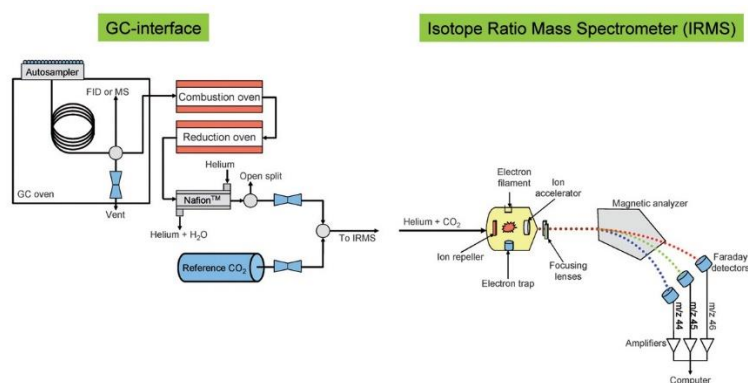




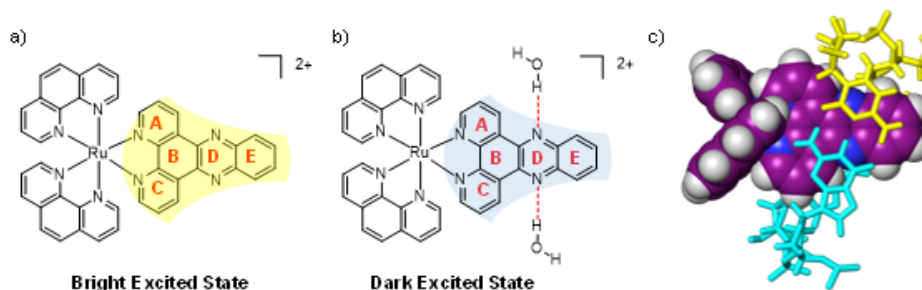
The Journal of the Institute of Chemistry of Ireland

Feature Articles

Detection of Prohibited Growth Promoters in Food Producing Animals: Challenges and Future Strategies



Ruthenium(II) Polypyridyl Complexes: Mechanistic Investigations and Applications in Chemical Biology



Winners:

Industrial Chemistry Award 017 Prof Tom Moody - Almac

Annual Lecture Series(Eva Philbin) - Prof Donal O'Shea - RCSI



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The Institute of Chemistry of Ireland

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**School of Chemical and
Pharmaceutical Sciences**

A message from the President

Colleagues

The Institute of Chemistry of Ireland is awarding the Annual Industrial award to Dr Tom Moody, who is representing a team from ALMAC. Meanwhile a series of lectures associated with the Eva Philbin Award will be delivered by Prof. Donal O'Shea (RCSI) starting this Friday 3rd November as part of the Irish Biological Inorganic Chemistry Society at their inaugural meeting in the University at Maynooth. In addition there is a Eurachem event in Dublin on 14th -15th May 2018, of interest to anyone interested in Quality Assurance.

It is with great sadness that I learnt of the passing of Philip Ryan. I had only known him for two years, through Institute of Chemistry of Ireland Council meetings. However as others who have known him for much longer attest, he was a true gentleman; his kindness and courtesy were always to the fore. He was a cornerstone of the Institute and promptly produced agenda, minutes and Annual reports.

He will be a huge loss to the Institute and I would like to convey my condolences to Fidelma, his wife on behalf of all the members of the Institute. *Ar dheis Dé go raibh a anam.*

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Editorial

This the 4th Issue this year and is the first that our Honorary Secretary, James Philip Ryan or Philip as we knew him, has not proof read draft versions for errors. Philip has been very supportive and helpful as ever with checking, emailing and posting ICN on our web site. He was a polite soft spoken chemist and person of many talents and has always encouraged me since I joined the Council of ICI. He will be greatly missed by all of us on Council. I expect to have an Obituary for him in a future Issue of ICN.

This Issue brings announcements of the Institute's Henkel Ireland sponsored Industrial for the 3rd year and our Annual Lecture Series Award (Eva Philbin). Also reported are some of the Pharma Industry Awards 2017 winners.

The spotlight is on two young chemists Amy Nagle of the State Laboratory and Fergus Poynton from Trinity's Biomedical Sciences Institute and as reported in Issue 3, the winner of the Irish RIA and international IUPAC-SOLVAY Award for Young Chemists.

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

Publishing Irish Chemical News is not getting any easier. I struggle to get papers on time and this Issue is lighter than I would like on academic type papers. Ideally I would have a pool of papers for publication in reserve so if there is a late paper I can take one from the pool and publish on time at a preannounced date. This is especially important if we are to charge for regular advertising or attempt to post job vacancies in the future.

I'm not sure what the problem is with chemists working in Ireland who do first class research work and are very happy to get research grants from the Irish tax payers and European funding. Sadly they are not very willing to communicate to a wider public and fellow chemists anything about their work. My view is that SFI and Horizon grants should require that researchers must provide general papers for publication in Irish publications. The significant announcements and discoveries would of course be the preserve of the peer reviewed international journals.

Again I see this disengagement reflected in the non-participation of Irish chemists and researchers in the EuCheMS Chemistry Congresses over the past 6 to 8 years. Hopefully this will change next year at the Liverpool Chemistry Congress which is a bit closer to home. The Institute will hopefully make a bid there to host the 2022 Congress in Dublin. We do need the support of Irish chemistry researchers and to make your presence felt in Liverpool. Hopefully Irish chemical researchers are not just "Atlanteans"[#] sitting out in the Eastern Atlantic on the edge of Europe. More details of the Liverpool Congress are in the following pages.

Physics is doing much better than chemistry at communicating their work to a greater public. Walk in to any good book shop to the Popular Science section and count the number of physics type books versus chemistry titles. Tonight for example I attended a lecture on Dark Matter at the Dublin Institute of Advanced Studies. It was well attended not just by physicists working in the area but by interested laypeople. What is the matter with communicating chemistry?

Maybe a first step in addressing these concerns would be for readers to encourage your colleagues to join the Institute and engage in promoting chemistry and if you are not a member to join. Membership forms are available on our website. www.chemistryireland.org

A last topic I would like to raise is about what we as chemists call ourselves. I have started to notice the term "Chemical Scientist" used in some publications including from our colleagues in the RSC. I would like to hear your views on this. Responses can be sent to:-

info@instituteofchemistry.org

[https://en.wikipedia.org/wiki/Atlantean_\(documentary_series\)](https://en.wikipedia.org/wiki/Atlantean_(documentary_series))

Patrick Hobbs MSc, FICI, CChem, CSci, MRSC.
Editor
31/10/2017



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#>



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

Paul Alivisatos, University of California, Berkeley, USA

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

Stefanie Dehnen, Philipps-Universität Marburg, Germany

Christopher Dobson, University of Cambridge, UK

Ben Feringa, University of Groningen, The Netherlands

Jin-Quan Yu, The Scripps Research Institute, USA

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

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

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



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

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

**The Institute of Chemistry of Ireland Announces the Winner of the
Industrial Chemistry Award 2017:-**



<https://www.almacgroup.com>

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

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

The Almac Group is an established contract development and manufacturing organisation that provides an extensive range of integrated services globally to companies within the pharmaceutical and biotech sectors.

Almac formed by Sir Allen McClay in 2002, born out of Galen Holdings Plc which he founded as Galen Ltd in 1968. Since then the Group has continued to grow organically and employs over 4,000 employees worldwide. The company headquarters is located at Craigavon, Northern Ireland.

Details of Award Ceremony and Lecture for December to be announced.

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

Check website: - www.chemistryireland.org



Institiúid Ceimice na hÉireann
Institute of Chemistry of Ireland



RCSI

Annual Lecture Series Award (Eva Philbin) 2017 Winner

Professor Donal O'Shea



Head of Department of Pharmaceutical & Medicinal Chemistry

RCSI

Research Overview

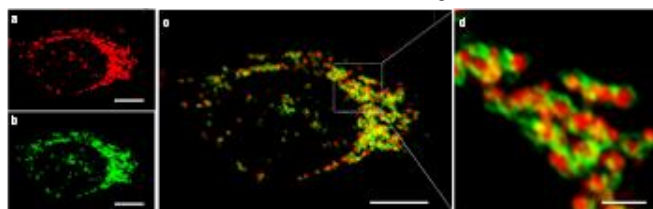
The central theme of his research lies in the advancement of new strategies for the synthesis and functional assessment of structurally complex molecules. Specific goals include the development of NIR fluorophores for fluorescence guided surgery, new light activated anti-cancer agents, and the generation of chemical tools to assist in gaining a molecular level insight into biological processes. His research has its foundations in synthetic chemistry and chemical biology with strong collaborative links with research and clinical imaging. Numerous industrial collaborative research projects have been carried out with companies such as Schering Plough, Janssen Pharmaceuticals, Alkermes Ltd and Ipsen Ireland. He has had four patents granted on light activated therapeutic agents and NIR-imaging agents and one filed on directed self-assembly of nanoparticles. He founded a spin-out company (HAE Therapeutics Ltd) to help exploit the intellectual property from his research work with license agreements enacted with companies based in the US, UK and China. Previous awards include the Royal Society of Chemistry, Inaugural 2012 North/South of Ireland lectureship award and he has been visiting Professor at Donghua University, Shanghai, the University of Rennes 1, the École Nationale Supérieure de Cachan, Paris, and at the CNRS in the Université Bordeaux 1.

