in May as the first oral proteasome inhibitor in Japan, indicated in combination with lenalidomide and dexamethasone for patients with relapsed or refractory multiple myeloma.

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Abbott and IDA Ireland announce investment of €10m to fund Sligo site relocation

May 31 2017 by Editor Denise Maguire

Global healthcare company Abbott will relocate its Irish Nutritional Devices business from its existing base at Ballytivnan, Sligo, to a new, purpose-built IDA Ireland Advance Technology building located in the Finisklin industrial estate.

The move will see a combined investment of almost €10 million and will enable the consolidation of manufacturing and business support within one building, enabling the creation of a medical nutrition device centre of excellence. This move also provides space for any additional manufacturing and support positions should they be created by the company in the future.

The aim is for the relocation to be completed in the first half of 2018 following work to extend the Finisklin building. This investment is supported by the Department of Jobs, Enterprise and Innovation through IDA Ireland.
Sean O'Hara, Abbott's Site Director at Ballytivnan said: "Our aim is to enable people to live fuller, healthier lives. The talent available in Ireland is key in enabling us to do so. This relocation and investment ensures our people in Sligo can continue to help people all over the world lead healthier lives full of unlimited possibilities."

CEO of IDA Ireland Martin Shanahan said: "IDA-supported multinational companies contribute significantly to Ireland in terms of direct employment, capital spend and developing Ireland's skills base. Abbott has a long history of investing in Ireland and valuing the talent and business infrastructure which is available nationally and in the business location of Sligo. Abbott is of key importance to Ireland's life sciences sector and contributes substantially to Ireland's export economy. The decision to proactively build properties to attract foreign investors into regional locations has been further evidenced by Abbott Nutrition's decision to move over 100 existing staff members into the newly built IDA Advance Technology building which will also provide scope for the company to grow in the future."

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GMIT to double its Innovation Hub space

May 23 2017 by Editor Denise Maguire

Galway-Mayo Institute of Technology (GMIT) is set to double the size of its Innovation Hub (iHub) building at the Galway campus following €5 million funding approval from Enterprise Ireland. Minister for Jobs, Enterprise & Innovation Mary Mitchell O' Connor announced the funding details during a visit to GMIT today (Thursday 18 May), welcomed by GMIT President, Dr Fergal Barry, Enterprise Ireland Director – West Region Barry Egan, and Dr Rick Officer, VP for Research & Innovation, GMIT.

Enterprise Ireland will contribute €3 million towards the cost of the building extension while GMIT will provide €500,000; Enterprise Ireland also approved funding of €1.8 million for the New Frontiers Programme 2016 – 2020 which is delivered in GMIT's two Innovation Hubs by New Frontiers Manager Tony O'Kelly.

New Frontiers is Enterprise Ireland's national entrepreneur development programme for innovative, early stage start-ups. Previous participants on the GMIT New Frontiers programme include DiaNia Technologies, Contego Sports, TaxHug, Allergy Lifestyle, Wildwood Vinegars, Rockfield Medical, BriteBiz and VT Networks.

GMIT's Building & Estates Office are in the process of appointing a design team for the extension works. It's hoped that construction work will commence in 2018. The proposed extension aims to increase the floor space of the iHub to 2,400 square metres from its current 1,150 sq m.

Welcoming the Minister, Enterprise Ireland staff and guests to the iHub, GMIT President, Dr Fergal Barry, said: "The Institute has further plans to develop enterprise and innovation space in all of its campuses. The extension of our iHub will allow GMIT to continue to support the development of export orientated Irish businesses with a particular focus in the Medical Device industry integrating our Innovation activity with our long establish excellence in research in this field and our newly launched undergraduate degree in biomedical engineering. Recently we also established a new Creative Hub for gaming projects, animation features and TV projects at our Centre for the Creative Arts and Media here in Galway city. We hope that the cumulative total of job creation supported though our Enterprise centres in all our campuses will double and that the number of companies supported annually will increase."

GMIT's Innovation Hubs have contributed significantly to the economic and social development of the region since their establishment in Galway and Mayo 10 years ago. The iHubs are currently fully occupied, accommodating some 46 enterprises. Client companies currently occupying the iHubs include Marvao Medical, OneTouch Telecare, Capsos Medical, Rockfield Medical, BlueDrop Medical, Kite Medical, GIRT, CALP, Cloud Strong, Siscin, Traffic Attic, Tr3Dent and Happy Media to name a few.

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Mallinckrodt to create 45 jobs at new Dublin Centre

May 16 2017 by Editor Denise Maguire

Pharmaceutical company Mallinckrodt has reported it is to create 45 high-skilled jobs at its new medical device engineering centre in Blanchardstown in Dublin. The jobs will be in a range of areas including product design, software development and electro-mechanical engineering.

The company's new centre in Blanchardstown has been set up to consolidate its global device research and development activities. An investment of €95 million has been made in the centre and the latest project is being supported by the Department of Jobs, Enterprise and Innovation through IDA Ireland.

Mark Trudeau, the company's president and CEO, said that Mallinckrodt has had a significant manufacturing and business presence in Ireland for almost a quarter of a century. "This new global device engineering facility allows us to centralise our device R&D skills and expertise in developing the next generation of products for a number of important and rare conditions to make a significant difference to the lives of patients," Mr Trudeau added.

Mallinckrodt has also said it has formed a new corporate partnership with the Coolmine Therapeutic Community. Coolmine provides day and residential services to men and women with problematic substance use and their families in Ireland. Mallinckrodt is granting initial financial support of €15,000 to Coolmine.

