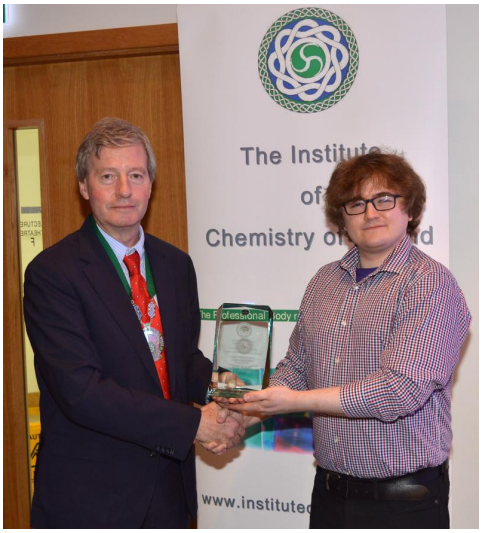
Irish Chemical News

A Journal of the Institute of Chemistry of Ireland

Institute of Chemistry Awards Ceremony 2025
UCD, O'Brien Centre for Science, Thursday 1st May 2025

Prod Paul Murphy Boyle Higgins Medal 2025
University of Galway

Prof Isabel Rozas Eva Philbin Award lecture 2025
Trinity College Dublin



Joint Winners Keerthi Nair and Fionn McNeill Dervilla Donnelly Postgraduate Award 2025
Atlantic Technological University Sligo and University College Dublin
Presentations by outgoing President ICI Prof Pat Guiry UCD

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The Professional Body representing Chemists in Ireland

The 10th Anniversary Issue with Current Editor

Title	Page

School of Chemistry & Chemical Engineering, QUB

A Message from the President

Dear Fellows, Members, Graduates and Associates.

This is my first opportunity for me to say to all our Members and Fellows how honoured I am to serve as President of the ICI. It will be a challenge to match the achievements of both my immediate predecessors who, in addition to our normal activities, brought the largest Chemistry conference ever run in Ireland to Dublin in 2024. This was a huge success academically and for the ICI in particular, since it showed how important the work it supports is for the whole chemistry community in Ireland. It is a testament to the organisational skills of all concerned that the EuChemS conference even generated a small surplus which we will certainly be able to put to good use. I am hoping that we will be able to build on this momentum during my term as President and raise the profile of the ICI both nationally and internationally. We have a lot to celebrate, and it is important that the work of the ICI and all its members is properly recognised. I am looking forward to working with our newly elected vice-President, Professor Anita Maguire of the University College Cork and the Officers and Council of the Institute in making that happen.

In this issue alone we have reports of several recent ICI-led academic meetings. These included the annual ICI Awards Day, which was held at University College Dublin on 1 May. This is a flagship event, and we had outstanding presentation from our awardees. Biographies of Professor Isabel Rozas of Trinity College Dublin, who received the ICI Eva Philbin Lecture Award and Professor Paul Murphy of the University of Galway, who received the ICI Boyle-Higgins Medal are included in this issue of ICN. In addition, the standard of applications for the ICI Dervilla Donnelly Postgraduate Award meant that we felt it appropriate to make awards to two postgraduate students. These were Keerthi Nair of ATU Sligo and Fionn McNeill of University College Dublin. Again, you can read about them and their work in the issue.

As well as the Awards Day other notable ICI meetings included the Inorganic Ireland Symposium was held on the 23rd of May 2025, at the University of Galway. This one-day meeting featured invited talks, oral flash presentations, and posters while Professor Stuart James (Queen's University Belfast) presented the ICI David Brown Lecture. This was followed by the 49th ICI Annual Congress, which had the theme "Electrochemical Horizons" and was organised by Professor Mike Lyons of Trinity College Dublin and

held in the School of Chemistry in TCD on the 4th of June 2025. This very successful event showcased the diversity and quality of electrochemical research which is being carried out right across the Island.

In addition to these recent meetings, we still have more events which will run in the near future. The IV Medicinal & Biological Chemistry Ireland Conference, which is organised by the ICI's Division for Medicinal & Biological Chemistry, will be held Queen's University Belfast, July 15-16, 2025. While our largest annual event, the 76th Irish Universities Chemistry Colloquium, will be hosted this year at Maynooth University on the 16th-17th June 2025 by the Department of Chemistry.

Of course, along with Meetings and Awards the ICI has many other activities. In particular, the ICI Young Chemists Network continues to be very active. Notably, in March this year Dr. Wiktoria Brytan from the University of Limerick represented the ICI-YCN at the European Young Chemists' Network 20th Delegate Assembly in Prague. The Delegate Assembly provides an excellent platform for young chemists across Europe to connect and network.

In closing, I would like to thank on behalf of our whole community, our Editor, Pat Hobbs, for his dedication and commitment in producing the ICN. I know that many of you do appreciate hearing about the activities of the ICI in this format, but it is particularly appropriate to highlight Pat's contribution now, since this edition of ICN marks 10 years of Pat's service as Editor.

With best regards,

President, Institute of Chemistry of Ireland

Prof Stephen bell FICI, FRSC

5/6/2025

Editorial

It's a time of change for the ICI and Irish Chemical News.

A big thank you to Prof Pat Guiry his wonderful contribution during his tenure as President of ICI. Prof Celine Marmion also steps back after her extended term as Immediate Past President.

The Institute and all of us on Council owe deep gratitude to both Prof Pat and Prof Celine for making the EuChemS Chemistry Congress (ECC-9) such a success last July. Their hard work and endless hours with the Scientific Committee formulating the Scientific Programme and getting commercial sponsorship and funding really paid off in terms of scientific content and made the Congress financially viable.

ICI has a new President and Vice-President. Both were elected at the AGM held in UCD on 1st May 2025.

The elected President is Prof Stephen Bell from Queens University, Belfast, having served as Vice-President for the past two years. Prof Anita McGuire, University College Cork, was elected Vice President. A big welcome to our two new officers. Inside you will find short biographies for both Stephen and Anita.

An important feature in this Issue is the **Awards Day** hosted in UCD on May 1st. This is covered along with photographs of Prof Pat Guiry presenting the Gold Medal and plaques to the awardees as one of his last duties before ending his Presidency. The lectures given were excellent and gave great insight into the quality of the work of these great researchers. As usual at this event day a reception is held after AGM and is an opportunity to catch up, meet new people and network.

You will notice the contents of ICN have changed. Many of the published papers in chemistry journals with links in the various topic sections of ICN were international authors with few featuring publications by researchers based on the Island of Ireland. The big change is that this Issue features Abstracts from researchers based on the Island of Ireland from our universities and research institutions. You will see that the contributions are arrange by university or institution rather than chemistry topic. In this Issue the focus is on the year 2024. In future Issues quarterly abstracts will feature, hopefully reducing its size.

Under each university, published papers for 2024 listed on their website, are compiled and presented in this Issue. Some colleges list these under author name in alphabetical order such as UCD while others are random. It's a major undertaking to find the papers for most colleges as they may be listed under different departments, research group or individual.

To enable a more efficient search system it would be a great help if all universities agreed to list their Chemistry and Medicinal Chemistry Publications in an easily accessible location on their website. Facilitating retrieval and allowing easier access, for publications such as ICN, which can then publicise and highlight the work of the individual researchers.

The Abstract format is as follows: the paper title, the author(s) list, journal name, number, volume, pages, DOI, and publication date. The DOI in dark blue takes you directly to the paper and most are open access. For authors two colours are used dark blue for an active link for information about the author(s) and light blue indicating that this link is text only, but the link is active in the actual paper in

most cases. Some journals only allow a text copy of the authors' name even though the link is active in the paper. It is not clear why this is.

You might note on the contents page that this Issue is the 10th Anniversary with current your Editor. The format had changed and evolved before, during and after the Covid pandemic when no meetings or conferences were happening in Ireland or abroad to report on. Papers however were being published, many with open access, hence the evolution to links to the open access papers. The more of these papers accessed, the more links followed by email from publishers and other sources and feeds from Chrome which then grew exponentially resulting in ICN becoming very large.

May/June is very active period for the Institute and there are several events especially in June after the Awards Day. We have the ICI Annual Congress on June 4th dedicated to electrochemistry in TCD and followed by the 76th Irish Universities Chemistry Research Colloquium 16-17 June 2025 hosted at Maynooth University. These events will be fully covered in the next Issue.

One of our ICI-YCN more active young chemists Dr Wiktoria Brytan was appointed to represent the young chemists in Ireland on the European Young Chemists' Network (EYCN). Wiktoria Brytan received the special recognition award for her contributions to the EYCN Communications Team. A short report is included in this Issue. The ICI-YCN have a new Chair, Francesca Adami University of Limerick. Francesca will take up her role at the YCN AGM during the Colloquium at Maynooth University.

There are other conferences supported by ICI along with internation specialist events of interest to chemists in Ireland posted in this Issue.

It is difficult to capture all the chemistry publications from the Universities and there is not a single list of research publications in one place on most university websites. Until this can be addressed do send a notification to the Editor's email with a link to your paper when it is published and then enjoy the extra credit by knowing the chemistry community here will be informed shortly afterwards. Apologies to anyone who published a paper, and I missed it. Any missed papers can be included in the next Issue.

This new format is not fixed in stone and can evolve further with suitable feedback. Please send your feedback suggestions to the Editor email address below.

Suggestions, Comments, Feedback and Responses are welcome and can be sent to the **Editor Email address: -**

editor@instituteofchemistry.org

Institute of Chemistry of Ireland (chemistryireland.org)

Patrick Hobbs MSc, FICI, CChem, CSci, MRSC.
Editor
Irish Chemical News

5th May 2025

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

The Institute of Chemistry of Ireland Young Chemists' Network (ICI YCN) is the young division of the Institute of Chemistry of Ireland and represents the interests of all young chemists in Ireland. A sub-committee of the ICI Council oversees all the activities of the YCN. The aim of the ICI YCN is to promote networking and collaboration opportunities for early-stage researchers by organising conferences and networking events for young chemists. It also aims to support young chemists by providing a platform to promote upcoming positions suited for young chemists.