Learning how to turn the lights on

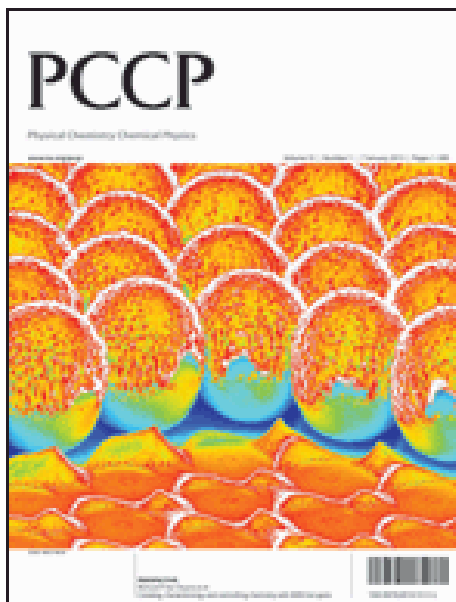
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Venues & Dates

Maynooth University:	Nov. 3 rd 2017
RCSI Dublin:	Dec. 2017
NUI Galway:	Dec. 2017
Limerick Institute of Technology:	Jan. 2018



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

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



IBICS Irish Biological Inorganic Chemistry Society

IBICS-1 Symposium

Maynooth University

3rd November 2017

John Hume Building JHL-4 and JHL-6

Programme

11.00-11.15	Opening Symposium	
		Chair: Celine Marmion
11.15-12.00	Walter Berger (Medical University Vienna)	Dissecting the mode-of-action of anticancer metal drugs: synergistic combinations and interaction with the anticancer immune response
12.00-12.45	Donal O'Shea (RCSI); Institute of Chemistry of Ireland Eva Philbin Award Lecture	Targeted and Responsive Agents for Fluorescence Guided Precision Surgery
12.45-13.45	Lunch	
		Chair: Matthias Tacke
13.45-14.05	Bernie Creaven (ITT)	Cu(II) Complexes: Pro or Anti-oxidant activity in Cancer cells?
14.05-14.25	Andrea Pettenuzzo (NUIG)	A sweet approach to the targeted anticancer chemotherapy: gold-based glycoconjugates
14.25-14.45	Orla Howe (DIT)	Piecing the puzzle: To decipher the biological mechanisms of novel copper-Phenanthroline complexes.
14.45-15.05	Reece Kenny (RCSI)	Design and Development of Novel Dual-Threat Metal Chemotherapeutics
		Chair: Denise Rooney
15.05-15.20	Flash poster presentation	<u>Anna Banasiak (DIT)</u> : Monitoring DNA Nuclease Activity of Bioinorganic Compounds using Electrochemical Biosensors

		<p><u>Eolann Kitteringham (RCSI)</u>: Development of a Novel Cytoplasmic Trackable NIR Platinum-Fluorophore Conjugate</p> <p><u>Aisling Crowley (DIT)</u>: The Mechanism of Action of a Copper(II) Folate-Phenanthroline complex in 2D and 3D cellular models</p> <p><u>Leila Tabrizi (NUIG)</u>: Synthesis and C–H Activation Reactions of Cyclometalated Copper(I) Complexes with NCN Pincer and 1,3,5-Triaza-7-Phosphaadamantane Derivatives: In Vitro Antimicrobial and Cytotoxic Activity</p> <p><u>Azeez Yusuf (DIT)</u>: Liposomal encapsulation of silver nanoparticles enhances cytotoxicity and causes induction of ROS independent apoptosis</p>
15.20-16.00	Coffee break	Poster Session
		Chair: Orla Howe
16.00-16.20	Sarah da Silva Ferreira (DIT)	A new mixed-valence Mn(II)Mn(III) compound with catalase and superoxide dismutase activities
16.20-16.40	Muhib Ahmed (MU)	Transition Metal Complexes of Novel Phenanthroline-based Ligands and their Antimicrobial Activity
16.40-17.00	John Kelly (TCD)	Probing Reaction Intermediates from Metal-containing Photosensitisers in Solution and in HeLa cells
17.00-17.20	Awatif Almoitary (DIT/NUIG)	Cellular effects of novel dual-acting Pt(IV) complexes based on cisplatin with phenylbutyrate
		Chair: Diego Montagner
17.20-18.05	Mike Hannon (Birmingham University)	Metallo-supramolecular cylinders that bind unusual DNA and RNA structures: from DNA nanoscience to bio-activity
18.05-18.10	Closing	
18.10-19.30	Banquet and wine reception	

To register or obtain further information email Dr Diego Montagner at Diego.Montagner@mu.ie

You can also register on the morning of the event.



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Detection of Prohibited Growth Promoters in Food Producing Animals: Challenges and Future Strategies

Dr. Amy Nagle, The State Laboratory



Dr. Amy Nagle obtained a Bachelor's Degree in Chemistry with Forensic Science from University College Cork in 2009. She then completed a PhD under Professor Jeremy Glennon at University College Cork on the design, synthesis and characterisation of novel liquid chromatography stationary phases with selectivity based on molecular recognition. She joined the State Laboratory in 2013, initially working in the area of confirmatory analysis of dioxins in animal feed and food of animal origin by HRGCMS. She now works as a Chemist in the Veterinary Toxicology section of the lab which provides an analytical and advisory service to the Department of Agriculture, Food and the Marine by analysing samples taken from food producing animals for veterinary drug residues such as steroids, sedatives and NSAIDs.

Natural steroids have been used in animal production for anabolic purposes to increase growth of muscle mass and improve feed efficiency and hence enhance meat production ^[1]. The European Commission published two reports in 1999 and 2002 which concluded that the presence of hormone residues in meat products are potentially harmful to human health through endocrine, developmental, immunological, neurobiological, immunotoxic, genotoxic and carcinogenic effects. However, they were unable to estimate the extent of any risk. Of the various susceptible risk groups, prepubertal children are of greatest concern as their endogenous levels of sex steroids, such as estradiol, are naturally low ^{[2][3]}. Subsequent reports such as those published by the UK Veterinary Products Committee Working Group have disagreed with this opinion. They concluded that the current scientific evidence does not indicate that the use of hormones in farming presents a risk to public health, however they agree that consumption of hormone residues in hormone-treated meat is an unnecessary additional exposure and is therefore unacceptable ^{[4][5]}.

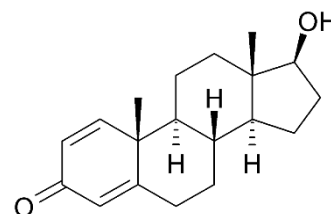
The use of hormonal growth promoters in food-producing animals has been prohibited in the European Union since 1988 under Council Directive 96/22/EC. Official control of residues of anabolic compounds in tissues of slaughter animals and food of animal origin is therefore undertaken in EU countries and must be performed in accordance with the requirements of Regulation (EC) No 882/2004. Compliance of EU Member States with the ban is checked by the analysis of samples collected at the slaughterhouse or on-farm under a National Residue Monitoring Plan as required by Directive 96/23/EC. The National Residue Monitoring Plan covers

all farmed food-producing species (bovines, sheep/goats, pigs, poultry, fish, horses and farmed deer) as well as food commodities such as milk, honey and eggs. The hormonal growth promoters are classified as Group A3 substances under Directive 96/23/EC. In Ireland, legislation is enforced by the Department of Agriculture, Food and the Marine (DAFM) under service contract to the Food Safety Authority of Ireland (FSAI). The State Laboratory is designated as a National Reference Laboratory for Group A3 substances and carries out multi-residue, mass spectrometry-based confirmatory analysis of samples for these compounds in a variety of matrices.

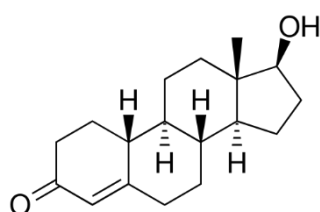
The analysis of growth promoting hormones in food is complicated by the presence of natural hormones in biological samples. For a range of compounds there can be multiple explanations for their presence in a sample: there may be endogenous production as part of the normal physiology of the species, the compounds may be produced in the sample as a result of the presence of certain bacteria or through instability or the animal may have been treated with the compound. Growth promoting hormones are usually administered in the form of synthetic steroid esters as there is a decreased rate of absorption of the drug from an injection site compared to the free drug, leading to a prolonged anabolic effect ^[6]. These esters are rapidly hydrolysed in vivo into substances which are also endogenously present in the urine of the animal. This poses a challenge in the enforcement of the ban on the use of growth promoting hormones in meat production. Some of the naturally occurring hormones used as growth promoters are discussed below.

Boldenone

17 β -Boldenone is an anabolic steroid with androgenic activity. Natural occurrence of 17 β -Boldenone has been found in non castrated male pigs and stallions while 17 α -Boldenone has been found in untreated male calves ^[7]. The presence of 17 β -Boldenone conjugates in the urine of young calves is used as proof of illegal administration however urine samples must be taken without faecal contamination as free unconjugated 17 β -Boldenone has been found in dried faeces on the fur of untreated calves ^[8]. Analytical results for Boldenone must also be specified as free or conjugated form and reference the animal species.

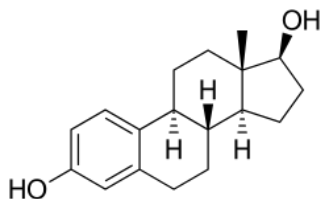


Nortestosterone



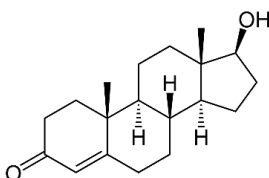
Also known as Nandrolone, 17 β -19-Nortestosterone is an androgenic anabolic steroid. 17 β -Nortestosterone is known to occur naturally in the urine of boars, stallions, sheep, goats and deer ^[7]. The main bovine metabolite is 17 α -Nortestosterone and natural levels are found in pregnant cows, horses and sheep and neonatal calves. It is not likely to be found in pigs of either sex however ^[9]. 17 α -Nortestosterone is used as the marker metabolite for illegal use in species/genders where there is no published data on endogenous presence.

Estradiol



17β-Estradiol is an estrogenic steroid. It has an active role in the normal development of the female sex characteristics during the lifetime of females. There are natural 17β-Estradiol levels present in porcines, equines, ovines and bovines [7]. Natural levels in cows have been found to vary greatly depending on the reproductive cycle and pregnancy. This poses a difficulty in detecting abuse of the steroid. At present, 17β-Estradiol itself is used as the marker residue for indication of illegal use.

Testosterone



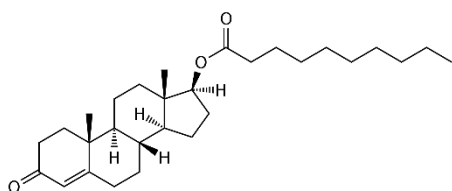
17β-Testosterone is an androgenic steroid. It is the main sex hormone secreted by males. Natural levels have been found in both bovines and porcines (male and female) as well as ovines and equines [7]. The levels are highly variable in all matrices and species: endogenous hormone levels in tissues vary with the sex and breed of the animal and also depend on whether the animals have been castrated or are pregnant. The main metabolite is 17α-Testosterone and has been found to be endogenous in bovines, ovines and equines [7]. Abuse of this hormone is hence difficult to detect.

