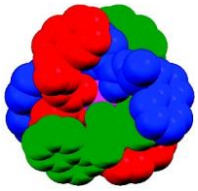
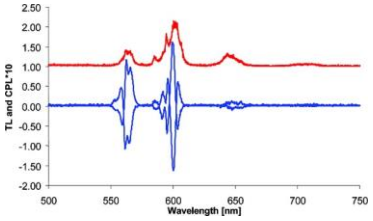
Irish Chemical News

The Journal of the Institute of Chemistry of Ireland

Feature Articles:-

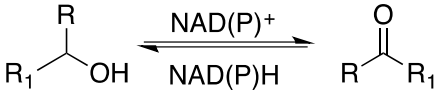




Metal ion directed supramolecular self-assemblies

X-ray crystal structure of the $Tb.1R_3$ complex showing the helical ligand arrangement

Novel Enzymes for the Synthesis of Chiral Alcohols and Amines



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Irish Chemical News

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

A Message from the President

Dear Fellows, Members, Graduates and Associates,

As we approach the end of the calendar year 2015, The Institute can look back on some highs and lows. Among the high points of the year was the introduction of our new Industrial Chemistry award, sponsored by Henkel Ireland. The recipient, Donal Coveney of TopChem, was presented with his award, at a special awards symposium held at UCD, on November 26th. Donal had already given his award lecture, during Science Week, at Sligo IT. There is a full report on both events in this issue, accompanied by photographs. We hope this will become an annual event and we are most grateful to Henkel for sponsoring this award and the good news is that the company will sponsor the award in 2016 as well. Calls for nominations for the 2916 Industrial Chemistry Award will go out early in the New Year.

A second award presented at the awards symposium was the now well-established Annual Chemistry Award (Eva Philbin Lecture Series). This award went to Michael Zaworotko, Bernal Chair of Crystal Engineering at the University of Limerick. He too, had already given the first of his lectures during Science Week, at UL. The third lecture will be given at NUIG on February 4th 2016. A full report of this award, with photographs, also appears in this issue.

I should like to congratulate both recipients on their awards. We hope to publish the text of both award lectures in this journal in due course.

Earlier in the year, we presented the Boyle-Higgins Award to Dermot Diamond of DCU. The award lecture was given in conjunction with the AGM at DCU. We also participated in a joint awards Seminar organized by the RSC at QUB and we had our Annual Congress, with the theme 'Asymmetric Synthesis' at UCD. These events have already been reported in previous issues of 'Irish Chemical News' and were all very successful and well attended. Another highlight was the annual Irish Universities' Chemistry research colloquium, hosted in June by NUI Maynooth.

In September, I was delighted to represent the Institute of Chemistry of Ireland at the EuCheMS General Assembly in Vienna. Unfortunately, there was some embarrassment, when I discovered that we had not paid our affiliation fees to EuCheMS. This was due to a serious cash flow problem, because many members are late paying their membership subscriptions. Our Honorary Treasurer spends a considerable amount of time and effort, as well as expense, sending out reminders, but still people forget. I would appeal to all members to consider completing the Direct Debit Mandate form, to ensure subscriptions can be collected in an efficient and timely manner. We manage to run a number of events throughout the year and present a variety of awards, thanks to our membership subscriptions, the contributions of our company members and a limited amount of industrial sponsorship. We also depend, to a huge extent, on the voluntary work of a small number of people who are actively engaged with the Institute. I am most grateful to all of our Council members, Committee members and event organisers for all the good work that they have done over the past year. They give freely of their time, on a voluntary basis. But there are costs involved and we do need our Members' subscriptions. So please do make a New Year's Resolution to pay your subscriptions on time. To those who are in the habit of doing so, a big 'Thank You"!

As well as recognizing significant contributions to Chemistry though our major awards, we also give awards to students, to encourage them in their study of Chemistry. Among these are: the Schools' Newsletter Competition, the Schools' Science Week Quiz, the medal awarded to the student (or students) who achieve the highest marks in the Honours Leaving Cert Chemistry examination each year, prizes in the Eurachem Analytical Measurement Competition, the annual Graduate Awards, and a prize for the best presentation at the Universities' Chemistry Colloquium.

Unfortunately, due to a number of circumstances outside our control, it was not possible to hold the Eurachem Analytical Measurement Competition in 2015. But the good news is that it will be back in 2016, when it will be hosted by Athlone Institute of Technology.

The year ended for us on a sad note, as we learned of the untimely passing of our former President and Registrar, Paraic James. The news broke on December 4th, on the very day of our final Council Meeting of the year. A vote of sympathy was passed at the meeting and several members of Council travelled to Sligo for the funeral. Our thoughts are with Paraic's family at this time and we extend our condolences to his former colleagues at DCU. Paraic will be greatly missed. May he rest in peace.

I wish you all a very Happy New Year and hope to see many of you at various Institute events in 2016.

Margaret Franklin, FICI, President.

Again we thank our Congress Sponsors:-

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Editorial

Earlier this year I committed to producing 3 issues of ICN and with this 3rd issue I have met that commitment. There is always room for improvement and next year I aim to have 4 issues at more regular intervals and hopefully the 4th will publish before Christmas rather than after. I'm working hard in the background to accumulate a pool of papers to publish at predetermined dates. I have attended a number of conferences and seminars and have been promised a number of articles which are wide ranging in topics of interest to chemists. Hopefully I will be able to bring these to you throughout 2016.

This issue has two academic papers one from Prof Thorri Gunnlaugsson last year's Annual Awards (Eva Philbin) winner and another from Dr Francesca Paradisi, Senior lectures at UCD. I do aim to have two academic papers per issue if possible.

I bring reports of a number of awards, our Institute Awards including for the first time our Industrial Chemistry Award, made possible by the generous sponsorship of Henkel Ireland, won by Dr. Donal Coveney founder of TopChem Pharmaceuticals, Sligo and a report on the Pharma Industry awards. The ISTA Senior Science Quiz is covered along with our Schools Chemistry Newsletter Competition.

I attended the National Sustainability Summit at the Aviva Stadium and report on that. BASF have provided a statement from their CEO Kurt Bock and a link to the full report "The United Nations Global Compact-Accenture CEO Study Special Edition: A Call to Climate Action". GSK Dungarvan have provided a case study on their efforts at sustainable CO_2 reduction by Adrian McCarthy.

The Government launched its strategy for Research and Development, Science and Technology at Innovation 2020 at the Convention Centre, Dublin on Tuesday 8th December and I report on this event. The Institute has issued a statement welcoming this strategy.

The Government has published a White Paper on Energy titled 'Ireland's Transition to a Low Carbon Energy Future 2015-2030'. The launch took place at The Mansion House, Dublin on 16 December 2015. I bring some initial comments on this and hopefully will have further commentary during 2016.

I have also procured a paper on the State Laboratory and its role in Irish society.

I do hope to establish ICN as a more popular and frequent publication for chemists working in Ireland to connect with a wider chemical community and the interested general public. Furthermore I have a concern and feeling that it is the separation of chemists from the wider chemical community, caused by their focus and the intensity of their research that leaves them reluctant to write general articles communicating their work and its importance to society in general. I feel that chemists receiving increasing amounts of tax payer's money do have a responsibility to communicate the purpose of their work and its benefits to society. I think that SFI and grant agencies should encourage more general communication of the importance of chemical research. I do urge researchers to explain and give better insight of their endeavors to the wider community by publishing in ICN.

I'm sure there is much that can be done to improve ICN and I welcome suggestions and comments. You can sent these to The Editor at:-

mailto:info@instituteofchemistry.org

Patrick Hobbs MSc, FICI, CChem, CSci, MRSC.

Editor ICN,

Immediate Past President.

Metal ion directed supramolecular self-assemblies: The 2014 Annual Award for Chemistry of the Institute of Chemistry of Ireland; The Eva Philbin Lecture

Prof. Thorfinnur Gunnlaugsson and Dr. David Caffrey

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

The University of Dublin

Introduction

Nature has developed some beautiful functional molecules through the use of complementary self-assembly processes; lipids, protein and DNA folding being examples of such macromolecular structures. Usually weak and none-covalent (or reversible) 'bonding' interactions, such as hydrogen bonding, π–π stacking and van der Walls forces are used to govern the self-assembly processes that take place in the constructions of such molecules, referred to as 'supermolecules'. Similarly chemists have developed many examples of molecules, or ligands that can self-assemble into novel architectures using the same methodology. The application of this chemistry is what is central to the field of supramolecular chemistry; the 'chemistry beyond the covalent bond' as it is often referred to; though today, the use of reversible bond-formations such as those as seen in imines, is commonly used to form large and functional molecules that can be considered as possessing function and properties seen for 'classically' defined supermolecules.

Supramolecular chemistry has become a powerful tool to generate functional structures and novel materials from simple building blocks (*e.g.* ligands) that are carefully designed to allow for such controlled self-assembly processes to take place and operate in solution; the resulting structures possessing function or physical properties that are different to those of the starting material. This kind of deign strategy has resulted in the formation of many examples of supermolecules that can find applications across disciplines and areas such as within, synthetic chemistry (e.g. in catalysis) and within various biotechnologies (such as in sensing, imaging and in drug delivers, to name just a few), materials and in medicine (in the construction of novel material for impaling and the coating of implants and medical devices, *etc*.). Often a key feature of these structures is the application of metal ions to direct the formation of such supramolecular self-assembles in addition to the forces referred to above. Metal ions such as transition and lanthanides are particularly attractive for use in the formation of such structures as these add specific directionality to the self-assembly formation/process and often these ions possess unique physical properties themselves, then these can also be capitalised on within the resulting self-assembly structures. Hence, the combination of weak self-assembly interactions and metal coordination can give rise to formation of highly novel and complex structures and materials, that would not be possible to form though classical covalent organic synthesis. At the School of Chemistry, and within the Trinity Biomedical Sciences Institute (TBSI), at Trinity College Dublin, we have focused a significant amount of our research efforts over the last decade on the development of novel and functional supramolecular structures using the above design strategy. In the following section, a select few examples of metal directed formation of supramolecular structures developed in our laboratory in recent times will be discussed, these being the ones that have laid the corner stones for the work currently being developed in our laboratory. A more comprehensive discussion can be found in some of our recent review articles.[1,2,3]

Recent developments

Applying metal directed self-assembly principles, we have designed a series of chiral mononuclear Ln(III) complexes from a variety of ligands. While in the past few years our attention has focused on two types of acyclic ligands, the once discussed in this article all consisting of an amide-substituted central pyridine coordinating unit. This binding motif serves as a successful revision of the di-picolinic adid (dpa) ligand

framework, and has been continuously elected for use in view of the presence of a tridentate cavity optimal for the assembly of homoleptic Ln(III) tris-chelates.

The story began in 2007, when we published the synthesis, crystallographic characterisation, and chiroptical spectroscopic behaviour of a collection of chiral supramolecular bundles, formed through separate complexation of the enantiomeric ligand pair **1S** (*S,S*) and **1R** (*R,R*), Figure 1, with a range of $Ln(CF_3SO_3)_3$ salts [Sm(III), Eu(III), Tb(III), Nd(III), and Yb(III)].[4]

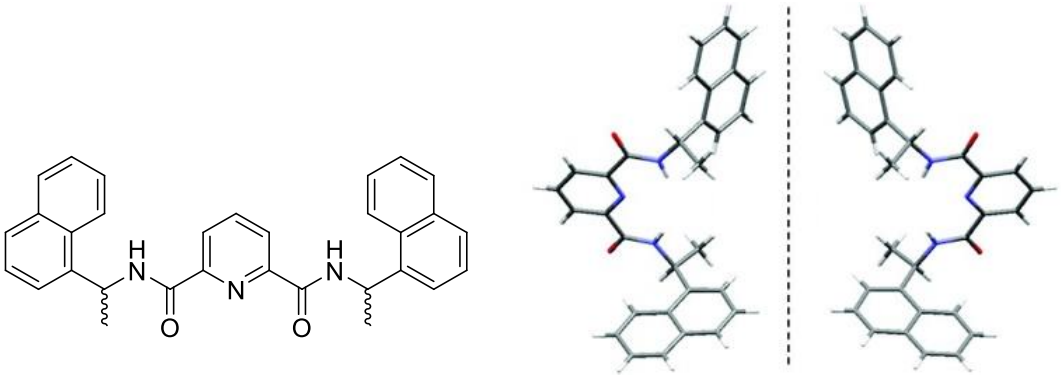


Figure 1. The chemical structure of **1S**(*S,S*) and **1R**(*R,R*) and their corresponding X-ray crystal structures that demonstrates their enantiomeric nature.

These two structurally simple ligands were synthesised in a single amide-coupling step, from commercially available starting material, whereby the chirality was introduced in the form of two flanking chiral naphthalene moieties, endowed with the ability to readily sensitise the Ln(III)-centred luminescence. Slow evaporation of the two ligands from CH_2Cl_2 afforded suitable crystals for X-ray diffraction studies, which clearly showed the C_2 ligand symmetry while simultaneously highlighting the enantiomeric relationship between the compounds, a fact reinforced by using circular dichromism (CD) spectroscopy.

Concerning the Ln(III) complexes, using both Nuclear Magnetic Resonance, or ^1H NMR, spectroscopy and electrospray ionisation (ESI) mass spectrometry confirmed the expected 1:3 (M:L) stoichiometry for all systems. This demonstrating that the metal ion directed the synthesis of the resulting bundles by coordinating to the central pyridine and the two amide moieties of each of the three ligands; giving an overall nice coordination environment around the metal ion. This would suggest that the metal ion was coordination saturated, i.e. no more ligands could be complexed and this was confirmed by determining the hydration state for the two systems, or the number of metal bound water molecules, the so called *q* values. For both, these were determined, by using photoluminescence spectroscopy, where the life-times and of the Ln(III) emitting moiety was monitored. For Eu(III), which emits in the *ms* time frame, the q-value was determined to be zero, confirming the coordinative saturation in aqueous media and consistent with the generation of a nine-coordinate Ln(III) species from the self-assembly of three ligands about a single metal centre.

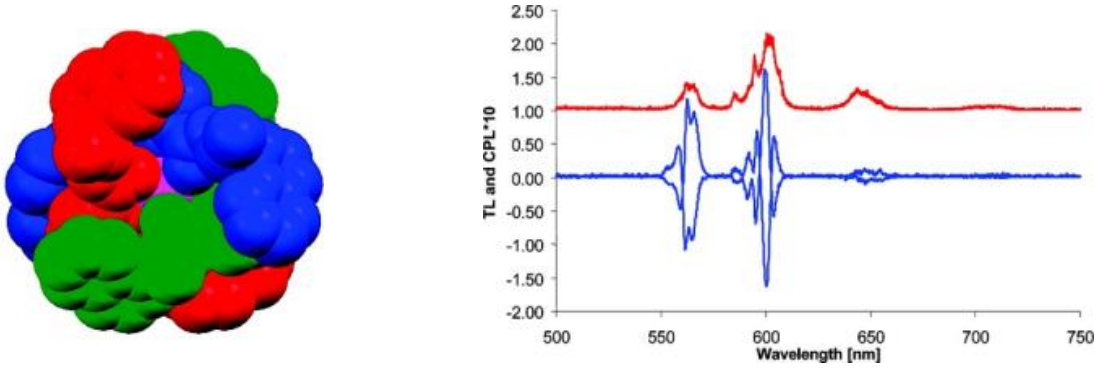


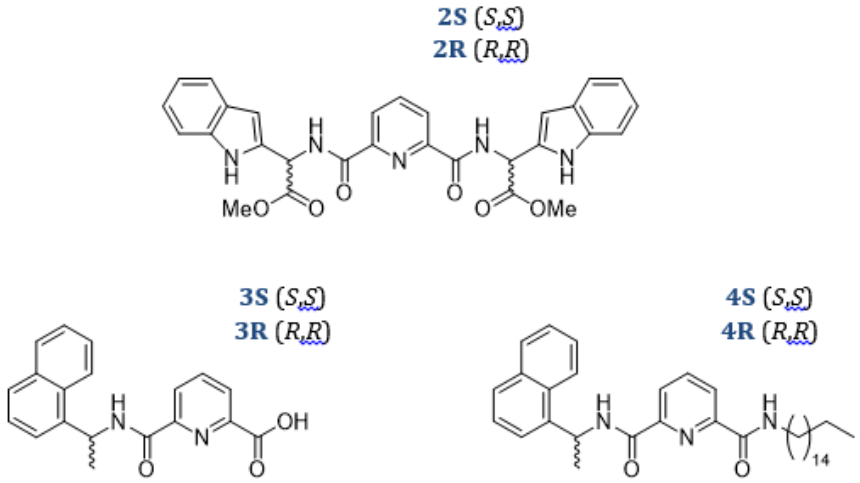
Figure. 2 a) X-ray crystal structure of the $Tb.1R_3$ complex showing the helical ligand arrangement. b) The luminescence emission spectrum of the $Sm.1S_3$ complex (red) and the circularly polarised emission spectra of the two Sm(III) complex enantiomers (blue).

