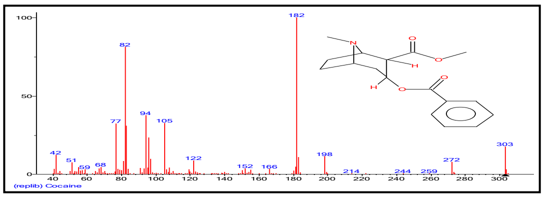
Irish Chemical News

The Journal of the Institute of Chemistry of Ireland

Feature Articles:-

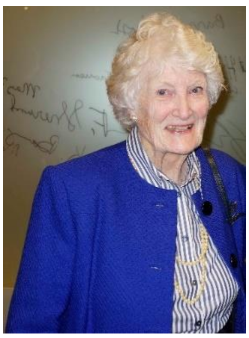
Eva Philbin Lecture 2016, Every Breath You Take, Prof John Sodeau

A Rapid Non-Destructive Extraction and GCMS Analysis Method for the Determination of Illicit Drugs



apc **Company profile**

Royal Irish Academy, Cunningham Medal, Prof Dervilla Donnelly



Irish Chemical News

Originated 1922
Incorporated 1950

The Institute of Chemistry of Ireland

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The Professional Body for Chemists in Ireland

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UHPLC
HPLC
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HPLC
<6000 psi
UHPLC
6000 – 15,000 psi
UPLC
9000– 15,000 psi
FLOW RATE
HPLC typically <3 mL/min
UHPLC typically <2 mL/min
UPLC typically <1 mL/min
OPTIMAL PARTICLE SIZE
HPLC ≥3.5 µm
UHPLC 1.5–5 µm
UPLC <2 µm
COST PER SAMPLE
HPLC
UHPLC
UPLC
OPTIMAL COLUMN I.D.
HPLC ≥4.6 mm
UHPLC 2.1– 4.6 mm
UPLC 1–3 mm

A Message from the President

Dear Fellows, Members, Graduates and Associates,

As I write this, I am nearing the end of my term of office. I should like to pay tribute to our Council Members who have served with me over the past two years. Thanks are due, in particular, to our long standing Honorary Secretary, Philip Ryan, who has served in this capacity for the past three decades. I also want to thank our Honorary Treasurer, John Keegan, who takes care of the finances. They are both assisted in their respective roles by our very efficient Executive Secretary, Maureen Moloney. I would like to thank her for her support in so many ways. I am most grateful also for the help and support of the Immediate Past President, Pat Hobbs, who handed over to me in 2015. In addition, he has taken on the role of Editor of this publication, 'Irish Chemical News' and has made it a great success, with a greater frequency of publication and a wide variety of content.

Apart from the officers and ordinary Council members, I acknowledge the work done by the various committees. We have standing committees dealing with Qualifications, Professional Affairs, Education, Environment, Recruitment, Industry, the Editorial Board and the Young Chemists' Group. We would welcome a greater input from our members into the work of the committees, as it so happens that the same handful of dedicated people are serving on several committees. For some of them, this has proved to be too much of a workload and as a consequence, some of the committees are not very active. We would like to have a greater input from members who work in industry and the public service, as most of our active members are from an academic background. In particular, we would welcome additional members to serve on the Professional Affairs Committee and on the newly formed Environmental Committee. If you have an interest or expertise in either of these areas, please let us know. Please note that it is not necessary to be on Council, in order to serve on a committee.

There are also *ad hoc* committees to organize events, such as the Annual Congress and the Awards. We have Regional Representatives, who organize events in the Regions and I would like to thank them for their dedication to the Institute and for their good work in promoting Chemistry outside of Dublin.

This issue of 'Irish Chemical News has a notice of our AGM, which will takes place in the Royal College of Surgeons on April 27th. I encourage as many members as possible to come along and make your voice heard. The Boyle-Higgins Award lecture will be given by Professor Henry Curran of NUIG on the same day, also at the RCSI and there will be a wine and finger food reception between the two events. Details of this award are also given in this issue. So please come along, enjoy the lecture and the refreshments and avail of the opportunity to do some networking with colleagues before the AGM. I look forward to seeing you there.

Margaret Franklin, FICI,

President,

The Institute of Chemistry of Ireland. February 2017

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Editorial

This, the first Issue for 2017 is I hope the first of 6 bimonthly Issues this year. It's a little delayed by something beyond my control and I expect the Issue 2 in late April. The regularity of publication is in large determined by timely receipt of papers. This is up to you members and contributors. I appreciate that most people are very busy but please try and submit in time for preparation and checking before publication.

The lead paper is from Prof John Sodeau, UCC, winner of this year's Annual Lecture Series Award (Eva Philbin Lecture 2016) titled "Every Breath You Take" presented with some humour, active links and some effort on you the reader to read deeper on the subject.

This is followed by an article on determination and analysis of illicit drugs by Dr Philip White GMIT. Then we have a profile on a very interesting new company APC, which was founded in UCD in 2011 by Prof Brian Glennon and Dr Mark Barrett from the School of Chemical and Bioprocess Engineering, UCD, and is now located nearby in South Dublin. This company employs many chemists and chemical engineers with close links and crossover between the two professions.

The Institute Council are delighted to hear that our former President Prof Devilla Donnelly has been nominated to receive this year's prestigious Cunningham Medal from the Royal Irish Academy. A short article on this award and Prof Donnelly is included. I hope to bring more on this in a later Issue.

Eurachem Ireland have provided 3 posters from the conference 'Food, Health and the Role of National Reference Laboratories' held in the State Laboratory last year. I have a number of reports provided by Industry and Business arm of Premier Publishing Ltd. This company organized a number of very large joint conferences in late January and mid February on Manufacturing & Supply, Sustainability and Research and Innovation. These were well attended with many chemistry topics and environmental presentations. I expect these events to generate some papers for publication in later Issues this year.
These events are free to attend and I encourage chemists to attend these annual conferences next year. This issues concludes with some IDA reports.

The Institute is delighted to announce the 3rd Industrial Chemistry Award 2017 sponsored by Henkel. See inside.

I would welcome feedback from readers and suggestions for improvement. Please let me know what topics you would like to have covered. I am always happy to receive chemistry papers about your research and your company whether national or multinational or a chemistry related service you provide.

I want to draw your attention to a number of events coming up and most important is our Boyle Higgins Gold Medal Award Lecture 2017 to be given by Professor Henry Curran in the RCSI on 27 April followed by our AGM. Our Annual Congress follows later in June at DIT Aungier Street. Two events are coming up in DCU, Pharmaceutical Regulatory Symposium on 15th of March and ESAFORM Conference on Material Forming – ESAFORM 2017 during from 26th – 28th April 2017. Eurachem Ireland have a workshop on April 25th. Somewhat later in 2018 the 7th EuCheMS Chemistry Congress will be held in Liverpool and researchers need to prepare now and be ready to make a big impression. There are flyers throughout this publication with more details of these important events.

I'm really not happy with the cover design so any suggestions for improvement are very welcome.
Send your ideas and suggestions to the institute email:-

info@instituteofchemistry.org

Patrick Hobbs
Editor
Irish Chemical News
Institute of Chemistry of Ireland

FIRST NOTICE

ANNUAL GENERAL MEETING

THURSDAY 27 APRIL 2017

Notice is herewith given that the Sixty-Eighth Annual General Meeting of the Institute of Chemistry of Ireland will be held in **THE ROYAL COLLEGE OF SURGEONS IN IRELAND, ST STEPHENS GREEN, DUBLIN 2, ON THURSDAY 27 APRIL 2017 at 6.30pm.**

All members of the Institute are invited to attend.

Members are entitled to submit nominations for Council on the accompanying form, which must be returned no later than Thursday 30 March 2017.

Candidates for election must be proposed and seconded by members of the Institute and indicate on the nomination form that they are willing to be on Council if elected.

Members with FICI, MICI or LICI may act as proposers or seconders. Members with FICI and MICI may serve on Council but only Fellows may serve as President or Vice President.

In accordance with Article 62 (a), the choice of Council for the office of President is Prof John F. Cassidy FICI (DIT) and the choice of Council for the office of Vice President is Prof Celine Marmion FICI (RCSI). This does not preclude other nominations.

In accordance with Article 34 (2), the Honorary Secretary, Dr James P Ryan FICI, EurChem, and the Honorary Treasurer, Dr John R Keegan FICI, EurChem, retire. Both have agreed to go forward for re-election.

There are three vacancies for Ordinary Membership of Council.

The full Agenda for the AGM, together with the ballot papers if necessary, will be made available after the close of nominations.

An electronic copy of the 2016 AGM Minutes is available to *bona fide* members of the Institute by sending an email request to the Honorary Secretary at < info@instituteofchemistry.org >.

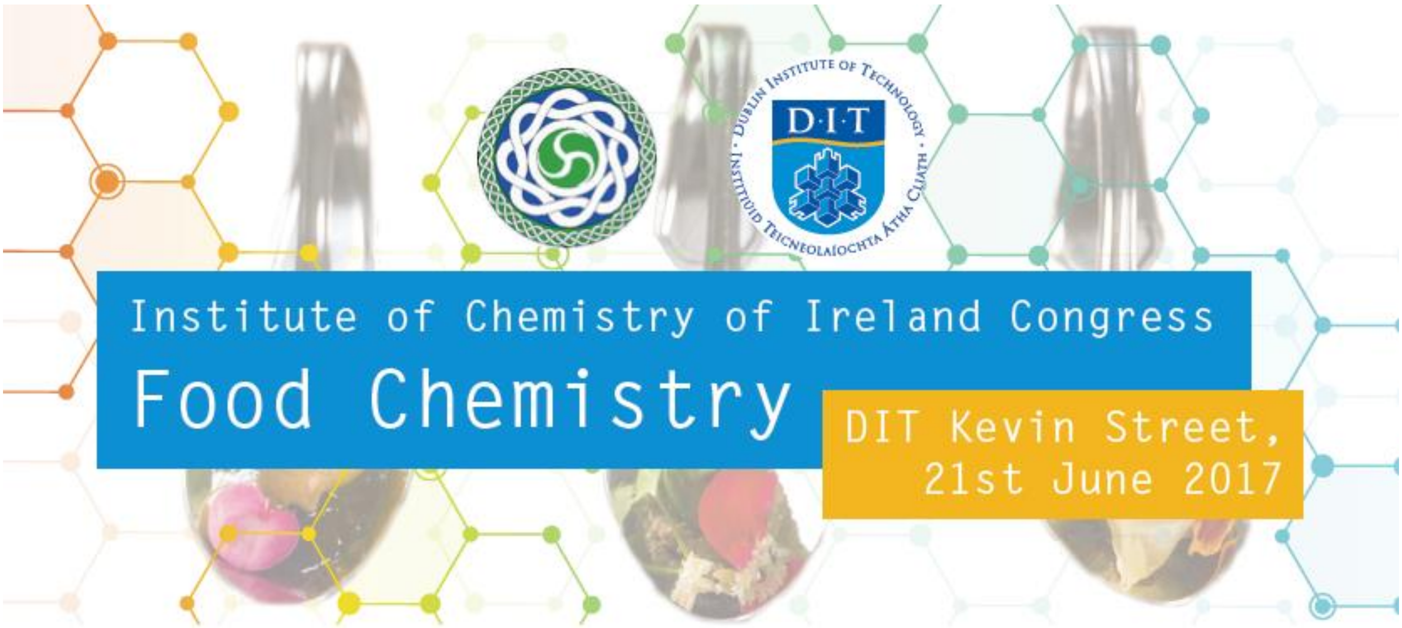
The AGM will be preceded by the 2017 Boyle Higgins Lecture given by Professor Henry Curran FICI (NUI Galway) at 5.00pm. This will be followed by a finger food reception. The title of this year's lecture is '*Developing Detailed Chemical Kinetic Mechanisms for Fuel Combustion*.'

Yours sincerely,

James P. Ryan

Dr James P. Ryan, FICI EurChem

Honorary Secretary



A full day conference consisting of Oral and Poster Presentations.

Sensory Aspects of food - Overview ; flavours, taste, colour, culinary aspects. Aesthetics of food related to chemical components; how are these are related to chemical components.

Sampling and analysis- challenges of sampling and analysing a heterogeneous material, quantitation of components, residue analysis, novel means of food characterisation

Functional Ingredients- Recent developments in the area, formulations, treatment of food, freeze drying; adulteration, nutraceuticals.

Oral presentations from

Dr. John Keegan (Public Analysts Laboratory)
Prof. Seamus O Mahony (UCC)
Prof.. Vitaly Buckin(UCD)
Dr. Maria Hayes (TEAGASC)
Prof. Jean-Christophe Jacquier (UCD)
Dr. Edward Malone (State Laboratory)
Dr Jesus Frias (DIT)
Ms. Charlene Connolly (Monaghan Mushrooms)
Mr. Tony McGorisk (Kerry Group) and plenary lecture from
Prof. Herve This (Institut National de la Recherche Agronomique)

Submission of poster titles to john.cassidy@dit.ie .

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).