In all cases for a specific species/gender where no prior information has been published indicating the endogenous presence of a compound or its marker metabolite, the confirmed presence can be considered proof of illegal administration, based on current knowledge [7].

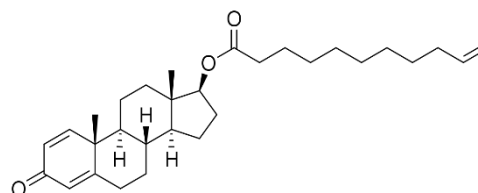
Proposed Strategies for the Detection of Abuse

Steroid Esters in Hair/Serum

Natural steroids are usually administered as synthetic steroid esters (e.g. testosterone decanoate and boldenone undecylenate, the chemical structures of which are shown below). As these steroid esters are not known to occur naturally, the presence of an ester in a biological sample is unambiguous proof of illegal administration [10]. The esters are rapidly hydrolysed in vivo into natural steroids therefore in urine it is hard to differentiate between the metabolites of endogenous natural steroids and those of the natural steroids from the administered steroid esters [11]. Previously the detection of steroid esters was limited to the analysis of tissue samples taken from the animal carcass at the alleged site of injection [7]. In recent years however, the alternative matrices hair and serum have been utilised to detect the intact steroid esters.



Testosterone decanoate



Boldenone undecylenate

Hair is considered to be an attractive matrix for prolonged detectability of drug residues ^[12]. In a study carried out in 2006, boldenone undecylenate, a long chain steroid ester, was detected in bovine hair samples up to 14 days after injection of a single dose of 2 mg/kg BW ^[11]. Residues can be incorporated into the hair from blood via the hair follicle, incorporated from sweat via the hair shaft or through pour-on treatment ^[10]. Sample preparation of hair involves digestion using a reagent such as tris(2-carboxyethyl)phosphine hydrochloride (TCEP) followed by extraction of the steroid esters and analysis by a technique such as LCMS/MS ^[13]. Difficulties associated with the analysis of hair samples include the risk of cross contamination of the hair from brushing against other animals and the large influence of pigmentation of hair on the amount of ester found. Compounds with a steroid-like structure have been reported to bind to melanin, the pigment responsible for hair colour, hence incorporation of the drug into pigmented hair is greater than its incorporation into non-pigmented hair ^[14]. A study carried out in 1997 found that in hair samples taken from bulls, testosterone was detected at a concentration approximately four times higher in black hair when compared to white hair ^[15]. Hair analysis is not yet widely used by EU member states as part of their routine monitoring programme.

It is more difficult to detect intact steroid esters in serum as they hydrolyse rapidly to release the natural steroid resulting in low concentrations of the steroid ester present in the serum. The detection time in serum after administration is very short (approximately 5 days). The detection window depends on the time needed for the steroid ester to reach the bloodstream, the efficiency of esterase activity in the blood and the length of the ester chain ^[7]. Modern MS techniques capable of lower limits of detection have allowed a longer window of detection. A derivatisation step in the sample preparation such as dansylation and sampling of the blood into sodium fluoride and potassium oxalate vacutainers have also been found to increase the detection limit ^[7] ^[16]. Sampling of blood from live animals in some EU Member States is considered too invasive however and is subsequently not used as a matrix ^[7].

Gas Chromatography – Combustion - Isotope Ratio Mass Spectrometry

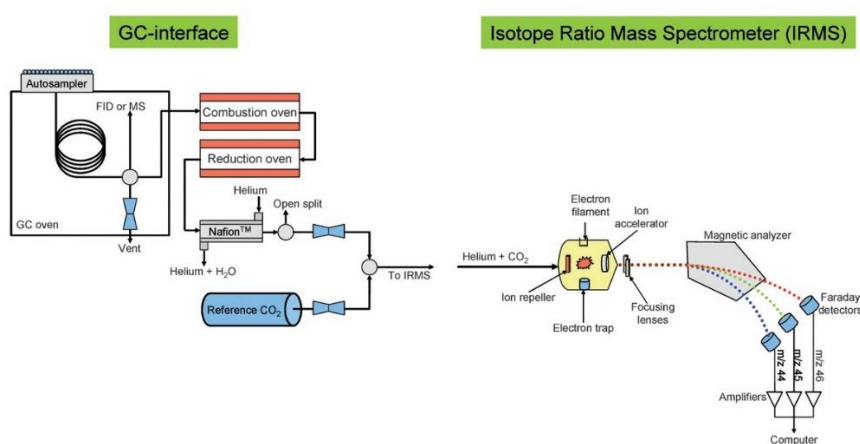
Isotope Ratio Mass Spectrometry (IRMS) measures the relative abundance of isotopes in materials. The carbon isotope ratio ($\delta^{13}\text{C}$ – see equation below) in an animal is influenced by the diet which normally consists of a variety of plant species ^[17]. Plants have differing $\delta^{13}\text{C}$ values depending on their photosynthetic cycle (C3 or C4). C4 plants such as maize have a higher ^{13}C content than C3 plants (e.g. wheat). Synthetic steroids are

usually synthesised from organic material derived from C3 plants (e.g. soy) while steroids produced within the body will derive carbon from the animal's diet which will consist of both C3 and C4 plants. Hence the $\delta^{13}\text{C}$ will be lower after exogenous steroid administration compared to the endogenous state ^[18]. The $\delta^{13}\text{C}$ value of the steroid or metabolite being measured by IRMS is usually referenced to an endogenous reference compound (ERC) such as DHEA that is not affected by exogenous steroid administration to ensure that the endogenous make-up of the animal has not been affected by factors such as diet so as to give low $\delta^{13}\text{C}$ values for all steroids ^[19]. A significant difference between the isotopic composition of the ERC and the metabolites indicates illegal administration ^[20].

$$\delta^{13}\text{C} = \frac{(^{13}\text{C} : ^{12}\text{C})_{\text{sample}} - (^{13}\text{C} : ^{12}\text{C})_{\text{reference}}}{(^{13}\text{C} : ^{12}\text{C})_{\text{reference}}} \times 1000 \text{ ‰}$$

Equation for isotopic ratio of Carbon ^[20]

A schematic of the GC/C/IRMS instrumentation is shown below. The sample elutes from the GC column into an oxidation chamber where it is combusted at elevated temperatures into a combination of gases including CO_2 , NO_x , and H_2O . These are transferred to the reduction chamber where the nitrous oxides are converted to nitrogen and excess oxygen is removed. Water is then removed by dried Helium passing through the Nafion membrane ^[21]. These dried gases pass through to the IRMS where they undergo electron-impact ionization. The resulting ions are separated according to m/z in the magnetic sector. For the analysis of CO_2 , three Faraday cups are positioned in the ion beam to collect the ions m/z 44 ($^{12}\text{C}^{16}\text{O}_2$), m/z 45 ($^{13}\text{C}^{16}\text{O}_2$) and m/z 46 ($^{12}\text{C}^{18}\text{O}^{16}\text{O}$). The sample is analysed alongside a reference gas and the relative isotopic abundance calculated ^[22].



Schematic of GC/C/IRMS instrument ^[21]

An advantage of GC/C/IRMS is the ability to use urine as a matrix for testing which can be easily sampled on-farm or at the slaughter house. As most screening methods are based on urine, it would also allow the same sample to be used for both screening analysis and confirmatory analysis by GC/C/IRMS ^[7]. Applications of IRMS to the detection of steroid abuse to date include the detection of testosterone abuse and estradiol abuse

in bovine urine via monitoring relative to DHEA ^[23] ^[24]. No thresholds of reference for $\delta^{13}\text{C}$ of steroid hormones have been established yet however, since their variations depend largely on the diet of the animal and also other factors such as age, sex or breed. There are also no criteria devoted to the interpretation of GC/C/IRMS results available in any official document such as EC/2002/657. Although IRMS is considered a suitable confirmatory technique, it is not currently widely used in the area of residue analysis as it is a very complicated technique to perform, the equipment is expensive and sensitivity of the instrument is not sufficient to reach the low levels of detection required by the EU.

Biomarkers

Biomarker approaches measure the biological effect of the steroid rather than the drug itself i.e. they do not detect the presence of a drug directly but detect its cumulative biological effect within the animal. Biomarkers (biological markers) are metabolites that are measurable indicators of some biological state or condition, for example physiological changes that appear in the animal due to the administration of an anabolic agent. Samples are analyzed searching for the presence of specific target analytes. Confirmation of steroid abuse is on the basis of a significant difference between data obtained for a particular animal and the corresponding reference population. Analytical techniques employed in metabolomics to collect data include GC-MS, LC-MS and NMR spectrometry ^[25]. Data processing is composed of four major steps; background noise correction, peak alignment, peak deconvolution and peak sorting. A large amount of data is generated during metabolomic fingerprinting therefore multivariate statistical techniques such as principal component analysis (PCA) are used to analyse data and to point out the potential biomarkers. Knowledge of statistics is hence required to calculate thresholds and determine compliance.

An advantage of the biomarker approach is that for all methods of doping used, a change in the mRNA, protein or metabolite profile should be detectable. However there are a number of disadvantages to the biomarker approach which have resulted in its lack of use in routine operation. Current EU legislation requires unambiguous evidence of drug administration such as classical targeted MS-based confirmatory approaches. The biomarker approach is based on scientific and statistical calculations and is an effect-based screening method i.e. it does not provide an indication of the presence of a specific compound. Official implementation would therefore require modification of the current legislation ^[26]. Metabolomic studies have been carried out on some species for particular veterinary drugs, for example Dervilly-Pinel and colleagues' metabolomic study of urine from cattle treated with a combination of steroids found changes in urinary metabolomic profiles compared to control animals ^[27]. However a considerable body of work is still needed to build up the large amount of control data needed for this approach. Complications also arise from the variation in biomarker concentrations due to age, breed, gender etc. of the animals.