Are you a chemist in Ireland aged between 18-35 years old? Want to be part of an exciting new network of young chemists and be part of a growing community? Join us today by emailing youngchemists@instituteofchemistry.org with your name, age, and where you study or work. If your institution is not listed below, you could even be part of our incredible committee.

Also see the International Young Chemists Network: https://www.iycnglobal.com

ICI's Young Chemists Network Committee for 2025/2026

Aaron McCormac, Chairperson of the ICI YCN, Director of the Institute of Chemistry Ireland, PhD student University of Galway.

Email: a.mccormac17@universityofgalway.ie youngchemists@instituteofchemistry.org

Committee Members 2025/2026

ICI-YCN at the 20th Delegate Assembly of the European Young Chemists' Network

As a member state of the European Chemical Society, the Institute of Chemistry of Ireland- Young Chemists' Network (ICI-YCN) elects a young delegate to represent the young chemists in Ireland on the European Young Chemists' Network (EYCN).

This year, the ICI Young Chemists' Network was represented by Dr. Wiktoria Brytan, University of Limerick, at the 20th Delegate Assembly in Prague, 20-22nd March 2025. Wiktoria received sponsorship from the ICI and EuChemS to attend the event.

The Delegate Assembly provides an excellent platform for young chemists across Europe to connect and network. Wiktoria has been working as part of the Communications Team on the EYCN for the last 2 years and has been supporting ICI-YCN events by communicating them through the EYCN networks and media.

Wiktoria Brytan receiving the special recognition award for her contributions to the EYCN Communications Team

The event was hosted by the Czech Chemical Society, and included workshops led by Elsevier, focusing on leadership skills and teamwork.

Marta Da Pian, Elsevier, leading a teamwork workshop (right).

Additionally, a session led by EuChemS president Angela Agostiano and EuChemS Science Communication and Policy Officer Chiara Capodacqua explored the 10th Framework Programme for Research and Innovation. A key moment of the assembly was the introduction of candidates for the next EYCN Board, who shared their visions for the future of the network.

Irish Delegate and ICI-YCN representative, Wiktoria Brytan was elected as the new Communications Team Lead, joining the Executive Board of the EYCN and forming the future of the network in Europe. Pictured below are the new Executive Board of the EYCN.

Pictured from left to right: **Jelena Kesic,** Membership Team Lead, **João António,** Executive Vice Chair, **Wiktoria Brytan**, Communications Team Lead, **Noah-Al-Shammery**, Executive Chair, Tatiana Sviriniuc, Global Connections Team Lead, **Carla Casadevall,** Networks Team Lead, **Monja Schilling**, Treasurer, and **Konrad Barnowski,** Science Team Lead.

The ICI is entitled to elect 2 delegates and 2 representatives on the EYCN panel. If you are interesting in connecting with European chemists and have your say on an international level, please contact : membership@eycn.eu.

ICI Awards Ceremony & Lecture Day May 1st, 2025, at UCD

Boyle Higgins Gold Medal Lecture Award 2025

Professor Paul Murphy, University of Galway

The ICI Annual Award for Chemistry (Eva Philbin Public Lecture Series)

Professor Isabel Rozas (TCD)

Dervilla Donnelly Postgraduate Award

Joint Winners:

Keerthi Nair (ATU Sligo)

Fionn McNeill (UCD)

Venue: UCD, O'Brien Centre for Science, SCIH 1.37 Lynch Theatre in Science Hub

2.20-3.00	Professor Isabel Rozas, Trinity College Dublin (Eva Philbin Award Lecture 2025) - "**Guanidinium, What a Wonderful Cation**"
3.00-3.20	Keerthi Nair, ATU Sligo – Dervilla Donnelly Postgraduate Award 2025 "**Development of Fe-based Functional Materials as Effective Catalysts in Advanced Wastewater Treatment**"
3.20-3.40	Fionn McNeill, University College Dublin – Dervilla Donnelly Postgraduate Award 2025 " **Enantioselective Synthesis of Sterically Hindered α-Aryl *O*-Heterocycles *via* Pd-Catalysed Decarboxylative Asymmetric Transformations**"
3.40-4.00	Tea/Coffee Break
4.00-4.40	Professor Paul Murphy, University of Galway (Boyle-Higgins Medal 2025) - " **Synthesis and Applications of Lectin Ligands. Insights from DFT Study Into Mechanisms Involved in Lewis Acid-catalysed Reactions of Protected Carbohydrates**"
4.40-5.30	ICI AGM and Wine Reception

The event was hosted by Prof Pat Guiry with assistance from Assoc. Prof Marcus Baumann and Dr Joseph Byrne both at UCD

Each award winner gave very a stimulating and interesting lecture on their respective research areas across four leading research institutions.

Boyle Higgins Gold Medal Award

Starting with the Boyle Higgins Gold Medal Award Winner Prof Paul Murphy here is a brief summary of his career:

Prof Paul V. Murphy being presented with the Boyle-Higgins Gold Medal by
Prof Pat Guiry, UCD, Outgoing President of ICI

School of Biological and Chemical Sciences, University of Galway, University Road, Galway

CAREER PROFILE (EDUCATION AND EMPLOYMENT)

2008-current Established Professor of Chemistry, University of Galway

2008-13 & 14-7 Head of School of Chemistry, University of Galway

1996-2008 Lecturer, Senior Lecturer, Associate Professor, University College Dublin (UCD)

1994-96 Chiroscience Postdoctoral Fellow, University of York, UK

1990, 1994 BSc, PhD, National University of Ireland (University College Galway)

SELECTED AWARDS, DISTINCTIONS, CONTRIBUTIONS

2001 Organizer Royal Society of Chemistry Carbohydrate Spring Meeting

2003-27 Science Foundation Ireland Investigator Award Holder

2005-12 Member Editorial Board of Carbohydrate Research

2005 Astellas USA Foundation Award

2013 Admitted as a Fellow of the Institute of Chemistry of Ireland

2019 University of Galway President's Award for Research Excellence (supervisor category)

2019-21 Chair of University of Galway School of Chemistry Self-Assessment-Team: Athena SWAN Bronze Award granted 2021-2025.

2024 SSPC Research Ireland Centre for Pharmaceuticals: Research Article of the Year 2023

2024 My Green Laboratory Certification

2025 Boyle-Higgins Gold Medal of the Institute of Chemistry of Ireland

RESEARCH INTERESTS AND MENTORING

1. Lectin ligand design, synthesis and application (glycomimetics). Currently includes development of ligands for galectins, siglec, macrophage galactose C-type lectin, hemagglutinin.

2. Development of Lewis acid promoted anomerisation (b to a-anomer isomerisation) for stereoselective synthesis of natural glycosides and glycomimetics. Currently focused on mechanistic study for anomerisation involving modern electronic theory (DFT).

3. Design and implementation of new reactions for C-N ring synthesis applied to preparation of pharmaceutically relevant iminosugars and to produce new iminosugars. Currently focused on study of stereoselective azide-alkene cycloadditions to give triazolines and their decomposition to aziridines at the anomeric centre, including use of flow chemistry to increase the efficacy of such reactions.

Prof Murphy has supervised 37 PhD & 8 MSc researchers to completion and 31 postdoc researchers. He and his group have published over 150 peer reviewed articles and reviews.

SELECTED PUBLICATIONS

Allylic Azide Rearrangement in Tandem with Huisgen Cycloaddition for Ring Formation. Stereoselective Synthesis of C-Iminosugars, L Moynihan, R Chadda, P McArdle, PV Murphy, Organic Letters, 2015, 17, 6226-6229. Open access link: http://hdl.handle.net/10379/5941

Lewis Acid Induced Anomerisation of Se-Glycosides. Application to Synthesis of a-Se-GalCer. AW McDonagh, MF Mahon, PV Murphy, Organic Letters, 2016, 18, 552–555. Open access link: https://aran.library.nuigalway.ie/handle/10379/5940

MUC1 Glycopeptide Vaccine Modified with a GalNAc Glycocluster Targets the Macrophage Galactose C-Type Lectin on Dendritic Cells to Elicit an Improved Humoral Response. A Gabba, R Attariya, S Behren, C Pett, J C van der Horst, H Yurugi, J Yu, M Urschbach, J Sabin, G Birrane, E Schmitt, S J van Vliet, P Besenius, U Westerlind, PV Murphy, Journal of the American Chemical Society, 2023,145, 24, 13027. Open Access link: https://pubs.acs.org/doi/full/10.1021/jacs.2c12843

Eva Philbin Lecture Award

Isabel Rozas was born in Madrid, Spain. After a B.Sc. in (Organic) Chemistry at the Universidad Complutense de Madrid (1981, Spain) she carried out postgraduate research at the Institute of Medicinal Chemistry (CSIC, Madrid, Spain) obtaining her PhD degree from the Universidad Complutense de Madrid in 1987. She performed post-doctoral research in the University of Saskatchewan (1989-91, Canada), followed by a second post-doctoral fellowship at Queen's University in Kingston (1993-94, Canada).

After working for 14 years as a researcher at the mentioned Institute of Medicinal Chemistry, in 2000 she moved to the School of Chemistry at Trinity College Dublin as a Lecturer in Medicinal Chemistry. In 2003, she became director of the Medicinal Chemistry course; in 2005, was elected Fellow of Trinity College Dublin, and in 2010, she became Professor in Chemistry.

Her main area of research is framed within the Medicinal Chemistry field, and, thus, her group works in the modelling, preparation and biophysical and biological evaluation of: (i) agents targeting nucleic acids (DNA minor groove and Guanine-quadruplexes) as anticancer or antiprotozoal therapies; (ii) guanidine-based inhibitors of protein kinases; (iii) compounds targeting adrenergic alpha2-adrenergic

receptors with application as antidepressants or antipsychotic agents; (iv) piperazine guanidinium derivatives as anti-tuberculosis agents; and recently (v) compounds targeting TMPRSS2 protease as potential anti Covid-19 therapies. In addition, she has an interest in the theoretical study of non-covalent interactions such as hydrogen bonds. She has published 175 papers and collaborates with several groups in Ireland, Spain, the UK, France, Germany, Italy, India, Canada and USA. Between 2019 and 2022, she was an Editor of Bioorganic and Medicinal Chemistry Letters and now is a member of the Advisory Board for both Bioorganic and Medicinal Chemistry and Bioorganic and Medicinal Chemistry Letters as well as Special Issue Editor for Results in Chemistry.