Institute of Chemistry of Ireland

Boyle Higgins Gold Medal Award Lecture 2017

will be given by

Professor Henry Curran

'Developing Detailed Chemical Kinetic Mechanisms for Fuel Combustion'

in the Royal College of Surgeons in Ireland, St Stephens Green, Dublin 2, at 5.00pm on Thursday 27 April 2017

The lecture will be followed by a **Reception** and the **ICI AGM**

Professor Henry Curran

Director of The Combustion Chemistry Centre
C-209, School of Chemistry
Professor, Department of Chemistry
Room 215, Arts/Science Building
NUI Galway

Abstract

Developing detailed chemical kinetic mechanisms for fuel combustion

Stricter emissions legislation combined with the need to reduce greenhouse gas emissions in order to militate against climate change drives fundamental research to produce cleaner, more efficient systems. Chemical kinetic mechanisms are used by relevant industries to predict and optimize the operating behaviour of combustion facilities used to produce energy such as internal combustion engines, gas turbines and other devices. By combining chemical mechanisms with computational fluid dynamics simulations allows for the accurate prediction of combustion which can lead to the design of cleaner, more efficient energy generation systems.

The Combustion Chemistry Centre, **C³** is engaged in fundamental research on the combustion of fossil- and bio-fuels. Combustion is the ultimate interdisciplinary field: it requires knowledge of chemistry, physics, fluid dynamics, thermodynamics and mathematics. In addition, combustion science has a well-defined purpose in society today, facilitating the study and analysis of problems associated with the generation of air pollutants. **C³** is concerned with the application of combustion research to the design of energy-efficient engine and gas turbine combustion systems and the impact of their use on toxic and greenhouse gas emissions, thus helping address the problems of urban air pollution and climate change.

The strategic goals of the Combustion Chemistry Centre are to:

- Promote the sustainable and efficient use of energy in transport

- Maximise energy efficiency and energy savings across the economy
- Deliver an integrated approach to the sustainable development and use of bio-energy
- Address global warming by reducing energy-related greenhouse gas emissions
- Accelerate energy research development and innovation in support of energy goals

The coupling of experimental chemical combustion studies in our shock tubes and rapid compression machine facilities, with detailed kinetic modelling is a unique feature of our research centre. In fact, the group is the only one in Ireland producing experts in the area of combustion. With the Government's decision to license large-scale incinerators for municipal waste, trained graduates with expertise in incinerator processes will be required. Currently, **C^3** is the only centre in Ireland with the expertise to train researchers for this growing industry.

However, in order to validate and produce accurate detailed chemical kinetic mechanisms in the first instance, a wide range of data is needed, and which is normally generated under well-controlled physical conditions of temperature, pressure, fuel/air ratio and dilution. These data include (i) ignition delay times recorded in shock tubes and in rapid compression machines, (ii) speciation data from flow reactors, jet-stirred reactors and flame experiments and (iii) flame measurements of laminar burning velocity. Typically, these mechanisms for hydrocarbon and oxygenated hydrocarbon systems are generated in a hierarchical way, starting first with the hydrogen/oxygen system, thereafter adding a carbon monoxide/carbon dioxide subset, followed by formaldehyde, methane and other larger C_1–C_n species.

This work will discuss the development of detailed chemical kinetic mechanisms in the context of hierarchy and range of validation. Some typical problems associated with these mechanisms will be discussed and some ideas on how they may be addressed will be explored. Moreover, the application of detailed kinetic mechanisms to fuel flexibility in gas turbines will be explored in some more detail.

Past Recipients

The Boyle Higgins Gold Medal and Lecture Award, instituted in 1985, is an award for research work carried out in chemistry under the headings: (a) Pure Chemistry, (b) Applied and Industrial Chemistry or (c) Chemical Education. The award is made for an outstanding and internationally recognised research contribution to the advancement of chemistry by a chemist of any nationality working in Ireland or by an Irish chemist working overseas.

Prof Duncan Thorburn Burns

Prof Albert Pratt

Dr Peter E. Childs

Prof Seán Corish

Prof M. Anthony McKervey

Prof Frank Hegarty

Prof David A. Brown

Prof Malcolm R. Smyth

Prof Richard N. Butler

Dr Sheila Willis

Prof Dervilla M.X. Donnelly

Prof Patrick J. Guiry

Dr John F. O'Sullivan

Prof Dermot Diamond

Prof Donald Fitzmaurice

Prof Henry Curran

Prof Rory More O'Ferrall

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#

Eva Philbin Lecture 2016

Every Breath You Take

John Sodeau

Department of Chemistry and Enviromental Research Institute

University College Cork

John Sodeau has been Professor of Physical Chemistry at UCC since 1998; he became Emeritus Professor there in September 2016. Before that time he worked as a postdoctoral Fellow and Lecturer at University California Irvine (UCI), later progressing to a Readership at the University of East Anglia in UK.

His research interests have been in the area of Photochemistry since his PhD work in identifying species generated by light and trapped at low temperatures. The studies naturally progressed to research in Atmospheric Science because the chemical processes involved are driven essentially by sunlight. Most of his research now is in real-time sensing of bioaerosols for application in pollen counting, hospital monitoring and green-waste site management.

Abstract

This article represents a flavour of the Eva Philbin lectures presented in 2016 and 2017 at University College Cork, Dublin Institute of Technology, Limerick Institute of Technology and Waterford Institute of Technology. However, some spices are added from a further lecture made at the National Sustainability Summit held in January 2017 called, "Facts, Fables and Fantasies about Climate Change".

Preamble

You can probably work out from the thumbnail sketch that my formative research years in photochemistry and atmospheric chemistry were between the mid-70s and early-80s. It was a period when I first heard the words, climate change, and the first time in my life that I smelt ozone made by a photochemical smog (in Los Angeles).

When I began writing the words that would become the Eva Philbin Lecture, three songs kept coming to mind from those years. One by the Hollies, one by Thunderclap Newman and one by the Police. Yes, pop trivia lovers they were: "The air that I breathe"; "Something in the air" and the one that I finally chose as a title. With that settled then I decided the talk would be an "edutainment" and not at all like my normal undergraduate or conference lectures. That was an important decision because, as the world made its Rake's Progress down 2016, "post-truth" became the Oxford Dictionaries "word of the year". So I became determined to play my part in telling clearly some "real truths" to the general public about the inseparable environmental issues that have been termed Climate Change and Air Pollution/Quality.

For those of you that want to see the pictures, videos and audio that are the lecture (at least the pilot version) then go to the crac.ucc.ie webpage and, I hope, enjoy. But in this essay I write down some more self-controlled thoughts than ever possible in a public lecture not only regarding the science but also on the roles that the media and general public have to play in protecting the air we breathe.

Air and atmosphere

The Sun, Earth and the other planets in our Solar System were born about 4.5 billion years ago. The dominant body is the Sun holding about 99.9% of the total Solar System mass. It is a nuclear reactor releasing energy equivalent to 100 trillion kg of dynamite exploding every second. Heat, light and solar wind reach all the planets from this continuous, dynamic process but it is only on one, Earth, where human life has developed. Why?

Of all the planets, Earth has the greatest density with its chemical composition being mainly iron and rock. The gravity that results helps hold on to the gases, vapours, droplets and solid particles released from the surface of the planet into a surrounding envelope we call the atmosphere. (That word is of Greek derivation from atmos meaning vapour and sphaira meaning sphere). In the beginning, volcanic activity released (outgassed) the initial atmospheric ingredients from Earth's mantle with the most important one being the lightest element, hydrogen. This gas subsequently fixed the other available simple elements, carbon, nitrogen and oxygen as methane (CH_4), ammonia (NH_3) and water (H_2O) molecules. However, the solar wind could then whisk our atmosphere away if not prevented. Fortunately for us, the flow of liquid iron in the Earth's core gives rise to a magnetic field, which serves to deflect the incoming charged particles from the Sun. Then photochemistry can take over.

In the prebiotic world, high-energy (ultra-violet, UV) sunlight broke the bonds of the simple molecules contained in our initial atmosphere, giving rise to other combinations of atoms, the most important of which was carbon dioxide (CO_2). The Sun also sends out lower energy, infra-red, IR light, which simply makes molecules hotter by causing them to vibrate. So once we developed a stabilized atmosphere with ingredients like water, methane and carbon dioxide, heat became trapped and Earth's surface could warm up, eventually, to the sort of temperatures we experience today. It's just how a Greenhouse works but with atmospheric ingredients rather than glass. If we had no atmosphere then our surface temperature would be about -18 C, like the Moon.

700 million years ago Earth was like a snowball or at least a slushie frozen drink. Water was trapped on the surface as ice until the carbon dioxide content of the atmosphere increased sufficiently to trap enough heat to turn the ice into liquid. Then complicated combinations of carbon, hydrogen, nitrogen and oxygen atoms could be made, eventually forming cyanobacteria. From their name it is obvious that they are coloured and

so can take up visible light from the Sun. And that was a turning point for life as we know it on Earth because these micron-sized photo-reactors turn carbon dioxide and water into oxygen gas. We term this process photosynthesis and is more familiar today to us in relation to the plant molecule called chlorophyll. Eventually DNA was formed, which acted as a building block to help construct a world in which plants and animals existed side by side in a mutually dependent relationship. We still take part in this vital connection with animals taking up oxygen and releasing carbon dioxide with plants doing the opposite.

Today, Earth is surrounded by a fluid atmosphere comprising a mixture of gases, vapours, droplets and small solid particles. Our worldwide average temperature is about 14-15 C. The chemical composition is dominated by molecular oxygen and nitrogen contributing 21% and 78%, respectively. (The missing 1% and the other components will be discussed in more detail later). The proportion of oxygen allows us to breathe effortlessly and not be too afraid of striking a match. We call this the Goldilocks mixture or more familiarly, Air. There is no Air on any other planet in our Solar System although they do all have atmospheres. For example, the atmosphere of Venus consists of about 96.5% carbon dioxide and 3.5% nitrogen. That atmosphere is not a mixture we should be aiming at breathing in!

Weather and Climate

We all know that the weather is an important, maybe the most important, topic of conversation in Ireland. Even Seamus Heaney wrote in 1979: “my people think money but talk weather”. Today he might have written “my people think money but talk climate change”. Countless articles about global warming and how the climes they are a changin’, have been written over the past few years. So where to begin here? Like many others I have chosen to outline first why we have climate and weather and what is the difference between them.

Planet Earth orbits around the Sun over a period of one year. It also rotates on an axis that is tilted toward the Sun at an angle that maximizes during June’s summer solstice. This causes a maximum amount of sunlight to reach the Northern hemisphere then. At the winter solstice, in December, the tilt away from the Sun is maximized leading to the longest nights. We divide the full year between toward, away and back to toward into four seasons with each day containing a differing amount of time between sunrise and sunset. The overall effect is for the Sun to score a concentrated direct hit on the equatorial region of the planet throughout the year. But at the poles the hit is much more spread out over area and time leading to much colder conditions being experienced there.

Heat flows from hot to cold and so the hot air over the Equator flows to the polar cold by means of the fluids we call our atmosphere and oceans. In the air the energy is transferred by winds caused by the motion of the Sun’s rays over the rotating Earth. To understand how winds develop imagine an area the size of Phoenix Park in summertime when the Sun is directly overhead and you feel very warm. After sunset the Sun will have moved on and you will feel cooler. The air experiences the same conditions but hot air rises because it becomes less dense exerting lower pressure (by the Ideal Gas Law), which will necessarily be replaced underneath by cooler, denser air as the Sun moves on its path. Wind results as the area equalizes the pressure between the low altitude cooler air and the higher altitude warmer air. Obviously, there will also be important but complicated interactions with the Oceans, for example the balance between water vapour, liquid and ice is temperature dependent. It is this overall complexity that makes accurate weather forecasting and climate predictions so difficult in parts of the world like Ireland.

We have about a half dozen measures to define our weather and climate: wind direction/speed; precipitation, temperature, sunshine, visibility and cloud. The difference between the label, weather, and the one we call climate is simple. The first reflects the measures in the short term (minutes, hours, days) and the second represents a much longer term average (30 years and more). The most intuitive way of thinking about it that I have ever read is to consider the weather as expressing a mood (like anger or joy) and climate, a personality (like calm or mercurial).

The winds act as an air-conditioning system for our planet moving in all directions at many speeds and so transfer heat from the equator to the poles. But they also transfer air pollutants over periods that vary from about 1-2 months within a hemisphere and about 2 years between hemispheres. That is at least in the air close to our surface. The time-scale contrasts with pollutants released from processes like combustion and agriculture to reach about 25 km altitude: they take 5-10 years for reasons related to the temperature structure of our atmosphere as discussed below.

Natural and Anthropogenic

Our atmosphere reaches an altitude of about 120 km but we do not think of it as one continuous covering. Rather we divide it into layers, not arbitrarily, but because of temperature profiles. The region that extends to about 10-12 km in altitude is called the troposphere (from the Greek meaning "changing"). It gets cooler as you move upwards because there is much lower pressure of atmospheric gases like oxygen. Climb a mountain and you will know what I mean. It is also a turbulent, highly mixed air because a balance is struck between the lower pressures at higher altitudes, hot air rising because of our everyday activities and sunlight hitting the surface. This essay focuses on activities in the lower region of the atmosphere but you probably have heard of the interesting chemistry that occurs in the warming layer that sits above the troposphere and we call the stratosphere (from the Greek meaning "layer"). Yes, I mean ozone depletion but that is for another day.

We owe the process of photosynthesis the main debt for producing breathable air containing 21% oxygen and we owe bacteria and volcanoes for the nitrogen content at 78%. Most of the rest is the inert gas, argon, at 0.9%. So, that leaves just 0.1% of trace gases to account for, including carbon dioxide. The sources of these chemicals are either from natural processes or anthropogenic/human activities. Many people are amazed that the most important aspects of atmospheric chemistry are related to these trace substances that may be present at levels as low as parts (trace molecules) per trillion (air molecules).