Conclusions and Future Perspectives:

Control of the use of natural steroids for growth promoting purposes is a complex area. Sampling of some animal species and gender combinations can prove futile due to high endogenous levels present in the animals. No threshold levels or action levels can be set in these cases and hence some countries have abandoned control of some steroids in certain animal species. More recently, growth promoting ‘cocktails’ with low concentrations of a number of compounds are being used to avoid detection which poses further challenges in the area ^[25]. Alternative strategies are being developed to allow discrimination between steroids of an endogenous or exogenous source but a lot of work remains to be done to allow routine use of these.

References:

- [1] Stephany R., Hormonal growth promoting agents in food producing animals. Handb. Exp. Pharmacol, 2010, 355-367.
- [2] Opinion of the Scientific Committee on Veterinary Measures Relating to Public Health: Assessment of potential risks to human health from hormone residues in bovine meat and meat products. 30 April 1999
- [3] Opinion of the Scientific Committee on Veterinary Measures Relating to Public Health: Review of previous SCVPH opinions of 30 April 1999 and 3 May 2000 on the potential risks to human health from hormone residues in bovine meat and meat products. 10 April 2002
- [4] Veterinary Products Committee (VPC). Executive summary and critical evaluation of the scientific reasoning and methods of argument adopted in the opinion of the Scientific Committee on Veterinary Measures Relating to Public Health which assessed the potential risks to human health from hormone residues in bovine meat and meat products.
- [5] Veterinary Products Committee (VPC). Risks Associated with the Use of Hormonal Substances in Food-Producing Animals. Report of the Veterinary Products Committee.
- [6] Kennedy D., Shortt H., Crooks S. et al., Food Addit. Contam. Part A Chem. Anal. Control Expo Risk Assess., 2009, 26(5), 683-691.
- [7] EURL Reflection paper: Natural growth promoting substances in biological samples. RIKILT Wageningen UR, Wageningen, 2014.
- [8] De Brabander H., Poelmans S., Schilt, R. et al., Food Addit. Contam., 2004, 21(6), 515-525.
- [9] Vandenbroecke M., Van Vyncht G., Gaspar P. et al., J. Chromatogr., 1991, 564(2), 405-412.
- [10] Stolker A., Groot M., Lasaroms J. et al., Anal. Bioanal. Chem., 2009, 395, 1075–1087
- [11] Nielen M., Lasaroms J., Mulder P. et al., J. Chromatogr. B, 2006, 830, 126–134.
- [12] Gray B., Viljanto M., Bright J. et al., Anal Chim Acta., 2013, 787, 163–172.
- [13] Hooijerink H., Lommen A., Mulder P. et al., Analytica Chimica Acta, 2005, 529, 167-172.
- [14] Hold K., Wilkins D., Crouch D. et al., J. Anal. Toxicol., 1996, 20(6), 345–349.

- [15] Gleixner A., Meyer H., Fresenius' J. Anal. Chem., 1997, 357, 1198-1201.
- [16] Anari M., Bakhtiar R., Zhu B. et al., Anal. Chem., 2002, 74 (16), 4136–4144.
- [17] Camin F., Bontempo L., Perini M. et al., Comp Rev Food Sci Food Safety, 2016, 15, 868 – 877.
- [18] Scarth J., Kay J., Teale P. et al., Drug Test. Analysis, 2012, 4 (Suppl. 1), 40–49.
- [19] Hebestreit M., Flenker U., Buisson C. et al., J. Agric. Food Chem., 2006, 54 (8), 2850–2858.
- [20] Scarth J., Akre C., van Ginkel L. et al., Food Additives and Contaminants, 2009, 26 (5), 640–671.
- [21] Muccio Z., Jackson G., Analyst, 2009, 134, 213-222.
- [22] Cawley A., Flenker U., J. Mass Spectrom., 2008, 43, 854–864.
- [23] ISOSTER project report GRD-2001-40085 executive summary. Determination of the origin of hormones in cattle. Coordinated by the Bundesinstitut für Risikobewertung. 2006.
- [24] Buisson C., Hebestreit M., Weigert A. et al., J. Chromatogr. A, 2005, 1093 (1-2), 69-80.
- [25] Regal P., Cepeda A., Fente C., Natural Hormones in Food-Producing Animals: Legal Measurements and Analytical Implications. InTech; 2012.
- [26] Dervilly-Pinel G., Courant F., Chéreau S. et al., Drug Test. Analysis, 2012, 4 (Suppl. 1), 59–69.
- [27] Dervilly-Pinel G., Weigel S., Lommen A. et al., Analytica Chimica Acta, 2011, 700 (1-2), 144-154.

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David Phelan, Managing Partner, Accreate presents the Pharma Leader Award 2017 to Brendan O'Callaghan.

Large Pharma Company of the Year



David Anchell, MD, Camida presents the Pharma Company of the Year - Large award to the Amgen Technology Ireland team.

SME Pharma Company of the Year



Pamela Quinn, MD, Kuehne + Nagel Ireland presents the Pharma Company of the Year - SME award to the EirGen Pharma team.

Innovation of the Year Award



Rachel Pallett, Sales & Marketing Director, EMEA, Watson-Marlow Fluid Technology Group presents the Innovation of the Year award to the Meda Rottapharm (a Mylan Company) team.

Pharma Project of the Year award



Tom Tobin, Customers Relations Director, Micro-Bio Ireland, presents the Pharma Project of the Year - Small award to the Cross Site Solvent Recovery Business - Pfizer Ringaskiddy team.

Sustainability Initiative of the Year Award



Ruth Appelbe, IWS, Sales Manager, Indaver presents the Sustainability Initiative of the Year award to the Pfizer Little Island team.

Research & Development Achievement Award



Mark Kelly, Business Manager 3M Life Sciences presents the Research & Development Achievement Award to Claire Lennon & Niall O'Reilly, PMBRC, WIT.

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Ruthenium(II) Polypyridyl Complexes: Mechanistic Investigations and Applications in Chemical Biology

Fergus Poynton

School of Chemistry and Trinity Biomedical Sciences Institute (TBSI), Trinity College Dublin,
The University of Dublin



Dr. Fergus Poynton studied Natural Science Trinity College Dublin, where he specialised in Chemistry and graduated with First Class Honours. During his undergraduate degree, under the supervision of Dr. Silvia Giordani, he investigated how the photophysical properties of single-walled carbon nanotubes could be modulated by their non-covalent functionalisation with photo-switchable spiropyrans, toward the development of nano-sized smart material.

Fergus then continued his studies at Trinity College and undertook his Ph.D. research under the joint supervision of Prof. Thorfinnur Gunnlaugsson and Prof. John Kelly from the School of Chemistry, where he examined the excited-state processes and reactivity of ruthenium(II) polypyridyl complexes in solution and in the presence of DNA, as highlighted in this article. In 2016, Fergus obtained his Ph.D. in Chemistry and was subsequently awarded both the Irish RIA and international IUPAC-SOLVAY Award for Young Chemists for the most outstanding Ph.D. thesis in the chemical sciences.

Recently, Fergus joined the research group of Prof. Seamas Donnelly as a post-doctoral researcher in the School of Medicine at Trinity College. He is now developing small molecule inhibitors of the cytokine macrophage migration inhibitory factor for the treatment of lung diseases and assessing the effectiveness of nanoparticle formulations to target these inhibitors to the lung in aerosol therapies.

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Introduction

The synthesis of Ru(II) polypyridyl complexes and investigation into their salient properties has become a major area of research over the past few decades.¹⁻⁵ This interest largely arises from their appealing photophysical and photochemical properties. Such complexes absorb visible light and emit long wavelength light within the red and near-infrared spectral regions. They possess long-lived triplet excited states and can show reversible redox processes. Moreover, their photophysical properties can be tuned by varying the nature of the ligands coordinated to the Ru(II) metal centre.⁶⁻⁹ Structurally, due to the octahedral geometry of a number of these complexes, chemists can readily gain access to molecules with complicated 3-dimensional architectures. In the case of octahedral complexes possessing three bidentate ligands, the configurations of these chelating ligands around the metal centre imparts chirality to the complexes, thereby giving rise to either a left-handed Λ -enantiomer or a right-handed Δ -enantiomer. In light of these features, such complexes have found increasing applications in biological systems, where they have been used to gain greater insights into the non-covalent binding of molecules to DNA,^{10, 11} as luminescent probes and new classes of light-activatable therapeutics.^{12, 13} However, in order to design and optimise new probes and photo-therapeutics, a detailed understanding of the underlying photophysical and photochemical processes involved in such applications is essential.

In the School of Chemistry, and within the Trinity Biomedical Sciences Institute (TBSI), at Trinity College Dublin, we have focused on exploring the photophysical processes and photoreactivity exhibited by Ru(II) polypyridyl complexes in solution and when bound to DNA, to understand the important factors which govern their activity and to examine their application as cellular imaging agents and photo-therapeutics.