Presently, she is the Chairperson of the Division of Medicinal and Biological Chemistry in the ICI (Institute of Chemistry of Ireland) and member of the Council of the European Federation for Medicinal Chemistry and Chemical Biology (EFMC).

Dervilla Donnelly Postgraduate Award

This year the Postgraduate Award has been renamed the **Dervilla Donnelly Postgraduate Award** in honour of the late Prof Dervilla Donnelly UCD. Of the contenders two stood out and the judging panel had great difficulty separating two of the contenders. It was agreed with the Institute that both would be deemed equal winners of this year's award.

In order of speaking there were **Dr Keerthi Nair, Atlantic Technological University Sligo**

Keerthi supervised by Prof Suresh C. Pillai of the Nanotechnology and Bio-Engineering Research Group during her PhD research. Keerthi's PhD research, conducted as part of the EU Horizon 2020 PANIWATER project, focuses on the development of Fe-based functional nanomaterials, particularly Metal-Organic Frameworks (MOFs) and their derivatives, as advanced catalysts for wastewater treatment. Her work addresses critical water contamination challenges and aligns with the United Nations Sustainable Development Goal 6, which aims to ensure clean water and sanitation for all.

ATU PhD Researcher Receives Prestigious Dervilla Donnelly Award 2025

Atlantic Technological University (ATU Sligo) PhD Researcher Keerthi M. Nair (Supervised by Prof. Suresh C. Pillai) of the Nanotechnology and Bio-Engineering Research Group has been honoured with the Dervilla Donnelly Postgraduate Award 2025 .

Keerthi worked for her PhD in cutting-edge research as part of the European Union's Horizon 2020 Research and Innovation Program, PANIWATER (Paniwater eu). This program emphasises the development of innovative solutions for water treatment, an area of utmost importance for environmental sustainability and human well-being. This recognition highlights Keerthi Nair's exceptional research in the development of Fe-based functional nanomaterials, particularly Metal-Organic Frameworks (MOFs) and their derivatives, as highly effective catalysts in advanced wastewater treatment processes.

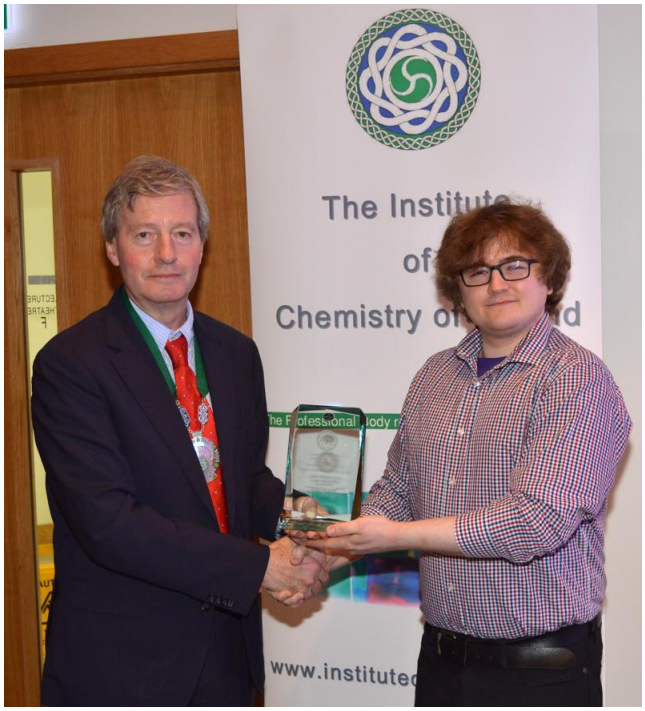
Beyond her research, Keerthi has dedicated considerable time to mentorship and education. As a teaching assistant, she has guided undergraduate students, fostering critical thinking and hands-on learning to enhance their academic experience. In addition, Keerthi has served as an active member and ambassador of the Current Chemistry Investigators (CCI), a pioneering science outreach initiative funded by Research Ireland and led by prestigious institutions such as Trinity College Dublin, ATU Sligo, University College Cork, and the Tyndall Institute. Keerthi's passion for public engagement also extends to large-scale science festivals. She has played a key role in organizing and facilitating three major public engagement events annually, each attracting over 2,000 attendees. These events include the ESB Science Blast in Dublin, the Cork Carnival of Science, and the Lifetime Lab Open Days, where she has helped to bring chemistry to life for diverse audiences.

Through her combined efforts in research, mentorship, and outreach, Keerthi continues to bridge the gap between scientific discovery and public understanding, ensuring that both knowledge and opportunities are accessible to all.

ATU President Dr Orla Flynn praised Keerthi's achievement, stating: "This recognition of Keerthi's work not only highlights her individual dedication and expertise but also reflects the high standards of research at ATU. Her work exemplifies our commitment to producing cutting-edge research with tangible global impact, reinforcing ATU's role in fostering scientific innovation and sustainability. Congratulations, Keerthi!"

Keerthi's recognition not only highlights her individual dedication and expertise but also serves as a testament to the high standards of research conducted at ATU. Her work exemplifies ATU's commitment to producing cutting-edge research that has a tangible impact on both scientific communities and global environmental challenges. The recognition further underscores ATU's role in fostering innovative research and cultivating talent that contributes to the broader field of science and sustainability.

The second **Postgraduate Awardee** was **Dr Fionn McNeill, University College Dublin** supervised by Prof Pat Guiry.



Fionn McNeill PhD lecture was titled *"The Enantioselective Synthesis of Oxygen-containing Heterocycles via Pd-catalysed Decarboxylative Asymmetric Transformations"* (Guiry Research Group, April 2025)

Short Biography

"I was born and raised in Dublin and very early on developed an interest in science which led me to pursue a career in chemistry. In 2016, I started my chemistry journey, enrolling in the Medicinal Chemistry and Chemical Biology course at University College Dublin. During this time, I interned at the Process Development lab at Takeda, Grange Castle and I completed my final year project with Dr. Paul Evans, studying the Staudinger-Ligation reaction for the synthesis of amides and enamides. Additionally, I was awarded the Frank Hegarty and Dervilla Donnelly medal for my undergraduate results, which I was very honoured to receive.

In 2020, I went on to pursue postgraduate studies, carrying out a PhD under the supervision of Prof. Pat Guiry at UCD. There I worked on lead mediated arylations of oxygen containing heterocycles and their application in palladium catalysed decarboxylative asymmetric transformations. The time in the Guiry group allowed me to flourish as a methodologist where I developed an interest in reaction scale up and product crystallisation and learned key skills in reaction optimisation, asymmetric chemistry and product characterisation. In 2023, I had the very exciting opportunity to study under Prof. Masayuki Inoue in the University of Tokyo, Japan, where I worked on the development of synthetic pathways towards natural products.

Last year, I was fortunate to publish my first paper on my work under a special collection for the 9th EuChemS Chemistry Congress in Chemistry: Chemistry A European Journal **https://doi.org/10.1002/chem.202401738** and present my work at the Convention Centre Dublin where the event was held. Earlier this year. I successfully defended my thesis, and I am due to start the next step in my career as a Process Development Scientist with APC."

The 76th Annual General Meeting of the Institute of Chemistry of Ireland

Immediately after the Award Lectures the Annual General Meeting took place in SCIH 1.37 Lynch Theatre, Science hub, O'Brien Centre for Science, UCD.

The main topic reported here is the change of President and Vice President. Prof Pat Guiry ends his Presidency and Prof Celine Marmion ends her Immediate Past President and both remail as Council members. Vice President Prof Stephen Bell QUB was duly proposed and elected as the new President of ICI. Prof Anita McGuire UCC was proposed and elected as Vice President.

Pat Guiry and Celine Marmion are due many thanks for their trojan work during a six year period in making the 9th EuChemS Chemistry Congress such a great success in Dublin last July 2024.

Prof Stephen Bell QUB. President ICI 2025-2027

Steven Bell is Professor of Physical Chemistry in the School of Chemistry and Chemical Engineering, Queen's University Belfast. He earned his PhD on time-resolved spectroscopy under the supervision of Professor John McGarvey. After postdoctoral work in the Rutherford Appleton Laboratory (Oxford, U.K.) with Professor Ron Hester, he was appointed to his first independent academic position as a lecturer in the University of York, before eventually returning to QUB.

His research interests centre on the development of Raman and surface-enhanced Raman spectroscopy for chemical analysis, but this has branched into areas as diverse as superhydrophobic materials and liquid-liquid interfaces. His work, which combines fundamental science with real-world applications, has been reported in over 200 publications. He pioneered Raman analysis of drugs of abuse, foodstuffs, and forensic evidence and has a long-standing interest making surface-enhanced Raman spectroscopy a robust quantitative technique.

He has a strong interest in the commercialisation of research and has been a Royal Society Industry Fellow. He was founder/director of Avalon Instruments Ltd, which manufactured user-friendly benchtop Raman systems and was ultimately purchased by Perkin-Elmer Inc.

Steven is a Fellow of the Institute of Chemistry of Ireland and the Royal Society of Chemistry. He is an elected Member of the Royal Irish Academy, where he sits on the Council as Vice President with responsibility for Research. He received the Royal Society of Chemistry's open prize in Analytical Chemistry , the Theophilus Redwood Award, in 2024.

Prof Anita McGuire UCC. Vice President ICI 2025-2027

Anita Maguire is currently Head of the School of Chemistry at UCC, having completed two terms as Vice President for Research & Innovation (2011-21). She is a Co-PI in SSPC, The Research Ireland Centre for Pharmaceuticals.

Following studies at UCC (BSc Chemistry 1985, PhD 1989), and postdoctoral research in Namur, Belgium then at the University of Exeter, UK, Anita returned to Cork in 1991 to establish an independent research team focusing on synthetic organic chemistry. Her research interests include development of new synthetic methodology, use of continuous flow, asymmetric catalysis, and the design and synthesis of bioactive compounds. 60 PhD students, 9 MSc and 47 postdocs have graduated from her team, many of whom have progressed to careers in the pharmaceutical sector in Ireland and internationally.