However, at this stage we did not have inside into the actual structure of the self-assembly in solution, and hence a valuable structural insight was gained through the use of X-ray crystal structure analysis of the solid state complexes, which not only exposed their highly symmetrical, bundle-type appearance, but also demonstrated the overall complex chirality arising from the helical ligand arrangement, Figure 2a. With regards to stability, a review of the crystallographic data found the central pyridyl ring of each ligand to intercalate between the naphthalene antennae of the other two, informing of the existence of stabilising π-π stacking interactions throughout the structures. From a chiral perspective, these results showed **1S** and **1R** to give rise to enantiopure Ln(III) bundles of opposite helicity, proof that the assembly process was in fact diastereoselective and hinged on the choice of ligand enantiomer. Upon assignment, this relationship was simplified to **1S** and **1R** conferring Δ and Λ metal stereochemistry, respectively. Indisputable spectroscopic evidence of the chirality transfer was provided using a unique spectroscopic technique, circular polarised luminescence, or CPL spectroscopy. This was carried out in collaboration with Dr. Robert D. Peacock at the School of Chemistry at Glasgow University; a collaboration that has been extremely fruitful over the years. With the metal ions now residing within a chiral pocket, the enantiomeric Ln(III) complexes predictably yielded CPL spectra consisting of emission signals of equal magnitude but opposite sign arising from the lanthanide ions, Figure 2b. This technique demonstrating that it was possible to probe the chiral nature of the self-assemblies by simply observing the nature of the CPL spectra arising from a metal ion that itself would not possess a chiral signature on its own.

However, this stoichiometry was thermodynamically driven as the 'complex' was formed by simply reacting one metal ion (e.g. Eu(III)) with three equivalents of either the *RR* or the *SS* enantiomers of **1**. Consequently it was important to be able to establish what was occurring in solution upon formation of the self-assembly, *i.e.* it was important to be able to determine the stepwise self-assembly formation in solution. The progression of the complexation process in solution was monitored by UV-vis (as the changes in the transitions assigned to the naphthalene units and the pyridine units could be monitored) and luminescence titrations (sine the ligand and the complex had luminescent signatures), which again accentuated the predominance of the **Ln.1S/R$_3$** system. From these measurements, it was possible to show that the initial formation of the 1:3 assembly occurred, in about 90% yield, but at higher ion concentration (e.g. the Ln(III) ion was titrated into a solution of the ligand) higher order self-assemblies began to form. From this titration experiments, the spectroscopic data (the stepwise changes in the spectrum upon addition of the lanthanide ions) could be fitted by using non-liner regression analysis and binding constants in the range of log $\beta_{1:3}$ = 20 – 22 were calculated for the Eu(III) complexes of **1S** and **1R** in acetonitrile. From the different binding constants obtained, a speciation distribution diagram could be formed that demonstrated the progression of the self-assembly pathway in solution.

In light of the good thermodynamic stabilities and strong chiral emissions arising from these structures, these enantiomeric monometallic bundles stood to represent a significant landmark in the advancement of Ln(III) self-assembly within our group. Owing to their shape and structure, they were named *The Trinity Sliotars*. Indeed, these original chiral sliotars have been heavily influential to the assemblies produced in the group since, where the goal has always been to modify the parent structure in new and exciting ways. Implemented to great effect, and distinguishing the ligand set **2** – **5**, was a modification strategy founded on variation of the chiral antennae of **1**. Replacing the naphthalene units for chiral tryptophan antennae, ligands **2S** (*S*,*S*) and **2R** (*R*,*R*) presented as a more radical departure from the original structure.[5] Unexpectedly, the trends and subsequent fitting of UV-vis and luminescence titrations confirmed the dominant formation of, on this occasion, the 1:2 (M:L) self-assembly formation for both Eu(III) and Tb(III). The complete absence of the anticipated 1:3 (M:L) stoichiometry, also apparent from mass spectrometry, was accredited to the relative increase in steric hindrance around the metal.

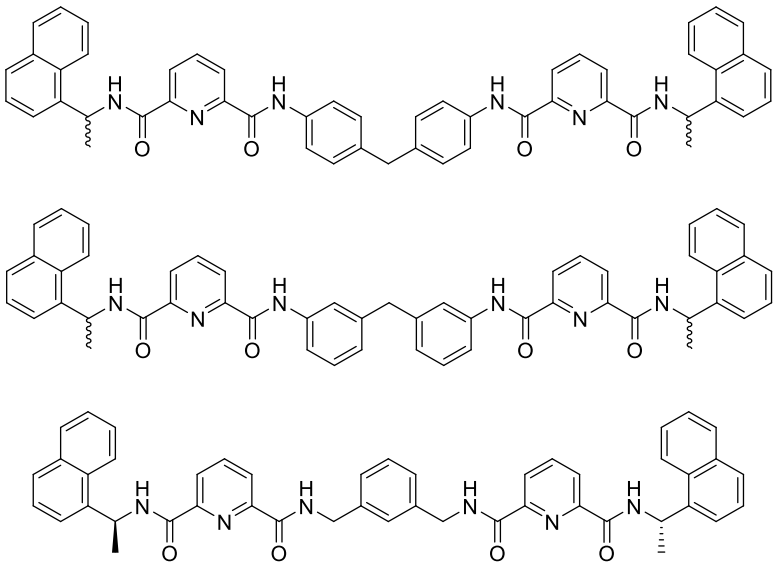
Carrying only a single naphthalene chromophore, the ligand pair **3** was developed as an asymmetrical analogue of **1**.[6] Utilising many of the same characterisation techniques, **3S** (*S*,*S*) and **3R** (*R*,*R*) were similarly shown to form 1:3 (M:L) complexes with several Ln(III) ions. Observation of phosphorescence spectral changes in the Eu(III) titrations of both ligands helped to identify luminescence intensity maxima upon the addition of 0.33 eq. of metal, evidential of the favoured formation of **Eu.3S/R$_3$** in solution. MM2 molecular modelling calculations were suggestive of a *half helicate* complex topology being most plausible, for which the three ligand antennae were positioned on the same side.



This has since then be confirmed by X-ray crystallography.[7] This model exhibited a more open structure to that seen for **1**, perhaps explaining the slight reduction in the binding constants. As before, the ability of the respective ligands to dictate complex chirality was demonstrated by CPL spectroscopy.

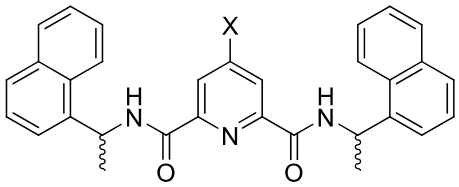
The synthetic attachment of a long hydrophobic hexadecyl chain to the carboxylic acid terminus of **3** was later performed to give **4S** (*S*,*S*) and **4R** (*R*,*R*), ligands perfectly equipped for the genesis of chiral amphiphilic Ln(III) self-assemblies.[8] Not only studied in solution, the enantiomeric **Eu.4S/R$_3$** systems were applied in the construction of stable self-assembled monolayers at the air-water interface. Employing Langmuir-Blodgett techniques, in collaboration with Prof. Martin Albrecht at University College Dublin, these chiral monolayers were then transferred to quartz slides to form luminescent Eu(III) films, from which the chiral emission was probed using CPL. The described systems, which acted as the first examples in their class, were designed with the view to satisfy the rising demand for supramolecular assemblies that can be further organised into functional devices. This movement into the realm of materials chemistry, therefore, reflects an enormous degree of versatility on behalf of chiral Ln(III) sliotar derivatives.

Through coupling of suitable spacer groups, the structure of **1** has since been adapted to include an additional binding pocket for the assembly of chiral bimetallic triple-stranded Ln(III) helicates, the first examples of which were developed from **5S** (*S*,*S*) and **5R** (*R*,*R*).[9] For this pair, the formation of **Eu$_2$.5S/R$_3$** helical species was ably demonstrated through rigorous analytical investigation. Significantly, the evolution of the metal-centred phosphorescence was monitored by Eu(III) titrations in acetonitrile, where the emission was observed to be most intense following the addition of 0.7 eq. of metal. This observation, allied with the NMR titration trends, emphasised the dominance of the desired 2:3 (M:L) stoichiometry in solution. In addition, excitation of the naphthalene antennae was found to sensitise Eu(III)-centred CPL emission of opposite sign, proving **Eu$_2$.5S$_3$** and **Eu$_2$.5R$_3$** to exist as enantiomers.



By incorporation of a *meta*-methylenediphenyl spacer that contrasted to the *para*-arrangement of **5** ligands **6S** (*S*,*S*) and **6R** (*R*,*R*) were designed with the intent of studying the effects of ligand structural isomerism on helicate formation.[10] Interestingly, fitting of the UV-vis absorption and luminescence titrations ascertained both ligands to form 2:3 (M:L) Eu(III) helicates of enhanced stability compared to those built before. An explanation for this improved binding was sought from MM2 models, which indicated the presence of a comparatively more *squeezed* complex cavity for **6**. This reduction in cavity size was foreseen to permit tighter coordination of the two Eu(III) ions in **Eu_2.6S/R_3**, with a concurrent increase in stabilising π-π forces. Switching to a xylene spacer, ligand **7S** (*S*,*S*) was also shown to form 2:3 (M:L) helicates of comparable stability with a series of Ln(III).[11]

While the above modifications have been centred on changing the spacers or the nature of the antennae the introduction of *para*-functionality to the dpa pyridine ring itself also represents a synthetic modification whose application to Ln(III) sliotar systems, though in its relative infancy, offers a major promise. Possessing the exact same core as **1** and differing only through substitution of the pyridyl 4-position, the enantiomeric ligand pairs **8** and **9** have been synthesised to pursue this strategy (X = OH and Cl, respectively), Figure 3a. Analysis of the Ln(III)



8S (*S*,*S*); **8R** (*R*,*R*): X = OH
9S (*S*,*S*); **9R** (*R*,*R*): X = Cl

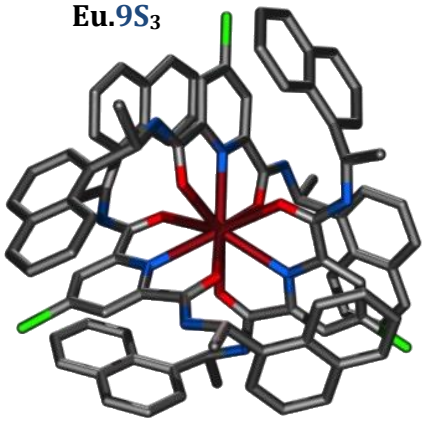


Figure 3. a) The structures of **8** and **9**. b) The crystal structure of the Eu(III) complex of **$9S_3$**.

complexation products of these chiral compounds in both solution and the solid state, Figure 3b, established the prevailing formation of 1:3 (M:L) bundles analogous to the original sliotar systems of **1**, with CD and CPL spectroscopy shedding light on the chirality transfer from ligand to later supramolecular system. Supplementary to this, the calculated log $\beta_{1:3}$ binding constants, being of the same approximate magnitude as those measured for **Ln.1S/R_3**, showed both substituents to have negligible effects on complex stability. Consequently, these *para*-positioned groups can be proposed as excellent reactive handles for the attachment of new and varied functionality anticipated to extend away from the metal ion centre, whilst having minimal effect on the overall stability of the luminescent self-assembly; being the stepping stones for introducing novel functionality and function to the resulting self-assembles.

The functionality and function can also be dictated by the changing the substituents on the amide sides; examples of that are of course the helicates shown above. However, a recent example from our group based on the same design idea is **10**, Figure 4, a simple di-benzoic acid derivative (**H_2L**) that we have shown to be able to form a 1:3 stoichiometry with ions such as Eu(III) and Tb(III); yielding structures such as those shown above for **9**. However, through the terminal carboxylic acids (that are easily deprotonated, giving **L^{2-}**) the structure can further self-assemble to give an extended self-assembly network of complexes bridged in three dimensions with lanthanide ions, these latter ions coordinating to the carboxylates. The consequence of this crosslinking is a formation of a network that in aqueous methanol solution gives rise to the formation of new material, a gel that is both highly luminescent, Figure 4b, but also self-healing, Figure 4c.[12] The material, a hydrogel, demonstrates that the lanthanide ions play now a pivotal role in both the self-assembly processes as well as in dictating the function of the resulting material. This material is reversibly formed, as

the gel can be 'dissolved' by adjusting the pH of the matrix; allowing for material to be released from the matrix.

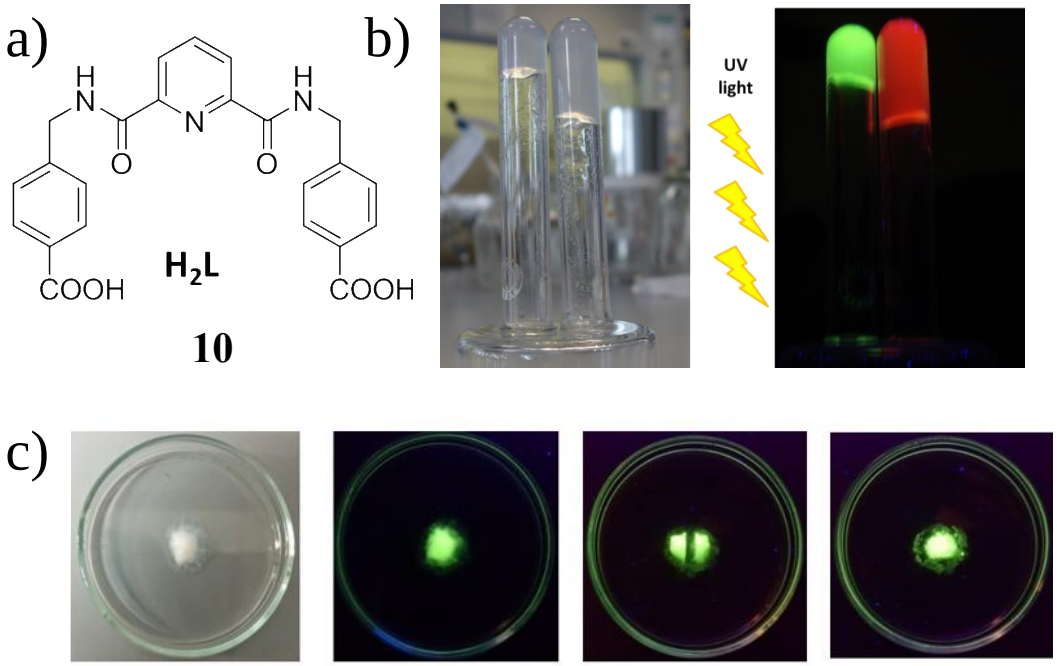


Figure 4. a) The structure of compound **10** in its di-acid form. b) The hydrogels formed from **10** upon deportation by Eu(III) and Tb(III) (red and green emissive, respectively). c) Demonstration of the self-healing capability of the Tb(III) gel.

Such delivery can also be achieved by simply incorporating complexes of the nature shown above into covalently formed (through radical polymerisation) hydrogels.[13] A phenomenon recently demonstrated in our laboratory where two types of emissive (Eu(III) and Tb(III) lanthanide self-assembly complexes were incorporated into HEMA based gel. The gel was highly luminescent, the emission of which could be modulated by external 'inputs' such as an anion (fluoride) or by changing the pH. The combination of both, was then used to demonstrate molecular logic behaviour within the gel, as the emission of either the Eu(III) or the Tb(III) centred emissions could be modulated by these 'inputs'.