Natural sources include lightning strikes to crack nitrogen in the air to produce nitrogen oxides or volcanoes to release sulfur gases and solids or even desert storms to transport sand and dust over many thousands of kilometres. Nature does not just release chemicals into the atmosphere and much research is now being done to monitor the release of biological materials like pollen, fungal spores and bacteria as it happens, in real-time because the information is of real use to at-risk members of the public like asthmatics. We create air pollution with transport (car, ships, aeroplanes) being important as well as domestic solid fuel (DSF) burning (coal, wood peat) and also agriculture (cattle, fertilizers, poor husbandry of livestock).

The resulting air pollutants have two main effects on life on Earth: (i) Health and Wellbeing; (ii) Climate Change. It is easy to write their names down but their effects can be many and varied. Anyway, here is my list: ammonia, nitrogen oxides (often termed NOx as the sum of nitric oxide and nitrogen dioxide), nitrous oxide (laughing gas), acid rain/sulfur compounds, carbon-containing particulate matter, hydrocarbon vapours and finally ozone and carbon dioxide. There is often debate about whether to call the final two chemicals, pollutants, because they are essential to life…..at the right levels. But I am including them and will discuss their less benign effects below.

The one ingredient of air that is most definitely not a pollutant is water, the essential of life. Its continual cycling thoughout the planet into plants, rivers, the air, the poles, oceans, whiskey and humans is entirely dependent upon temperature. Its environmental behaviour may prove to be an insuperable problem for us to solve if, eventually, the average surface of planet Earth moves to 20 C or more.

So do we wish to face desertification, extreme weather events, flooding, polar ice cap and Greenland melting? Or increase cancer rates, cardiovascular problems, dementia and asthma? I think not but we are moving on that pathway mainly because of our demand for carbon-based energy and the combustion process used since stone-age times. It is time to move on, world, and to include a blend of nuclear, wind and solar.

Climate Change and Air Pollution

Although the terms are often separated, Climate Change and Air Pollution are inseparable. They go together like bacon and eggs or pie and mash if you happen to come from the East End of London. The most obvious chemical connection between them is carbon-containing particles that are released in a variety of combustion processes. We often term these materials soot or black smoke or, more recently, particulate matter (PM) but no matter the name or even the exact composition, which can range from elemental carbon to thousands of organic compounds, they affect both our health by breathing in and also our climate by absorbing heat radiation.

The intimate connection between the two terms has been unappreciated by politicians in the past. That is why, in Ireland at least, diesel fuel and car taxes are so much cheaper than petrol equivalents. Although part of the decision may be due to the powerful trucking and agricultural lobby in Ireland a lot is due to the scientific ignorance of most government Ministers about atmospheric chemistry. Hence diesel is somewhat better kilometer for kilometer than petrol in releasing carbon dioxide but it is far worse for emitting toxic nitrogen dioxide (and often carbon particles too). Climate change and health do battle in this scenario and the public's day-to-day well-being suffers as a result.

Having said that I am actually going to separate the two topics because it is easier to explain them that way.

Climate Change

It has always struck me as amusing that somebody called Cole Porter wrote a song called "It's too darn hot". And although the burning of fossil fuels will take a central role in my discussion of the global warming we are experiencing today, I am going to start 700,000,000 years ago when our planet was frozen and compare it to our blue planet of today, if only to say that Earth has experienced climate change in a purely natural way. As discussed above the atmosphere developed over that time span crucially included carbon dioxide and water vapour that, because of their molecular structures, could let high energy UV light through to the surface where photosynthesis was promoted (and therefore life). Some of the sunlight energy is used up in that process and what is left is the much less energetic wavelengths we call IR, which cannot escape the planet as natural re-radiation because the water and carbon dioxide are not transparent to heat; rather they absorb it. The overall process is now often called the Natural Greenhouse Effect. Over the very long time-span between pre-historic times and pre-industrial revolution times (~1750-1830) the Earth reached a state that was not too hot and not too cold to sustain a temperate existence for us and other life on Earth.

After 1830 though when carbon combustion became central to our energy, industrial and economic demands the amount of carbon dioxide released increased dramatically from a value of 280 parts per million (ppm) then to over 400 ppm today. One Nobel Prize winning chemist (Svante Arrhenius) predicted in 1896 that a mean increase for temperature on the planet of 5-6 C would occur if we doubled the carbon dioxide level to ~560 ppm. So we have known for some time what might happen if fossil fuels were burnt unchecked.

Climate change is happening; it is inevitable with the pathway we are on. Countless graphs, models and diagrams show the inexorable increase of global temperatures over the last 150 years with the most dramatic increases being measured in the last 10 years. As I write this article NOAA (National Oceanic and Atmospheric Administration) is once again reporting that the year I have just lived in, 2016, was the hottest on record….like last year was and the year before that. [1, 2] At the same time the Observatory on Mauna Loa, Hawaii showed that the annual increase of carbon dioxide measured there was 4.5 ppm. The figure is worrying because over the last 60 years of measurement the average annual rates of increase were about 1-2 ppm. Last year we reached a peak of ~407 ppm at Mauna Loa in May and at no point, over the whole year, was the amount measured to be lower than 400 ppm. [3]

So what is happening as a result and what might happen in the future? We can term what is going on currently an Enhanced Greenhouse Effect. The best way I have of describing it is to make the comparison of Earth's atmosphere acting as a thin woolen shawl with holes in it up to 1750-1830. After that time by adding more carbon dioxide (increasing the thickness of the wool) and by filling in some of the holes (other pollutant Greenhouse Gases, GHG, like methane, nitrous oxide and chlorofluorocarbons) we are beginning to overheat.

The final results of our behavior, in the not too distant future, might be catastrophic leading to millions of climate refugees. In the meantime we are seeing cold seas like Bering warming and in so doing disrupting the plankton/fish food chain causing the Puffin population to be killed off. Sea-ice volume at the Arctic is now just 20-25% what it was in 1979. Droughts in Dafur and Syria have led to food insecurity, famine and war.

And what do our leaders and politicians and media do? Look at the Dail record for May 2016 to experience the quality of the contributions from one Irish politician on the subject of climate change. Then remember the Australian Senator who blamed climate change on a United Nations conspiracy in collaboration with the World's Banks. And who can forget the new President of the USA blaming the Chinese for the problem. We deserve better.

But scientists have to put their case much more clearly and without jargon, whenever possible. The media must show objectivity every time an indefensible fantasy is expressed by a politician no matter how amusing. And the public must learn to listen and discriminate between the truth and lies no matter where they got their information.
Greenhouse gases are not the only problem, particles like black carbon are too. Volcanic eruptions also spew many particles into the atmosphere sometimes with great vigour. And they can actually have a cooling effect on the planet because sulfur particles can reflect sunlight out from the Earth. When that has happened in the past, say 1740 and 1814, harsh winters and crop failures have followed. It will be interesting to see what violent volcanoes do to moderate our enhanced heating budget now we are well into the industrial age throughout the world.

Where there's life there's hope and the Paris agreement signed in late 2015 and now in force gives us some hope for keeping the planet temperature increase well below Arrhenius' prediction to 2 C or so. But most modelers I have spoken to are not hopeful that this can happen in the time available to us and most believe the 3-4 C increase above the pre-industrial time scenario by 2100 is more realistic. Keep an eye out for the Mauna Loa data on carbon dioxide levels on the internet over the next year because that may be our earliest warning that we are already too late to do anything to keep the planet as we currently enjoy. Anyway, who cares as long as we've got our health?

Air pollution

Air pollution has been noted since Roman times but the first recorded ban on coal burning was in 1273 when Edward I of England acted to curb urban smoke. Although "smoke" is still a term we employ to describe the quality of our air we now know a lot more about the ingredients that accompany the combustion process be they from coal, wood, peat, diesel, kerosene, propane bottles or natural gas. There are a number of common emissions that can do harm to us in a variety of ways. The main ones are nitrogen oxides (including nitric acid), sulfur oxide chemicals (including sulfates and sulfuric acid), ozone and oxygenated radicals like hydroxyl, metals and metal ions, carbon-containing particles and often related organic compound vapours like formaldehyde and aromatics. Actually, I could list thousands if I needed to name them and had the time, energy and will.

Regarding our health and well-being, the main air pollutants that I have selected to briefly discuss here in terms of air quality (or the air that we breathe in other words) are: Particulate matter (PM) of various sizes/compositions and nitrogen dioxide.

The combustion process of solids produces much PM. They are of a wide range of sizes and we define the main ones as ultrafines (about 500 of them could sit side by side in the width of a human hair), fine that is $PM_{2.5}$ (30-40 in a hair) and finally, coarse, PM_{10} (5-10 in a hair). Clearly, these are all of a size to enter into us through our nose or mouth with differing effects depending on the size and composition. The largest get into our upper respiratory tract and lead to associated problems particularly for at-risk groups like asthmatics. The $PM_{2.5}$ group can move further down and enter our arterial system causing cardio-problems. Finally the ultrafines, although less well-studied in terms of their health effects, are likely associated with blood/brain crossover and dementia.

The mechanism by which the damage occurs to blood flow is that the smaller particles can cause inflammation on arterial cell walls likely by the production of free radicals from the oxidation of cellular hydrogen peroxide. Plaque builds up as a result and heart attacks can follow. Very recently, a similar type of mechanism has been proposed to explain why the presence of air-borne ultrafine particles can cause an increase in dementia for those living 100 m or less from busy roads. It has been suggested that tyre and brake pad wear give rise to nanoparticles consisting of the iron oxide, magnetite. This material contains Fe (II), which acts in a Fenton's reagent type way on cellular hydrogen peroxide in the brain leading to free radical production, plaque build-up and brain cell degeneration.

Deaths are easier to count than incidence of diseases like asthma, COPD and cancer on a national scale in many countries. So our attempts at relating air pollution events and air quality levels to mortality is in a much greater state of reliability than other medical associations. This type of work was kicked off in the USA during the 1980s with a study called the Harvard Six Cities study.[4] It was shown conclusively, after much searching for confounders and high-level peer-review, that there is indeed an association between $PM_{2.5}$ long-term exposure and death. Depending on the level of particles in the local air some 5-10 years was shown to be taken off from life-span. These type of data are now used to show the weeks/months reduction in lifetime depending upon pollutant exposure in particular regions. The total months reduced are added up to give some estimate of life expectancy and increase in mortality at a particular place. By these statistical methods it has been estimated that fine particulate matter led to 3.15 M premature deaths globally in 2010 with 375,000 occurring in Western Europe. (In Ireland the estimate is 1200 per year).

The main culprits for making particulate matter are well-known: (i) exhaust and non-exhaust emissions from cars, trucks and buses; (ii) coal, wood and peat burning in open fires. For more specifics on the chemistry and sources of these pollutants in Ireland then go to the crac.ucc.ie webpage and look at the SAPPHIRE project sponsored by the EPA. I am only going to pass on one surprising fact to you. Burning smoky coal produces 4.3 kg/1000kg burnt of primary $PM_{2.5}$. Peat produces 4.5 kg and wood 9.0 kg. Go figure.

But smoky coal is not a good guy by any means because of its sulfur content. Its burning leads to sulfuric acid that turns into particles when it encounters the increasing amount of ammonia that is being released to our air by agricultural activities. Indeed this formation process to make ammonium sulfate particles is thought to be one of the world's biggest killers by air pollution. Farmers beware.

Nitrogen dioxide is also a killer because its chemical structure also promotes the formation of highly reactive free radicals in our blood circulation system. And the "extra" release of nitrogen dioxide was the crime that VW should not be forgiven for (along with some other car manufacturers). The story needs no repeating here but they gamed ("fiddled") their electronic emission systems results to indicate artificially low levels of the gas from their diesel cars. A criminal act?

Past and future

Air Quality has not been a high priority to monitor in Ireland over the last ten years. The number of real-time monitoring stations operating reliably throughout the country can be counted on the fingers of one hand. The comparison between that effort and Northern Ireland, UK, even Tasmania is embarrassing. Up to date information about air quality in many localities throughout Europe is passed on to the public by means of phone apps and web sites. (http://aqicn.org/map/europe as an example). Check out Ireland's contribution to the data.

The problem is not just the EPA's; local authorities must play a part too at a much greater level of activity and enthusiasm than is currently shown in most places (Wexford is an honourable exception). But what is required is legislation like most other countries have around the World that is not simply aimed at living within EU or USA directed limits. First and foremost should be concern for the health of the population. And for that to happen Ireland needs to scrap its Air Pollution Act with all its negative connotations and introduce the positive message associated with a Clean Air Act. Then local authorities will do something and prioritise their resources for us all.

Things can only get better and the EPA is currently working on the introduction of a National Ambient Air Quality Network for 2017. They deserve our full support

And we can all do our bit: buy an electric car; make sure local authorities install more electric chargers; use natural gas if you are on the grid; ensure careful husbandry and use less nitrogenous fertilizer if you are a farmer; if you have to burn wood use a very high temperature enclosed stove. I could fill a page with a wish-list but instead I will finish this article the way the lecture ends, with a quote by Edmund Burke:

Nobody made a greater mistake than he who did nothing because he could do only a little.

Postscript

As far as I am aware, there are no "alternative truths" in the above essay. I made a conscious decision to include few traditional references because it is not an academic paper, more an informed opinion piece. The article is designed to be thought provoking and I hope readers will go away and check the facts for themselves. Fact checking is a habit that we all must begin to do much more of in order to bring "post-truthers" to task.