She was the inaugural Chair of the National Forum on Research Integrity in Ireland established in 2015 until the end of 2024.

International activities include Chairing the ERC Advanced Grants Evaluation panel PE5 – Synthetic Chemistry & Materials, membership of the International Advisory Board, EPSRC CDT React, Imperial College London, and as an Adjunct Professor in the University of Bergen, 2011-16.

She was elected as a Member of the Royal Irish Academy in 2014, Vice President of the Royal Irish Academy for 2019-22 and chaired the Diversity Committee of the RIA for 2019-2023.

Social & Networking after the Award Lectures and AGM

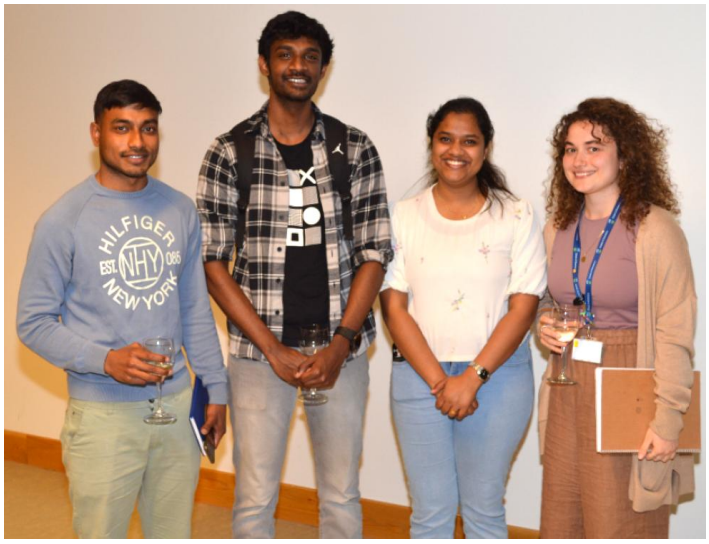
Prof Eoghan McGarrigle, UCD, Prof Paul Murphy, Prof Grace Morgan (facing back) UCD, Celin Marion

Prof Mary J. Meegan, Margaret Franklin, Odilla Finlayson

L-R John Keegan, Margaret Franklin, Odilla Finlayson

L_R Dr Marco Minneci, Isabel Rozas, Emeritus Prof Mary J. Meegan TCD

L-R Celine Marmion, Emeritus Prof Michael McGlinchey UCD, Grace Morgan Stephen Bell



L_R Bodhayan Biswas UCD, Guru Vigknesh Anantharaj UG, Aiswarya Siby UG, Elisabetta Panichelli UCD

L_R Dr Keerthi Nair, Prof John Kelly, Prof Suresh Pillai

L-R Prof Stephen Bell, Prof John Kelly, Prof Celine Marmion

Sharali Malik, UCD & Laura Cunningham, University of Galway

The 22nd European Carbohydrate Symposium
6th-10th July 2025, Gdansk, Poland
The 22nd European Carbohydrate Symposium in Gdansk – eurocarb22 (eurocarb2025.com)

Abstract Submissions extended to 28 February

Welcome to EUROCARB 2025

It is a pleasure to invite you to **22nd EUROCARB** to be held in Gdańsk on **July 6th-10th, 2025,** hosted by the Faculty of Chemistry, University of Gdańsk, under the auspices of the` European Carbohydrate Organization.

The first **EUROCARB** symposium was organized in Austria in **1981**. As a biennial meeting, it has evolved from a carbohydrate chemistry forum to a glycoscience meeting which also includes glycobiology and biological chemistry. Nowadays, **EUROCARB** is positioned as a leading symposium at the forefront of Glycosciences in Europe.

The **EUROCARB 2025** program will try to consolidate the interplay between chemistry and biology, to be attractive to both communities, and reinforce the needed interaction between glycochemistry, glycobiology, and applied glycosciences. The conference will be organized in several topics that cover all aspects of Glycosciences, aimed at showing the latest developments in the field, provide a forum for discussions and networking and highlight the challenges and future trends in carbohydrate-related scientific disciplines and applied technologies.

EUROCARB 2025 will gather academia and industry to burst innovative technologies into application in a large diversity of fields, including medicine, nutrition and food sciences, material sciences, chemistry, biotechnology and bioeconomy.

The symposium is also an opportunity to visit **Gdańsk**, which is located on the Baltic coast of northern Poland. Either before or after the symposium you'll be able to enjoy the city, its architecture and museums.

On behalf of the Organizing Committee, I invite you to the 22nd EUROCARB in **Gdańsk in 2025.**

Zbigniew Kaczyński

Chair of the Organizing Committee

Contact: For the e-mail correspondence, please use the e-mail address: **eurocarb22@ug.edu.pl**

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

Physical Chemistry Chemical Physics
Phys. Chem. Chem. Phys.,
28 March 2025, Volume 27, Issue 12
Page 5935 to 6374
https://doi.org/10.1039/d4cp04689g

Support our Institute by publishing your new research results in this prestigious peer reviewed journal.

Scope

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

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

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

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

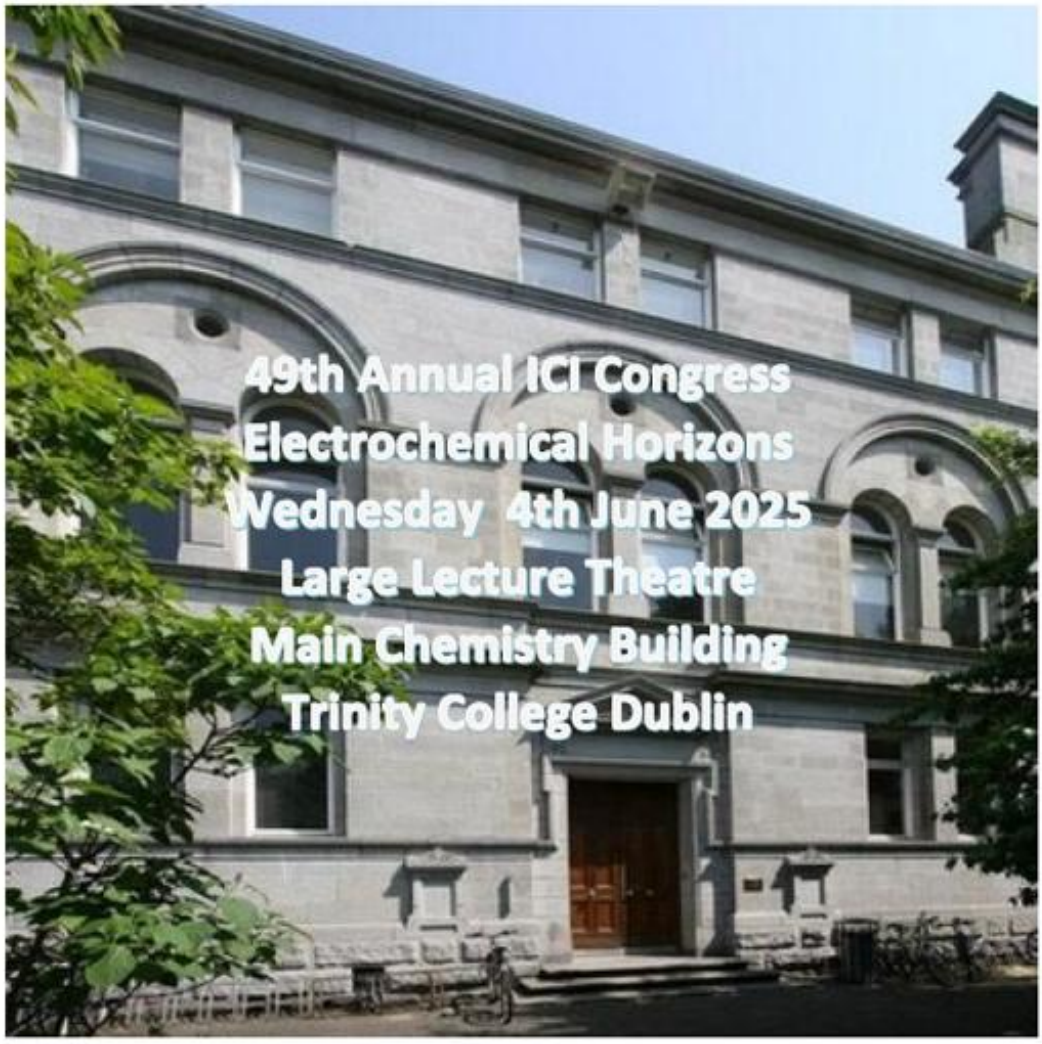
ICI Annual Congress 2025

TCD on June 4th organised by Professor Lyons (TCD)

Large Lecture Theatre, Main Building School of Chemistry in TCD

Topic: Electrochemical Horizons

This event is a one-day meeting. This symposium will address important current topics in Electrochemical Science and will be of broad general interest.



Trinity College Dublin
The University of Dublin

Institute of Chemistry of Ireland

49th Annual ICI Congress
Electrochemical Horizons
Wednesday 4th June 2025
School of Chemistry TCD

10.00-10.55 **Tea and Coffee / Registration**

11.00- 11.05 Welcome: **Professor Mike Lyons, School of Chemistry & AMBER, Trinity College Dublin**
Electrochemical Horizons: will the final frontier be ever reached?

11.05-11.40 **Professor Carmel Breslin, Maynooth University**
Electrochemistry and its Environmental Applications for a Greener Future

11.40-12.15 **Ass. Professor Chris Batchelor McCauley, School of Chemistry, Trinity College Dublin**
New Frontiers in Electrochemistry, from Neutrons to Protein Modification

12.15 -13.00 **Professor Valeria Nicolosi , School of Chemistry, CRANN, AMBER & I-form, Trinity College Dublin**
2D nanomaterials inks for energy applications

13.00 - 14.00 **Lunch (local venues)**

14.00 - 14.35 **Professor Paula Colavita, School of Chemistry, Trinity College Dublin**
Functional thin film carbon electrodes as platform materials for fundamental studies of interfacial reactivity.