Conclusion

The above account demonstrates that not only unique structures can be formed from structurally simple ligands by using metal directed self-assembly formation, but it also shows that such self-assemblies can generate novel functional material that otherwise could not be formed. The phenomenon of 'metal directed self-assembly' structures is thus a powerful tool to generate new material that has functions unique to the self-assembly pathway used and different to that of the ligands it is made from. This type of supramolecular chemistry has major advantages over many exciting chemistry protocols and technologies as it often allows for more control to be achieved, as well as the products are often formed in a reversible manner. Hence, the future of this type of chemistry is very bright.

Acknowledgement

The above research was supported by the Irish Research Council for Science, Engineering & Technology (IRCSET), the Irish Research Council (IRC) and The Science Foundation Ireland (SFI).

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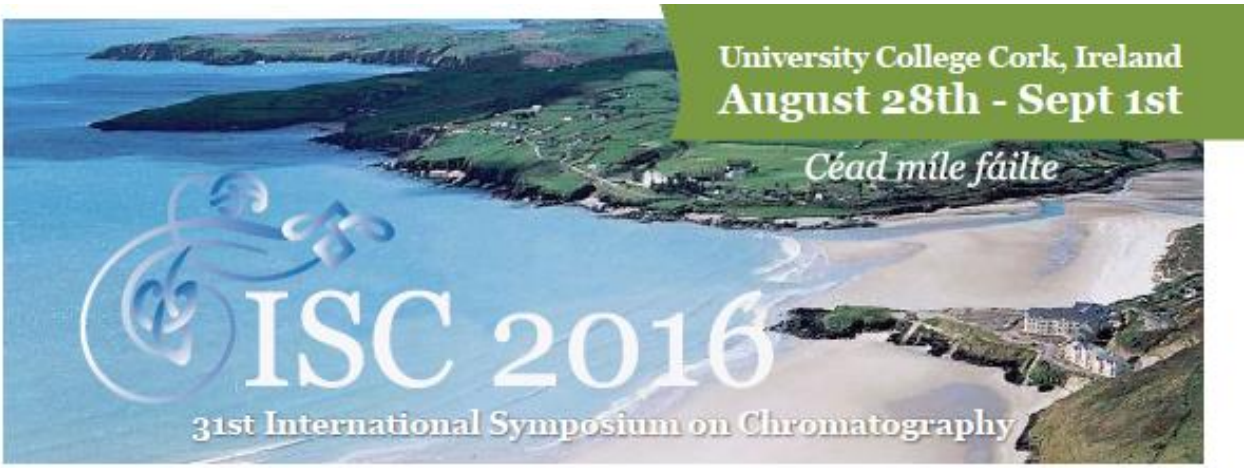

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Dear Colleagues,
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Cork City has a rich history, dating back to a monastic settlement founded by St Finbar in the sixth century and between 915 and 922, when Viking settlers established a trading community. The River Lee flows through the beautiful city, an island in the river forming the main part of the city centre just before the Lee flows onward into Cork Harbour, the world's second largest natural harbour, after Sydney Harbour, Australia. The City still retains the pleasant charm and friendliness of a country town and nearby at Cobh, you can stand at the last port of call of the Titanic, on its fateful maiden journey.

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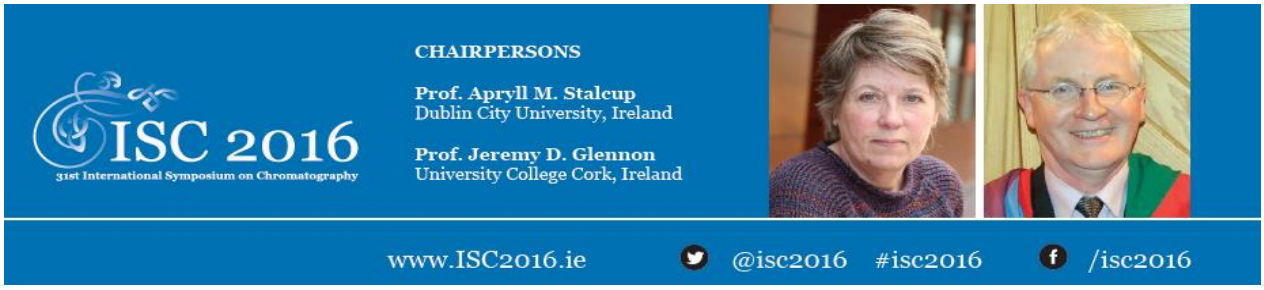

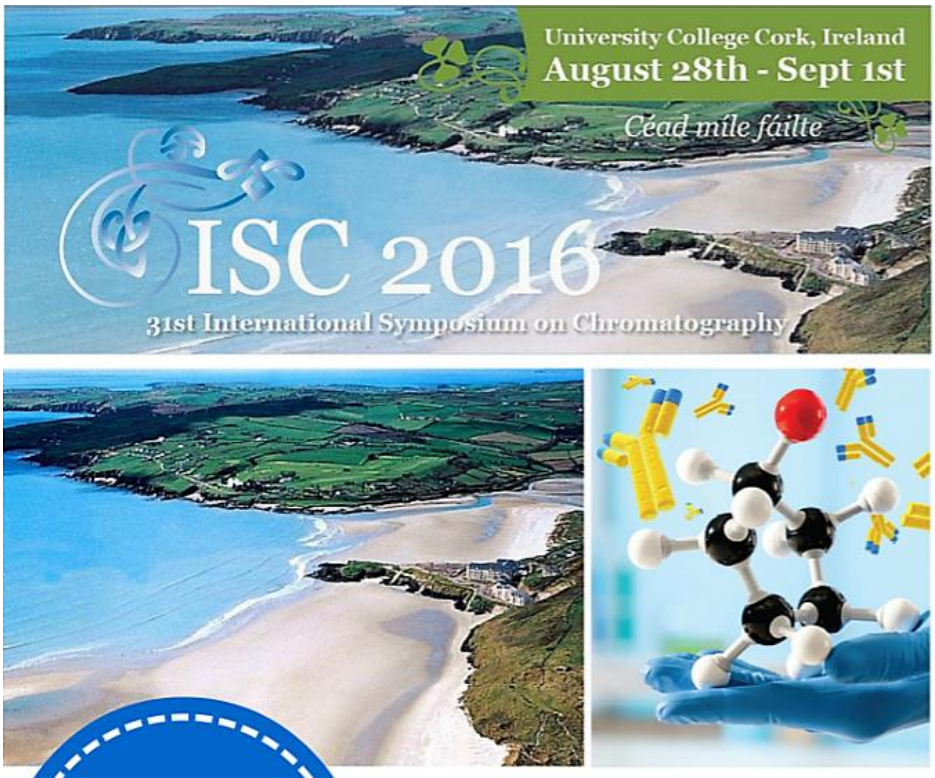

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Novel Enzymes for the Synthesis of Chiral Alcohols and Amines

Francesca Paradisi

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Dr. Francesca Paradisi obtained her MSc and PhD from the University of Bologna (Italy) where she developed new syntheses for non natual amino acids with potential biological activity. In 2001 she joined the group of Prof. Paul Engel in the Department of Biochemistry in UCD (now the UCD School of Biomedical and Biomolecular Sciences) where she started to work on enzymes and their synthetic applications. In 2006 she joined the School of Chemistry in UCD as Lecturer in Chemical Biology. She developed her own independent research particularly focussing on oxidoreductases and transaminases from extreme organisms which offer great potential for biotechnology. In parallel, she is also maintaining a more synthetic research stream currently looking at the incorporation of geometrically constrained amino acids into biologically active peptides as novel anticancer drugs. In 2014 she was promoted to Senior Lecturer. In 2015 she was a visiting academic at UC Davis in California where she worked on glycosyl hydrolases.

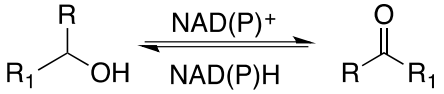
Abstract

We have investigated a variety of halophilic enzymes from halophilic organisms to date (including one halo-tolerant bacterium) with the specific aim of identifying new and robust biocatalysts able to withstand the presence of a variety of organic solvents, and with an interesting substrate scope. Halophilic alcohol dehydrogenases (ADHs) and amine aminotransferases (AAT) alike show an unusually broad substrate scope, excellent tolerance to organic solvents and ease of manipulation. The enzymes have been successfully immobilized on an epoxy-resin which allows for reusability of the biocatalysts over 10 times.

Introduction

The possibility of using enzymes in organic solvents offers numerous advantages when compared to traditional aqueous enzymology; higher solubility of hydrophobic substrates being key, as well as the elimination of microbial contamination in the reaction mixture.[1] Enzymes in organic solvents are often denatured and stripped of the essential water layer [2,3] which allows for both structural stability and catalytic activity. Retention of stability and activity in this medium remains a significant challenge. Solvent-tolerant enzymes that naturally remain stable in organic solvents have come to be very useful biocatalysts for non-aqueous enzymology.[4,5] Halophilic enzymes function under extremely high salt concentration and they have been reported to be stable under "dry condition" (low water concentration).[6] Studies have suggested that the halophilic adaptation strongly correlates with the enzyme structure; halophilic enzymes possess a higher pro-ratio of acidic amino acids and lesser pro-ratio of hydrophobic amino acids when compared to corresponding mesophilic enzymes.[7–9] As salt tends to greatly reduce water activity of the medium, halophilic enzymes may become the choice for biocatalytic processes performed in low water activity environments like aqueous/organic and non-aqueous media.[1]

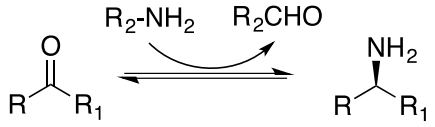
Alcohol dehydrogenases (ADHs) are enzymes highly relevant in biotechnology and have been investigated for decades for their applications in fermentative processes as well as synthesis of valuable pharmaceutical intermediates such as chiral alcohols.[10,11] These biocatalysts are co-factor dependent and are capable of interconverting alcohols into aldehyde/ketones (Scheme 1).



Scheme 1: general scheme of an ADH catalyzed reaction

A vast number of ADHs has been characterized and more recently ADHs from extremophilic organisms have raised interest for their ability to carry out reactions at high temperatures or in the presence of organic solvents.[12,13] Similarly amino transaminases are a family of enzymes with high potential in biotechnological applications. They can be very useful for the enantioselective production of a series of compounds such as chiral amines and enantiopure amino alcohols often needed for the synthesis of biologically active compounds. ω-Transaminases play a central role in the biocatalytic preparation of enantiopure amines for their generally high turnover rate, broad

substrate specificity and no requirement for external cofactors.[14,15] ω-Transaminases stereospecifically introduce an amino group from an amino donor to a carbonyl acceptor (Scheme 2) and the range of donors and acceptors varies significantly among transaminases.



Scheme 2: general scheme of an ω-transaminases catalyzed reaction

Here we summarise our recent findings on two alcohol dehydrogenases from *Haloferax volcanii* (*Hv*ADH1 and *Hv*ADH2) and an amino transaminase from *Halomonas elongata* (*He*AT).

ADH1 and ADH2 from *Haloferax volcanii*

His-tagged *Hv*ADH1 and *Hv*ADH2 were cloned, homologously overexpressed and purified from *H. volcanii* strains.[16] *H. volcanii* is an extremely halophilic archaeon isolated originally from the Dead Sea. The production of *Hv*ADH1 and *Hv*ADH2 is highly efficient due to the selection of transformed *H. volcanii* cells by *pyr*E2 and *hdr*B markers, that maintain plasmids in rich medium without the requirement for antibiotics, known to impair cell growt.[17] Both enzymes are soluble and exhibit alcohol dehydrogenase activity that is approximately 10-fold greater than that previously reported for ADH12 from *H. marismortui*. [18] *Hv*ADH1 was exclusively NAD^+-dependent, while *Hv*ADH2 displayed a strong preference for the phosphorylated coenzyme. Both *Hv*ADH1 and *Hv*ADH2 are strongly haloalkaliphilic (3-4M KCl and pH 10 is required for optimal activity in the oxidative reaction) and the apparent dissociation of *Hv*ADH1 and *Hv*ADH2 tetramers into less active dimers is observed when the enzymes are eluted in 1 M NaCl.

*Hv*ADH1 and *Hv*ADH2 were assayed for activity against methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 2-propanol, 2-butanol, isoamyl alcohol, glycerol and benzyl alcohol. The results are here expressed as relative activities (%) (**Fig.1**). Interestingly, there is an apparent negative correlation between the substrate chain length and the salt concentration required for optimum *Hv*ADH2 activity. The enzyme is maximally active with ethanol with 4 M KCl. It is maximally active with 1-propanol with 2 M KCl and with 1-butanol and 1-pentanol with 1 M KCl. Optimum *Hv*ADH2 activity with the secondary alcohols, 2-propanol and 2-butanol, is observed with 3 M KCl and 2 M KCl, respectively, and with isoamyl alcohol in the presence of 1 M KCl. Maximum activity with benzyl alcohol is detected with 2 M KCl. Both *Hv*ADH1 and *Hv*ADH2 catalyse the reductive reaction optimally at pH 6.0, with 4 M KCl in the case of *Hv*ADH1, and with 1 M KCl in the case of *Hv*ADH2.

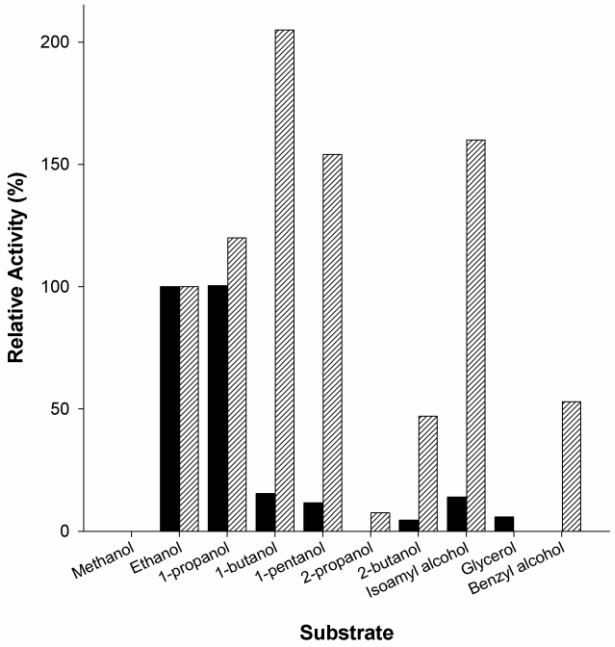


Figure 1: *Hv*ADH1 (black bars) and *Hv*ADH2 (striped bars) activity against a range of alcohol substrates

Both haloarchaeal enzymes described here are found to be highly thermoactive. *Hv*ADH1 exhibits maximum activity at 80°C while *Hv*ADH2 is maximally active between 85°C and 90°C.

With respect to *Hv*ADH1, the stability of *Hv*ADH2 is remarkable. While *Hv*ADH1 (crude and purified) is inactive after two weeks, crude *Hv*ADH2 retains half of its original activity following incubation at −20°C for 75 days and purified *Hv*ADH2 retained almost one third of its original activity following incubation for 42 days.