Please read the above alongside the graphics and videos presented in my on-line Eva Philbin lecture (http://www.ucc.ie/en/crac/newsevents/fullstory-717902-en.html). A picture tells a thousand words but we should not lose the ability to read 1000 words or more, uninterrupted, on a subject with the consequences that climate change and air pollution have for us all.

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A Rapid Non-Destructive Extraction and GCMS Analysis Method for the Determination of Illicit Drugs of Abuse on Irish Bank Notes using Chromatographic Deconvolution.

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Biography

Dr. Philip White graduated from GMITs Chemistry and pharmaceutical science programme in 2008. He undertook his doctoral work at DIT in conjunction with the Marine Institute working on the use of passive samplers as environmental monitors of Persistent Organic Pollutants (POPs). After a successful introduction of passive samples as part of Irelands monitoring programme to satisfy Irelands legislative requirements under the water Framework Directive he helped the Marine Institute to gain accreditation in the analysis of POPs in marine matrices. In late 2015 he joined GMITs school of science as an assistant lecturer in chemistry and forensics. He currently has a number of PhD students in the area of environmental contaminants analysis including microplastics and POPs. His areas of interest have broadened to include forensics analysis as evidenced by this work. He is the current chair of the Irish Mass Spectrometry Society.

Abstract:

A successful preliminary investigation was undertaken into the possibility of using a rapid, non-destructive extraction technique on a number of bank notes to determine the presence or absence of illicit drugs of abuse, in this case cocaine. A number of 5, 20 and 50 Euro bank notes were extracted (2 of each) using the rapid, non-destructive technique and then analysed using Gas Chromatography Mass Spectrometry (GCMS) in a scan mode (50 – 550 *m/z*). Analysis was completed on an Agilent Gas (GCMS) instrument with an 'NIST' Mass Spectral Library in conjunction with 'Masshunter' software equipped with chromatographic deconvolution. A peak found in the chromatogram of one of 20 Euro notes analysed was shown to be consistent with cocaine.

Introduction:

A study was envisioned to test the concept and usefulness of chromatographic deconvolution in conjunction with a rapid non-destructive extraction technique, in the analysis of GC chromatographic spectra for the presence of illicit drugs of abuse. The use of cocaine dramatically increased in Ireland during the 'Celtic Tiger' period with An Gardaí Siochana statistics showing that during this period cocaine overtook opiates and amphetamines to be the second most widely used illicit drug in Ireland. [1] A study completed by Bones *et al* [2] in DCU in 2007 stated that 100% of the notes tested were found to have traces of cocaine present. The Bones *et al* [2] study was found to have used a small sample size of 45 notes. The findings suggest that only 62% of the notes had cocaine present at greater than 2 ng/note. The remainder of the notes had only trace amounts of cocaine present and so it has been suggested that these notes may have been contaminated by close proximity to notes which were used in the illicit consumption of cocaine. This would suggest that 62%, rather than 100% of the notes were contaminated directly through usage in cocaine inhalation which would make Ireland comparable to other studies of this kind. [3].

The study by Bones *et al* [2] used LC/MS/MS to check for a number of different types of illicit narcotics. Other studies indicate a number of techniques can be used including GCMS. [3, 4] The study by Esteve-Turrillas *et al* [4], upon which the extraction element of this study is based, analysed a number of Spanish bank notes using a rapid extraction technique followed by targeted GCMS/MS analysis for quantification. With recent advances in the field of structural elucidation and chromatographic deconvolution for GC, the question of whether GCMS could be used in association with chromatographic deconvolution, rather than direct quantification methods such as Single Ion Monitoring (SIM), to identify the presence of cocaine since the reported levels and high percentage of positive tests of cocaine on bank notes makes it the ideal compound for analysis of this type.

General quantification of an analyte in a complex sample requires a large amount of method development work not to mention the associated QC work. This type of analysis is usually preceded by an exhaustive extraction step, in relation to the use of consumable (solvents etc.) and preparation time. Recent advances in automated sample preparative instruments have resulted in a reduction in both consumables and laboratory time, but come at great cost in the initial outlay for instrument purchase. Conversely, advances in the use of (MS) mass spectrum instruments has resulted in lower and lower LOD/LOQ measurements coupled with reductions in background noise and matrix interferences. In fact the use of high resolution mass spectrometry (HRMS) instruments when analysing samples in the SIM or MRM (Multi-Residue Monitoring) mode can reduce background noise and matrix interferences to a non-interfering level in most applications. GC, when combined with MS when using the electron ionization (EI) mode can allow for the identification and quantification of volatile and thermally stable compounds because the fragmentation of metabolites during EI are highly characteristic of the chemical structure. The resulting mass spectra, when compared to mass spectral libraries, can result in positive identification of the compound in question.

However, one of the most overlooked advances in MS technology is that of chromatographic deconvolution algorithms, has huge potential to tap into the data that is discarded when running in SIM and MRM modes. All forensic samples, as well as food science and environmental samples, have the capability of being run in a regular MS scan mode (50 – 550 m/z) which will provide supplemental sample details which the SIM or MRM method will not record. The MS scan method, when coupled with powerful advances in the use of chromatographic deconvolution algorithms, means that the analytical chemist now has a very useful and underutilised new tool for analysis. Chromatographic deconvolution methods have the capability to scan an unprocessed sample and potentially identify a compound present in a ‘crowded’ chromatogram. The potential for this type of analysis has still not been fully explored outside the areas of proteomics and metabolomics where non targeted screening using GCMS in EI (Electron Ionisation) mode is used to identify and even quantify metabolites present in samples. [5]

MS-based metabolomics experiments using the deconvolution technique are generally conducted using non-targeted metabolic profiling - where the identity and relative quantity of as many metabolites as possible are obtained.[6] Techniques also used include targeted profiling - where the absolute quantity of a pre-selected smaller set of metabolites, typically related by chemical or biological similarity, are obtained using internal standards and reference compounds and metabolic fingerprinting – in this case a global snapshot of the metabolism is acquired and compared without performing quantification and chemical identification. In this experiment a non-targeted approach was used, where the identity of a compound in a sample could be determined, thus indicating its presence or absence. [5]

For GC-MS data the deconvolution process of computationally separating co-eluting components and creating a ‘pure spectrum’ for each component has been discussed in the literature and it is not the aim of this investigation to go into great detail. Briefly, for each observed TIC that results from two or more components, deconvolution calculates the contribution of each component by calculating a number of parameters. Noise analysis, is a process where the software calculated the noise from the chromatogram by calculating the average random deviation from a detector signal in areas of the chromatogram which are free from any analyte peaks. The second step is ‘component perception’ where the software recognises the clustering of ions of a certain magnitude which represent the presence of an analyte. Next, the instrument software compares the peak to a model peak shape for a component. The final step, ‘deconvolution’, extracts the ‘purified’ spectra from individual ion chromatograms for each component using the model shapes and the least-squares method. [7]

The initial question as to the usefulness of chromatographic deconvolution in detecting the presence of an illicit compound, in this case cocaine for the reasons already outlined, was undertaken.

Experimental

Each banknote (5, 20 and 50 euro notes – 2 of each) was placed in a clean plastic bag after collection from general circulation and stored at room temperature. The samples (notes) were placed in separate 15ml centrifuge tubes and 12ml of methanol was added. Tubes were capped, agitated by vortex for 5 minutes and spun in a centrifuge at 800rpm for 15 minutes. The bank notes were removed and allowed to dry. Samples were evaporated to near dryness by vacuum evaporator under nitrogen (max 10 psi) at 35^{0}C and reconstituted with methanol for further analysis by GC/MS. An Agilent GC-MS (5977E) run in EI mode with a J&W DB-1 30 m 0.25mm x 0.25um column was used. The inlet was operated in splitless mode with the temperature at 260°C, the ion source at 230°C and the quadrupole at 150°C. The auxiliary transfer line was set at 280°C. Column oven temp programme was 100°C - ramp 5°C per minute for 30 minutes. Helium was used as the carrier gas. The extracts (2 µL) were then injected directly on to the instrument. The resulting chromatograms were then subjected to chromatographic deconvolution software on the 'Mass hunter' platform. The deconvolution software results were then investigated and any compounds of interest, were then identified using the compound identification software.

Results

One of the resulting chromatograms is shown below in Figure 1. This chromatogram is one of the 20 euro notes that was analysed. This is an example of a complex chromatogram.

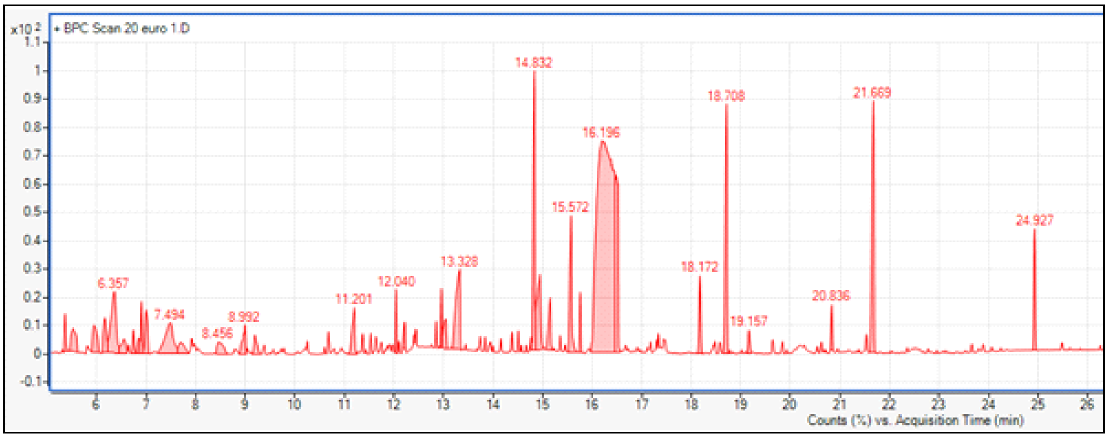

Figure 1: Chromatogram of a 20 euro note analysed on an Agilent 5977E instrument run in scan mode (50 – 550 *m/z*) using a J&W DB1-MS 0.25 x 0.250um column.

With many co-eluting and overlapping peaks present the detection of a compound, particularly in low concentration is problematic. The tendency for the analytical chemist would be to try and extract an individual ion, or groups of ions using the software, however this does not always produce the desired result as many compounds may contain similar ions if they elute in the same time frame. The deconvolution software was then applied to the chromatogram from Figure 1 and separates the chromatogram into 'pure spectra' for each individual peak in the chromatogram as shown below in Figure 2.

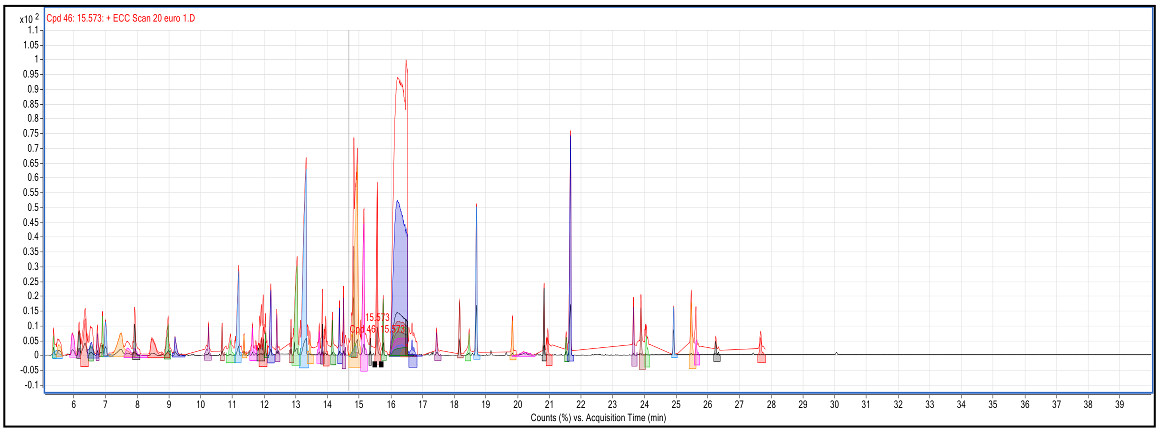

Figure 2: Chromatographic deconvolution of the chromatogram of the 20euro note which is shown in Figure 1.

The deconvolution software has resolved a number of different compounds from the complex chromatogram all of which can now be investigated individually or sorted based on the base peak or a number of ions expected and can be identified using the identification software. Conversely, as was the case in this study, the base peak for cocaine was noted as 182 m/z and a search was made for this peak in the above Figure 2. A peak at 15.57 minutes was found to have a base peak of 182.1 m/z and this peak was then further investigated. The MS fragmentation pattern for the peak at 15.57 minutes with the base peak of 182.1 *m/z* from Figure 2 can be seen in Figure 3.