14.35-15.10
Professor Micheal Scanlon, Department of Chemical Science & the Bernal Institute, University of Limerick
Electrosynthesis of Conducting Polymer Thin Films at a Polarized Liquid/Liquid Interface

15.10- 15.45 **Assoc. Professor Robert Johnson, School of Chemistry University College Dublin**
Non-Aqueous Solvent Confined within a Nanopipette: Applications in Pharmaceutical Analysis

15.45-16.15 **Dr Paul Kavanagh, School of Chemistry & Chemical Engineering, Queens University Belfast**
Insights into Organic Electrosynthesis Through Electroanalytical Approaches.

16.15- 17.00 **Professor Robert Forster , School of Chemical Sciences Dublin City University**
Reimagining Medicine: Health through Wire-free Electroceuticals

17.05-17.50 Poster session and mixer

17.55- 18.10 Poster Prize Presentation and Closing Remarks: **Professor Steven Bell, School of Chemistry and Chemical Engineering, QUB, President, Institute of Chemistry of Ireland**

Registration details

Registration closes 2/6/25

Registration Fees

ICI Member	**€50**
Non-member	**€75**
Student/Post-Doc	**€25**

The student registration fee will include a voucher, which can be used to cover the cost of one year's subscription fee for membership of the ICI.

Payment will be collected through the following link:

https://clr.ie/138214

choosing which category of registration you require and asking for credit card details. A range of different credit cards are acceptable.

Posters

Students or ECRs who wish to present a poster should send the title of the poster to melyons@tcd.ie by 2/6/2025.

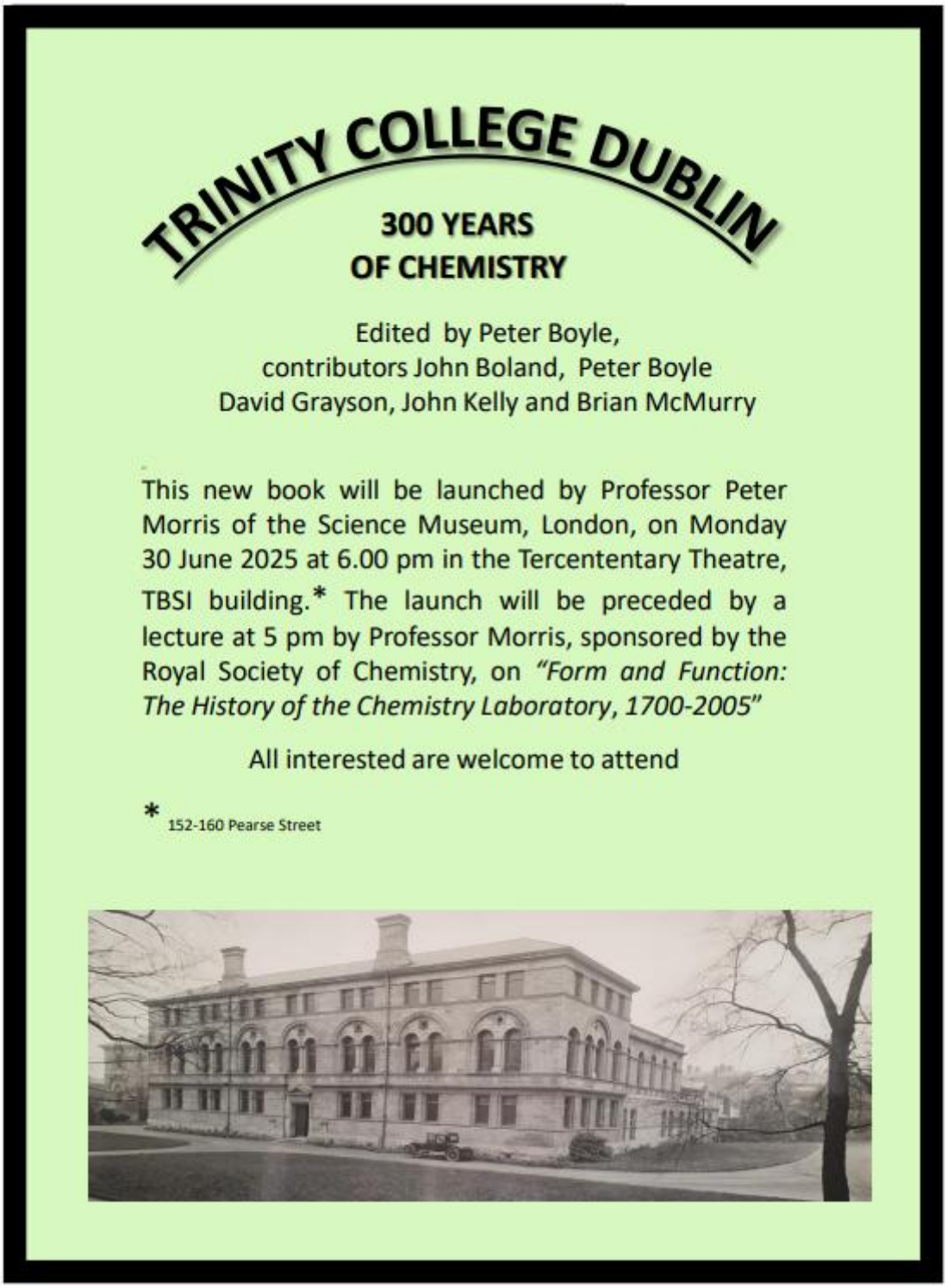
Dietary Requirements

Delegates with dietary requirements are asked to note this in the dedicated section of the registration app.

Updates and revisions to the program will be posted on the ICI website: https://www.chemistryireland.org/

and on the School of Chemistry website TCD:

https://chemistry.tcd.ie



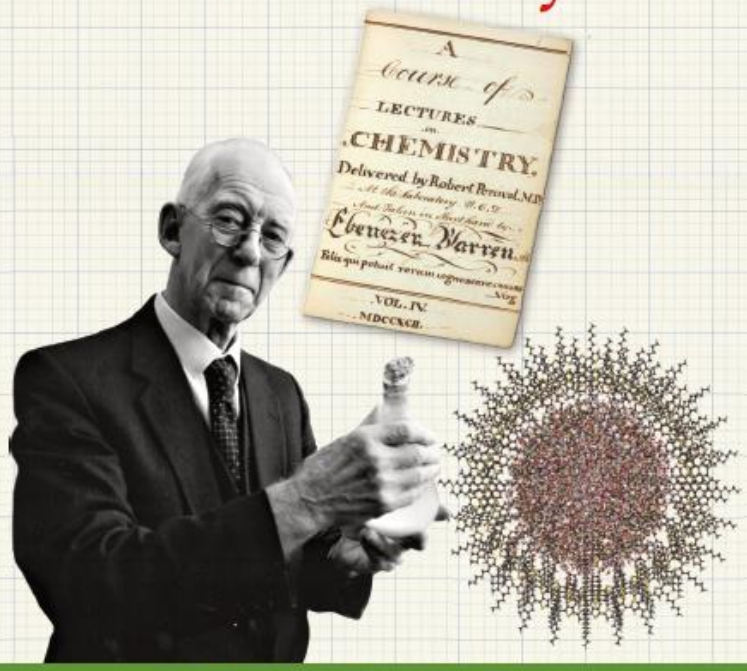
This invitation to members and colleagues at the Institute of Chemistry of Ireland to the launch of our book "Trinity College Dublin – 300 years of Chemistry", which will be held at 5pm June 30 in the Tercentenary Theatre of the Trinity Biosciences Institute on Pearse Street.

The launch will be followed by a wine reception where copies of the book will be available.

Prof John J. Boland
School of Chemistry
SFI AMBER Research Centre
Trinity College Dublin

TRINITY COLLEGE DUBLIN

300 YEARS OF Chemistry



This is the history of 300 years of chemistry at Trinity College Dublin, from its beginnings in the early years of the eighteenth century to the present day. The narrative also serves as a history of the development of chemistry as a science and the part played by Trinity in this development. The first chemistry lecturer in the College was appointed in 1711 whose job was to teach chemistry to medical students, and since that humble beginning over 300 years ago chemistry in Trinity has blossomed into a major interdisciplinary subject with a primary input into other areas such as biochemistry, genetics, immunology and materials science. Trinity has also played its part in the development of hugely important industrial concerns such as the enormously valuable pharmaceutical industry. As well as chronicling these advancements, the book also focuses on the individual people who worked on chemistry in Trinity over the past three centuries, and tells the stories of the many brilliant, idiosyncratic, and clever personalities who were responsible for the well-being of chemistry within our walls. It is hoped that the many chemistry graduates of Trinity will find pleasure in these pages.

JACKET FRONT:
Wesley Cocker, Professor 1947-78
The lecture notes of Robert Perceval 1792
Computer simulation of an electroactive micelle to study the dynamics of ions in the central spherical cavity

TRINITY COLLEGE DUBLIN
300 years of Chemistry
PETER BOYLE *Editor*

HINDS

John Boland • Peter Boyle • David Grayson
John Kelly • Brian McMurry
Editor Peter Boyle

The authors of this book are either current or former members of the academic staff of the School of Chemistry in Trinity, so that they bring to their task a first-hand knowledge of their subject. Three of the authors are Trinity graduates. **Peter Boyle**, who edited this volume, graduated from Trinity in 1960 and carried out his PhD studies in Trinity under the aegis of Professor Cocker. He deals with the first two centuries of the Department's existence, a period during which chemistry was closely aligned to the medical school. **David Grayson** and **Brian McMurry** also graduated from Trinity, in 1968 and 1953 respectively. They too studied for their PhD degrees under Cocker, and they take up the story from the early years of the 20th century to when Cocker retired in 1978. The last two chapters of the book, contributed by **John Kelly** and **John Boland**, chronicle the fortunes of the School leading up to and beyond the new millennium. Kelly, a graduate of Manchester University, covers the rapidly evolving teaching and research missions of the School and the impact of new hires and research funding. Boland, who conceived the idea of this book, deals with chemistry as the central science in an interdisciplinary world, its impact on School development and the challenge to be visible on the international stage. In 2025 the department was rated as amongst the top 100 chemistry departments in the world.