In the following section, the progress we have made in these efforts is presented, which include the development of a new technique for probing the binding site of the excited states of these complexes in DNA and, for the first time, carrying out time-resolved infrared (TRIR) studies in crystals. A more comprehensive discussion can be found in some of our recent articles.¹⁴⁻¹⁶

Luminescent Probes for DNA

In 1990 it was demonstrated that Ru(II) complexes incorporating the dipyrido[3,2 *a*:2',3' *c*]phenazine (dppz) ligand were non-emissive in aqueous solution, but highly luminescent in the presence of double-helical DNA or in aprotic organic solvents. This “off”→“on” emission behaviour in the presence of an analyte is highly attractive for both diagnostic and imaging applications due to the extremely low limit of detection achievable with such systems: down to a single molecule.¹⁷ This behaviour was coined the “DNA light-switch” effect and has led to the development of numerous Ru(II) complexes based on this ligand for use as luminescent probes for biomolecules such as DNA, RNA and amyloid- β aggregates, both in solution and within live cells.^{10, 13} It has been proposed that the “light-switch” mechanism arises from the conversion of the emissive “bright” excited state of the complex to a non-emissive “dark” excited state, as a result of water molecules coordinating to the complex, shown in Figure 1, which rapidly deactivate the excited state. However, the nature of this dark excited state and its interactions with the coordinating water molecules

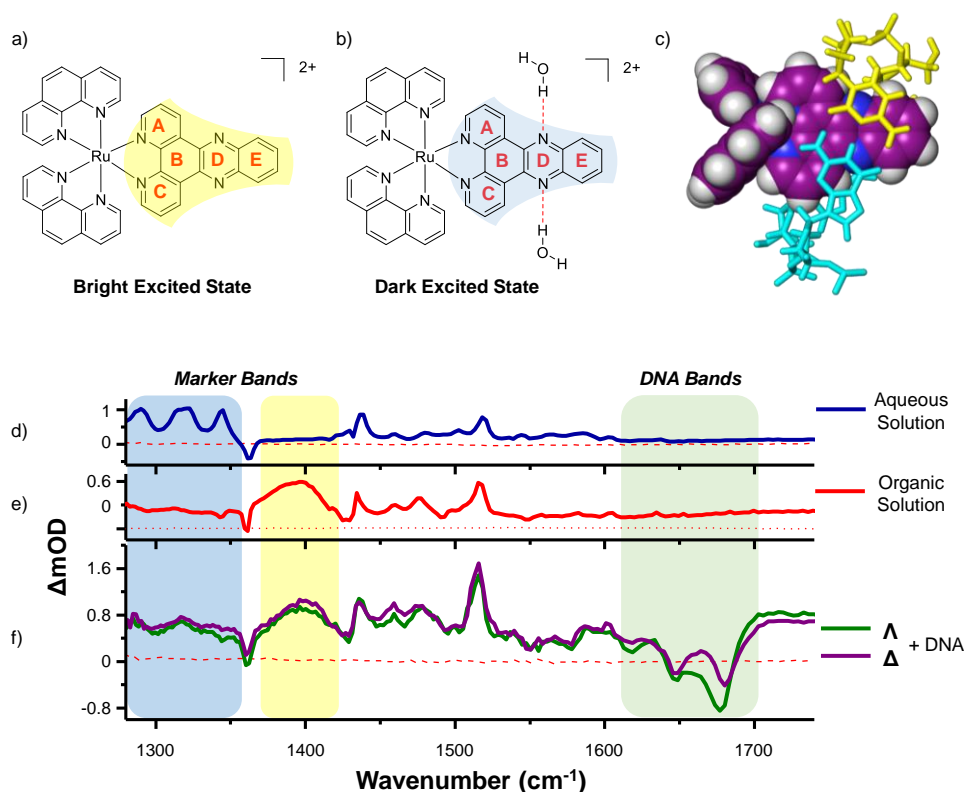


Figure 1: Schematic diagrams showing the structure of **Ru.1** a) in aprotic organic solvent, b) in water and c) when bound to DNA at a CC/GG step by intercalation of the **dppz** ligand. The ring lettering used to define the **dppz** ligand is shown and the yellow and blue highlighted regions represent the presence of the emissive bright and non-emissive dark excited states, respectively. TRIR spectra recorded 35 ps after 400 nm excitation of d) **Ru.1** (500 μ M) in aqueous solution, e) **Ru.1** (500 μ M) in aprotic organic solution and f) Δ - and Λ -**Ru.1** (400 μ M) and a duplex DNA oligonucleotide d(TCGGCGCCGA)₂ (500 μ M duplex) in deuterated potassium phosphate buffer (50 mM) pH 7. The blue and yellow coloured regions highlight the characteristic marker bands for the dark and bright excited states of **Ru.1**, respectively, while the green coloured region highlights the vibrational bands associated with the DNA base pairs.

have yet to be fully established, which represents a significant challenge towards the design and optimisation of new luminescent probes based on this system. With this in mind we investigated the excited-state

properties of the “light-switch” complex $[\text{Ru}(\text{phen})_2(\text{dppz})]^{2+}$ (**Ru.1**) (phen=1,10 phenanthroline, shown in Figure 1) by ultrafast TRIR spectroscopy.

By probing specific vibrations of the excited states of **Ru.1**, we demonstrated for the first time, characteristic spectral features for both the emissive bright excited state in aprotic organic solvent and the non-emissive dark excited state in aqueous solution, shown in Figure 1d-e. Furthermore, by combining these solution measurements with density functional theory calculations it was found that both the coordination of two water molecules to the nitrogen atoms of the **dppz** ligand (ring D in Figure 1b) as well as the high polarity of the surrounding solvent medium were required to convert the bright excited state into the dark excited state. Moreover, these calculations revealed that vibrations within the excited state of **Ru.1** coupled with the water molecules coordinated to ring D, which facilitated efficient coupling with vibrational states of the bulk solvent, thereby providing a possible mechanism by which the dark excited state is efficiently deactivated in aqueous solution.

The spectral features of the bright excited state of both the left-handed Λ - and right-handed Δ -enantiomer of **Ru.1** were also observed when the complexes were bound to double-stranded DNA. In addition, photo-excitation of **Ru.1** was found to perturb the DNA bases in the direct vicinity of the bound complexes, shown in Figure 1f, which facilitated the identification of the bases at the binding site of the complex. Furthermore, the perturbation of the DNA bases was specific to each enantiomer, which highlighted the different nature in their interactions with DNA. This demonstrates that TRIR spectroscopy can be a valuable technique for determining the identity and nature of the binding site of molecules to mixed sequence duplex DNA.

Photo-Reactive Complexes

The photosensitised oxidation of guanine is an important method to study one of the processes that results in DNA damage, and also represents a mechanism of action for novel photo-therapeutics. When two π -deficient 1,4,5,8-tetraazaphenanthrene (**TAP**) ligands are coordinated to the Ru(II) metal centre, the excited state of **Ru.2** (Figure 2a) becomes highly oxidising and capable of oxidising the guanine residues of DNA. We employed time-resolved visible and infrared spectroscopy to monitor this electron-transfer process on the picosecond and nanosecond timescales in order to characterise the important factors that govern the reversible photo-oxidation of guanine by this class of complex. These studies revealed that the chirality of the complex had a significant impact on the electron-transfer process of **Ru.2** bound to DNA. For Λ -**Ru.2**, both the rates and yield of photo-oxidation of guanine were highly sensitive to the sequence of DNA. Intriguingly, however, Δ -**Ru.2** showed no such sensitivity.

A considerable challenge to researchers investigating the photo-oxidation of DNA in solution by non-covalently bound photosensitisers is the inherent uncertainty regarding the location and orientation of the bound photosensitiser. These factors are extremely important to the photo-oxidation process and, to overcome such limitations, we probed the photo-oxidation reaction of guanine by Λ -**Ru.2** in crystals of the complex bound to a DNA duplex of defined sequence, shown in Figure 2b-d. By combining X-ray crystallography with ultrafast spectroscopic data, the rates of the different steps of the reversible photo-oxidation of guanine in DNA were characterised for a system in which the geometry of the reaction site was known with atomic resolution and importantly, allowed the individual guanine undergoing the oxidation reaction to be proposed. This now represents a means by which researchers can gain new insights into electron-transfer processes in biomolecules in the crystalline state and opens the possibility to probing these processes within cells.

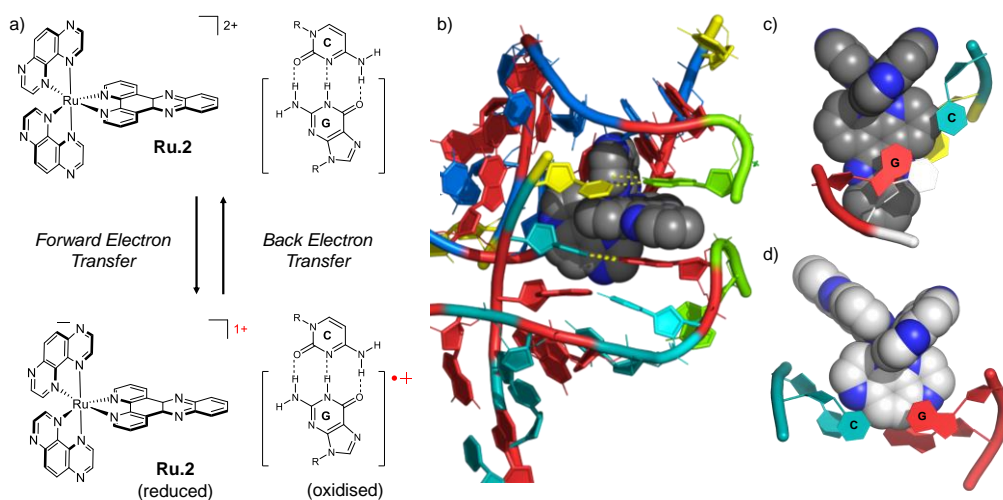


Figure 2: a) illustration of the reversible photo-oxidation of a guanine site in DNA by **Ru.2**, b) the structure of Λ -**Ru.2** bound to two DNA duplexes in the crystal structure of Λ -**Ru.2** bound to duplex decamer, c) the structure of the **dppz** ligand of Λ -**Ru.2** intercalated into the terminal G_9A_{10}/T_1C_2 step and d) the structure of the ancillary **TAP** ligand of Λ -**Ru.2** intercalated into the G_3G_4/C_7C_8 step in the crystal structure of Λ -**Ru.2** bound to DNA. Colours: nitrogen atoms of the complex are blue, T is yellow; G is red, A is green, C is cyan.

photo-oxidation of guanine in DNA were characterised for a system in which the geometry of the reaction site was known with atomic resolution and importantly, allowed the individual guanine undergoing the oxidation reaction to be proposed. This now represents a means by which researchers can gain new insights into electron-transfer processes in biomolecules in the crystalline state and opens the possibility to probing these processes within cells.