In addition to its impressive stability, the tolerance of *Hv*ADH2 following overnight incubation at 4°C with 10% and 20% organic solvents, DMSO and ACN, was significantly greater than that reported for *Hm*ADH12, HLADH and YADH. [18] To properly investigate the behaviour of *Hv*ADH2, we further examined the effect of water-miscible organic solvents such as dimethyl sulfoxide (DMSO), tetrahydrofuran (THF), acetonitrile (ACN) and methanol (MeOH) in aqueous solution on the activity and conformational stability of this halophilic ADH.[13]

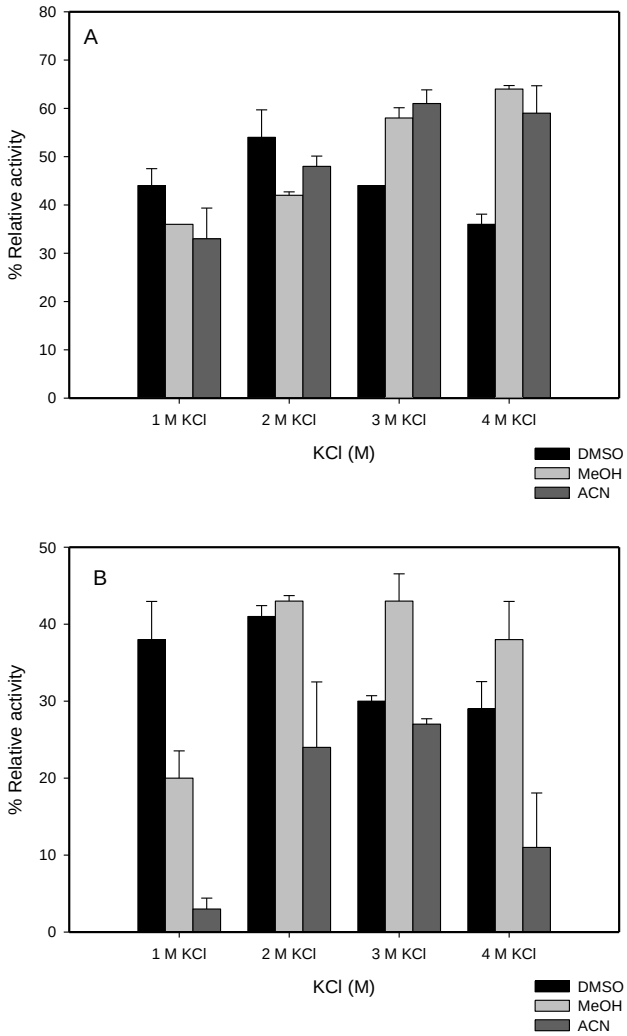


Figure 2: Organic solvents effect on the activity of *Hv*ADH2 at different KCl concentration. (A) Effect of 5 % (V/V) organic solvents. (B) Effect of 10 % (V/V) organic solvents. Enzyme activity was assayed under standard assay conditions and the results were expressed as relative activities (%) with respect to that observed in the absence of solvent at 4M KCl.

In the presence of 5% (V/V) acetonitrile (ACN) and methanol (MeOH) the optimal *Hv*ADH2 activity is once again recorded at 4M KCl though 3M KCl appears to be very similar (**Fig. 2.A**). Interestingly, 5% DMSO has a remarkable effect on the optimal salt requirements, yielding the best activity with only 2M KCl (suboptimal salt concentration) which declines steadily at higher salt concentrations. Increasing the solvent ratio to 10%, lowers in all cases the salt requirements (**Fig. 1B**). DMSO and MeOH are the best co-solvent and the enzyme retains over 40% of catalytic efficiency at a suboptimal salt concentration. However, the presence of organic solvents has no effect on the optimum pH for the oxidative reaction.

*Hv*ADH2 has also been successfully covalently immobilized on metal-derivatized epoxy Sepabeads. This was the first reported example for a halophilic protein. A significant increase in the stability of the immobilized enzyme was achieved by blocking the unreacted epoxy groups with ethylamine. The immobilization process increased the enzyme stability, thermal activity and organic solvents tolerance when compared to its soluble counterpart, indicating that the immobilization enhances the structural and conformational stability. At 60 ˚C the immobilized enzyme showed 20% higher activity compared to the free form, for example, and following incubation for 24 h with 30% DMSO and 30% methanol immobilized *Hv*ADH2 retained 55% and 60% respectively. Upon increasing the incubation time to 72 h the immobilized enzyme still retained 55% and 45% activity respectively. One step purification–immobilization of this enzyme has been carried out on metal chelate-epoxy Sepabeads, as an efficient method to obtain immobilized biocatalyst directly from bacterial extracts.

Amino transaminase from *Halomonas elongata*

The *spuC* gene was identified as a putative aminotransferase from *H. elongata*. *H. elongata* is a moderate halophile which evolved an organic-osmolyte strategy to overcome the high osmotic pressure of its natural environment,[19] *it* does not exhibit the extensive adaptation of the intracellular macromolecules present in archaea halophiles, which preferentially evolved to maintain their proper osmotic pressure by the accumulation of high cytoplasmic concentration of potassium chloride.[20] On the contrary, *H. elongata* preserves an appropriate cytoplasm osmotic pressure by accumulation and/or biosynthesis of organic solute. The gene was cloned into the vector *pRSET B*, expressed in *E. coli* BL21(DE3) and purified by metal affinity chromatography.[21] The His-tagged enzyme was characterized at different temperatures, pHs, salt concentrations and in the presence of different cosolvents and additives. The substrate specificity of the transaminase was studied against a library of amino donors and amino acceptors and compared with the □-TA from *V. fluvialis* and *C. violaceum*.

The effect of pH on HEWT activity is reported in **Figure 3**.

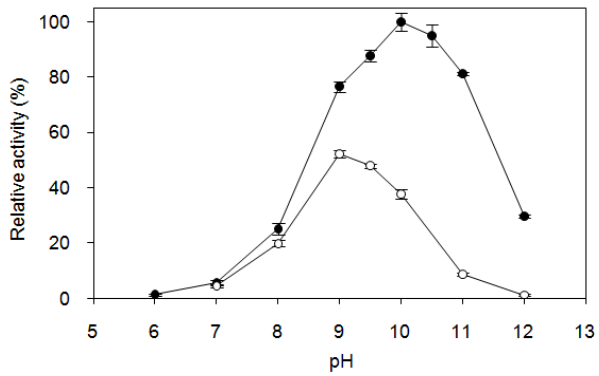
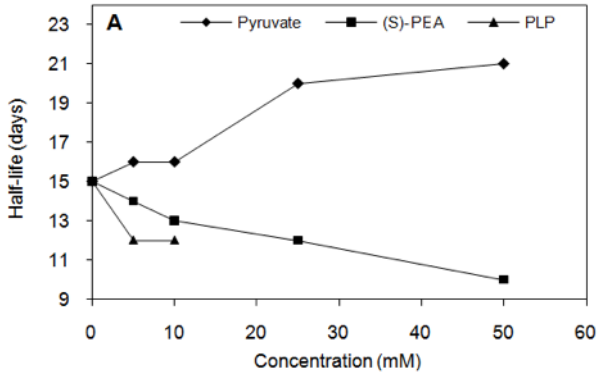


Figure 3: pH effect on enzyme activity (●) and stability (○).

*He*WT activity reached the maximum at pH 10, but the catalyst is more stable at lower pHs. The optimal balance between activity and stability was found around pH 8-9.

HeWT was tested at different temperature and the highest activity was reached at 50 °C while its stability is well preserved for temperatures up to 35 °C over 24 hours.

The stability of HEWT in the presence of organic molecules involved in the standard reaction was determined. The enzyme was stored with different concentrations of (*S*)-(−)-1-phenylethylamine, pyruvate and pyridoxal 5′-phosphate (PLP) at 25 °C and the activity was monitored over time under standard conditions (**Figure 4.A**). An increase in the enzyme stability was found at increasing pyruvate concentrations, while increasing the amine concentration resulted in a progressive inactivation of the catalyst. The destabilizing effect of (*S*)-(−)-1-phenylethylamine is, in any case, significantly lower with respect to what reported for *V. fluvialis* ω-TA: in that case the enzyme was completely inactivated when the concentration of the amine was higher than 5 mM.[22] The simultaneous presence of PLP with (*S*)-(−)-1-phenylethylamine alleviates the inactivating effect of the aromatic amine (**Fig. 4.B**).



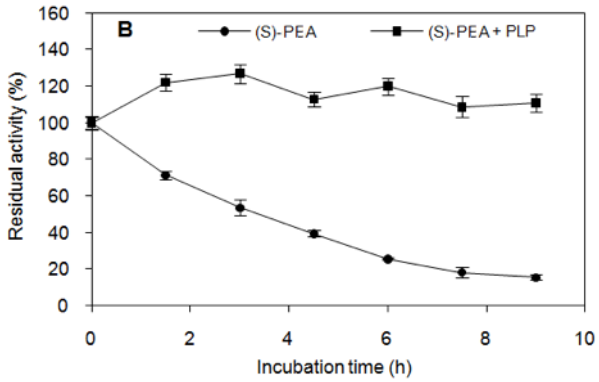


Figure 4: Enzyme stability at different additive concentrations (**A**). Stability interaction of pyridoxal 5′-phosphate and (*S*)-(−)-1-phenylethylamine (PEA), both 5 mM, on the enzyme (**B**).

The addition of a co-solvent to the reaction mixture was expected to affect both enzyme activity and stability. The effects of a selection of common water-miscible organic solvent were investigated (**Table 1**). In all cases, a decrease in enzyme activity was observed. However, the transaminase stability was unaffected by organic solvents.

Co-solvent ratio	Relative activity (%)			
	10 %		20 %	
Incubation time	0 h	22 h	0 h	22 h
No co-solvent	100 ± 3	100 ± 6	100 ± 3	100 ± 6
MeOH	78 ± 4	68 ± 2	48 ± 4	47 ± 4
DMSO	51 ± 1	42 ± 2	38 ± 2	27 ± 5
EtOH	40 ± 1	46 ± 4	23 ± 5	25 ± 2
*t*BuOH	34 ± 6	36 ± 3	19 ± 1	20 ± 3
*i*PrOH	28 ± 1	30 ± 1	16 ± 6	16 ± 1
ACN	26 ± 3	n.d.	8 ± 1	n.d.
*n*PrOH	17 ± 4	n.d.	0	n.d.
THF	4 ± 5	n.d.	0	n.d.
Not determined (n.d.)				

Table 1: Co-solvent effect on HEWT activity and stability.

The effect of different salt concentrations on enzyme stability and activity was also investigated. In all conditions, enzyme activity decreased with the increase of salt concentration, when compared to the enzyme at pH 8.0 in 50 mM phosphate buffer. On the other hand, the salt presence shows little to no effect on the stability of the enzyme

(results not shown). This is a clear difference between *He*WT and the *Hv*ADHs discussed above.

We investigated also a range of amino donors and, interestingly, this enzyme accepts isopropylamine as amino donor with a relative initial rate 3-4 times higher respect to *C. violaceum* and *V. fluvialis* ω-TAs with 41% of final conversion. *He*WT is highly (*S*)-selective, being able to fully convert (*S*)-1-phenylethylamine to acetophenone and showing no detectable activity with the opposite enantiomer; a resolution of the racemate stops at 50% of conversion permitting the recovery of (*R*)-1-phenylethylamine with e.e.>99% (E>100).

A library of compounds was selected in order to investigate the characteristics of the new amine transaminase in comparison to the two well-known structural homologues from *C. violaceum* and *V. fluvialis.*[23] In spite of a higher sequence identity with the former, HEWT shows initial rates that are more comparable with the *V. fluvialis* ω–TA activity. Higher initial reaction rates were measured for pyruvate, propanal and phenylacetaldehyde.

As expected, the reactivity with aldehydes and α-ketoacids is higher with respect to the ketones due to the relative low electrophilicity of their carbonyl group compared to aldehydes and ketoacids. Bulky aldehydes such as vanillin, cinnamaldehyde, and 2-phenylpropionaldehyde are well accepted by the enzyme.

Of particular interest are the activities with 1,3-dihydroxyacetone and L-erythrulose. Usually, in fact, α,α'-dihydroxyketones are not accepted by TAs; two notable exceptions are the ω-TAs from *C. violaceum* [24,25] and *P. aeruginosa*. [26]

Five amino acceptors were tested with isopropylamine and *o*-xylylenediamine to assess the synthetic scope of *He*WT. Although the equilibrium is unfavourable, increasing the amino donor equivalents or using *o*-xylylenediamine shifts it towards the products. *He*WT had moderate conversions across the range of amino acceptors with isopropylamine (IPA) and *o*-xylylenediamine including acetophenone, cinnamaldehyde, vanillin and 2-phenylpropion-aldehyde. Very efficient usage of isopropyl amine and *o*-xylylenediamine was found when benzaldehyde was employed as acceptor with 90-95% conversion (**Table 2**).

The enantiospecific reaction of *He*WT with acetophenone and IPA was investigated by chiral HPLC. The (*S*)-enantiopreference was highlighted with an excellent ee > 99% towards the production of (*S*)-(−)-1-phenylethylamine.

	Isopropylamine		*o*-Xylylenediamine
	Conv. 1 eq. (%)	Conv. 20 eq. (%)	Conv. 1 eq. (%)
Acetophenone	9.7 ± 0.4	13.0 ± 0.1	29.2 ± 0.2
Benzaldehyde	85.4 ± 2.2	95.3 ± 0.1	90.9 ± 2.0
Cinnemaldehyde	20.1 ± 0.7	21.8 ± 0.1	28.5 ± 0.1
Vanillin	10.2 ± 0.7	13.2 ± 0.4	15.6 ± 0.1
2-Phenylpropion aldehyde	6.0 ± 0.9	19.0 ± 2.0	22.7 ± 1.8

Table 2

Conclusions

We have reported here on the characterization of two halophilic ADHs and one halo-adapted amino transaminase. In all cases the substrate scope is remarkably broad and we will continue to investigate the potential of these enzymes for synthetic applications.

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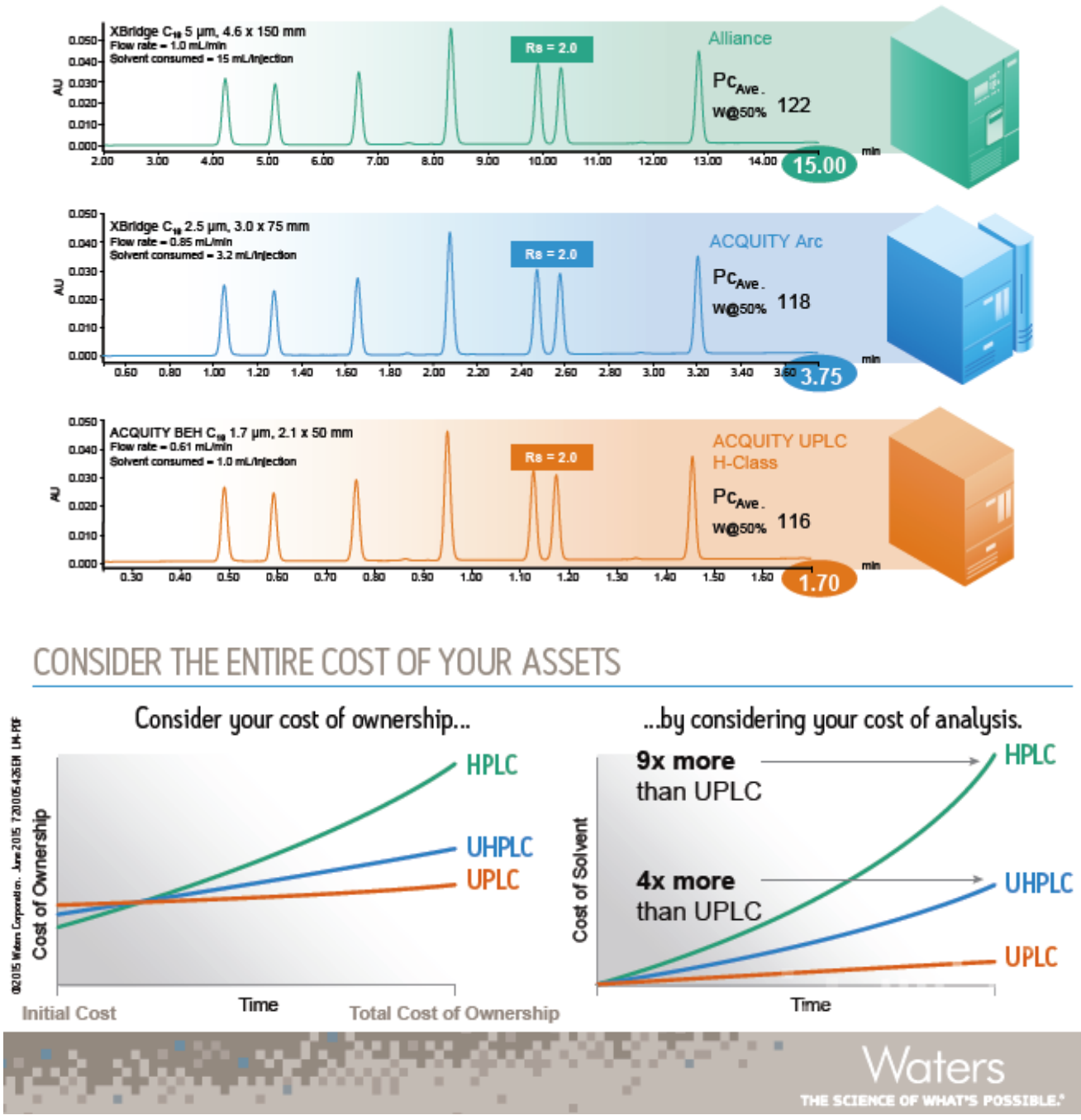