Trinity College Dublin appointed its first lecturer in chemistry in 1711 so that its chemistry department can claim to be amongst the oldest in the world. The lectureship was elevated to a full professorship in 1785 and this book traces the development of chemistry in Trinity from its beginnings in the eighteenth century to what it is today. In those early years, chemistry was taught in universities as an adjunct to medicine and was often called "the hand-maid of medicine", so that our first chemistry lecturer was not a chemist at all. Rather he was a distinguished doctor, and until the end of the eighteenth century chemistry in Trinity was still dominated by medicine. However, with the appointment in 1850 of James Apjohn to the Professorship, chemistry in Trinity became an important subject in its own right and by the end of that century could hold its own with the best in Europe. For a while after that, in the period covered by the two world wars, chemistry in Trinity languished in the doldrums but the appointment of Cocker to the chair in 1947 brought with it a massive injection of energy, enthusiasm, and initiative, and under him the Department was revitalised. A whole chapter of this book is devoted to Cocker, and many graduates will have personal reminiscences of these years. After Cocker, the Department continued to rise in stature and the final two chapters bring the story up to modern times when today chemistry in Trinity is highly ranked on the international scene.

JACKET BACK:
1887 Chemistry building

International Chemistry Events

European Chemistry Thematic Network ECTN

JAGIELLONIAN UNIVERSITY IN KRAKÓW

Eurolecturer Academy

Summer School
Question-Driven Learning in STEM
29 June – 1 July 2025 | Krakow, Poland

Although student-centered learning is widely embraced, many academic teachers still face challenges in implementing active learning strategies.

Discover innovative approaches at the **'Question-Driven Learning in STEM'** Summer School, featuring international expert **Prof. Mauro Mocerino** (Curtin University, Perth, Australia), who integrates questioning techniques and collaborative learning into his teaching—moving beyond traditional lecturing.

Take this opportunity to develop materials for your own teaching practice.

Organized by the **ECTN Eurolecturer Academy**, this Summer School equips lecturers and programme directors with the knowledge and skills to confidently apply active learning strategies, enhance the use of questioning techniques, and support collaborative learning among students.

Master active learning - join the 'Question-Driven Learning in STEM' Summer School!

Enhance teaching skills

Meet international experts

Share knowledge

Develop teaching material

This Summer School is recognized by

EuChemS
European Chemical Society

Information, Programme, and Registration
ECTN ELA Summer School

IV Medicinal & Biological Chemistry Ireland Conference

Queen's University Belfast, July 15-16, 2025

The IV Medicinal & Biological Chemistry Ireland conference will be hosted in Queen's University Belfast, UK on July 15-16, 2025.

Organised by the Division for Medicinal & Biological Chemistry of the Institute of Chemistry of Ireland (ICI), this meeting will take place with support by the European Federation of Medicinal Chemistry and Chemical biology (EFMC).

This biennial meeting will showcase a wide panel of international and national keynote speakers from various fields of medicinal chemistry and chemical biology, and early career researchers will have the opportunity to:

– showcase their research through poster and flash oral presentations
– attend a careers fair including presentations from stakeholders within the pharmaceutical industry

Deadline for registration and abstract submission: 1st June 2025

We look forward to welcoming you to Belfast in July!

Resister here:-

Link to Registration, Abstract Submission & Scientific Programme

IV Medicinal & Biological Chemistry Ireland Conference, July 15-16th, Queen's Univ. Belfast (UK)

QUEEN'S UNIVERSITY BELFAST

Institute of Chemistry of Ireland

EUROPEAN FEDERATION FOR MEDICINAL CHEMISTRY AND CHEMICAL BIOLOGY

Organized by the Medicinal & Biological Chemistry Division of the Institute of Chemistry of Ireland

Confirmed speakers:

Donald Weaver (U. Toronto); Angela Russell (U. Oxford); Mark Bradley (Queen Mary U. London); Nicholas Mitchell (U. Nottingham); Daniel H O'Donovan (AstraZeneca); Graham Cotton (Almac); Lorraine Martin (QUB) Eddie Myers (U. Galway); Joe Byrne (UCD); Joanna McGouran (TCD); Trinidad Velasco-Torrijos (Maynooth U.).

Registration, Poster Abstract Submission, Scientific Programme
https://medicinalchemistryireland.wordpress.com/

Deadline for Registration and Abstract Submission: 20th June 2025

ALMAC | ThermoFisher SCIENTIFIC | SK biotek | Royal Society of Chemistry Republic of Ireland Local Section | AstraZeneca

European Chemistry Thematic Network ECTN

Eurolecturer Academy

NICOLAUS COPERNICUS UNIVERSITY IN TORUŃ

5th STEM-CPD Summer School

15 - 19 September 2025 | Toruń, Poland

Passionate about advancing STEM education? Do you believe that continuous professional development (CPD) in teaching and learning is important for enhancing university education?

The **5th STEM-CPD Summer School** equips you to design impactful professional development activities for STEM lecturers at your university.

Through this **intensive program**, you will enhance your expertise in STEM teaching and learning, gain **an international perspective**, and collaborate with a global network of educators.

Organized by the **ECTN Eurolecturer Academy** and **Nicolaus Copernicus University in Toruń**, this summer school offers more than just learning- it is a gateway to a dynamic community.

Join us and take your commitment to STEM education to the next level!

Empower STEM education

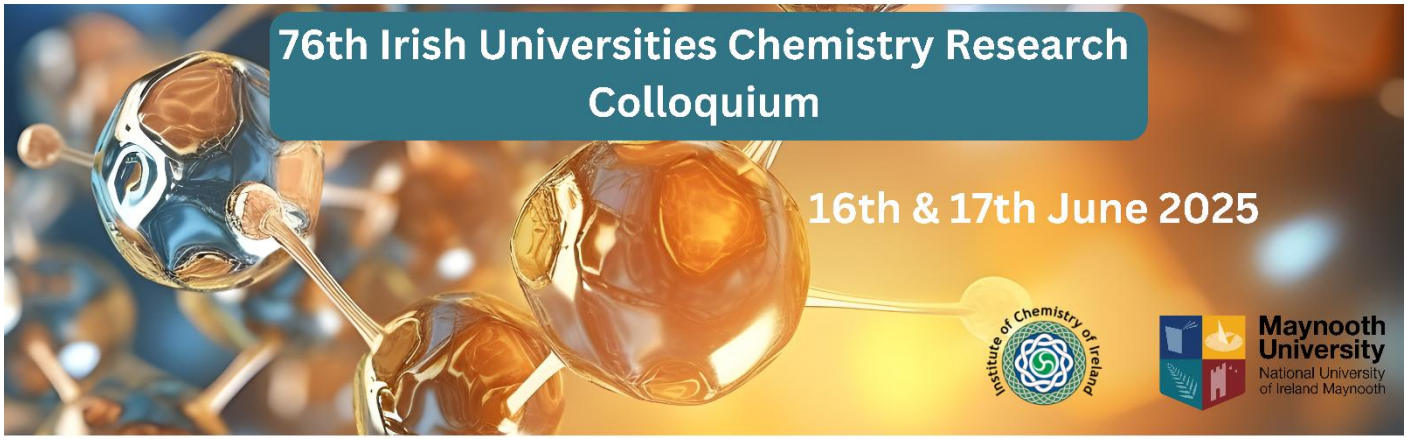
Join international CPD community

Become CPD-Ambassador

This Summer School is recognized by

EuChemS
European Chemical Society

Information, Programme, and Registration
5th STEM-CPD Summer School



Welcome

The 76th edition of the Chemistry Colloquium run annually under the aegis of the Institute of Chemistry of Ireland will be hosted this year at Maynooth University on the **16th-17th June 2025** by the Department of Chemistry.

Speakers will include:

- Dr Michelle Browne, Helmholtz-Zentrum, Berlin
- Professor Steven Bell, Queen's University, Belfast

Format for the Colloquium. We will follow the successful format of recent years. All final year PhD students are welcome to present their research. To achieve this, there will be multiple parallel sessions. For other postgraduate and postdoctoral researchers, there will be a poster session and combined drinks/dinner reception in the evening of the 16th of June. All participants will be welcome to a BBQ dinner and drinks at the MSU Building on campus, in the evening of 16th June.

Oral and Poster Presentations

All final year postgraduate students are encouraged to submit an abstract and are guaranteed an oral presentation slot.

All other students who submit an abstract for an oral presentation may be allocated a speaking slot if sufficient slots are available. If there are not sufficient slots available, these students are guaranteed an opportunity for a poster presentation .

All students and post docs who submit an abstract for a poster presentation are guaranteed that opportunity.

Theme Areas for Abstract Submission

- Organic Synthesis
- Medicinal Chemistry
- Materials

- Sustainable and Environmental Chemistry
- Reaction Mechanism and Computational Chemistry
- Electrochemistry

Oral Presentations should be either 15 or 20 minutes in length (tbc) including time for questions.

Poster Presentations should be printed in standard format A0 or A1 size.

Full details on the list below are available on the Colloquium web site:

https://www.maynoothuniversity.ie/chemistry/76th-chemistry-colloquium-2025#:~:text=The%2076th%20edition%20of,Browne%2C%20Helmholtz%2DZentrum%2C%20Berlin

Location
Plenary Speakers
Registration and Payment Details
Accommodation
Abstract Submission Information
Programme and Book of Abstracts
Sponsors

Sincere Gratitude To All Our Sponsors

We are very grateful to our many Sponsors without whom the 76th Colloquium would not have been possible.