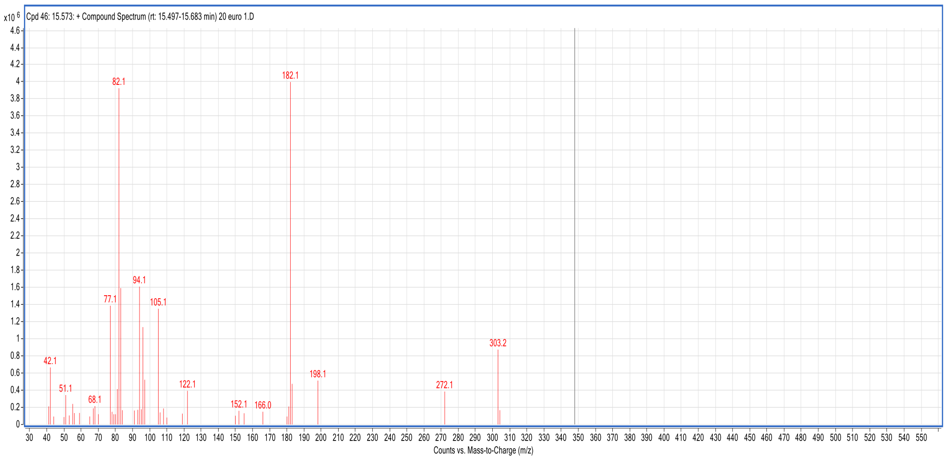

Figure 3: Mass fragmentation pattern for the peak located at 15.57 mins in the chromatogram shown in Figure 2.

The identification software was then applied to identify this compound. Figure 4 below is the EI MS fragmentation pattern found by the software which identifies the fragmentation pattern in Figure 3 as consistent with that of cocaine. The match and R match found by the software is 944 out of 1000 with the % probability being 58.2%. This would indicate a high probability that the fragmentation pattern in question found at 15.57 minutes in Figure 2 is indeed similar to that of cocaine.

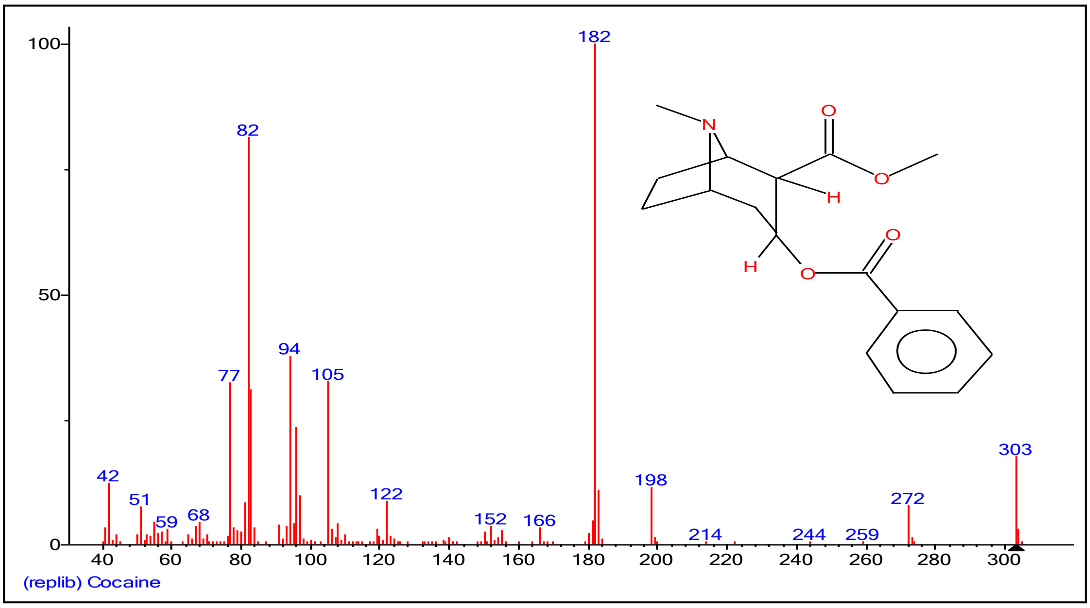

Figure 4: MS fragmentation pattern of cocaine from the 'NIST MS Identification software'

Discussion:

The rapid, non-destructive technique for the extraction of bank notes reported by Esteve-Turrillas *et al* [4] can indeed be described as such since all of the notes, once allowed to dry after the extraction process, exhibited no detectable deterioration and were returned to general circulation. The technique itself was indeed rapid with each sample prepared and ready for analysis in under an hour. The resulting chromatograms were found to be complex as indeed no clean-up process was undertaken during the extraction procedure. Nevertheless identification of the possible presence of cocaine on one of the bank notes analysed suggests that, in association with the extraction technique, chromatographic deconvolution can be used in this fashion to give a positive or negative result for cocaine.

From the resulting chromatogram (Figure 1), as previously mentioned, the tendency for the analytical chemist might be to try and extract an individual ion, or groups of ions using the software however, this does not always produce the desired. When the deconvolution software was applied the chromatogram it then separates the spectra into 'pure spectra' which can then be assessed individually. This allows the analytical chemist to identify all the compounds present using the identification software or to concentrate on a single or group of compounds. As much of the analysis performed on GC and LC MS is completed with the instrument in SIM or MRM mode, many compounds present in a sample which may be of interest could be missed. The technique of chromatographic deconvolution therefore can prove useful in a number of analytical fields including forensics and environmental analysis.

The draw backs in the technique as currently presented are obvious and relate to a number of shortcomings in the experimental design. As an initial step only this technique shows promise however, it would require extra method development to ensure that the results are consistent within a larger number of samples. Also to be determined would be the limits of detection and the possibility of quantification. Further work will concentrate on these issues as well as the determination of other illicit compounds.

Conclusion:

The rapid, non-destructive method followed by analysis with the use of chromatographic deconvolution software used in this preliminary investigation has proven useful in identifying a compound consistent with that of cocaine in one of the samples. Positive identification will require further study. The technique of chromatographic deconvolution followed by structural analysis on MS systems can be a useful supplementary technique to those used to identify compounds in samples which are currently missed using quantitation MRM or SIM methods.

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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

Accelerating the delivery of quality, life-changing medicines to patients

APC Ltd partners with global bio/pharmaceutical industry to accelerate the delivery of quality, life-changing medicines to patients. APC achieves this goal through integration of fundamental chemical and process engineering principles, innovative technology platforms and scientific expertise to enable its partners deliver optimized manufacturing processes for their medicines.

APC was founded by Prof Brian Glennon and Dr Mark Barrett from the School of Chemical and Bioprocess Engineering, UCD, Ireland in 2011.

Born of collaborations in pharmaceutical process and manufacturing optimisation, within Ireland, APC has significantly expanded to become a global pharmaceutical and biotech process research company.

As pharmaceutical companies strive to become more efficient and profitable, information attainment and knowledge management is becoming an increasing necessity to enable the launch of their medicines to patients faster. Since its establishment, APC has been meeting this key global market need with the completion of over 300 projects on more than 100 medicines and has established significant strategic partnerships with 8 of the top 10 global pharmaceutical companies and 5 of the top 10 global biotech companies.

APC has established itself as a global leader in process research, development and innovation. APC's state-of-the-art facility in Cherrywood, Dublin, enables the highly qualified team to deliver valuable process information to our clients facilitating significant reductions in operating costs and cap-ex expenditure, delivering processes that are safe to bring to plant and that are reliable with minimum batch-to-batch variances.

View into APC Process Development & Small Molecule Labs

State of the Art Facility

The Taoiseach, Enda Kenny officially opened the APC world-class, process research facility in Cherrywood, Dublin in February 2016 with the announcement of 100 new jobs. The 6,000m^2 premises serves as APC's new headquarters.

APC Reception with view into Process Development Lab - Large Molecule

An important demonstration of the success of APC in delivering technical and commercial excellence is the significant and unprecedented expansion of APC itself. APC boasts a 100% customer retention rate, with year-on-year growth of over 100% since 2011. It now strategically partners with global pharmaceutical industry leaders on multi-million euro projects to deliver process knowledge for their medicines. This growth has been built on relationships across multiple business units within our partners' global organisations. APC has realised a geographic spread across Ireland, UK, EU (& Switzerland), USA, Asia and Australasia and exports approximate to 80% of turnover.

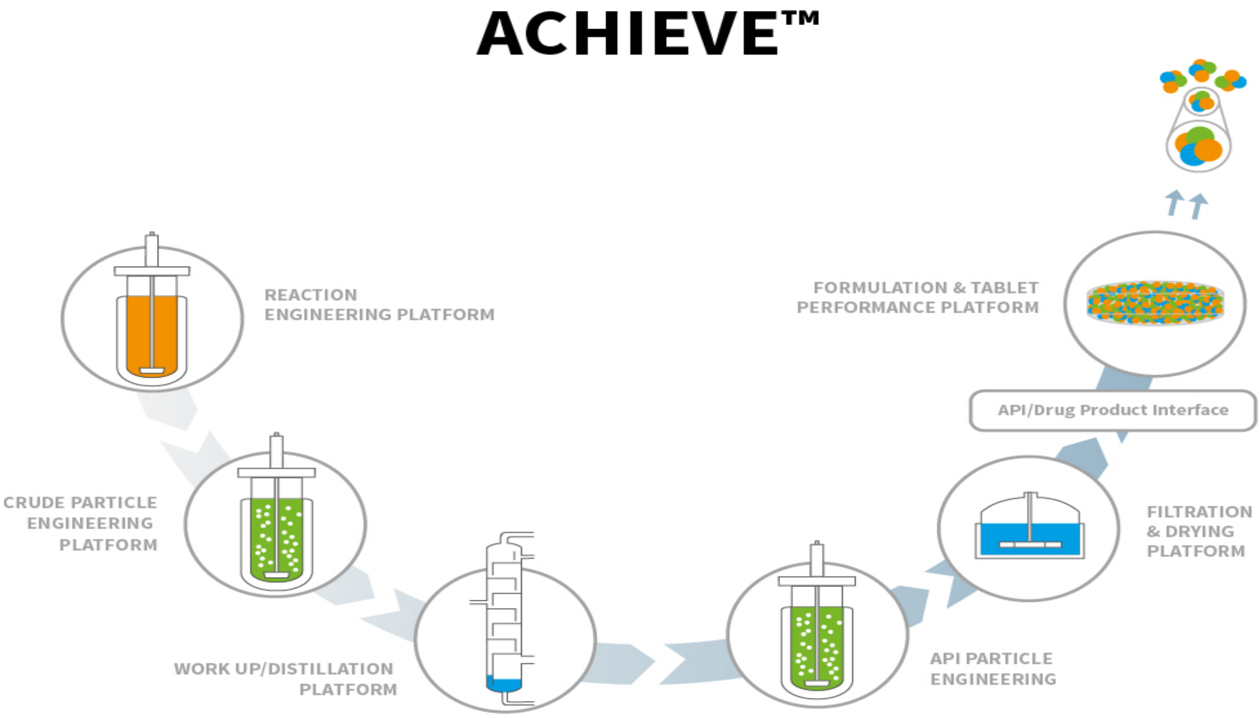
Through these partnerships, APC has defined and understood the significant information drivers of the market. These include ownership of the process knowledge, meeting regulatory requirements for better control over medicine quality & risk mitigation over the entire manufacturing supply chain.

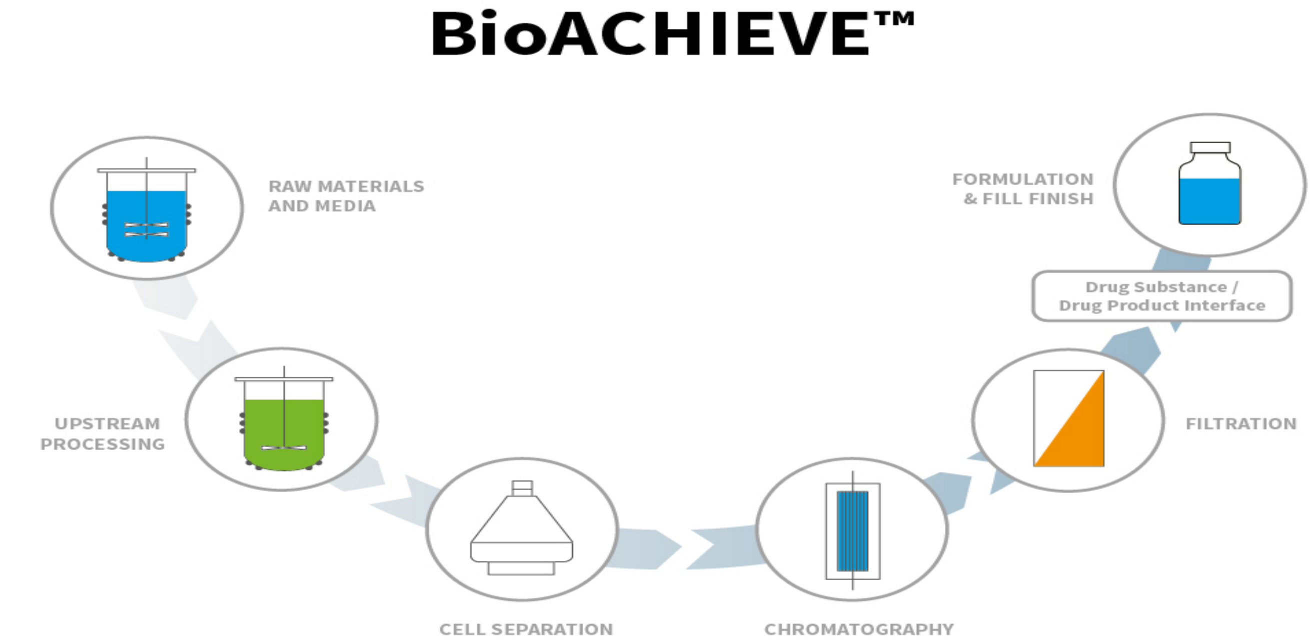
Technology & Innovation

Innovation is at the heart of what APC does. APC uniquely specializes in integrating process engineering performance across the full life cycle of a medicine, from route synthesis and early Phase development to manufacturing support and next generation development. APC reduces the time, risk and cost associated with the commercialization of new and existing medicines.