Development of Cellular Imaging Agents and Light-Activatable Therapeutics

In addition the mechanistic investigations discussed above, we have developed a number of Ru(II) polypyridyl complexes for use as cellular imaging agents and light-activatable anti-cancer agents. Unfortunately, the “DNA light-switch” complex **Ru.1**, is poorly internalised by live cells, thereby limiting its application as a cellular probe.¹⁸ To address this issue, we extended the surface area of the **dppz** ligand, as shown in Figure 3a, to increase the cellular uptake of the resulting complexes, as well as enhance their binding affinity for DNA. After substitution of the **dppz** ligand of **Ru.1** for this new extended ligand, designated **pdppz**, the “DNA light-switch” effect of the resulting complex (**Ru.3**) was preserved, as illustrated in Figure 3b, whereby the complex is non-emissive in water, but highly emissive when bound to DNA. Moreover, in addition to its activity as a solution-based DNA probe, **Ru.3** was shown to effectively stain cellular DNA, as seen by the red emission of the complex in Figure 3c, from isolated intact cell nuclei, stained with the complex. Furthermore, **Ru.3** was shown to be internalised and successfully imaged within live cells, where it can be seen to cluster next to the cell nucleus as shown in Figure 3d. In addition, the complex showed low toxicity towards cells in either the absence or presence of light, and has therefore been the focus of further research and optimisation.¹⁹

In the case of the **pdppz**-analogue of the photo-reactive complex **Ru.2**, the photo-reactivity of the resulting **pdppz** complex **Ru.4** was exploited to develop an anti-cancer agent, whose activity could be “switched on” using light. This mode of therapy, termed photochemotherapy, involves the administration of an inactive drug to patients, which disperses throughout the body. The drug can then be activated in a spatially and temporally controlled manner by selectively illuminating specific areas of the body (*e.g.* a tumour) with light of the appropriate wavelength to activate the administered drug. In the case of cancer therapies, such a treatment modality avoids many of the side effects and collateral toxicity to non-cancerous cells that is seen with traditional chemotherapy treatments. Indeed, when live HeLa cervical cancer cells were incubated in the dark with **Ru.4** at a concentration of 100 μ M for 24 hrs, little toxicity was observed in cells. However, if

the cells were subsequently exposed to visible light, the internalised **Ru.4** was activated and became extremely toxic to the cancer cells, resulting in the controlled cell death of the irradiated cancer cells.

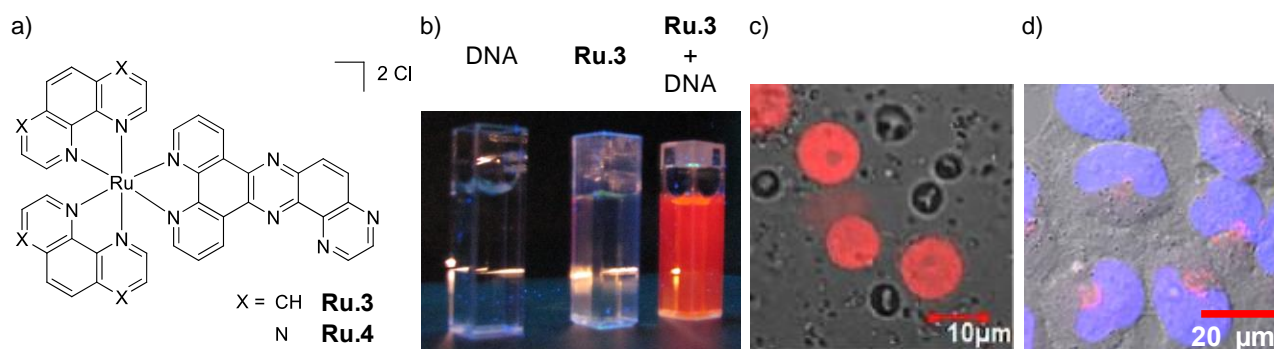


Figure 3: a) chemical structure of the pdppz-complexes **Ru.3** and **Ru.4**, b) images showing the change in luminescence of **Ru.3** when in phosphate buffered solution (10 mM) at pH 7.4 in either the absence or presence of DNA. Confocal microscopy images of c) isolated cell nuclei, stained with **Ru.3** (red) and d) HeLa cervical cancer cells treated with **Ru.3** (100 μ M) for 24 hrs (red) and the commercial nuclear stain DAPI (blue).

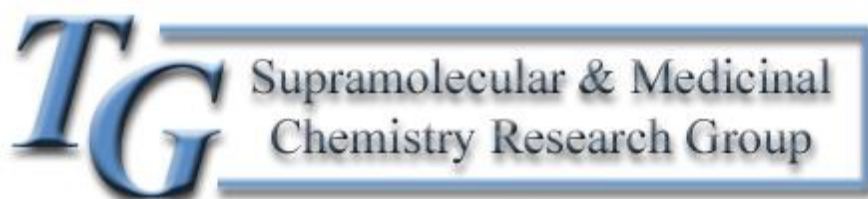
Conclusion

The above account demonstrates some of the rich photochemistry of Ru(II) polypyridyl complexes and how they can be exploited to design new diagnostic probes and therapeutics. Indeed, Ru(II) polypyridyl complexes, with targeted intracellular localisation, have now been developed as imaging and diagnostic agents for both cellular and *in vivo* applications.¹⁰ Moreover, this year the first Ru(II) polypyridyl complex entered clinical trials for the treatment of bladder cancer with light, which will undoubtedly pave the way for exciting new developments within the field in the years to come.²⁰

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This work is the result of a number of close collaborations between research groups within Dublin and the UK, namely the research groups of Prof. Clive Williams in the School of Biochemistry and Immunology at Trinity College Dublin, Dr Susan Quinn at University College Dublin, Prof. Conor Long at Dublin City University, Prof. Christine Cardin and Dr John Brazier at the University of Reading, UK, and the Central Laser Facility at Rutherford Appleton Laboratory, UK.

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School of Chemistry:

<http://www.tcd.ie/Chemistry/>

TBSI:

<http://www.tcd.ie/biosciences/>

References

1. J. G. Vos and J. M. Kelly, *Dalton Trans.*, 2006, 4869.
2. V. Marin, E. Holder, R. Hoogenboom and U. S. Schubert, *Chem. Soc. Rev.*, 2007, **36**, 618.
3. C. Daniel, *Coord. Chem. Rev.*, 2015, **282-283**, 19.
4. S. Fantacci and F. De Angelis, *Coord. Chem. Rev.*, 2011, **255**, 2704.
5. J. P. Paris and W. W. Brandt, *J. Am. Chem. Soc.*, 1959, **81**, 5001.
6. S. Campagna, F. Puntoriero, F. Nastasi, G. Bergamini and V. Balzani, *Top. Curr. Chem.*, 2007, **280**, 117.
7. D. W. Thompson, A. Ito and T. J. Meyer, *Pure Appl. Chem.*, 2013, **85**, 1257.
8. M. Abrahamsson, H. Wolpher, O. Johansson, J. Larsson, M. Kritikos, L. Eriksson, P.-O. Norrby, J. Bergquist, L. Sun, B. Åkermarck and L. Hammarström, *Inorg. Chem.*, 2005, **44**, 3215.
9. L. Zayat, O. Filevich, L. M. Baraldo and R. Etchenique, *Philos. Trans. R. Soc., A*, 2013, **371**, 20120330.
10. M. R. Gill and J. A. Thomas, *Chem. Soc. Rev.*, 2012, **41**, 3179.
11. B. J. Pages, D. L. Ang, E. P. Wright and J. R. Aldrich-Wright, *Dalton Trans.*, 2015, **44**, 3505.
12. C. S. Burke, A. Byrne and T. E. Keyes, in *Advances in Imaging and Sensing*, eds. S. Tang and D. Saeedkia, CRC Press, Florida, USA, 2016, ch. 11, pp. 227.
13. N. P. Cook, V. Torres, D. Jain and A. A. Martí, *J. Am. Chem. Soc.*, 2011, **133**, 11121.
14. F. E. Poynton, J. P. Hall, P. M. Keane, C. Schwarz, I. V. Sazanovich, M. Towrie, T. Gunnlaugsson, C. J. Cardin, D. J. Cardin, S. J. Quinn, C. Long and J. M. Kelly, *Chem. Sci.*, 2016, **7**, 3075.
15. P. M. Keane, F. E. Poynton, J. P. Hall, I. P. Clark, I. V. Sazanovich, M. Towrie, T. Gunnlaugsson, S. J. Quinn, C. J. Cardin and J. M. Kelly, *Faraday Discuss.*, 2015, **185**, 455.
16. S. M. Cloonan, R. B. P. Elmes, M. Erby, S. A. Bright, F. E. Poynton, D. E. Nolan, S. J. Quinn, T. Gunnlaugsson and D. C. Williams, *J. Med. Chem.*, 2015, **58**, 4494.
17. K. Rurack and U. Resch-Genger, *Chem. Soc. Rev.*, 2002, **31**, 116.
18. C. A. Puckett and J. K. Barton, *J. Am. Chem. Soc.*, 2007, **129**, 46.
19. B. C. Poulsen, S. Estalayo-Adrian, S. Blasco, S. A. Bright, J. M. Kelly, D. C. Williams and T. Gunnlaugsson, *Dalton Trans.*, 2016, **45**, 18208.
20. Theralase Technologies Inc., *Theralase Successfully Achieves Primary and Secondary Objectives for First Three Patients Treated Using Anti-Cancer Technology for Bladder Cancer*, <http://theralase.com/pressrelease/theralase-successfully-achieves-objectives-for-patients-treating-using-anti-cancer-technology-for-bladder-cancer/>, (accessed June 2017).

First circular



Scientific Workshop in connection with Eurachem General Assembly 2018

**Data - Quality, Analysis
and Integrity**

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



Local organising committee

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

Scientific committee

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

Registration

Registration is open from 1st OCTOBER 2017 at

www.eurachem2018.com

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

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

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

Aims

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

Topics covered during the workshop will include:

Current Practices

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

Future Challenges

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

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

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

Workshop Programme

Monday 14th May 2018

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

Tuesday 15th May 2018

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

For more details on the workshop
and to register visit

www.eurachem2018.com

Invited contributions

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

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

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

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

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

Early bird registration rate closes:
March 31st 2018

Exhibition

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

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

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IDA Press Release 25 Oct 2017



Frances Fitzgerald, Tánaiste and Minister for Business, Enterprise and Innovation and Niall O'Leary, Vice President and Site Head, IOPS Raheen – Regeneron

Limerick, Ireland (October 25, 2017) -- Regeneron Pharmaceuticals, Inc. (NASDAQ: **REGN**), one of the fastest-growing companies in the global biotechnology industry, today announced further expansion of its Limerick Industrial Operations and Product Supply (IOPS) bioprocessing campus with an additional 300 jobs and investment of \$100 million, bringing the total expected employment at the site to 800 people and total investment to \$750 million. The project is supported by the government through IDA Ireland.