Universities Research & Publications in Ireland

University College Dublin, School of Chemistry, Publications 2024, Focus on Journal Articles

* Principal Contact

Expedited access to β-lactams via a telescoped three-component Staudinger reaction in flow

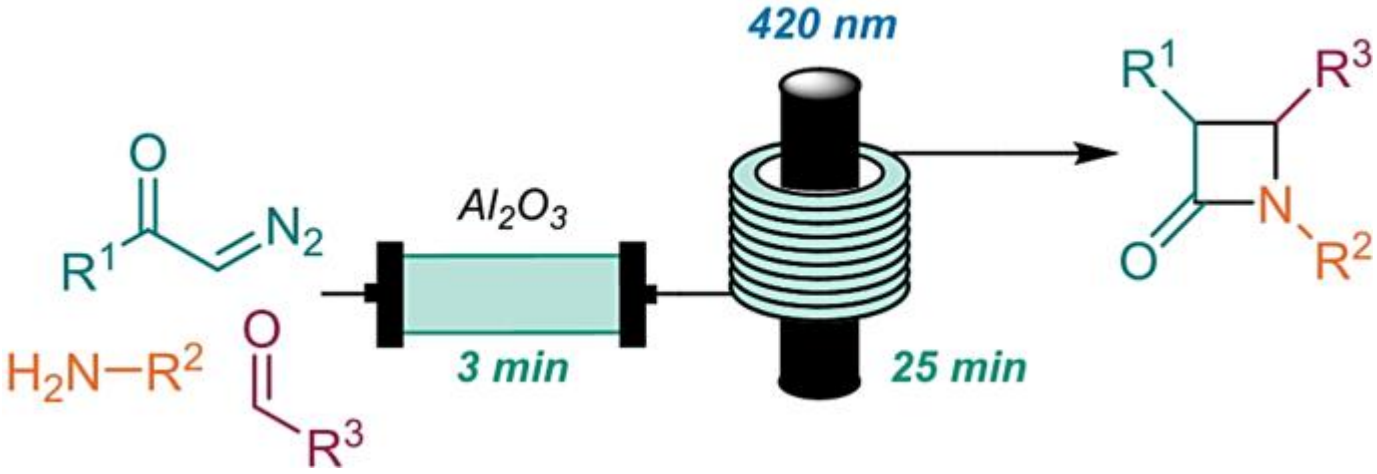
Federica Minuto, Andrea Basso & Marcus Baumann*

J Flow Chem **14**, 615–621 (2024).
https://doi.org/10.1007/s41981-024-00333-0 or https://rdcu.be/eiCrc
Published 23 August 2024
Open Access

Abstract

The Staudinger reaction is widely used for the generation of β-lactams *via* the thermal cycloaddition of imines with ketenes. Traditionally, it cannot be performed as a multicomponent reaction between aldehydes, amines and ketenes, thus limiting its versatility. Recently we reported for the first time a three-component Staudinger reaction in batch, exploiting a photochemical Wolff rearrangement of diazoketones and an in-situ generation of the imine. Here we report an expedited continuous flow approach that generates the crucial ketene intermediate prior to its telescoped reaction with an imine component at ambient temperatures. The imine is prepared by an in situ dehydration between amines and aldehydes in a packed bed reactor containing basic alumina as drying agent. The resulting telescoped flow approach features a fast dehydration reaction (t_{Res} ca. 3 min) as well as an efficient Wolff rearrangement using LEDs (420 nm) to afford the desired β-lactam products in less than 30 min which compares favourably with reaction times of several days in batch mode. Flow processing thereby affords a safe and streamlined entry to these important targets and allows their effective generation on gram scale. Moreover, this approach exploits several homogeneous and heterogeneous transformations under mild conditions that generate water and nitrogen gas as the only by-products.

Graphical Abstract



Acyl-1,4-Dihydropyridines: Universal Acylation Reagents for Organic Synthesis

Karthikeyan Manoharan[1] and Bartosz Bieszczad[1,2,*]
[1] Centre for Synthesis and Chemical Biology, School of Chemistry, University College Dublin, Belfield, D04 V1W8 Dublin, Ireland
[2] School of Chemical and Pharmaceutical Sciences, Technological University Dublin, City Campus, Grangegorman, D07 H6K8 Dublin, Ireland
[*]Author to whom correspondence should be addressed.
Molecules 2024, 29(16), 3844
https://doi.org/10.3390/molecules29163844
Published: 13 August 2024
Open Access
(This article belongs to the Special Issue Featured Reviews in Organic Chemistry 2024)

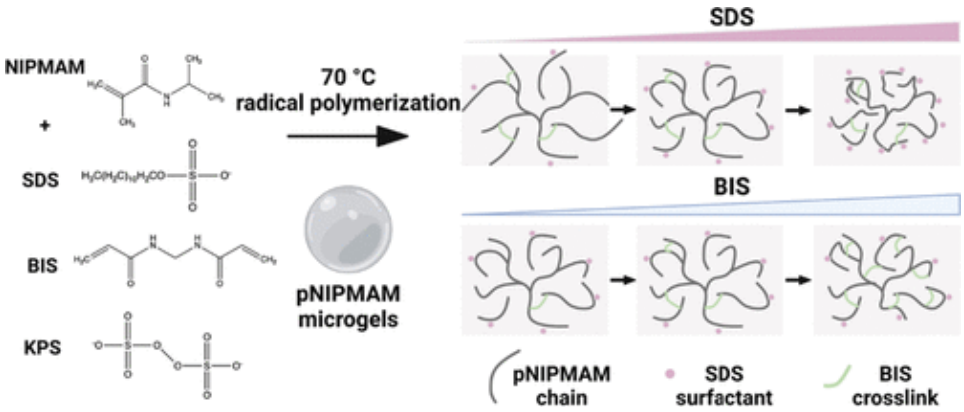
Abstract
Acyl-1,4-dihydropyridines have recently emerged as universal acylation reagents. These easy-to-make and bench-stable NADH biomimetics play the dual role of single-electron reductants and sources of acyl radicals. This review article discusses applications of acyl-1,4-dihydropyridines in organic synthesis since their introduction in 2019. Acyl-1,4-dihydropyridines, activated by photochemical, thermal or electrochemical methods, have been successfully applied as radical sources in multiple diverse organic transformations such as acyl radical addition to olefins, alkynes, imines and other acceptors, as well as in the late-stage functionalisation of natural products and APIs. Release of acyl radicals and an electron can be performed under mild conditions—in green solvents, under air and sunlight, and without the use of photocatalysts, photosensitizers or external oxidants—which makes them ideal reagents for organic chemists.

Thermoresponsiveness Across the Physiologically Accessible Range: Effect of Surfactant, Cross-Linker, and Initiator Content on Size, Structure, and Transition Temperature of Poly(N-isopropylmethacrylamide) Microgels

Danielle Winning, Jacek K. Wychowaniec*, Bing Wu, Andreas Heise, Brian J. Rodriguez Dermot F. Brougham*
ACS Omega 2024, 9, 34, 36185–36197
https://doi.org/10.1021/acsomega.4c02115
Published August 12, 2024

Abstract
The influence of surfactant, cross-linker, and initiator on the final structure and thermoresponse of poly(*N*-isopropylmethacrylamide) (pNIPMAM) microgels was evaluated. The goals were to control particle size (into the nanorange) and transition temperature (across the physiologically accessible range). The concentration of the reactants used in the synthesis was varied, except for the monomer, which was kept constant. The thermoresponsive suspensions formed were characterized by dynamic light scattering, small-angle X-ray scattering, atomic force microscopy, and rheology. Increasing surfactant, sodium dodecyl sulfate content, produced smaller microgels, as expected, into the nanorange and with greater internal entanglement, but with no change in phase transition temperature (LCST), which is contrary to previous reports. Increasing cross-linker, *N*,*N*-methylenebis acrylamide, content had no impact on particle size but reduced particle deformability and, again contrary to previous reports of decreases, progressively increased the LCST from 39 to 46 °C. The unusual LCST trends were confirmed using different rheological techniques. Initiator, potassium persulfate, content was found to weakly influence the outcomes. An optimized content was identified that provides functional nanogels in the 100 nm (swollen) size range with controlled LCST, just above physiological temperature. The study contributes chemistry-derived design rules for thermally responsive colloidal particles with physiologically accessible LCST for a variety of biomedical and soft robotics applications.

Graphical Abstract



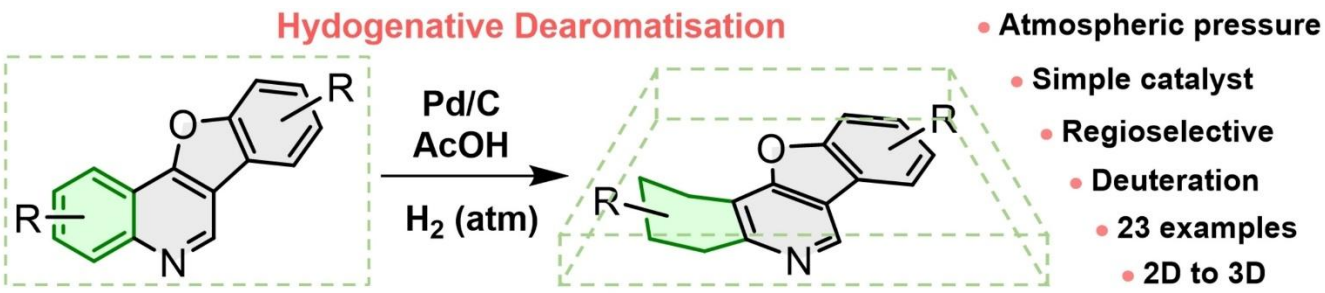
Regioselective Partial Hydrogenation and Deuteration of Tetracyclic (Hetero)aromatic Systems Using a Simple Heterogeneous Catalyst

Roberta A. Kehoe, Dr. Amy Lowry, Dr. Mark E. Light, Dr. David J. Jones, Dr. Peter A. Byrne, Dr. Gerard P. McGlacken* (UCC, SSPC-UL, University of, Southampton, University of Edinburgh, UCD),

Chemistry A European Journal Volume30, Issue17 March 20, 2024 e202400102
https://doi.org/10.1002/chem.202400102
First published: 12 January 2024

Abstract
The introduction of added '3-dimensionality' through late-stage functionalisation of extended (hetero)aromatic systems is a powerful synthetic approach. The abundance of starting materials and cross-coupling methodologies to access the precursors allows for highly diverse products. Subsequent selective partial reduction can alter the core structure in a manner of interest to medicinal chemists. Herein, we describe the precise, partial reduction of multicyclic heteroaromatic systems using a simple heterogeneous catalyst. The approach can be extended to introduce deuterium (again at late-stage). Excellent yields can be obtained using simple reaction conditions.

Graphical Abstract
The introduction of added '3-dimensionality' through late-stage functionalisation is a powerful synthetic approach to biologically significant moieties. Herein, a hydrogenative, regioselective dearomatisation of extended (hetero)aromatic systems is described, using a simple Pd catalyst at atmospheric hydrogen pressure. Deuteration is also demonstrated, and some initial mechanistic insights are revealed.