This USP is delivered via APC's proprietary research programmes, ACHIEVE™ and BioACHIEVE®™

These platforms, for small and large molecule manufacturing respectively, are underpinned by fundamental chemical engineering approaches of experimental measurement, process modelling and kinetic and thermodynamic understanding, delivering knowledge which can be scaled and applied directly to improved process for medicine development and manufacture.





APC bring together a variety of platform technologies with our team of chemical engineers, scientists, analysts and formulators to enable chemical and biological process design.

APC's information and research framework allows us to systematically design, optimise and provide scale independent process solutions. The derived information deliverables, which are clinical phase appropriate, allow APC to create processes that are optimised, robust and, most importantly, portable. By creating portable processes, it allows our partners to have a flexible supply chain.

How we do it…….Information

APC has had key market success with innovations in Model Predictive Control (MPC), Continuous Processing and Informatics. In the Biotech sector, MPC takes the application of Process Analytical Technologies to the next level by enabling real-time control of complex processes through a virtual feedback loop between the bioreactor and feed controller. Continuous processing enables our clients to deliver high quality medicines, with reduced manufacturing footprint and costs. Informatics tools developed by APC underpin the transformation of process data into process knowledge, facilitating significant process efficiencies.

In order to sustain its innovation roadmap, APC dedicates approximately 15% of its resources to on-going internal innovation programmes, led by PhD-qualified teams in Chemical & Bioprocess Engineering and Process Chemistry. In addition, APC is a partner in a number of major academic/industrial consortia, including the Synthesis and Solid-State Pharmaceutical Centre (SSPC) and the Pharmaceutical Manufacturing Technology Centre (PMTC), financially supporting research and hosting PhD programmes.

This collaboration was highlighted recently when APC hosted a live tour of continuous technology as part of the "Adopting Continuous Manufacturing 2017 Workshop" which was held on 22nd – 23rd February 2017 in association with the SSPC. In particular, the tour highlighted the integration of continuous technology into APC'S ACHIEVE™ platform technology. The main topics covered during the tour included:

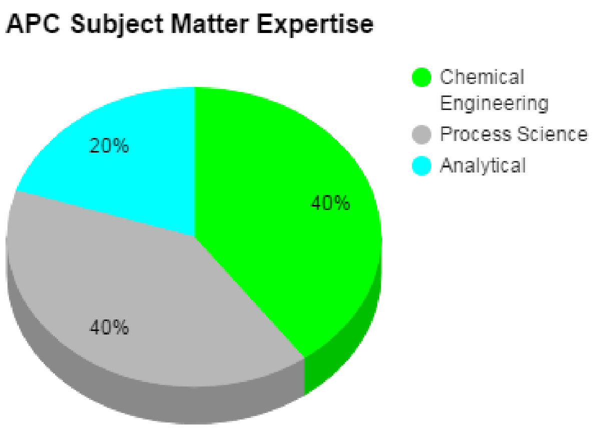
- Continuous Crystallization Platform Overview
- Continuous Chemistry Platform Overview
- Integration of Continuous Technology into Process Development: Lessons Learned
- Continuous Reactor Technology: Criteria for Selection
- Modelling for Continuous Process Development

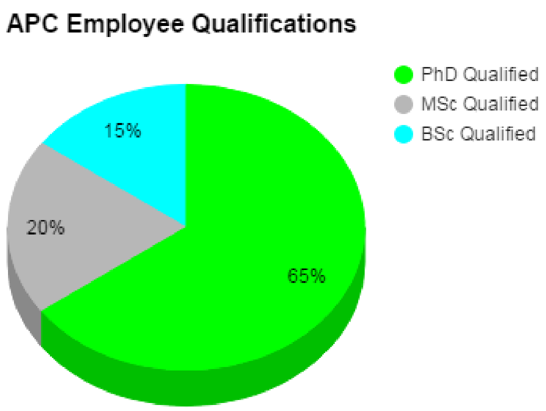
Research Scientist Dr Damien Carr demonstrates Continuous Chemistry to CM2017 delegates

People

APC Team in Sorrento Park, overlooking Killiney Bay, Dublin

From the recruitment of its first staff in late 2011, APC employee numbers have grown to a full-time staff of 100+ chemical engineers and scientists, with on-going recruitment to double staff numbers in 2017. APC is nationally the largest employer of PhD qualified chemical engineers.





APC have also deployed a recruitment strategy to allow us attract the brightest and best minds both nationally & internationally. 30% of our team is now international which underpins a diverse level of experience, expertise & culture, that contributes to a vibrant working environment.

Recent Awards

APC won the prestigious Pharma Company of the Year- SME award in 2016. This is the second-time APC has won this award, having previously been a recipient in 2014. The Pharma Industry Awards is the premier awards ceremony for recognising and celebrating the most original and innovative individuals and companies that demonstrate excellence in the Irish Pharma sector.

Professor Brian Glennon receives the award from Barry Joyce – MD @ VWR

Other recent awards for APC include:

- Science Foundation Ireland 2016 – Entrepreneurship Award
- Irish Times InterTradeIreland 2014 - Innovation Award (Bioscience)
- Pharma Industry Awards 2014 - Innovation of the Year

Recent Conferences/Publications

- Characterization of an Integrated Continuous Cooling Crystallization Process with an in-Situ Wet Mill System for Particle Size Reduction. D. Acevedo, V. K. Kamaraju, B. Glennon and Z. K. Nagy. 462030 AIChE Annual Meeting, 11th-13th Nov 2016, San Francisco, USA.
- Model Predictive Control: A Process Development Tool for Mammalian Cell Culture Processes. J. Whelan, M. Barrett, B. Glennon and S. Craven. 461029 AIChE Annual Meeting, 11th-13th Nov 2016, San Francisco, USA.
- The Development of Integrated Continuous Drug Substance Processes. 461095 AIChE Annual Meeting, 11th-13th Nov 2016, San Francisco, USA.
- API Particle Formation: Technological Approaches to Forming Unique API Characteristics. J. Whelan, M. Barrett and B.Glennon. 461101 AIChE Annual Meeting, 11th-13th Nov 2016, San Francisco, USA.
- A Quality-by-Design Approach To Upstream Bioprocess Interrogation And Optimisation S. Craven, J. Whelan, M. Barrett and B. Glennon. 3333253 ESBES 11th – 14th Sep 2016, Dublin, Ireland
- Continuous Processing: Application to Process Design and Material Supply J.Whelan, M. Barrett, and B. Glennon 416697 AIChE Annual Meeting, 8th-11th Nov 2015, Salt Lake City, Utah USA
- Application of Raman to Pharma and Bio-Pharma Process Design J. Whelan, M. Carr, M. Barrett & B. Glennon, IFPAC Annual Meeting, Washington, USA, January, 2015
- Process Analytical Technology and Quality-by-Design for Animal Cell Culture S. Craven, J. Whelan *Cell Engineering* Vol 9 pp 647-688 Nov 2014
- Glucose concentration control of a fed-batch mammalian cell bioprocess using a nonlinear model predictive controller S. Craven, J. Whelan and B. Glennon *J.Proc.Con.* 04/2014; 24(4):344–357.

To find out more, please visit our website*:*

www.approcess.com

Acadamh Ríoga na hÉireann
Royal Irish Academy

Former Institute President and Boyle Higgins Gold Medal Winner Professor Dervilla Donnely will be honoured by the Royal Irish Academy with its highest award The Cunningham Medal.

Royal Irish Academy

Cunningham Medal Presentation

to Professor Dervilla M. X. Donnelly, MRIA

7 March 2017

Prof Donnelly at the 2015 Institute of Chemistry of Ireland, Industrial Award Chemistry Award in UCD

UCD chemistry graduate Dervilla Donnelly has led a multi-faceted career combining outstanding contributions in research and teaching with leadership in science policy and broader public service. Following her B.Sc and Ph.D. from UCD and postdoctoral studies at UCLA, she returned to UCD as a lecturer in chemistry in 1956. She rapidly gained international renown in her field of phytochemistry, the study of chemicals with biological activity derived from plants, and was appointed professor of phytochemistry in 1979. Wood chemistry was a particular interest, and she applied her research to a variety of problems encountered within the Irish forestry industry.

Donnelly's commitment to European research saw her elected chairman of the European Science Research Council and vice-president of the European Science Foundation. She was the first woman president of the Royal Dublin Society and chairman of the Dublin Institute for Advanced Studies, the Custom House Docks Development Authority and the National Education Convention.

In 2000 Dervilla Donnelly received the UCD Charter Day medal, for her many contributions to the country and to the university. Of these contributions, she is particularly proud of her eighty Ph.D. students, many of whom have themselves won considerable distinction in academia, industry and business.

WITS Women in Technology and Science

WITS presented its inaugural Lifetime Achievement award at a gala ball in Dublin on Saturday June 25th 2011, in recognition of the significant contribution made by Irish women in the area of technology and science. Professor Dervilla Donnelly, Emeritus Professor of Organic Chemistry at UCD was the winner of the inaugural award, chosen from a list of twelve nominees drawn from a wide spectrum in the scientific world, noted for their work on a global level and recognised as key advocates in promoting the cause of increasing the number of women studying for careers in the world of science, technology and engineering and maths (STEM). The judging panel was led by the Chief Scientific Adviser to the Government, Professor Patrick Cunningham.

Professor Dervilla Donnelly (President, Institute of Chemistry of Ireland 1994–1996.

ICI Gold Medal Award: 2000 Professor Dervilla M.X. Donnelly (Pure Chemistry)

The Cunningham Medal is the Royal Irish Academy's premier award and its history goes back to the earliest years of the Academy, which first met in Dublin on 18 April 1785.

Four years after that meeting, in 1789, Timothy Cunningham, a barrister of Gray's Inn and a writer on legal subjects, bequeathed the sum of £1,000 and his library to the Royal Irish Academy to enable it to award premiums for the 'improvement of natural knowledge and other subjects of their institution.'

Between 1796 and 1885 the Cunningham Medal was awarded thirty-five times in each of the three areas of Academy interest (Science, Polite Literature and Antiquities). Many of Ireland's most important figures, in this golden era of the Academy, received the Cunningham Medal. They included: in astronomy, John Brinkley; in chemistry, Sir Robert Kane; in Egyptology, Edward Hincks; in Irish studies, John O'Donovan; in seismology, Robert Mallet. William Rowan Hamilton, himself a world renowned mathematician, won the medal twice and the great antiquarian, George Petrie, received it three times, once for an essay on the history and antiquities of Tara Hill and, most famously, for his landmark essay on Ireland's round towers. Sir William Wilde, father of Oscar, accepted the Cunningham Medal for his many services to the Academy, particularly the cataloguing of the Academy's large museum collection, which was exhibited in Academy House in the 1850s before being transferred to the National Museum of Ireland.

From 1880, the Academy decided to use the Cunningham Bequest both for the awarding of medals and for the publication of research papers, in a valuable series of substantial volumes, known as the Cunningham Fund Memoirs, which continued until 1967.

The Medal itself is a notable example of the medallist's art. It is considered to be the finest work of William Mossop who was a pioneer Irish medallist born in Dublin in 1751. The Medal shows on the obverse side a bust of the first President of the Academy, Lord Charlemont, in the uniform of the Volunteers and on the reverse *Hibernia* holding with her right hand a shield showing the harp and Irish crown and with her left hand a rod with a cap of liberty.

After a break of almost 100 years, the Award was briefly revived in 1989 when a Cunningham Medal was awarded to Frank Mitchell. In 2000 the Academy Council agreed to revive the presentation of the Cunningham Medal as an occasional award to recognise outstanding contributions to scholarship and to the objectives of the Academy, by a Member of the Academy (the Medal is only awarded to Members of the Academy). Since then the Cunningham Medal has been awarded at three yearly intervals, by turn in each section of Science or the Humanities and Social Sciences (Polite Literature and Antiquities).

Cunningham Medal Awardees

1796	Thomas Wallace
1800	Theophilus Swift
1805	William Preston
1818	John Brinkley
1828	John D'Alton
1830	George Petrie
1833	George Petrie
1834	William Rowan Hamilton
1838	James MacCullagh
1839	James Apjohn
	George Petrie
1843	Robert Kane
1848	William Rowan Hamilton
	Samuel Haughton
	Edward Hincks
	John O'Donovan
1858	Edward J. Cooper
	George Salmon
	Charles William Wall
	William Reeves
1862	Humphrey Lloyd
	Robert Mallet
	Whitley Stokes
	John Thomas Gilbert
1873	William R. Wilde
1878	Aquilla Smith
	John Casey
	Edward Dowden
	George James Allman
1879	William Archer
	Robert Stawell Ball
1881	Howard Grubb
1883	Edward Perceval Wright
1884	John Birmingham
1885	John Christian Malet
1989	George Francis Mitchell
1989	George Francis Mitchell
2001	Daniel J. Bradley
	Maurice Craig
	Bernard Crossland
	David B. Quinn
2005	Denis L. Weaire
2008	Seamus Heaney
2011	John V. McCanny
2014	Patrick Honohan
2017	Dervilla M. X. Donnelly

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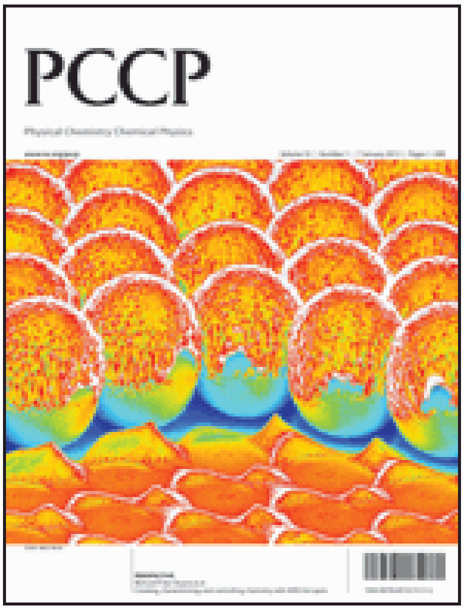


Support our Institute by publishing you new research results in the prestigious peer reviewed journal.