Since 2013, when Regeneron first announced plans to invest in operations in Ireland, the company has consistently exceeded job and investment projections for its Irish Operations. In October 2015, Regeneron projected employment in Ireland would reach 500 by the end of 2017. As Regeneron's Irish expansion continues with employment expected to rise to 800 by the end of 2018, recruitment is ongoing for high-end specialist positions in commercial manufacturing, process sciences, quality assurance/control/validation and various support functions.

Regeneron's 400,000 square foot, state-of-the-art production facility in Limerick is the largest scale bulk biologics production facility in Ireland and one of the largest biologic production operations in the world. The additional \$100 million investment will support the construction of a number of manufacturing suites to increase drug substance production capacity and enable the company to meet demand for its life-transforming medicines for patients with serious diseases.

Welcoming the investment and jobs announcement **Taoiseach Leo Varadkar TD said**; "I'm delighted to

welcome additional highly skilled and diverse Regeneron jobs to Limerick. Regeneron's decision to expand so significantly is testament to the talent pool and attractive business environment available to companies in Ireland. This planned further expansion by Regeneron in Limerick is a significant contribution to the rejuvenation of the region."

Tánaiste and Minister for Business, Enterprise and Innovation Frances Fitzgerald TD said;

"Regeneron, a leader in the global biopharma industry, set up in Limerick in 2014 and has created a world-class science hub to produce medicine for millions of people. I am delighted to see the great progress made to date giving rise to further substantial investment and additional jobs to be created in Limerick. It is great news for Limerick and the wider region."

Dan Van Plew, Executive Vice President and General Manager of Industrial Operations and Product Supply (IOPS) at Regeneron, said;

"Gut feel is a large portion of any site selection. When we picked Limerick years ago, we simply felt good about the community, universities and people. A few years and a lot of experience later, I can now confidently say I *know* Limerick is a place where you can build and thrive as a biotech. We are proud of what has happened here and the vast majority of this work has been completed by people who come from Munster. These folks built, validated and began production in a way I'd put up against any other team on the planet. We feel at home here and the way we have been welcomed has made our ongoing growth and investment in Limerick rewarding on the most personal levels."

Niall O'Leary, Vice President and Site Head, IOPS Raheen, said; "Limerick offers an exceptionally good location for U.S. multinationals. Located just 30 minutes from Shannon Airport with a five hour time difference from New York, Ireland is also a midway point for U.S. executives linking into our partners, such as Bayer in Germany and Sanofi in France. In addition, the very favourable business environment along with the support provided by IDA Ireland and Limerick City and County Council make the city an ideal home for Regeneron."

Speaking of the investment, **Martin Shanahan, CEO, IDA Ireland, said;** "An additional \$100 million investment and 300 jobs commitment by Regeneron is a huge boost for the Mid-West Region. The Irish Government is committed to continuing to invest in our education, research and broader ecosystem to ensure that Ireland remains the competitive location of choice for new biotech manufacturing operations. Combined with the regulatory and licencing regime applying to pharma in Ireland, Ireland is a hot-spot location for biologics investment and career opportunity in biologics."

In addition to the production facility in Limerick, Regeneron's European Business Operations for IOPS, the company has a growing Dublin office, currently employing 30 people and serving as the company's European Business Administration headquarters. Regeneron's total headcount in Ireland is expected to approach 850 by the end of 2018.

For further information:

IDA Press Office: 01 6034258

<https://www.idaireland.com>

<https://www.regeneron.ie>

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Excellence is our Passion

IDA Ireland welcomes news of Henkel Additive Manufacturing Operation in Tallaght



IDA Ireland today welcomed the news that **Henkel Ireland, will establish a major Additive Manufacturing project in Tallaght, Dublin**, where the global company already has a significant manufacturing and R&D operation for a wide range of adhesive technologies, serving a global market. Henkel, which also owns beauty care, laundry and home care divisions, is the world's largest adhesives manufacturer.

Henkel's Additive Manufacturing (3D Printing) project, which is supported by the Irish Government through IDA Ireland, will employ 40 highly skilled scientists and engineers who will develop new advanced materials for use in precision manufacturing industries, such as medical devices, automotive and aerospace.

Henkel's Adhesive Technologies business unit is developing novel materials customized for various 3D Printing processes and technologies and is constantly expanding partnerships with global technology leaders. Ireland was selected because of the country's strength in high value medical device R&D and manufacturing, coupled with a growing investment profile in Additive Manufacturing. Henkel's R&D team based in Tallaght has a wealth of scientific knowledge and experience in developing adhesive technologies with existing capability to develop 3D printing materials.

Welcoming the announcement, **An Tánaiste and Minister for Business, Enterprise and Innovation Frances Fitzgerald TD** said: "This is very welcome news by Henkel, which already employs 400 people in its operations in Dublin. The development of this new Additive Manufacturing Centre of Excellence, employing 40 highly skilled staff, will further consolidate the company's operations in Ireland. Additive Manufacturing is a new and very innovative development for the manufacturing sector and this technology is likely to have a significant impact globally when its potential is fully developed. We very much appreciate Henkel's investment and the quality jobs being provided, which will help put Ireland at the forefront of a new and exciting chapter in manufacturing".

Henkel Technology Centre Director, Dr Matthew Holloway, said: "I'm excited that the IDA is supporting this R&D Project. Additive Manufacturing will be a significant disruptor to future manufacturing methodologies and it is important for the team in Ireland to help shape this change. We have a proven track record of developing world-class adhesives and look forward to focusing our expertise on creating new chemistries and technologies for 3D Printing. Henkel recognises the strength of relationships with the research community in Ireland and this will enhance our capability to innovate."

Speaking following the announcement **Martin Shanahan CEO of IDA Ireland** said: "As a long-standing client employing 400 people, IDA Ireland works very closely with Henkel. This move is a significant departure for Henkel into a new emerging technology. I have no doubt that the company will be able to successfully utilise their wealth of scientific knowledge with adhesive technologies to produce innovative additive manufacturing technologies. Henkel's investment will help to further develop a pronounced national competency in high performance materials for additive manufacturing.

Ireland is ranked as one of the best countries in the world for business with top rated resilient supply chains which has enabled companies like Henkel to thrive and succeed here."

About Henkel:

Henkel operates worldwide with leading brands and technologies in three business units: Laundry & Home Care, Beauty Care and Adhesive Technologies. Every day, millions of customers and consumers use products from Henkel with brands such as Loctite, Sellotape and UniBond; Bloo, Dylon and Colour Catcher; Schwarzkopf, LIVE, Got2B and RightGuard.

In Ireland, Henkel employees circa 400 staff and has three sites; Tallaght (Adhesives R&D, production, bottling & packaging), Ballyfermot (adhesives manufacturing) & Little Island, Cork (DYLON Colour Catcher manufacturing).

In 2016, Henkel reported global sales of €18.7bn and an adjusted operating profit of €3.2bn. Its shares are listed in the German stock index DAX.

For further information:

IDA Press Office: 01 6034258

<https://www.idaireland.com>

<https://www.regeneron.ie>



Minister Halligan congratulates ENBIO on €1.5m win from Horizon 2020



Irish SME receives €1.5m from EU to clean up metal coating industry

Mr John Halligan T.D., Minister of State for Training, Skills & Innovation congratulated ENBIO, an Irish SME with facilities in Dublin and Clonmel, Tipperary on winning €1.52 million from the European Commission to develop a green alternative to the toxic chemicals necessary to coat metals.

Their work will be focussed initially on the space sector but has wide-ranging applications in aerospace, automotive and general industry, as well as public infrastructure and civilian applications. The funding is provided under the EU's Horizon 2020 SME Instrument Phase 2.

European environmental legislation (REACH) is reducing the use of hazardous chemical treatments widely used to prepare metal surfaces for bonding or coating in the space sector. However, it is not just the space sector that needs a replacement but any European industry using wet hazardous metal pre-treatments such as chromate conversion processes, which is important to the aerospace, automotive, and industries in general.

Congratulating ENBIO on its success, Minister Halligan stated, “ENBIO is an excellent example of the large numbers of SMEs successfully applying to Horizon 2020, giving Ireland the second highest success rate in Europe for the Horizon 2020 SME Instrument with a 13% success rate compared to a European average of 5.5%. Not only are Irish companies like ENBIO being successful, they are also targeting larger sums of money than comparable companies across Europe. To date, this represents an investment of €54.1 million in innovative Irish SMEs, enabling accelerated growth of these companies.”

ENBIO has developed a proven alternative coating process – their patented CoBlast process. The European Commission funding will enable ENBIO to accelerate their development and launch of a chemical replacement metal treatment. ENBIO's alternative uses no hazardous chemicals and meets or exceeds existing industry standards and performance requirements.

ENBIO has already gained significant experience in the Space sector with the European Space Agency (ESA) – the company has provided two protective coatings for the ESA’s most advanced spacecraft, Solar Orbiter, one of which will become the closest man-made object to sun. ENBIO is supported in this work by Enterprise Ireland, who have been pivotal in helping ENBIO to position themselves in the space sector.

Once ENBIO has proven their process in the space sector, they plan to extend the technology to applications on earth and help clean up the coatings sector across numerous industries and the thousands of acres of metal requiring protection from the elements. The SME Instrument funding will enable ENBIO’s accelerated breakthrough into these global markets. This will place ENBIO at the forefront of green coating technology internationally and put CoBlast on the path to world-wide adoption.

“The SME Instrument is quite a different call to the traditional H2020 funding routes. At a launch event in Brussels, the key message was as much about backing the company as it was about backing the idea. The grant will have a massive impact in scaling the CoBlast process for the space sector and beyond and gives ENBIO the opportunity to invest in the capital equipment and team needed to do this work.” – Dr. Barry Twomey, CTO, ENBIO.

“We are thrilled to have been granted this funding to accelerate CoBlast for adhesive bonding for the space sector and beyond – the sunset dates are fast approaching and ENBIO are dedicated in offering a solution.” – Dr. Paolo Fiorini, Head of Operations, ENBIO.

“Receiving the SME instrument funding is an enormous boost for ENBIO. It validates the potential of our technology and gives us the momentum to help change the world for the better through greener coatings – both in space and back here on earth. Assisted by Enterprise Ireland, the ENBIO team has been developing a suite of exciting new coatings and this funding will help us to bring those to market quickly” – Dr. Kevin O’Flynn, General Manager, ENBIO.