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SFI to invest €72 million in new Research Centres

May 03 2017 by Editor Denise Maguire

Science Foundation Ireland has announced it will invest €72 million over the next six years in four new world-class SFI Research Centres in Ireland. The new SFI Research Centres will be supported by 80 industry partners who will provide an additional €38 million to support cutting-edge basic and applied research with strong industry engagement, economic and societal impact. The decision follows a comprehensive international peer review process involving leading industry and academic experts over the last 12 months.

Innovation 2020, the Government's five-year strategy for research and development, science and technology, directs that the network of SFI Research Centres should be further developed to build critical mass in strategic areas of research strength and address enterprise needs.

The announcement marks the third tranche of funding under the SFI Research Centres Programme. The first seven SFI Research Centres were established in 2013 and a further five were established in 2015. These 12 world-leading SFI Research Centres are recognised internationally for research excellence; attract talent and capital to Ireland; anchor, attract and spin-out businesses; consolidate excellent basic and applied research across Higher Education Institutions; and secure EU and other international funding.

The four new SFI Research Centres will address the following:
– Smart manufacturing IT and industrial automation systems, led by Prof Conor McCarthy, University of Limerick
– Biological resources as alternative materials to finite fossil resources, led by Prof Kevin O'Connor, UCD
– Innovative techniques and processes in Additive Manufacturing, led by Prof Denis Dowling, UCD
– Diagnosis, monitoring and treatment of chronic and rare neurological diseases – led by Prof David Henshall, RCSI (Project Title – Future Neuro).

Professor Mark Ferguson, Director General of Science Foundation Ireland and Chief Scientific Advisor to the Government of Ireland said: "Our existing 12 SFI Research Centres are outstanding international examples of applied and basic combined (ABC) research. They are making important scientific advances, enhancing enterprise and industry, developing critical skills, supporting regional development, and enhancing Ireland's international reputation. They are drivers of Ireland's increased rankings in research and innovation over the last number of years. They are also an important engine for the economy; companies engaged with the SFI Research Centres are located all over Ireland and globally. The commitment of industry and academic bodies to come together to develop these new SFI Research Centres clearly demonstrates the potential economic and societal impact of the planned research. I look forward to working with the four new SFI Research Centres on their road to becoming world-class centres of research excellence."

Four further SFI Research Centre proposals were approved in principle by the SFI Board following stringent assessment by international peer review. SFI is seeking additional funding to support these centres over the next six

years. These proposed SFI Research Centres involve collaborative partnerships with over 100 companies who have committed €60 million funding to the centres.

The new SFI Research Centres will be formally launched in September 2017.

MSD to invest in Tipperary plant

May 03 2017 by Editor Denise Maguire

US drug company MSD is set to invest €40 million in its manufacturing facility in Co Tipperary this year, as it installs new technology used to improve a number of products. The investment will bring the total MSD has spent over a three-year period upgrading the Tipperary facility to €75 million.

New technology being installed includes a spray drying facility, which is used in the production of a number of new products to increase their solubility and improve how they are absorbed by patients. The MSD plant has been operating for 41 years and exports to 30 countries, including destinations in Europe as well as the US and Japan.

Ger Carmody, the site lead at the MSD plant in Ballydine, said the investment reflects the growing importance of MSD Ireland's operations in the group's global network. He said the workforce at the plant was "leading the way" in the development of new medicines including MSD's treatment for Hepatitis C, which is being manufactured at the factory.

The company employs more than 1,800 people in Ireland across its facilities here, which include manufacturing, commercial, global finance services, and marketing.

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Diaceutics signs multi-million-euro partnership with BioReference Laboratories

Irish data insights and solutions company Diaceutics has announced a five-year multi-million-euro partnership with US-based BioReference Laboratories. The partnership will see Diaceutics acquire real-time testing data from BioReference, allowing it to help pharmaceutical companies achieve faster rollouts of new drugs through better understanding of the US diagnostics market.

Through its partnership with BioReference, which works with 30,000 healthcare providers across the US, Diaceutics will have access to data from 50,000 patient samples per day. Coupled with insights from BioReference, the real-time data will help improve patient testing by ensuring that pharmaceutical companies better understand the testing patterns of physicians considering precision medicine therapies for patients.

Currently, Diaceutics estimates that pharmaceutical companies are missing out on more than 20% of cancer patients every year in the US due to the challenging diagnostic landscape. With 70% of new drugs in the next five years expected to be test-dependent, Diaceutics expects that percentage will increase.

Peter Keeling, CEO, Diaceutics, said: “Diagnostic data from laboratories like BioReference helps pharmaceutical companies better understand the testing journey that patients go on in the often difficult search for a targeted therapy. That information allows pharma to pinpoint patients that need to be on a specific – and often life-changing – drug, accelerate speed to market for new drugs and improve patient outcomes.”

Diaceutics will integrate the data gathered from BioReference with its existing lab data accumulated through partnerships with other labs. Together, the data will allow Diaceutics to provide pharma with more complete, aggregated testing data that meets their very specific requirements – helping them to close the 20% patient gap in the oncology testing market and achieve a better return on new drug investments.

Keeling continues: “Timing is key for many patients Diaceutics strives to increase the number of patients correctly tested, therefore increasing the demand for new drugs – an attractive prospect for pharmaceutical companies – and ultimately significantly improving patient outcomes.

“We have seen first-hand the improved decision-making by our pharma clients when presented with the relevant data trends in specific disease areas. Enriching our real time and retrospective analytics with BioReference’s knowledgebase allows us to further map the diagnostic journey of patients and help pharmaceutical companies better understand how testing impacts precision prescribing. With this information, we can simply enable better decision making and investment in patient, physician and laboratory education.”

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