Waters

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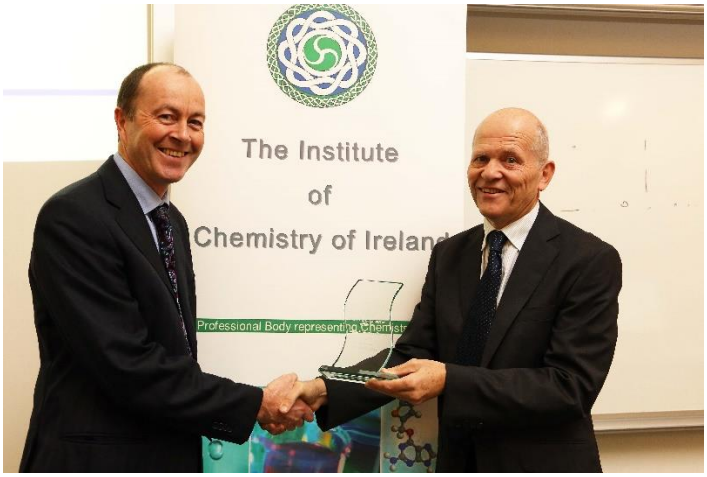
IT Sligo's Science Week

Science Week 2015 at IT Sligo was a special one for Dr Donal Coveney, Managing Director of TopChem Pharmaceuticals Ltd. Dr Coveney was presented with the Institute of Chemistry of Ireland Industrial Chemistry Award 2015, sponsored by Henkel Ireland Ltd. This new award has been introduced by the Institute of Chemistry to recognise the contribution of chemists working in their industry field.

The presentation was made by the Immediate Past President and Editor Irish Chemical News of the Institute of Chemistry, Patrick Hobbs at IT Sligo where Dr Coveney was one of the guest lecturers for the Institute's Science Week. His talk entitled: 'Jumping through hoops and chasing our tails' examined the challenges in securing market approval of pharmaceutical products.



IT Sligo's Science Week, which is now into its 16th year, takes place every November and is an annual week-long celebration of Science. It begins with the hugely popular Family Science Fair – which provides a day of science related performances, interactive displays and demonstrations for all the family to enjoy. This event alone attracts about 2,500 people of all ages to the Institute's campus each year.

"It's all about making science accessible for people of all ages," explains Dr Jeremy Bird, Head of the School of Science at IT Sligo. "The Institute's annual Science Fair has become a very strong community event – and that's reflected in the number and range of people attending."

Volunteer Geraldine O'Rourke lights up proceedings during the Dragon Show (presented by Sue McGrath) at the IT Sligo Science Fair in November.

The Institute's series of Science Week lectures on topics of public interest each evening was also hugely popular. Among the special guests this year was renowned astrophysicist, Professor Jocelyn Bell Burnell from the University of Oxford, who has helped the world expand its understanding of the universe. She gave an inspiring talk on 'Black holes in Space'.

The setting for Science Week was IT Sligo's impressive 72-acre modern campus, which boasts some of the finest Science facilities in the entire Institute of Technology sector in Ireland. The new €17million MacMunn Science Building, named after famous Sligo-born scientist Charles MacMunn, was officially opened by the Taoiseach in September 2014.

Anna, Dhani and Jay Keane with Owl from Eagles Flying at the 16th Annual IT Sligo Science Fair.

The new 4,200m2 space boasts an 80-station first year laboratory, seven other teaching laboratories and four research laboratories.

Main Entrance IT Sligo

IT Sligo's "Main Concourse"

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LENNOX

November was an exciting month for the Institute with two Institute Awards presented to two very well deserving recipients for excellent achievements in chemistry. The awards were presented at a ceremony at UCD's Centre for Synthesis and Chemical Biology CSCB.

First presented was Dr Donal Coveney of TopChem Pharmaceuticals for his achievement in founding his indigenous Irish owned pharmaceutical company. Donal was the first chemist to win the **Institute's** new **Industrial Chemistry Award 2015** sponsored by Henkel Ireland Ltd.

TopChem Pharmaceuticals develops generic pharmaceutical products mainly for the US market. While these products are known chemical entities, TopChem develop synthetic processes, delivering high quality pharmaceutical grade active ingredients. The company faces many challenges. Even though most of these products have been on the market for many years, as a new entrant they are quite rightly judged by the highest standards. This leads us to into a labyrinth of analytical investigations in an effort to track and trace potential impurities. Donal's lecture focused on some case studies, which touched on synthetic and analytical challenges encountered in product development. Donal delivered his lecture with some style initially during Science Week in IT Sligo and again on the Awards night at UCD. The lecture was titled:-

"Jumping through hoops and chasing our tails – challenges in securing market approval of pharmaceutical products".

Donal was presented with his cheque for €1000 and Plaque by Dr Patricia Cullen, Director Product Development, Henkel Technologies, AG Industry.

Donal is the founder and managing director established TopChem as an indigenous manufacturer to develop & manufacture API's for supply to the global pharmaceutical industry. He has led the company to FDA & EU GMP certification. The company has filed 4 Drug Master Files & secured business from global players Mylan, Sandoz and Perrigo. He currently employs 15 chemists.

To date more than 90 chemists, Grads and Post-Grads have been employed since inception in 2007 and many have gone on to find employment in the multinational sector. The Company also offers technical services to the Pharma sector including process development, technical support and troubleshooting.

Donal is a graduate of UCC, and obtained his PhD in Organic Chemistry under Prof Dervilla Donnelly in 1987. He has also been a President of the Institute from 2007-9. He has published a number of papers and is holder of 6 patents.

Donal with Prof Dervella Donnelly on the awards night UCD

Longer term we would hope to make this a prestigious annual event with support from the Irish pharmachemical industry to recognise the contribution chemists in Ireland make to Ireland and our economy. The institute is delighted with the offer from Henkel to sponsor the Industrial Chemistry Award again in 2016. We will be announcing this news and inviting nominations of chemists and groups early in the New Year.

President Margaret Franklin, Mr Hugh Finlay, Dr Patricia Cullen at the Awards

Annual Lecture Series Award (Eva Philbin)

Professor of Bernal Chain of Crystal Engineering at UL's SSPC

This year's winner of the Annual Lecture Series was Professor Michael Zaworotko. President Margaret Franklin presented him with the plaque at UCD at our Awards Ceremony. The Professor has given his first lecture at UL, and the second at UCD on the Awards night. The third will follow early in the New Year at NUI Galway facilitated by Dr Niall Geraghty on Thursday, February 4th at 4.00 p.m. in the Dillon Lecture Theatre, hosted by An Cumann Ceimice.

Professor Zaworotko was appointed to the Bernal Chair of Crystal Engineering at the University of Limerick in 2013. Originally from Wales. Professor Zaworotko comes to UL from the University of South Florida and is among of the top 20 research chemists in the world. Previously Prof Zaworotko was Dean of Arts and Science at the University of Winnipeg, Professor of Chemistry and Department Chair at St Mary's and has held research positions at the University of Victoria, University of Alabama and Imperial College, London.

This appointment is the first under the Science Foundation Ireland (SFI) Research Professorship Programme which aims to attract iconic research talent to Ireland. The programme includes funding of €6 million to support a body of research critical to our pharmaceutical industry and enhancing Ireland's reputation as a centre for excellence. Professor Zaworokto is in demand as a consultant to several major pharmaceutical companies many of whom have supported his research. He is a Member of UTEK Corporation's Scientific Advisory Council, Member of Thar Pharmaceuticals Scientific Advisory Board and a Member of Alkermes Scientific Advisory Board. He holds 6 patents and a further 10 are pending. Professor Zaworotko is a prolific publisher of high quality peer reviewed journals. His h-index is 68. He has published over 300 original research articles and these have been cited over 21,000 times. He is among the top 20 most cited chemists in the ISI database, was Elected Fellow of the American Association for the Advancement of Science in 2011 and is a reviewer for Science, Nature, JACS and Angewandte Chemie.

President Margaret Franklin presents Prof Zaworotko with his Award plaque at UCD

Professor Zarorotka's lecture was lively and interesting and particularly relevant at this time with the Climate Change Summit in Paris and The National Sustainability Summit in Dublin. He covered the chemistry, structure, synthesis of these new materials and their ability of absorb CO_2 from the atmosphere or emission sources and the potential to recover useful alcohols by bioprocessing of the captured carbon load. He also covered the issues of water vapour absorption by these materials. He addressed the use of these structured materials for the delivery of pharmaceutical drums to patients. His lecture was titled:-

"Crystal Engineering of Task-Specific Materials: Addressing Pharmaceutical Materials"

That composition and structure profoundly impact the properties of crystalline solids has provided impetus for exponential growth in the field of *crystal engineering* over the past 20 years. This lecture will address how crystal engineering has evolved from structure design (form) to control over bulk properties (function). Strategies for the generation of **m*ulticomponent pharmaceutical materials, MPMs***, which can serve as drug substances, will be highlighted by three case studies, including one that addresses brain bioavailability of lithium.

Part of the new Bernal Building with its distinct geometric pattern.

EuCheMS European Chemical Sciences

Integrating CO2 in the Value Chain: the Role of Chemistry

This workshop, which took place on the 3 March 2015 at the European Economic and Social Committee in Brussels, explored the ecological and economic possibilities of integrating CO2 in the value chain.

Chaired by MEP Julie Girling and opened by Mindaugas Maciulevičius, from the European Economic and Social Committee, it counted with a presentation from EuCheMS President, Prof. David Cole Hamilton.

This event was an opportunity for participants to learn from the ESCA winners of 2014, Prof. Dr. Walter Leitner and Prof. Dr. Jürgen Klankermayer, who not only provided evidence on the rich possibilities of CO2 conversion but also transmitted a clear message on sustainability: “If you want to go fast, go alone. If you want to go far, go together." In addition the European Commission´s activities on these topics was delivered by José Lorenzo Valles from DG R&I.

The Workshop was co-organised with the European Parliament Intergroup on Climate Change, Biodiversity and Sustainable Development and brought together European policy-makers, the chemical sector, the academic world and civil society in order to discuss the opportunities of turning waste into fuels, basic chemicals, polymers, and even fine chemicals and pharmaceuticals.

- Final Report
- Agenda
- Presentation from Prof. David Cole-Hamilton (*EuCheMS President*)
- Presentation from José Lorenzo Valles (*Head of Unit, DG R&I, European Commission*)
- Presentation from Prof. Walter Leitner and Prof. Jurgen Klankermayer (*Institute for Chemical Technology and Macromolecular Chemistry, 2014 ESCA Winners*)

Contact Information **EuCheMS Office** Rue du Trône 62 1050, Brussels, Belgium Email: secretariat @euchems.eu

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The National Sustainability Summit took place on the 3rd November in the Aviva Stadium, Dublin.

http://www.sustainabilitysummit.ie

The event took place at a pivotal time – in the run-up to UN climate change summit in Paris this December. It's expected this climate conference will conclude a groundbreaking international agreement on emissions which, for the first time, will cover all nations of the world.

Given such a legally binding deal could be implemented as early as 2020, the National Sustainability Summit provides the ideal platform to discuss and debate what this will mean for Irish business, regulatory bodies and government.

It's clear that sustainability is no longer an optional add-on for business. In a commercial world of 5 and 10 year plans, adapting to climate change is now an imperative. Companies need to know that their supply chain is both secure AND sustainable. Shareholders and customers are increasingly demanding to know where their products are coming from. Market advantage will flow to those companies which can prove it.

EU emissions reduction targets are already influencing business planning in all sectors of the Irish economy, construction, manufacturing, IT, food, aviation, energy, water, retail, hospitality, logistics and supply chain. Innovations and entrepreneurial skills have already begun to create a more sustainable Ireland, and this will be reflected in the National Sustainability Summit.

The purpose of the National Sustainability Summit is to create a forum where business leaders, innovators, regulators and government can examine both the commercial opportunities in the emerging green economy as well as the challenges in achieving sustainability goals. Our aim is to create an annual event which will chart how industry is progressing and how Ireland can secure competitive advantage.

This is not just a social call-to-action but a wake-up call for Irish business – something which will only become more apparent in the event of an international deal in Paris. A collaborative approach to sustainability is called for. Key stakeholders need to work together to achieve very challenging targets, including those already set by the European Union. There will be significant penalties for government and losses for business in the event of failure.

The speaker line up was drawn from senior management from the largest and most influential Irish and international companies who have delivered quantifiable eco results. Speakers come from areas such as pharmaceutical, food, aviation, retail, hospitality, food, construction, manufacturing, IT, logistics, supply chain and energy sectors and academia. It will deliver compelling case studies that will help you create a sustainable business of your own or adapt your current business model.

Above Text provided by Colin Murphy, MD National Sustainability Summit

Some 1000 delegates attended on the day with 80 speakers on the main stage and four other parallel sessions with 38 exhibitors. The topics were varied and wide ranging. Paul Cunningham Editor, This Week In Politics, RTE was MC and introduced the French Ambassador, who with elegance and conviction gave the opening speech and explained the overriding need for sustainability and France's role in ensuring the COP21 Climate Change Summit took in Paris this December.

Our National Sustainability Summit took place shortly before the historic Conference of Parties COP21 or if you prefer 2015 Paris Climate Conference. This was a great leadership achievement for the French Presidency. With 196 countries agreeing to limit CO_2 emissions to a legally binding and universal agreement on climate change, with the aim of keeping global warming well below 2°C and aiming for 1.5°C above pre-industrial levels by 2100.

The agreement calls for developed countries to take the lead in reducing greenhouse gas emissions and developing countries are "encouraged" to reduce emissions. A tracking system has been put in place to track and report progress on emissions reductions. But the agreement still only sets targets, not mandates. The agreement makes clear that rich countries are responsible to provide funding for adaptation, loss and damages to poor and vulnerable nations. A figure $100 billion per year has been suggested. But the devil is in the detail, there is cautious optimism of success but a lot of more work lies ahead.

Below two companies at the National Sustainability Summit have kindly provided articles for this issue of ICN and a number of others have committed to provide papers during 2016. BASF have provided a copy of their CEO's Kurt Bock statement "A Call to Climate Action" from The United Nations Global Compact-Accenture CEO Study along with a link to the full document. GSK Dungarvan have provided a case study by Adrian McCarthy, Site Energy Champion outlining their efforts and plans to achieve carbon neutrality.

Following closer to home after the Paris Conference our own Government have published a White Paper on Energy titled 'Ireland's Transition to a Low Carbon Energy Future 2015-2030'. The launch took place at The Mansion House, Dublin on 16 December 2015. The paper takes into account European and International climate change objectives and agreements, as well as Irish social, economic and employment priorities.

Minister Alex White T.D. *Minister for Communications, Energy and Natural Resources* indicated in his forward to the paper that "this White Paper sets out a vision for transforming Ireland's fossil fuel-based energy sector into a clean, low carbon system by 2050.

Taoiseach Enda Kenny T.D. wrote "Ireland's access to secure, clean and affordable energy is essential to keep our recovery going. This White Paper on energy is an essential part of the Government's overall recovery plan that charts the future development of the Irish economy and energy sector."