What is Horizon 2020?

Horizon 2020 is the biggest EU Research and Innovation programme ever with nearly €80 billion of funding available over 7 years (2014 to 2020) – in addition to the private investment that this money will attract. It promises more breakthroughs, discoveries and world-firsts by taking great ideas from the lab to the market. Enterprise Ireland leads Ireland’s participation in Horizon 2020.

Horizon2020 - the SME Instrument

The SME instrument has been designed specifically for single or groups of highly innovative SMEs with international ambitions, determined to turn strong, innovative business ideas into winners on the market. Visit www.horizon2020.ie to learn more.

ENDS

For more information on ENBIO visit www.enbio.eu/OSMOSIS

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Launch of €6.7 Million Climate Change Research Initiative Led by University College Dublin



October 16th 2017

Pictured (l-r) at University College Dublin are Professor William Gallagher, Director, UCD Conway Institute; Professor Andrew J. Deeks, President, UCD; Seán Kyne TD, Minister of State for Community Development, Natural Resources and Digital Development; Professor David Kay, Aberystwyth University and Professor Wim Meijer, Head, UCD School of Biomolecular and Biomedical Science, who is leading the Acclimatize project.

The Government has officially launched the 5-year Acclimatize project (www.acclimatize.eu/), a new €6.7 million climate change research initiative, with Professor Andrew J. Deeks, President, University College Dublin (UCD). The project has been part-funded by the European Regional Development Fund through the Ireland Wales Programme 2014-2020.

The overall objective of the project, led by UCD in partnership with Aberystwyth University, is to improve the quality of coastal waters in both Ireland and Wales, boosting local tourism and supporting marine industries, such as shellfish harvesting.

The goal of the Acclimatize project is to identify pollution streams and their impact on coastal waters, in both urban and rural settings, and the impact of climate change on pollution.

With this data real-time models will be developed to inform the effects of climate change, through altered weather patterns, including rainfall, temperature and tides which impact the quality of water in coastal areas.

The project aims to develop a range of practical management methods, including smart real-time predictive tools, to improve the quality of such coastal waters to ensure compliance with regulations to protect human health and the marine environment.

Seán Kyne TD, Minister of State for Community Development, Natural Resources and Digital Development, said: “With Budget 2018 we have secured a 43% increase in funding for energy and climate action initiatives to help us on our journey to a low carbon economy. Research initiatives such as Acclimatize are very important in assisting Government and other stakeholders in making informing decisions which maximise the effectiveness of the funding available. Acclimatize is also a very positive example of how EU funds are being used to support local economies to address pollution in our coastlines and mitigate the impacts of climate change.”

Professor Andrew J. Deeks, President, UCD, said: “University College Dublin is delighted to be taking part in another collaborative partnership with Aberystwyth University. The ability to sustain our environment, to use natural resources wisely and to manage waste is central to our society and economy. In this regard the Acclimatize research project, which we are officially launching today, will help to bridge the knowledge gap in relation to the pollution of at-risk bathing waters in Dublin Bay, and in a number of bays around Wales, by identifying and quantifying the pollution streams entering these bays and determining the impact on these waters through a dynamic period of climate change.”

The Acclimatize project will focus on designated and ‘at-risk’ bathing waters in two complementary environments, a large scale urban and a rural agricultural environment.

The large scale urban environment is represented in the project by ‘at-risk’ bathing waters in Dublin Bay (Sandymount, Merrion and Dollymount strands), whereas the rural agricultural environment will focus on ‘at-risk’ bathing waters in Wales; Wiseman’s Bridge (Pembrokeshire), Newquay North and Aberystwyth South (Ceredigion, Aberdyfi (Gwynedd) and Rhyl (Denbighshire).

Initial fieldwork at Cemaes Bay in Anglesey was successfully completed in the 2017 bathing season and provides an excellent platform on which to build predictive modelling. This has already been presented to the international science and policy communities with an invited keynote talk in New Zealand in September 2017. It was also presented in a report to the WHO and EU on the science-base supporting revision of the WHO and EU water quality criteria for bathing waters which will be considered by international experts in early 2018.

Professor Wim Meijer, Head, UCD School of Biomolecular and Biomedical Science, who is leading the Acclimatize project, said: “Climate change is predicted to produce more weather extremes and, in particular, storminess in North West Europe including the Irish Sea. This will have negative impacts on coastal water quality in the period to 2100 which will threaten the sustainable use of coastal waters which form the economic basis of coastal tourism and shellfish harvesting industries.”

He added: “Improvement of bathing waters is often complicated, or prevented altogether, by a lack of knowledge of the pollution streams that contribute to non-compliance. Climate proofing of regulatory and infrastructural decisions affecting bathing water quality is therefore a policy challenge urgently needing the policy evidence-base which we will provide in the Acclimatize project.”

Professor David Kay, Centre for Research into Environment and Health, Department of Geography and Earth Sciences, Aberystwyth University, who is leading the project in Wales, said: “The first year of Acclimatize in Wales is progressing well with excellent support from relevant local authority and resource agency partners. The Acclimatize Cemaes Bay study location was chosen to assist with sustainable compliance of this site against the EU bathing Water Directive using the latest real-time modelling strategies to protect public health through cutting-edge modelling and management approaches.”

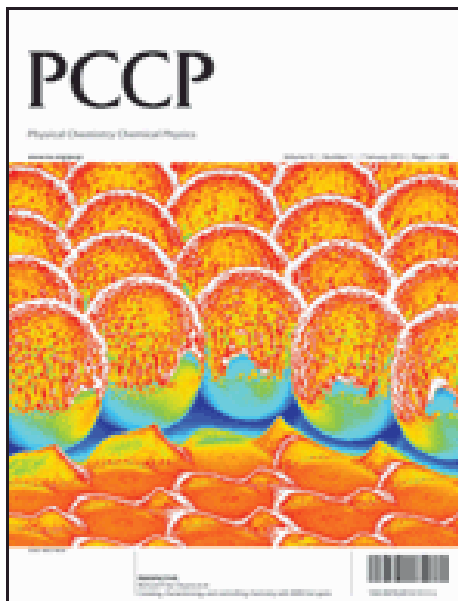
“The work has generated significant international interest already and early field data have been communicated to the WHO and EU policy and scientific communities including a presentation to the UK inter-agency bathing waters biennial conference in November 2017 in Wrexham. Follow-on work at additional sites, together with an examination of climate change impacts, will commence with our project partners in the autumn of 2017.”

Professor William Gallagher, Director of the UCD Conway Institute in which Professor Meijer is one of over 90 Conway Fellows, commented, “The Acclimatize project builds on years of hard work by Professor Meijer and his colleagues and I am delighted that a Fellow from our Institute is co-leading on such a key European initiative with obvious and tangible impacts on people’s daily lives.”

At UCD Professor Meijer is collaborating with Professor John O’Sullivan, UCD School of Civil Engineering and Professor Gregory O’Hare, UCD School of Computer Science on the Acclimatize project.

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NUI Galway is Named University of the Year



October 10th 2017

NUI Galway has been named The Sunday Times University of the Year. Trinity College Dublin is the runner-up in The Sunday Times Good University Guide 2018. Athlone Institute of Technology is The Sunday Times Institute of Technology of the Year, while Letterkenny IT is the runner-up. The guide contains Ireland's only league table that measures the performance of all 21 multi-faculty third-level institutions.

NUI Galway is the University of the Year for the third time since the guide was first published in 2002. The university first won the award in 2002 and again in 2009.

The university, which excels across the arts and sciences, has seen considerable recent investment. Michael D Higgins, President of Ireland, opened the O'Donoghue Centre for Drama, Theatre and Performance in April and a medical academy has come on stream in Donegal, in the grounds of Letterkenny University Hospital.

The university has a reputation as a centre of excellence in relation to medical technology, as evidenced by the launch in September 2016 of Curam, Science Foundation Ireland's (SFI) centre for research in medical devices. The centre promotes links between academia and industry partners. The SFI and various companies will invest €49m over six years, with €19m more in funding coming from the EU's Horizon 2020 programme.

The quality of academic staff at NUI Galway is also crucial to the university's success, with a number of professors such as Henry Curran, Colin O'Dowd, Donal O'Regan and Dr Ronan Sulpice named among the

world's most highly cited researchers in an analysis of published research by multinational group Clarivate Analytics.

Research citations have helped the university rise further up the international university rankings this year. Academics garnered around €89,000 per head in research income in the Good University Guide's latest survey of research power.

NUI Galway boasts the best job prospects of any university in the republic with an impressively low three per cent graduate unemployment rate, together with one of the best progression rates, which sees 88% of students complete their studies.

"We are very well attuned to the needs of the country and the region," says Dr Jim Browne, President of NUI Galway. "We try to orient our programme for the needs of our economy in the longer term. We also try to have an appropriate balance of traditional academic scholarship and work-based learning. We have a target that 80% of our undergraduate students would have experiential learning."

More than 260 students took part in NUI Galway access and foundation courses this year, with 150 receiving an offer of entry. In total, the access programme office has 1,100-plus undergraduates on its books.

NUI Galway's openness to alternative means of teaching and learning is evident, too, in its work with the Irish language. The university is close to the Connemara Gaeltacht, the largest Irish-speaking area in the country and as such NUI Galway celebrates and promotes the Irish language offering classes from beginner to advanced level as well as programmes taught through the medium of Irish.

Alastair McCall, Editor of The Sunday Times Good University Guide, says: "In the eight years since NUI Galway last won our University of the Year award it has continued to grow its global reputation as one of the great seats of learning. Some of its academics are among the most cited in the world and its reputation spans the arts and the sciences. The university brought in more than €65m of research income last year, evidence of the cutting edge at which many of the academics operate.

"It is also pivotal to the regional economy, rooted in its community and playing an active role at all levels. Its students are encouraged to volunteer and be part of that community and not just come to Galway as educational tourists. When Galway is the European Capital of Culture in 2020, the university will be at its heart; the newly-opened O'Donoghue Centre for Drama, Theatre and Performance a bold statement of the importance of the arts to the university."

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