Scope

PCCP (*Physical Chemistry Chemical Physics*) is an international journal for the publication of cutting-edge original work in physical chemistry, chemical physics and biophysical chemistry. To be suitable for publication in *PCCP*, articles must include significant new physical insights; this is the prime criterion that referees and the Editors will judge against when evaluating submissions.

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.

Impact factor: 4.493*
Publishing frequency: 48 per year
Indexed in MEDLINE and Web of Science

http://pubs.rsc.org/en/journals/journalissues/cp#!recentarticles&adv

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**

Your local contact:

Andreina Moran
Account Manager
Sigma Aldrich Ireland Ltd

086 389 8647
andreina.moran@sial.com

TrainMiC Metrology in Chemistry Part III

Workshop - 25 April 2017

The Shared Facilities Building,

Backweston Laboratory Campus, Celbridge, Co.Kildare

Eurachem Ireland will host a TrainMiC workshop on Metrology in Chemistry. The workshop will be delivered by two of Ireland's TrainMiC trainers, trained at a European level to deliver these workshops in Ireland. This workshop covers Part III of the TrainMiC syllabus. Note that attendance at Part I and/or Part II is not required to attend Part III.

Please note that, due to the mathematical nature of the statistics modules, the number of participants in this workshop will be kept to a maximum of 30.

Programme

9.30-10.00	Registration with tea/coffee		
10.00	Introduction to TrainMiC and Eurachem Ireland update	Barbara O' Leary	Eurachem Ireland
10.10	Introduction to Metrology	Teri Donaghy	TrainMiC Trainer
10.50	Sampling, as a part of the measurement procedure.	Joe Fitzsimons	TrainMiC Trainer
11.30	Tea/coffee break		
Participants will be divided into two groups for the statistics modules.			
12.00	Statistics for Analytical Chemistry – Part I	Group 1: Teri Donaghy Group 2: Joe Fitzsimons	Location: Lecture Theatre Location: Upstairs meeting room.
1.15	Buffet style sandwich lunch		
2.00	Statistics for analytical chemistry – Part II	Group 1: Joe Fitzsimons Group 2: Teri Donaghy	Location: Lecture Theatre Location: Upstairs meeting room.
3.15	Ends		

Completed registration forms should be emailed to eurachem@statelab.ie by 6 April. Registration forms can be requested by emailing eurachem@statelab.ie.

Fee €90 Students/Unwaged: €50

Who should attend?

The workshop will be of interest to early-career chemists; chemists interested in refreshing their metrology knowledge; post-graduate chemistry students; scientists and engineers working in chemistry metrology.

Eurachem Ireland Introduce TrainMic Workshops

Eurachem Ireland is an organisation for people in Ireland working in, and studying, chemistry, particularly focusing on analytical chemistry. We operate a mailing list to keep members abreast of developments and events in Ireland and internationally. Eurachem Ireland promotes the objectives of Eurachem which is a network of organisations in Europe with members from 32 countries. It aims to establish a system of international traceability for chemical measurements and promotes good quality practices. As such Eurachem Ireland is pleased to facilitate the running of a TrainMiC workshop annually.

What is TrainMiC?

TrainMiC is a European Programme that aims to provide harmonised training to those working in analytical chemistry throughout Europe. Metrology in chemistry simply means making chemical measurements and every time we carry out analysis we make measurements. The TrainMic workshops, therefore, are applicable across all sectors – food, forensics, water analysis, environment to name a few, and to students, to regulatory laboratories, to those working in industry and in academia. The purpose of TrainMic is to *facilitate the training of metrology in chemistry to laboratory staff, researchers, educators, decision-makers and accreditation assessors, in order to strengthen the measurement infrastructure (ec.europa.eu/jrc/en/trainmic).* Attendance at a TrainMiC workshop should help to improve the quality of chemical measurements and also help with interpreting requirements of ISO 17025.

The training courses are developed, validated and regularly updated by a team of experts from across Europe. In Ireland there is a team of trainers under the direction of a team leader. The trainers have been intensively trained themselves in a European *Train the Trainer* training event where they become very familiar with the presentations which they then disseminate to workshop participants. The TrainMic syllabus currently consists of nine modules divided into 11 presentations as follows:

- Introduction to Metrology in Chemistry
- Traceability of Measurement Results
- Single Laboratory Validation of Measurement Procedures
- Uncertainty of Measurement – Part I Principles
- Uncertainty of Measurement – Part II Approaches

- Selection and use of Reference Materials
- Interlaboratory Comparisons
- Internal Quality Control
- Sampling as a part of Measurement Procedures
- Statistics for Analytical Chemistry – Part I
- Statistics for Analytical Chemistry – Part II

Eurachem Ireland run a TrainMic workshop every year, usually in the Spring. The full list of presentations above are given across three workshops. Part I was run in 2015, Part II in 2016 and Part III will run in Spring of 2017. It is therefore possible to cover the entire TrainMic syllabus over a three year period. The workshops are arranged so that they do not have to be attended in order. You can choose to attend a single workshop or to start with Part III before continuing with Parts I and II. Each workshop is run over a single day with breaks for coffee and lunch where the topics covered in the presentations can be discussed with the trainers and the other participants.

Bring TrainMic to You

If you are a company, research institute, college or university and you feel you have a large number of staff or students who would benefit from the TrainMic training course material, TrainMic can present a workshop, on site, and can cover the modules you feel will be of most benefit to you. Please contact us at Eurachem Ireland and we will be happy to put you in touch with the TrainMic Ireland Team Leader to organise a tailored, on site workshop.

For details of upcoming workshops and current costs (typically not more than €100 per attendee per workshop), please check our website: http://www.statelab.ie/eurachem.html or contact us via email at eurachem@statelab.ie.

More information on the TrainMiC programme can be found at https://ec.europa.eu/jrc/en/trainmic.

Eurachem Ireland A Focus for Analytical Chemistry in Europe

Food, Health and the Role of National Reference Laboratories Conference (Feb 3rd - 4th 2016) at the State Laboratory.

The conference was organised by the Department of Agriculture, Food and the Marine, the State Laboratory, HSE Public Analyst's Laboratory, Dublin, the Food Safety Authority of Ireland and the Marine Institute. There were a diverse range of speakers from the EU Commission, EU Reference Laboratories, the Food and Veterinary Office, FVO and leading international academics, as well as nationally based experts.

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.

Eurachem Ireland, provided the following posters for inclusion in the Irish Chemical News. These posters were presented as part of the 'Food, Health and the Role of National Reference Laboratories' conference which was held at the State Laboratory in February 2016.

Feidhmeannas Seirbhíse Sláinte
Health Service Executive

National Reference Laboratory – Food Contact Materials

Public Analyst's Laboratory, Dublin

NRL Functions:

- Provide expert analytical services to organisations such as HSE-EHS, FSAI, DAFM, SFPA, LAs, etc.
- Determine the specific migration for a range of substances from Food Contact Materials using methods that are accredited to ISO 17025 (2005)
- Participate in regular Proficiency Tests (PT) organised by the EURL and other organisations e.g. FAPAS, CHEK
- Participate in the EURL workshops and other activities
- Provide advice to the Competent Authority

The Public Analyst's Laboratory, Dublin has been designated as the National Reference Laboratory for Food Contact Materials (FCMs) under Article 33 of Regulation 882/2004.

Any material intended to come into contact with food, that is already in contact with food, or that can reasonably be expected to come in contact with food, is considered to be a *Food Contact Material.*

Food Contact Materials include packaging materials, cutlery, dishes, containers, processing machinery, cutting boards etc.

The list of materials includes active and intelligent materials (AIM) and articles, adhesives, ceramics, cork, glass, ion-exchange resins, metals and alloys, paper and board, printing inks and colours, regenerated cellulose, rubbers, silicones, varnishes and coatings, waxes, and wood.

Principal Legislation (Food Contact Materials):

Commission Regulation (EC) No 1935/2004 on materials and articles intended to come into contact with food

Commission Regulation (EC) 2023/2006 on good manufacturing practices for materials and articles intended to come into contact with food

Commission Regulation (EU) 10/2011 on plastic materials and articles intended to come into contact with food

Council Directive 84/500/EC relating to ceramic articles intended to come into contact with foodstuffs

Import Controls:

Commission Regulation (EU) No 284/2011 laying down specific conditions and detailed procedures for the import of polyamide and melamine plastic kitchenware originating in or consigned from the People's Republic of China and Hong Kong Special Administrative Region, China

Analysis performed for:
Semicarbazide
Isopropylthioxanthone
Lead and Cadmium
Chromium and Nickel
Epoxidised soybean oil (ESBO)
Phthalates
Photoinitiators
Primary Aromatic Amines
Melamine
Formaldehyde
Benzophenone and 4-methylbenzophenone
Bisphenol A
Seven Metals of Annex II–Reg. 10/2011

Analysis of non-intentionally added substances (NIAS):

Food Contact Materials can be analysed directly using simulants for migrating substances OR

Foods can be analysed directly for substances that have migrated into them

EU 'Safe for Food Contact Symbol'

Feidhmeannas Seirbhíse Sláinte
Health Service Executive

National Reference Laboratory
Mycotoxins including other Plant Toxins

Public Analyst's Laboratory, Dublin

NRL Functions:

- Provide expert analytical services to organisations such as HSE-EHS, FSAI, DAFM, SFPA, LAs, etc.
- Determine the levels of mycotoxins and plant toxins in a variety of matrices using methods that are accredited to ISO 17025 (2005)
- Participate in regular Proficiency Tests (PT) organised by the EURL and other organisations e.g. FAPAS, CHEK
- Participate in the EURL workshops and other activities
- Provide advice to the Competent Authority

The Public Analyst's Laboratory, Dublin has been designated as the National Reference Laboratory for Mycotoxins under Article 33 of Regulation 882/2004.

Mycotoxins are toxic secondary metabolites produced by organisms of the fungi kingdom, commonly known as moulds. The term 'mycotoxin' is usually reserved for the toxic chemical products produced by fungi that readily colonize crops. One mould species may produce many different mycotoxins, and the same mycotoxin may be produced by several species.

In 2015 the scope of the EURL on Mycotoxins was extended to include responsibility for other Plant toxins.

Plant toxins are toxic secondary metabolites which naturally occur in food, feed, weeds and ornamental plants. The chemical diversity is tremendous. Aromatic plants which are used as ingredients in food (herbs, spices), scents and flavours (essential oils) or traditional herbal remedies are examples where plant toxins are found.

Principal Legislation (Mycotoxins):

Commission Regulation (EC) No 401/2006 laying down the methods of sampling and analysis for the official control of the levels of mycotoxins in foodstuffs

Commission Regulation (EC) No 1881/2006 setting maximum levels for certain contaminants in foodstuffs

Import Controls Legislation (Mycotoxins):

Commission Regulation (EC) No 669/2009 implementing Regulation (EC) No 882/2004 of the European Parliament and of the Council as regards the increased level of official controls on imports of certain feed and food of non-animal origin and amending Decision 2006/504/EC

Mycotoxins controlled:

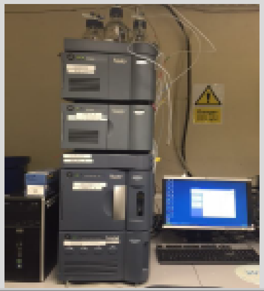
Aflatoxins B_1 B_2 G_1 G_2
Aflatoxin M_1
Ochratoxin A
Deoxynivalenol (DON)
3- and 15-Acetyl DON
Nivalenol
Fumonisin B_1 B_2 B_3
Patulin
Diacetoxyscirpenol
Zearalenone
T-2 and HT-2 toxins
Citrinin

Plant toxins controlled:

Ergot alkaloids
Pyrrolizidine alkaloids
Tropane alkaloids

Foods tested:

Nuts
Seeds
Cereals
Cereal-based Baby Food
Infant formula and follow-on formula
Milk
Dried Vine Fruits
Apple Products
Food Supplements
Spices



Principal Legislation (Plant Toxins):

Commission Regulation (EU) 2015/1940 amending Regulation (EC) No 1881/2006 as regards maximum levels of ergot sclerotia in certain unprocessed cereals and the provisions on monitoring and reporting

Commission Recommendation (EU) 2015/976 on the monitoring of the presence of tropane alkaloids in food

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Feidhmeannas Seirbhíse Sláinte
Health Service Executive

National Reference Laboratory – Polycyclic Aromatic Hydrocarbons including other Process Contaminants.

Dublin Public Analyst's Laboratory

NRL Functions:

- Provide expert analytical services to organisations such as HSE-EHS, FSAI, DAFM, SFPA, LAs, etc.
- Determine the level of PAHs and other process contaminants using methods that are accredited to the ISO 17025 standard.
- Participate in regular Proficiency Tests (PT) organised by the EURL and other organisations e.g. FAPAS, CHEK.
- Participate in the EURL workshops and other activities.
- Provide advice to the Competent Authority .