The White paper is some 126 pages with 9 chapters plus annexes. Frank McDonald in the Irish Times Thu, Dec 17, 2015 commented ……. "provides no clear road map" and ….. "One would expect a White Paper to be full of clarity and firmness of purpose, unlike a Green Paper, which discusses issues and puts forward a series of options to address them. In effect, what Minister for Energy Alex White has produced is a Green Paper".

Given that the paper has just been published we can expect much further commentary on our energy policy and informed comment and articles are invited for publication in ICN.

The United Nations Global Compact-Accenture CEO Study

Special Edition: A Call to Climate Action

Kurt Bock
CEO, BASF

"Limiting [global] warming to 2C involves substantial technological, economic and institutional challenges".

This quote from the Fifth Assessment Report of the Intergovernmental Panel on Climate Change points out the scale of progress demanded from our society to address climate change. As a business, we will play an important role to find the answers to this challenge and related issues, such as the availability of water and raw materials.

The challenge will be to develop solutions, which enable the growing world population to attain a high standard of living while using resources most efficiently. With an adequate regulatory framework in place, and guided by an agenda for sustainable development as laid out by the UN, the economy will be able to act as a "broker" and facilitate the best possible distribution of limited resources.

At the same time, substantial technological innovations are required to enable every human being to lead a "good life" without overusing the resources. These technological innovations are mainly driven by enterprises: in order to be able to assert themselves in competition, they invest in research and development and introduce new technologies into the market.

Both the incremental further development of existing products as well as game-changer innovations are key contributions to this end. For example, BASF has continuously been improving and developing insulating materials that help in significantly lowering the energy demand of houses. At the same time, we have been innovating in order to reduce the fossil fuel demand and associated carbon emissions in transportation radically, starting with lighter materials. Realizing that electric cars with an increased battery performance will allow for larger cruising ranges and thus "change the game", we began to work intensively on materials for more efficient batteries.

Just as we drive product innovations, we also further develop our own production processes. Since 1990, we have reduced the greenhouse gas intensity of our production by 74%. In order to continue on this path, we just set ourselves the new corporate target to implement energy efficiency management systems at all our production sites by 2020. However, we have to realize that the technological improvement of existing processes has physical limits. That is why we are also looking for disruptive innovations for our production processes. In this respect, I am convinced that cross-sectoral co-operations play an important role. Together with ThyssenKrupp and Linde, for example, we are working on a new process for the production of hydrogen (a basic material for the chemical industry) that is much more carbon efficient than the conventional process and at the same time delivers metallurgical carbon for use in the steel industry. Similarly, we have teamed up with other chemical companies in a Low Carbon Technology Partnership initiative. Jointly we are analysing the potential of various game changing innovations for carbon emission reduction in chemical production.

The potential that enterprises have for driving technological innovations for a low-carbon future can also be seen in our R&D expenditure. BASF spends more than 50% of its annual R&D budget of 1.9 billion euros on solutions in the area of climate protection and energy and resource efficiency.

And this is where we come full circle – back to the regulatory framework mentioned at the beginning. The investments in R&D are always long term oriented with the ultimate target to improve processes or go for new technologies. At COP-21, politicians have the chance to set up a long-term, reliable emission reduction framework, enabled by low-carbon technologies. The national contributions to this framework need to be globally harmonized. This is key as the economy will only be able to fulfill its role as a "broker" for the best possible global distribution of the limited carbon emission budget, if we have comparable levels of greenhouse gas reduction efficiency globally rather than regionally diverging concepts and measures.

I am convinced that with such an agreement in place, investments into incremental technological improvements as well as into R&D for breakthrough innovations would further increase. Creative minds in business all over the world would have a clear picture of the low-carbon future they are innovating for, finding answers to the substantial challenges we are facing.

You can read or download the full pdf document here including Kurt Bock's letter within it.

https://www.accenture.com/t20151111T221550__w__/us-en/_acnmedia/Accenture/Conversion-Assets/DotCom/Documents/Global/PDF/Strategy_7/Accenture-UNGC-CEO-Study-A-Call-to-Climate-Action.pdf#zoom=50

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New approaches and technology have been introduced in recent years that have created significant organisational and process improvements. The aim of the conference is to showcase such innovative approaches and to disseminate the cutting edge research that underpins them. The conference will be of interest to senior management, established practicing engineers and researchers together with those that are much earlier in their careers.

Delegates have registered from leading food, pharmaceutical, medical, chemical, electronics and engineering manufacturing sectors. Manufacturing on this island of Ireland has some of the best people, products, brands and innovation. We deserve nothing less than the best business environment to chart a new economic course to growth. But government needs to set the climate and conditions to allow this to happen. Manufacturers small and large from across the country will gather to challenge political decision makers to deliver a business environment which manufacturing deserves. Delegates attending the conference will:

– gain industry insights to help their business plan ahead

– share good practice and learn from each other's experience

– connected with senior business leaders to find new business opportunities

– meet with key technology providers in the dedicated exhibition area

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Energy Kaizen Event, GSK Dungarvan.

Adrian McCarthy

Introduction

GSK Dungarvan recently presented at the National Sustainability Summit on how it has developed a 4year plan to reduce CO2 emissions by 66% by the end of 2017. This was completed through an Energy Kaizen event which was held onsite in December 2013.

Background

GSK Ireland operations make an important contribution to our global business. They employ 1,500 people in four locations throughout the country. There are manufacturing sites in Cork, Dungarvan and Sligo producing high quality products and distribute them through a global network. The Pharmaceutical and Consumer Healthcare business provide a huge range of medicines, vaccines and consumer products to Irish people.

GSK Dungarvan produces a variety of well-known 'over-the-counter' pharmacy and oral care products including, Panadol, Polygrip, and Corega. In fact 7.5 billion Panadol tablets are produced in Dungarvan each year – that's 150 Panadol tablets a second! – and are exported to over 70 countries worldwide. Four tubes of Polygrip and 80 Polident/Corega denture cleanser tablets are made in Dungarvan every second.

Energy Kaizen Event

GSK globally have ambitious goals for carbon, water and waste. Since 2010 the overall carbon footprint has reduced by 18% with a targeted reduction of 25% by 2020, water has reduced by 20% and there is a target of zero operational waste to landfill by 2020.

At Dungarvan the site energy kaizen event was held in conjunction with GSK Central Utilities team, a host of external vendors, site leadership, production operators, quality teams and site engineering. It was a 5 day structured event which is designed to identify energy saving opportunities, quantify plan and to identify resource and support. The results not only identify capital intensive projects but also simple actions, quick wins. The GSK Central Utilities team have conducted >80 of these events globally with average saving opportunities of 20-30%. They can be used as an initiative program or as a momentum regain for mature programs.

The key to a successful kaizen event is preparation. Site energy maps and detailed system information on display in the meeting room allows key areas get maximum attention.

Day 1

The first day consist of introductions and description of the agenda. Familiarisation of the site to the operations and utilities are completed. 'Walk the Walls' process is completed in teams where system information is analysed through charts which are on display in the meeting room. This will range from general electrical supply data in daily and monthly format, HVAC and BMS live system information, chilled water loop info and compressed air data etc...

Historical site cost, usage and trends for SEU's (significant energy users) can be reviewed. Team members will highlight and comment on areas of interest from their expertise and experience for further investigation. These will allow development of areas of opportunity.

Day 2

The second day of the event is where the teams go out onsite to GEMBA areas and processes that have been identified the previous day. This gives the opportunity to talk with those closest to the process in question for real life issues and opportunities. Dependant on the site size and the team size there will be a number of

groups formed with a cross-functionality in each. Teams are given fixed durations to GEMBA their area and a time is allowed for presentation to the group of the findings. This may offer further ideas and identification areas of improvement or implementation of new technologies.

Day 3

The third day is split into two; the first session is where new technologies or renewable energy could be utilised onsite. Prep work on this session can prove useful for experts to complete desktop studies. The findings of the studies can be discussed with the experts and the site engineering teams for a best fit and compatibility of the technologies. Main areas of focus for this are usually renewable technology or HVAC operations. With renewable technologies, some research into available grants or schemes will be beneficial in the financial review of the identified options.

Later in the day there will be planned breakout groups focussing on standard work practices. Areas of operations and maintenance are reviewed in through a process map and discussed with those working with the process in hand.

Day 4

The size of the team is reduced for the fourth day as this is when the identified projects and recommendations are quantified for cost, savings, resources and benefits. Project lists are developed, estimated capital investment and required resources are planned.

Once this has been compiled the final out-brief can be prepared.

Day 5

This is when the findings are shared with the site leadership team for further analysis and approval. Members of the team will present various sections in the out-brief presentation.

This will outline the costs, benefits and opportunities for the site over the four year plan.

Benefits found in GSK Dungarvan

The successful kaizen event in Dungarvan identified 53 projects and 173 quick wins. This are planned to be completed over a 4 year period from the start of 2014 to the end of 2017. There has been a significant amount of projects already implemented in the first two years ranging from HVAC enthalpy control and air change reductions to LED lighting upgrades, chilled water and steam system optimisation projects.

The range of projects will continue over the next two years with work having commenced on the largest of these. A woodchip boiler is under construction and planned for completion in Q4 2016. This will provide steam to both of the sites in Dungarvan and will replace 5 existing oil burners. This project alone will deliver 33% of the CO2 emissions (5,500 tonne/CO2).

Artistic Impression of the Woodchip Boiler in Dungarvan which is currently under construction.

Other iconic renewable projects are in progress with full planning permission granted recently for a 2.3MW wind turbine which will reduce the CO2 emissions by a further 15%, and also desktop surveys of solar PV arrays being completed.

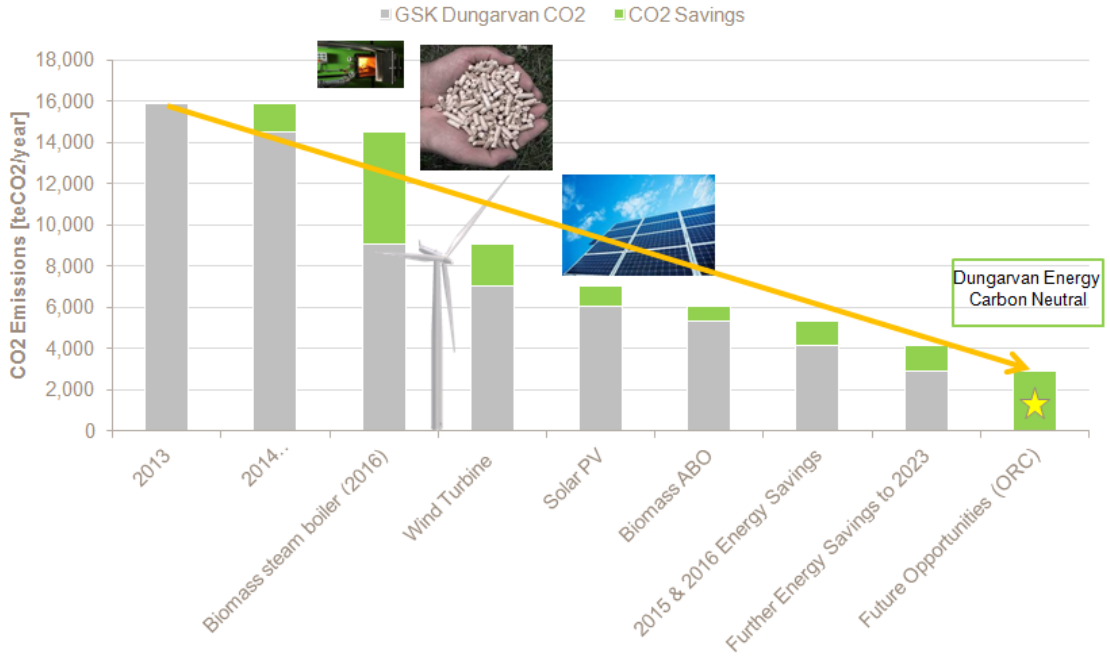
GSK Dungarvan is currently on target to reduce CO2 emissions by 66% from 2013 levels.

Conclusion

A site energy kaizen is a proven method of developing plans and projects for site emission reductions. The cross functionality allows innovative thinking and problem solving with support from vendors, specialists, local experts and site leadership.

The kaizen event can be easily adaptable and replicated for different sites with differing operations and outputs to produce viable energy reduction plans.

GSK Dungarvan are planning the next energy kaizen for 2017 to further identify opportunities for the next 4 years and for the site to get closer to the goal of carbon neutrality.



Dungarvan's vision for future carbon neutrality

The Pharma Industry Awards presentations took place on October 22th at the Ballsbridge Hotel, Dublin. The awards are an annual event and will be held again in 2016. There were a total of 16 awards presented to the leaders and organizations from Ireland's pharma industry. The categories are listed in the table below.

Award Categories 2015
Pharma Industry Company of the Year 2015
Pharma Leader of the Year 2015
Pharma Company of the Year 2015
Biopharma Company of the Year 2015
Biotech Company of the Year 2015
Pharma Research Centre of the Year 2015
Pharma Contract Services Company of the Year 2015
Pharma Start-up Company of the Year 2015
Innovation of the Year 2015
Partnership Alliance of the Year 2015
Health & Safety Award 2015
Sustainability Initiative of the Year 2015
Operational Excellence Award 2015
Research and Development Achievement Award 2015
Pharma Education & Training Award 2015
Supply Chain Achievement Award 2015

Reporting on the event in the Sunday Business Post, November 8 2015 Graham Clifford interviewed some of the Awards winners. His full article can be viewed on line here:- http://www.businesspost.ie/awards-reflect-irelands-role-as-centre-of-pharma-innovation and below follows a condensed version.

MSD won five of the prestigious awards including Pharma Industry Company of the Year, Pharma Company of the Year, Biopharma Company of the Year, and Sustainability Initiative of the Year, and their online Health News and information Service for healthcare professionals, Univadis, won the Innovation of the Year award.

Ger Carmody, Site Lead at MSD in Ballydine, Co Tipperary, explained why these award wins are important to the company. “These awards are a significant benchmark and a valued achievement for MSD. Our success this year speaks to our ongoing commitment to Ireland, to our innovative pipeline; and to our future growth and development plans,”

The Pharma Leader of the Year Award, which recognises the significant contribution of individuals in the growth and sustainability of the Irish Pharmaceutical sector, went to Dr. Reg Shaw from the National Institute for Bioprocessing Research and Training (NIBRT). In his lifetime’s work with numerous bodies, Dr Shaw has played a pivotal role in developing the sector on our shores.

MSD

Joe Haugh, Deputy CEO, Zenith Technologies presents the Pharma Industry Company of the Year award to the MSD team.

Dr Reg Shaw

David Phelan, Life Science Practice Leader, Accreate, presents the Pharma Leader of the Year award to Dr.Reg Shaw.

Other winners include Genzyme, a Sanofi Company, which was named Biotech Company of the year. It also won the Health and Safety Award for its ‘Pioneering Resilience’ project. With its Irish base in Waterford, Genzyme currently employs over 600 staff and has been in Ireland for 14 years.

Ruth Beadle, the Site Head in Waterford, said she and the staff at Genzyme were “thrilled with these awards from our peers at a national level and added “they are an endorsement of what our great team do at work right through the year. It’s particularly satisfying to be named Biotech Company of the Year as that’s a sector where Ireland has attracted several of the world’s best organisations. The award for our Resilience Programme is also very welcome as it’s something innovative that a lot of people at the site put a great deal of work into creating and delivering.”

BioKinetic Europe won the Pharma Contract Services Company of the Year; The Biopharmaceutical Industry Technical Group were named Partnership Alliance of the Year.

Pfizer Ireland Pharmaceuticals Grange Castle received the Operational Excellence Award. Grange Castle is Pfizer’s largest single investment in Ireland, a €1.8 billion biotechnology facility located on a 90-acre site in South County Dublin, with buildings and facilities extending to more than one million square feet.

Waterford-based Q1 Scientific was named Start-Up Company of the Year with its CEO Louise Grubb describing the award as “hugely significant” and “a great aid in helping us to attract more potential customers”.

Synthesis and Solid State Pharmaceutical Centre (SSPC) won the Research and Development Achievement award. Jon O’Halloran, General Manager said its award would help bring the work of the collaborative group to a wider audience.

Pharma Research Centre of the Year

Synthesis and Solid State Pharmaceutical Centre

Matt Moran, Director, PharmaChemical Ireland and Awards Judging Co-Ordinator, presents the Pharma Research Centre of the Year award to the Synthesis and Solid State Pharmaceutical Centre team.

Innovation of the Year

Univadis - MSD

Dr. Niall Hoey, Chief Executive, Portalis, presents the Innovation of the Year award to Ger Carmody, MSD for Univadis.

Other winners included the National Institute for bioprocessing research and training (NIBRT) which won the Pharma Education and Training Award. A global centre of excellence for training and research in bioprocessing NIBRT is located in a world class facility in Dublin beside UCD and closely replicate a modern bioprocessing plant with state of the art equipment. NIBRT is based on an innovative collaboration between University College Dublin, Trinity College Dublin, Dublin City University and the Institute of Technology in Sligo.

The Supply Chain Achievement Award went to the TCP Group which dispenses and distributes specialised medication to patients with rare conditions in their home.

More details and photographs about the Pharma Industry Awards 2015 are available at the web page:-

www.pharmaawards.ie / Event Strategies Ltd. www.eventstrategies.ie

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ISTA Senior Science Quiz Final 2015 - Sponsored by the institute of Chemistry of Ireland

The National Finals of the annual ISTA Senior Science Quiz took place in Trinity College on Saturday 21st November. The Edmund Burke theatre was filled to capacity with 48 teams of Leaving Certificate science students from all around Ireland along with their teachers who are members of the Irish Science Teachers' Association – the professional association for teachers of science subjects in the Republic of Ireland. Over 1000 students took part at a Regional level during Science Week Ireland and the winners were invited to the **PharmaChemical Ireland** sponsored National Final.

In recent years ISTA has linked up with a charity for the final and this year it was **'The Caroline Foundation'** in aid of Cancer Clinical Research Trust. The purpose of the Foundation is to support the work of Professor John Crown. Like ISTA it is a voluntary organisation and all donations go directly to the research.

A special thanks to **Dr Conor O'Brien**, current President of ISTA, **Dr Aoibhínn Ní Shuilleabhain** who acted as quizmaster, **PharmaChemical Ireland** sponsor, **Trinity College** who provided the venue, Dublin Branch of ISTA who organised the Final and last but not least the students, teachers and parents who attended.

Congratulations and well done to ALL who participated.

1st **Presentation Brothers College**, The Mardyke, **Cork**. Teacher: ***Ms Claire Lynch***

2nd **Christian Brothers College**, **Cork**. Teacher: ***Ms Jane O'Connell***

3rd **Summerhill College**, **Sligo**. Teacher: ***Mr John McGetrick***

4th **Calasanctius College**, Oranmore, **Galway**. Teacher: ***Ms Maura Conneally***

5th **St Andrew's College**, Booterstown, **Dublin**. Teacher: ***Ms Hilary Rimbi***

1st: Presentation Brothers College, The Mardyke, Cork
Team: John Fehilly, Alex O'Carroll, Jimmy Costello
Teacher: Ms Claire Lynch

2nd Christian Brothers College, Cork
Team: Niall McCarthy, Colm Power, Rory Doyle
Teacher: Ms Jane O'Connell
Quiz Coordinator: Mary Mullaghy

The **Institute of Chemistry of Ireland** gave **€200** towards spot prizes. At each of the 12 Regional Rounds a

€15 book token was presented to a Leaving Certificate student and a slide advertising the ICI Chemistry Schools Newsletter Competition was made available to over 1000 students and their teachers. At the National Final in Trinity College a €20 book token was used as a spot prize and again the ICI newsletter competition details were advertised to the audience. Next year we hope to expand the quiz to have 13 venues to include Wexford. Venues this year included: **Athlone IT, Carlow IT, IT Tralee, GMIT, LYIT, Limerick IT, NUI Maynooth, Sligo IT, Trinity College, UCC, Waterford IT and Loreto College, Monaghan.**

Schools Chemistry Newsletter Competition Results 2014/15

Topic: *'Crystallography'*

First Place: Katie Ward, St Andrews College, Booterstown, Co Dublin.
Joint Runners-Up:
Fionn O'Leary, CBS Secondary School, Mitchelstown, Co. Cork.
Alice Drayne, St Andrew's College, Booterstown, Co Dublin.

Joint Highly Commended:
Bronagh Harkin, Megan McGlone, Katie McGurk and Orla Mallon, St Mary's Grammar School, Derry.
Amy Burgess, St Andrews College, Booterstown, Co Dublin.
Emily Fenton, CBS Secondary School, Mitchelstown, Co. Cork.
Oscar Maltby, St Andrew's College, Booterstown, Co Dublin.
Richard Neville St Andrew's College, Booterstown, Co Dublin.

Ms Hilary Rimbi (Chemistry teacher), (Principal of St Andrew's College), Richard Neville, Oscar Maltby, Amy Burgess, Alice Drayne & Katie Ward.

Fionn being awarded his certificate and cheque by Mary Mullaghy on behalf of the Institute of Chemistry of Ireland at the ChemEd Conference in UCC.

Fionn from CBS Secondary School, Mitchelstown with his parents Mary & Michael O'Leary

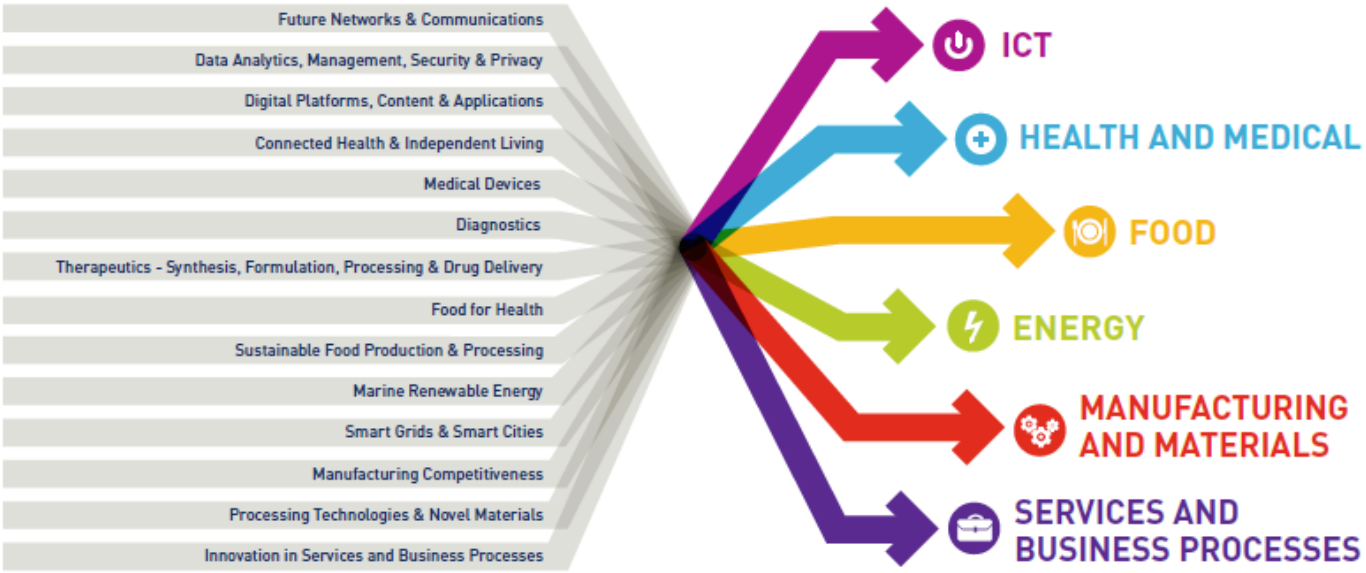
Vision

Ireland - a Global Innovation Leader driving a strong sustainable economy and a better society

The Government launched its strategy for Research and Development, Science and Technology at Innovation 2020 at the Convention Centre, Dublin on Tuesday 8th December. The Taoiseach T.D., Enda Kenny, Minister for Jobs, Enterprise and Innovation, Richard Bruton T.D., and Minister for Skills, Research and Innovation, Damien English T.D. spoke at the launch event. This reflects the Government's vision for Ireland becoming a Global Innovation Leader. The policy document along with a shorter booklet and leaflet are available to read and download at:-

https://www.djei.ie/en/Publications/Innovation-2020.html

The strategy covers six main sectors and their sub-sectors nicely illustrated in their document graphic:-



An important goal for the Strategy is to increase total investment in R&D in Ireland, by Government and enterprise, to 2.5% of GNP versus 1.81% GNP in 2013. It is estimated that, this would mean investing €5 billion per year in R&D by the private and public sectors by 2020. This will represent almost doubling current levels of investment o €2.9 billion in 2014.

Some of the objectives to be delivered by the programme strategy are:

- the number of research personnel in enterprise will be increased by 60% to 40,000
- research masters and PhD enrolments will be increased by 30% to 2,250;
- private investment of R&D performed in the public research system will be doubled
- 40% increase in the share of PhD researchers transferring from SFI research teams to industry
- Ireland's participation in International Research Organizations will be expanded – we will apply for full membership of ELIXIR, and we will explore membership options for CERN and ESO
- the network of Centres will be further developed, building critical mass and addressing enterprise needs;
- a successor to the Programme for Research in Third Level Institutions will be rolled out to include investment in the creation of new, and the maintenance and upgrading of existing, facilities and equipment and ensure full utilization;
- €1.25 billion funding under the EU Framework Programme Horizon 2020 will be drawn down;
- a new Programme of Funding for Frontier Research will be introduced, providing resilience and responsiveness to meet new challenges or opportunities as they emerge;
- challenge-centric research will be initiated to stimulate solutions-driven collaborations bringing together enterprise, higher education institutions and public sector to identify and address national challenges
- horizon-scanning – in the coming years a formal horizon-scanning exercise will be undertaken to identify areas of strategic commercial opportunity for Irish-based enterprises. This process will feed into the next research prioritization exercise in 2018
- international benchmarking – a series of structures will be put in place to benchmark Ireland's performance in these areas against other comparable economies, and develop steps to improve our comparative performance

Playing a critical role in delivery Science Foundation Ireland (SFI) will undertake to explore and develop the following new initiatives during 2016:

Challenge-based funding M**echanisms.**

SFI Research Centres

SFI Investigators Programme

SFI President of Ireland Future Research Leaders Programme

PhD funding programme

http://www.sfi.ie/news-resources/press-releases/government-publishes-ambitious-innovation-strategy-innovation-2020-excellence-talent-impact.html

http://www.sfi.ie/news-resources/press-releases/science-foundation-ireland-welcomes-new-government-science-strategy-innovation-2020.html

The Institute of Chemistry of Ireland welcomed the Government's Strategy as indicated in Innovation 2020 in a statement:-

The Institute of Chemistry of Ireland *"welcomes **Innovation 2020**, the new government strategy for research and development in the areas of science and technology. The Institute particularly welcomes the government's commitment to increase total investment in R&D in Ireland to 2.5% of GNP which would result in over €5 billion being invested per year by 2020. The clear investment in human capital,*

infrastructure and Frontiers research represented by the significant increase in postgraduate and post-doctoral research funding and a successor to the programme for research in third level institutions, will allow Ireland to continue to compete for funding at an international level. While this new strategy is good news for the research community, it also good news for the country as a whole since the outputs from this research investment will translate into innovations across all aspects of Irish society including health, technology, environment as well as the economy through direct foreign investment in the commercial sector and increased employment'

Taoiseach Enda Kenny T.D.

Minister Rechard Bruton T.D.

Minister Damien English T.D.

In addition to the Innovation 2020 launch **Damian English TD** also launched an updated directory of research supports **"Directory of Innovation Supports, Research Centres and Technology Centres"** and can be downloaded:-

https://www.djei.ie/en/Publications/Directory-of-Innovation-Supports-Research-Centres-and-Technology-Centres-2016.html

Directory of Innovation Supports, Research Centres and Technology Centres 2016

Knowledge Development Box and 6.25% Tax Rate

"Ireland will introduce the first Organisation for Economic Co-operation and Development-compliant Knowledge Development Box (KDB) in January 2016. The KDB offers a 6.25% tax rate on income arising from eligible intellectual property assets, and will require that a company evidence the link between RDI activity/expenditure in Ireland, and the income derived from the resulting intellectual property.

The Finance Act will set out further details relating to eligibility and Revenue guidelines will be issued in due course."

Some 2000 delegates attended the **Innovation 2020** event. Some 14 information hubs were set out and most Universities and Institutes of technology were present to promote their research, technology centres and commercialization efforts. Knowledge Transfer Ireland, the Irish Research Council, Enterprise Ireland Science Foundation Ireland, Industrial Development Authority and Horizon 2020 amongst others were present to promote their activities.

Paul Cunningham, RTE was MC and did the introductions. He introduced Ms Julie Sinnamon CEO Enterprise Ireland who talked about introduced the Big Ideas and introduced the Big Ideas presentation Icon. Paul then introduced each of 12 Start Up companies under an Enterprise Ireland scheme called "BIG IDEAS

Investor-Ready Start-Ups. He invited a representative from each company to give a 2 minute summary of their company on the centre stage and they had an opportunity to talk with investors afterwards.

This was followed by a Speakers Session where 3 senior executive speakers Bill Kearney, IBM, Julie Spillane, Accenture and Frank Wilson, Ceramicx spoke about their experiences in running technology companies. This was followed by a discussion and question and answer session.

Compiled by Patrick Hobbs MSc FICI CChem CSci MRSC
Editor Irish Chemical News
Institute of Chemistry of Ireland

Minister English announces UL's Matthew Gleeson as Winner of SFI Research Image of the Year Competition

KILKENNY - 2nd November 2015 – Minister for Skills, Research and Innovation Damien English TD, today announced **Matthew Gleeson, postgraduate researcher at the University of Limerick, as the winner of Science Foundation Ireland's Research Image of the Year** competition for his picture 'Lightning Wires' at the SFI Science Summit in Kilkenny. The winning image was selected from over 40 submissions and will appear on the front of the 2015 SFI Annual Report.

The SFI Research Image competition celebrates images captured by SFI-funded researchers during the course of their research. Matthew is a researcher at the University of Limerick. His winning entry in the competition is of hydrothermally synthesized sodium niobate micro-wires. The image was taken using differential interference contrast on a light microscope, the image being about one hundred microns across. The sodium niobate micro-wires were grown using a method similar to pressure cooking called hydrothermal synthesis. The image shows the largest of the wires which have widths fractions the diameter of a human hair. This optical image shows Sodium Niobate micro/nano wires, grown using a method similar to pressure cooking, called hydrothermal synthesis. The image shows the largest of the wires have widths fractions of the diameter of a human hair. The bright white color of the wires is due to the wires properties, refractive index. The contrast is due to the difference in refractive index between the wires and supporting glass slide. The wires are grown for novel ICT technologies, such as using light to transfer information in microchips and optical information processing. The image was taken as part of a PhD project under the supervision of Dr. Ning Liu and Dr. Christophe Silien at the University of Limerick.

Lightning Wires

Speaking at the SFI Science Summit, which was attended by 300 researchers, **Minister English** said: "Matthew's image 'Lightning Wires' demonstrates that science has the capacity to surprise. His striking mage allows us to see what is not visible to the naked eye and it really captures the viewer's attention. I congratulate him on this success." Congratulating Matthew, **Professor Mark Ferguson, Director General of SFI and Chief Scientific Adviser to the Government of Ireland**, added: "The SFI Research Image competition offers researchers the opportunity to show the rest of the country what their research looks like and to showcase their work. This image shows the creation of very small artificial wires which can be used for novel applications in future microchips and computers. I congratulate Matthew on his win and wish him continued success with his research at the University of Limerick."

www.sfi.ie

240 jobs at risk in Roche pharmaceutical facility Co. Clare

Posted on 13 November 2015. Tags: Jobs, Pharmaceuticals, Roche

The Roche facility in Clarecastle, Ennis, Co. Clare

Pharmaceuticals company Roche is pulling out of four of its facilities worlwide, including its site in Clare, with 240 jobs set to go unless a replacement firm is found.

The company's Clarecastle site has 240 employees who are now at risk of losing their jobs, with the company looking for a buyer to take on the facility and staff.