The Dublin Public Analyst's Laboratory has been in existence as an analytical laboratory since 1862. It was designated as the National Reference Laboratory for Polycyclic Aromatic Hydrocarbons (PAH) under Article 33 of Regulation 882/2004 in 2006 and was awarded INAB accreditation for PAH determination by GC-MS in 2007.

PAHs are a group of carcinogenic compounds produced by incomplete combustion of organic matter. Commission Regulation 1881/2006 defines the maximum permitted levels of PAHs in specified foods such as smoked meat and fish, herbs and spices, oils and fats, cocoa products, food supplements, baby food and infant formula.

In 2015 the scope of the EURL on PAHs was extended to include responsibility for other process contaminants. These contaminants are generated during the processing of food and are absent from the raw materials.

There is no strict definition for a process contaminant but there could potentially be a long list of compounds e.g. acrylamide, furan, 3-MCPD, fatty esters with MCPD and glycidol, ethyl carbamate, nitrosamines, trans fat, benzene in soft drinks, perfluorinated compounds, hydroxymethylfurfural, extraction solvents and perchlorate.

Laboratory Staff:

Dublin Public Analyst
Dr. Michael O'Sullivan

PAHs:

PAHs are a class of compounds with multiple fused aromatic rings that are formed during the incomplete combustion of organic material; many are highly carcinogenic. They can enter the food chain from processes such as smoking (in the case of fish and meats) or cooking over a naked flame or inappropriate drying (as with herbs, spices, food supplements and cocoa beans). They can also be present as a result of environmental contamination.

Commission Regulation 1881/2006 controls the limits of PAHs in certain foods with maximum levels for benzo[*a*]pyrene and the sum of PAH4 (sum of benzo[*a*]pyrene, benz[*a*]anthracene, benzo[*b*]fluoranthene and chrysene).

Acrylamide:

Acrylamide was first reported in food by Swedish scientists in 2002 and is classed by the IARC as a probable carcinogen. It is a Maillard reaction product produced when starchy food is heated above 120°C. Susceptible Foods are those made from potatoes or wheat, which are rich in reducing sugars and the amino acid asparagine.

There is currently no maximum EU wide limit for acrylamide in food; however Commission Recommendation 2013/647/EU sets out indicative values for acrylamide in certain foods which triggers an investigation if exceeded.

Monochloropropandiol and glycidol esters:

The use of acid pre-treatment or roasting, followed by solvent extraction can produce MCPD esters by the action of the acid on fats. It is estimated that there is 100% bio-availability of MCPD and glycidol from fatty esters.

Glycidyl fatty acid esters (GE) are generated during the deodorisation of edible oil. Glycidol is categorised as probably carcinogenic to humans.

There are currently no maximum limits for MCPD or glycidyl esters in food, however EFSA are collecting monitoring data on their levels in food.

Furan:

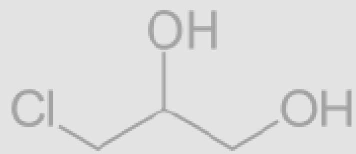
In 2004 the US-FDA reported finding furan in food in sealed jars and cans. Furan is a small molecule with a boiling point of 32°C and is classified by IARC as a possible carcinogen. The mechanism of production is uncertain; furan is thought to be produced by several routes involving heat degradation of sugars, polyunsaturated fatty acids and ascorbic acid (vitamin C) during cooking/processing.

There is currently no maximum limit for furan in food.

3-MCPD:

3-Monochloropropandiol (3-MCPD) is produced by the action of hydrochloric acid on fats during the manufacturing of soy sauce. 3-MCPD is classified by the IARC as a possible carcinogen.

The maximum limit for 3-MCPD in soy sauce is 20 µg/kg as defined in Commission Regulation 1881/2006.



Industry and Business
Promoting Manufacturing Excellence

What Needs to Change in Ireland if we Want to be a Real Global Leader in R&D

Post written by Ian Collins, Partner at EY Ireland. Previously published on Fora.ie

The burden for small firms investing in research should be lifted.

Ireland's tax regime already ranks among the best in class internationally and allows companies to claim significant cash refunds for their research efforts – in turn facilitating the creation of jobs and ultimately driving the economy.

The resulting cash benefits through this tax relief enables companies to increase their cash flows – something which is essential, in particular, for SMEs – and thus invest further in more research and development (R&D).

From the perspective of global multinationals operating in Ireland, the regime provides incentives for companies to bring their R&D activities here.

However, while the uptake of the R&D tax credit has grown significantly in the past decade, Ireland is still falling behind other developed countries in terms of the amount spent relative to the size of the economy – currently ranking 12th within the EU.

In tandem with this, there are likely big changes on the horizon such as Brexit, possible US tax reform and competition increasing within the EU.

It is imperative, therefore, that more must be done to ensure Ireland can continue to compete on the global R&D stage in order to become a world leader and a major hub for scientific and engineering research.

Steps to make Ireland an R&D hub

One of the key areas that must be examined is human capital. This means creating an environment where the very best, home-grown talent has incentives to stay in Ireland and move into areas of innovation and R&D, while foreign talent is also attracted to move here.

For Irish workers, this can be done by fostering the uptake of STEM (science, technology, engineering and maths) subjects in schools and universities so that we develop a pipeline of R&D talent.

Meanwhile, for experienced hires and senior executives both here in Ireland and those considering moving here, our domestic income tax rates are still far too high when compared to our European competitors.

We therefore need to put in place incentives and reliefs so that we can compete as a top destination for the best talent within Europe – in particular during a time when the employment market is becoming more and more mobile.

In addition to focusing on the area of human capital, Ireland must give companies further incentives to invest in R&D so that we can climb our way up the EU investment rankings.

To move this dial, there are a number of steps that could be considered:

Foster greater collaboration between industry and academia – At the moment, the cap on R&D relief for subcontracting to universities sits at 5%, compared to 15% for third parties subcontracted to carry on R&D on a company's behalf.

A change to equalise this cap would avoid apparent discrimination and also help to drive the government's commitment to create greater linkages between businesses and third-level institutions.

Lessening the burden on small companies – For SMEs, any delay in the issuing of R&D refunds by the Revenue can have a detrimental impact on their ability to trade.

Therefore, it would be a welcome development for SMEs to be given the opportunity to avail of their cash refunds immediately, as opposed to the current regime which sees this take place over a three-year period.

This would serve to encourage more small businesses to engage in R&D by easing any concerns they may have on the potential impact of a delayed refund – while, at the same time, creating a cycle whereby they have incentives to inject that cash back into further R&D investment.

In addition to this, there should be a reduced administrative burden placed on SME's to encourage greater participation.

Encouraging FDI through Ireland's R&D tax regime – Growing Ireland's investment in R&D cannot solely rely on spend by Irish indigenous companies, but rather we must actively sell our R&D offering to the international business community to ensure that we are attracting FDI in this space.

As such, aligning the R&D tax credit regime with R&D grant relief offered by the IDA could offer companies availing of these grants greater certainty with respect to their overall cost of doing R&D in Ireland, thus making a compelling business case to house those projects on our island.

An essential contributor

R&D activity is an essential contributor towards the ongoing prosperity of the domestic and global economy. It is therefore essential that we as a country do everything in our power to facilitate increased R&D, both amongst our Irish indigenous companies and through the attraction of FDI.

In doing so, we will be better positioned to compete with our international counterparts who are also vying for their piece of the pie.

Industry and Business
Promoting Manufacturing Excellence

OncoMark Secures €2.1 Million Investment to Commercialise Breast Cancer Diagnostic Test

OncoMark, a University College Dublin (UCD) spin-out company, announced on Wednesday that it has secured €2.1 million to fund the commercialisation of OncoMark's lead product, OncoMasTR, which it plans to launch in 2018. OncoMasTR is a novel prognostic test for early-stage breast cancer that will reduce the number of breast cancer patients receiving unnecessary chemotherapy.

OncoMark CEO Des O 'Leary said: "In the absence of accurate tests, the majority of early-stage breast cancer patients are treated with chemotherapy despite many not benefiting from the treatment. This exposes individuals to severe side effects and results in significant costs to healthcare systems worldwide. Approximately 70% of patients do not require chemotherapy after initial surgery, but it has been difficult to identify these individuals. The OncoMasTR test is designed to enable a more personalised approach to patient care, helping clinicians to determine which patients should not receive chemotherapy, ultimately improving their quality of life."

The funding round included; Kernel Capital, through the Bank of Ireland Kernel Capital Venture Funds, the Irrus Investments syndicate, the Galway HBAN MedTech syndicate, private investors and Enterprise Ireland.

OncoMark was previously awarded €2.7 million, through the Horizon 2020 SME Instrument Phase 2, to clinically validate the OncoMasTR test. This new funding round will allow the translation of the test from clinical validation to regulatory approval and full commercialisation.

Dr Tom Kelly, Head of Division, Industrial, Lifesciences and Consumer, Enterprise Ireland said, "The thriving Irish medtech sector continues its story of success and the development of innovative products such as OncoMasTR contributes significantly to Ireland's reputation as a leading global cluster for medical technologies. Companies like OncoMark are the future of the Irish economy. They have used Ireland's extensive innovation ecosystem and worked with the Enterprise Ireland commercialisation team to bring the fruits of academic enquiry to market and profitably".

OncoMark is focused on the development of novel panels of cancer biomarkers, to aid treatment decisions and allow more tailored patient management, ultimately improving the quality of life for cancer patients.

OncoMark, which was co-founded by Professor William Gallagher and Steve Penney as a spin-out from UCD's School of Biomolecular and Biomedical Science, is headquartered at NovaUCD, the Centre for New Ventures and Entrepreneurs.

The OncoMasTR test is based on a panel of genetic 'drivers' of breast cancer. The original research that resulted in the identification of the panel was led by Professor Adrian Bracken, Smurfit Institute of Genetics, Trinity College Dublin and researchers at the UCD Conway Institute, led by Professor William Gallagher. The OncoMasTR technology was subsequently exclusively licenced by both universities to OncoMark.

The [2017 Research and Innovation Conference and Exhibition] in Citywest, on February 14th

The day was a great success. Over 1200 delegates gathered to listen to over 100 inspiring and informative talks and meet with exhibitors that can help them in the R&D Journey.

If you are interested in pre-registering on the website for complimentary pass for the 2018 event you can do so here.

The video of the day as well as the presentations will up uploaded next week and a link will be emailed to all delegates.

www.innovateireland.ie

These joint events held at Citywest on January 31st.

Bigger than the Innovation Conference with some 2500 delegates attending and many topics covering chemistry topics.

The institute of Chemistry of Ireland Annual Lecture Series Award winner Prof John Sodeau gave an interesting talk based roughly around his article in the Issue. It is expected these events will generate a number of papers for future publication in ICN.

To exhibit or to be considered for a speaking spot for these conferences in 2018, you can contact:

John Bent or Colin Murphy

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IDA Ireland http://www.idaireland.com

Wexford, Ireland – February 3, 2017 – Waters Corporation (NYSE:WAT) officially opened a new site expansion at their state-of-the-art manufacturing and assembly facilities in Wexford, Ireland.

"The Manufacturing Centre of Excellence in Wexford, Ireland is instrumental to our global manufacturing strategy. We strive to consistently develop reliable products that not only meet our customer's needs, but also contribute to their success," said Christopher J. O' Connell, President and CEO, Waters Corporation. "This expansion will allow for significant increases in operations, services and development functions onsite."

This year marks Waters' 20th anniversary in Wexford. Since commencing operations in 1997, the company has seen continuous and sustained growth. Presently, over 300 people are employed in the 145,000 square foot facility that manufactures chromatography columns, solid-phase extraction devices and mass spectrometry instruments. To read more Ctrl+click:-

http://idaireland.us3.list-manage1.com/track/click?u=1742b1fc555505427ce19d986&id=d114f38390&e=0ec98a7f8c

Friday, January 27th 2017: Element Six, a world leader in synthetic diamond super-materials and member of The De Beers Group of Companies, has today announced the creation of a further 100 jobs at its Shannon facility as part of a €7million investment at the plant this year.

Read the full article Ctrl+click:-

http://idaireland.us3.list-manage.com/track/click?u=1742b1fc555505427ce19d986&id=f548a5d5d5&e=0ec98a7f8c

January 27th 2017 Craigavon based global contract pharmaceutical development and manufacturing organisation, Almac Group, has secured new premises in Dundalk, County Louth to support its ongoing global expansion plans in response to increased client demand.

Almac will make a multimillion investment in the new facility at IDA Business Park. The expansion has been supported by the Department of Jobs, Enterprise and Innovation through IDA Ireland, Ireland's inward investment promotion agency.

The facility will be utilised by Almac Pharma Services and Almac Clinical Services, both of which are registered to operate in the Republic of Ireland. The new premises increases the Group's European footprint by 32,000sq ft and provides continued presence within the European Union in the long term.

This investment comes just weeks after Almac confirmed ambitious plans to expand its operations at its global Headquarters in Northern Ireland with the construction of a new laboratory and additional office facilities. The company simultaneously announced investment at its North American site creating an additional 300 new, full time jobs. These investments will see an increase of Almac's global headcount to over 5,000 by the end of 2017. Read the full article Ctrl+click:-

http://idaireland.us3.list-manage.com/track/click?u=1742b1fc555505427ce19d986&id=a3e2e28471&e=0ec98a7f8c

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