The giant pharmaceutical operator is spending around $1.6bn on restructuring its business with parent company, Roche Holding, withdrawing from facilities in Ireland, Spain, Italy and the US.

There will be 1,200 job losses worldwide, with plans to withdraw from the sites to be completed by 2021.

Roche has been in operation in Ennis for over 40 years and the news appears to have come completely out of the blue.

Roche's profits, at €9.45m last year, were down €2m on 2013, with revenues falling 20 percent.

The company's portfolio is shifting toward biologics, with a new generation of "specialised medicines based on small molecules" requiring a whole new operation.

This shift has resulted in Roche Holding investing in a new Swiss facility, while major investment has gone into its biologics manufacturing capacity in the past two years.

MD Gerry Cahill said the decision was taken as a result of a drop in requirement for the product the plant manufactures.

He said they would continue to manufacture drugs but in much smaller volumes and therefore a smaller site would be needed.

Mr Cahill said failure to find a buyer would result in the first redundancies being offered next year.

Posted in company news, PharmaceuticalComments Off on 240 jobs at risk in Roche pharmaceutical facility Co. Clare

Almac buys out Athlone's Arran Chemicals

Posted on04 November 2015. Tags: acquisition, Almac, Armagh, Arran Chemicals, Athlone, Chemical, pharma

Almac's headquarters are in Craigavon, Co. Armagh and it has operations in the US, Singapore and Tokyo

Pharmaceutical giant, Almac has bought out Arran Chemicals, a privately-owned company based in Athlone.

The Northern Ireland company currently employs 57 people, and the move increases Almac's global workforce to more than 4,000.

Almac says it will invest in the Roscommon plant as the two companies have been working together on projects for the past five years.

Arran Chemicals specialises in making pharmaceuticals, flavoured and fragranced products for the personal care market and other chemical and industrial products.

Dr Stephen Barr, managing director at Almac Sciences, said: "This is a very exciting development. Based on our combined strength, scale and technology, we will be able to offer finished commercial products and partly processed pharmaceutical materials or intermediates using our current world leading biocatalysis technology platform."

Anthony Owens, managing director of Arran Chemical Company, said: "We are very pleased with this significant development which enables us to continue to deliver high quality products to our global customer base in addition to offering a broader range of solutions.

"This move builds on our established presence in the industry and we look forward to merging our expertise and experience with Almac's undoubted success to match the increasing requirements of customers across the whole spectrum of the industry."

Almac made profits of £12.6m last year and increased its turnover by 5%. Almac is one of Northern Ireland's leading exporters.

Its headquarters are in Craigavon, Co. Armagh and it now has operations in the United States, Singapore and Tokyo. Almac provides services to other pharmaceutical firms, as well as developing its own products, mainly in cancer diagnostics.

http://www.industryandbusiness.ie

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

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

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

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

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Over 200 delegates attend PharmaChemical Ireland Conference in Cork

Posted on25 September 2015. Tags: Industry and Business, Little Island, pharmaceutical, PharmaChem, Sean Sherlock

At the PharmaChemical Ireland Conference at the Radisson Blu Hotel, Cork were L to R., Colin Murphy MD, Industry and Business Magazine and Matt Moran, Director, PharmaChemical Ireland. Picture, Tony O'Connell Photography.

Minister at State, Sean Sherlock TD opened the fifth PharmaChemical Ireland (PCI), Parenteral Drugs Association (PDA), International Pharmaceutical Engineers (ISPE) Conference in the Radisson Hotel, Little Island, Cork on Wednesday the 23rd of September.

The conference, entitled Continuing the Innovation Journey throughout the Lifecycle, brought together 200 delegates to discuss the latest regulatory and innovation developments facing the sector. An international panel of speakers from Ireland, the EU and the US discussed and debated the very latest ideas and thoughts that affect the industry globally at all stages of the evolution of medicines, from discovery to the market place.

Speaking at the conference PCI Director Matt Moran pictured with Managing Director Industry & Business Magazine Colin Murphy said: "These are very exciting times for the industry in Ireland. Over €3 billion worth of capital investment has seen the sector bounce back from the patent cliff environment into a period of sustained growth. We have seen a number of high profile investments especially in the biotechnology sector. Existing sites such as Pfizer, MSD, Allergan, Brsitol Myers Squibb, Mylan and Eli Lilly have invested significant sums in expansion. They have now been joined by new entrant to the Irish market, such as Alexion, Regeneron , Jazz and Biomarin.

"As we undergo such rapid expansion the need for skills has never been greater, over 2500 new jobs will be created in the next few years. State funded initiatives such as The National Institute for Bioprocessing Research and Training (NIBRT) and pharmachem Skillnets have vital role to play in this regard. I am optimistic that if industry, Government and the academic community work together we can meet this challenge and go onto even better times ahead."

"A taxation environment that supports enterprise, investment and R&D remains of critical importance to this sector. The Government's stated support for the 12.5% rate of corporation tax in this country is very welcome."

http://www.industryandbusiness.ie

Portable benchtop NMR spectrometer from GPE for Fluorine, Proton or Dual NMR

The spectrometer offers spectroscopic resolution at a fraction of the size and maintenance of current NMR instrumentation. The design brings analytical performance and point-of-need utility to the benchtop, fume hood or glovebox due to the compact size of the machine.

The NMReady was the first 60 MHz spectrometer available on the benchtop NMR market. Given its small footprint (Dimensions: 9.5 x 11x 17 inches) and light weight nature (only 45 lbs), the spectrometer is ideal for incorporation directly into the laboratory. The NMReady is compatible with all standard consumable 5mm NMR tubes, also available from GPE Scientific, so sample preparation is simple and fast.

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

Contact Information:

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

Phone: +44(0)1525 382277

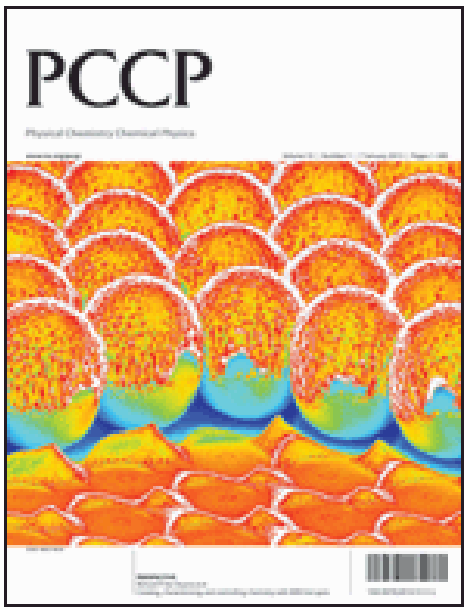
E-mail: info@gpescientific.co.uk

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

Company Information:

GPE Scientific Ltd was established in 1962 and is a leading distributor and manufacturer of laboratory equipment, glass blowing products and specialised glass components for the industrial, laboratory and research markets. There are many reasons to choose GPE Scientific above our competitors; we pride ourselves in stocking thousands of products from leading suppliers providing you with the best selection of laboratory equipment on the market. This includes being the exclusive distributors for Chemglass Life Sciences and Chemical Reactors, Norell NMR Tubes and Accessories and the portable Nanalysis NMReady Benchtop Spectrometer.

Institute of Chemistry of Ireland as a Co-Owner Benefits when you publish in PCCP



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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

The State Laboratory: 10 Years in Backweston

Written by Michael O'Gorman, State Laboratory

Introduction

The State Laboratory provides an analytical and advisory service to Government Department and Offices in support of their policies and regulatory programmes. It is under the aegis of the Department of Public Expenditure and Reform.

The Laboratory has been in its present location in Backweston, Co Kildare for over a decade. It traces its origins to 1924, when the Laboratory of the Revenue Commissioners and the Chemistry Laboratory of the Department of Agriculture were amalgamated.

The Laboratory is mandated as the Central Government Laboratory to provide a chemical and advisory service to Government Departments and Offices. Its functions have expanded from its origins in Revenue and Agriculture to embrace most aspects of Government legislative activity which require the application of chemical analytical expertise. The State Chemist has enforcement and referee status under various Acts of the Oireachtas (including the European Communities Acts) and their relevant implementing regulations. Being a service provider, the State Laboratory's activities and strategies are driven by the requirements of its clients in an evolving regulatory environment.

Government Departments use the services of the State Laboratory for a variety of purposes:

- to gather revenue for the State
- to protect the consumer against fraud and counterfeit products
- to provide evidence for litigation
- to confirm the eligibility of products for EU aid
- to safeguard the quality of food and agricultural products
- to prevent residues, contaminants and indigenous toxins entering the food chain
- to underpin the free movement of goods and the globalisation of world trade
- to assist in the protection of our cultural heritage
- to assist Coroners' investigations into causes of death.

The State Laboratory fulfils its mandate as the Government's Central Analytical Chemistry Laboratory by assisting Government Departments and Offices in the implementation of their policies and directives through the provision of a holistic service which includes:

- sample analysis
- evaluation and interpretation of analytical data, vis-à-vis regulatory specifications
- providing expert evidence for legal proceedings
- negotiating and advising on technical legislation

The Laboratory's central strategy is the provision of an efficient, cost effective, state of the art, quality analytical service which is responsive to the needs of its clients and commensurate with the political and societal requirements of the 21st century.

The Laboratory in Merrion Street

The State Laboratory came into existence in April 1924, when pre-existing Revenue and Agriculture laboratories were merged. For 60 years it was housed in what had been the College of Science building in Merrion Street in Dublin. It shared the building with government offices and with part of UCD.

In the 60 years following its establishment, the biggest change in the Laboratory was a large increase in work which followed Ireland's accession to the then EEC. Additional staff were recruited to cope with the added workload. The Merrion Street laboratory was becoming too small to accommodate the work and people.

The Laboratory in Abbotstown

In the early 1980s a major refurbishment of the entire Merrion Street block was undertaken, to provide offices for government, and it was impractical for a chemical laboratory to share the building any longer.

It was decided that the State Laboratory would move from Merrion Street. A site for a new building was provided on government land on the Abbotstown estate, near Castleknock. Klaus Unger designed the new Laboratory, and the building work was overseen by the OPW.

The Abbotstown laboratory, which opened in 1984, was a modern purpose-built chemical laboratory. However, with the passage of time, as the workload increased, as new analytical equipment was bought, and as staff numbers continued to grow, the building was approaching capacity. In response to this, it was decided to extend the Laboratory, to provide conference facilities, and building commenced. However, this decision was overtaken by a government decision to use the Abbotstown site for other purposes.

The move to Backweston

The second relocation of the State Laboratory was precipitated by the Government's decision in 2001 to build a National Football Stadium on the Abbotstown site. It was therefore necessary to build the new laboratory quickly, and to move all operations to a new site by 2005. The new location chosen for the Laboratory was in Backweston, Celbridge, Co Kildare, on land already owned by the Department of Agriculture.The new laboratory was designed by a team of OPW architects led by Ciaran O'Connor (now the State Architect). The management of the State Laboratory were heavily involved in designing the brief for the architect.

Opportunities and new facilities

The new building offered opportunities to take advantage of new building technologies, and the new laboratory was built to contemporary building, scientific and safety standards. It is considerably larger than the old Abbotstown laboratory, with more laboratory and office space. The new building is on two floors. It avails of natural light to the greatest possible extent. A distinctive feature of the structure is the use of natural wood. The surroundings are

landscaped and provide a pleasant working environment for staff. The building includes a large meeting room, laid out in a cabinet table configuration. There are, in addition, other meeting rooms within the building.

Many of the day-to-day functions and responsibilities related to the building that had previously fallen directly on the State Laboratory, were handed over to a facilities management company.

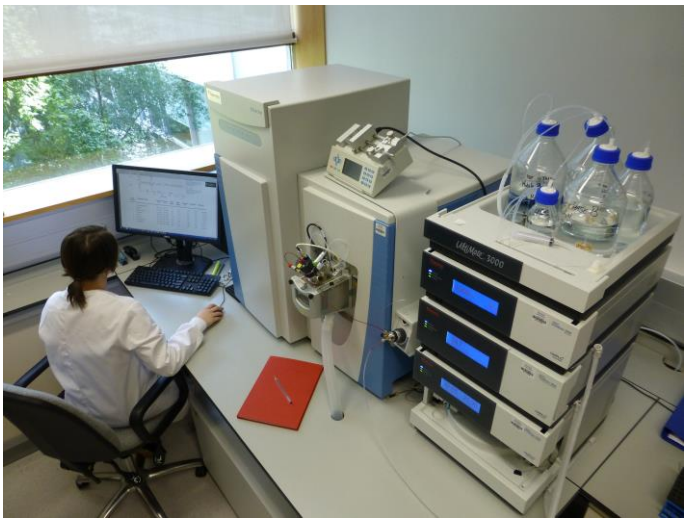
Laboratories of the Department of Agriculture, with which the State Laboratory had shared the Abbotstown site, also moved to Backweston. In addition, administrative civil servants were relocated to the site. The State Laboratory and these other institutions avail of a Shared Facilities building. This building houses a large lecture theatre, meeting rooms and a restaurant. Official meetings, scientific conferences and other events can be accommodated in the Shared Facilities building.

The move to Backweston provided a timely opportunity for the State Laboratory to modernise its ICT systems. A sophisticated computer network was designed to support the analytical, organisational and managerial work of the laboratory.

The logistics of moving

The move to the new laboratory was complicated by the impossibility of the Laboratory temporarily ceasing its analytical work for clients. Considerable effort was required to manage the move to the new site. Staff moved on a phased basis over four months to the new laboratory. Services to clients were maintained throughout the move, with analysis continuing in Abbotstown while equipment was installed and commissioned in Backweston. A great effort was made to move equipment from Abbotstown to the new laboratory, despite the difficulties that this entailed.

The State Laboratory suspended its Accreditation status for the duration of the move, as required by INAB.



In addition to moving to a new physical location, the State Laboratory continued the process of transforming itself organisationally, as it implemented the managerial innovations that were required by central government.

The Economic Crisis

The economic downturn and the crises that occurred over the past decade required the State Laboratory to provide its services with reduced financial resources. It was necessary to “do more with less.” The laboratory continued to provide a full service to its clients, despite reduced resources. Management, in consultation with the Laboratory’s clients, conducted a continual process of review of the work of the Laboratory.

For several years, staff numbers fell, because of the retirement of staff and the embargo on recruitment. Retirements meant there was some loss of corporate memory and loss of expertise. In more recent years, the resumption of

recruitment has brought new expertise and skills to the Laboratory. The State Laboratory remains a highly desirable place of employment for appropriately qualified people.

The State Laboratory in 2015

Over the past decade, the Laboratory has concentrated on chemical analysis. In addition, the general trend away from classical chemical analysis to more complex and sophisticated instrumental techniques has

continued. The Laboratory provides a consistently relevant and up-to-date service by using emerging technologies to meet the evolving needs of client departments.

The Laboratory has a robust Quality System in place, supported by the Paradigm 3 Compliance Management system. The Laboratory was awarded INAB (Irish National Accreditation Board) accreditation in 2003. The number of tests accredited by INAB has now risen by 2015 to 48 test methods covering 406 individual analytes.

The LIMS (Laboratory Information Management System) is a crucial component for organising work of the laboratory, for both senior management and other staff.

The Laboratory has the skills and the instrumental resources to respond quickly to crises that can occur in regulated industries or elsewhere in the environment. Among these in the past decade have been suspected dioxins in animal feed, the occurrence of horsemeat in beef, and illegal fuel laundering.

Laboratory staff are heavily involved in scientific cooperation with other agencies in Ireland and abroad. Staff represent Ireland's interests at EU and other meetings of international bodies.

Though the laboratory building is different, and the techniques employed are much more complex, the State Laboratory continues to provide a scientific service to its clients, as it did in 1924. It has in the intervening years acquired several new clients, notably the coroners, the State cultural institutions and the Health Products Regulatory Authority. Yet, more than 90 years since it was established, the State Laboratory is still supporting the work of the Revenue and providing an important service to the Department of Agriculture.

Detailed information on the work of the Laboratory is available on the State Laboratory website, www.statelab.ie, where the Annual Report and other publications may be found.

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