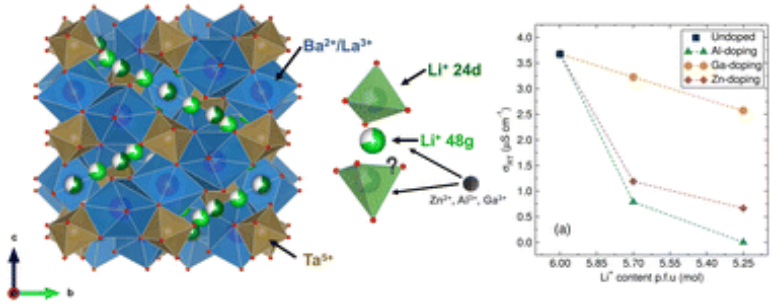
The effect of aliovalent dopants on the structural and transport properties of Li6La2BaTa2O12 garnet Li-ion solid electrolytes†

Marco Amores, *[a] Peter J. Baker, [b] Edmund J. Cussen [c] and Serena A. Cussen *[d]
(University, Geelong, Australia, Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, UK, Technological University Dublin, University College Dublin)
Mater. Adv., 2024,**5**, 8826-8835
https://doi.org/10.1039/D4MA00679H
First published 01 Oct 2024

Abstract

Li-rich garnet solid electrolytes are promising candidates for all-solid-state batteries, allowing for increased energy densities, compatibility with Li-metal anodes and improved safety by replacing flammable organic-based liquid electrolytes. Li-stuffed garnets typically require aliovalent doping to stabilise the highly ionic conductive $Ia\bar{3}d$ cubic phase. The role of dopants and their location within the garnet framework can greatly affect the conduction properties of these garnets, yet their impact on the structure and resulting ion transport is not fully understood. Here, we evaluate the effect of aliovalent doping with Al^{3+}, Ga^{3+} and Zn^{2+} in the $Li_6BaLa_2Ta_2O_{12}$ (LBLTO) garnet material. A combination of PXRD and XAS reveals a linear cell parameter contraction with an increase in doping and the preference of the 24d Li^+ sites for Al^{3+} and Zn^{2+} dopants, with Ga^{3+} occupying both the 24d and 48g Li^+ sites. Macroscopic ionic conductivity analyses by EIS demonstrate an enhancement of the transport properties where addition of small amounts of Al^{3+} decreases the activation energy to Li^+ diffusion to 0.35(4) eV. A detrimental effect on ionic conductivities is observed when dopants were introduced in Li^+ pathways and upon decreasing the Li^+ concentration. Insights into this behaviour are gleaned from microscopic diffusion studies by muon spin relaxation (μ^+SR) spectroscopy, which reveals a low activation energy barrier for Li^+ diffusion of 0.16(1) eV and a diffusion coefficient comparable to those of $Li_7La_3Zr_2O_{12}$ (LLZO) benchmark garnet materials.

Graphical Abstract



- This article is part of the themed collection: Celebrating International Women's day 2025: Women in Materials Science

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Investigation of sodium insertion in hard carbon with operando small angle neutron scattering†

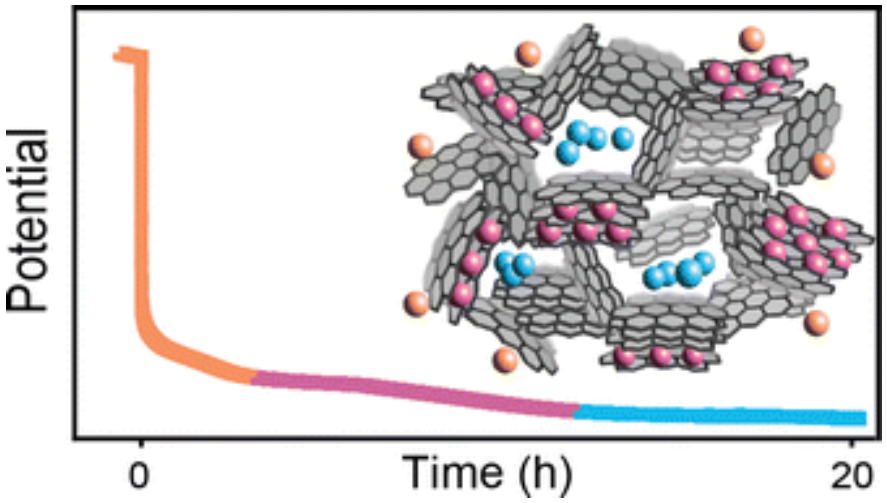
Emily M. Reynolds, [ab] Jack Fitzpatrick,[ac] Martin O. Jones,[ab] Nuria Tapia-Ruiz,[ac] Helen Y. Playford, [ab] Stephen Hull,[ab] Innes McClelland, [ad] Peter J. Baker, [ab] Serena A. Cussen ‡[ad] and Gabriel E. Pérez *[ab]
J. Mater. Chem. A, 2024,**12**, 18469-18475
https://doi.org/10.1039/D3TA04739C

Abstract

Sodium-ion battery technology is a promising and more sustainable alternative to its more conventional lithium-ion based counterpart. The most common anode material for these systems is a disordered form of graphite known as hard carbon. The inherent disorder in these carbons results in multiple possible pathways for sodium storage making the characterisation of sodiation

mechanisms during cycling highly challenging. Here, we report an *operando* small angle neutron scattering (SANS) investigation of sodiation in a commercial hard carbon using a custom electrochemical cell. We demonstrate that it is possible to discern different sodiation mechanisms throughout cycling and provide supporting evidence for a three-stage model in which sodium ions are first adsorbed onto the surface of particles, then intercalated into the graphene layers, and finally inserted into the nanopores during the electrochemical stage known as the plateau region. This study showcases the unique capabilities of *operando* SANS for the characterisation of sodiation mechanisms of carbon-based, disordered, porous materials.

Graphical Abstract



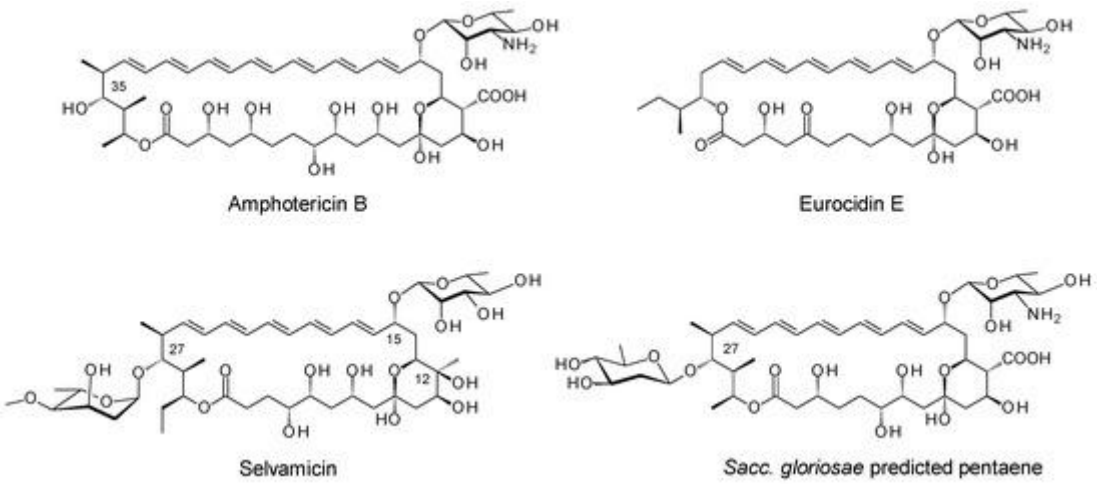
Characterisation of Modular Polyketide Synthases Designed to Make Pentaene Analogues of Amphotericin B

Yuhao Song [1], Mark Hogan[1], Jimmy Muldoon [2], Paul Evans [2] and Patrick Caffrey [1,*]
1.School of Biomolecular and Biomedical Science, University College Dublin, D04 V1W8 Dublin
2.School of Chemistry and Centre for Synthesis and Chemical Biology, University College Dublin
Molecules **2024**, *29*(6), 1396
https://doi.org/10.3390/molecules29061396
Published: 21 March 2024

Abstract

Glycosylated polyene macrolides are important antifungal agents that are produced by many actinomycete species. Development of new polyenes may deliver improved antibiotics.
Here, *Streptomyces nodosus* was genetically re-programmed to synthesise pentaene analogues of the heptaene amphotericin B. These pentaenes are of interest as surrogate substrates for enzymes catalysing unusual, late-stage biosynthetic modifications. The previous deletion of amphotericin polyketide synthase modules 5 and 6 generated *S. nodosus* M57, which produces an inactive pentaene. Here, the chain-terminating thioesterase was fused to module 16 to generate strain M57-16TE, in which cycles 5, 6, 17 and 18 are eliminated from the biosynthetic pathway. Another variant of M57 was obtained by replacing modules 15, 16 and 17 with a single 15–17 hybrid module. This gave strain M57-1517, in which cycles 5, 6, 15 and 16 are deleted. M57-16TE and M57-1517 gave reduced pentaene yields. Only M57-1517 delivered its predicted full-length pentaene macrolactone in low amounts. For both mutants, the major pentaenes were intermediates released from modules 10, 11 and 12. Longer pentaene chains were unstable. The novel pentaenes were not glycosylated and were not active against *Candida albicans*. However, random mutagenesis and screening may yet deliver new antifungal producers from the M57-16TE and M57-1517 strains.

Graphical Abstract



Advances in the Chemistry and Biology of Specialised Pro-Resolving Mediators (SPMs)

Lucy Byrne and Patrick J. Guiry
Centre for Synthesis and Chemical Biology, UCD School of Chemistry, University College Dublin
Molecules 2024, *29*(10), 2233
https://doi.org/10.3390/molecules29102233
Published 10 May 2024

Abstract

This review article assembles key recent advances in the synthetic chemistry and biology of specialised pro-resolving mediators (SPMs). The major medicinal chemistry developments in the design, synthesis and biological evaluation of synthetic SPM analogues of lipoxins and resolvins have been discussed. These include variations in the top and bottom chains, as well as changes to the triene core, of lipoxins, all changes intended to enhance the metabolic stability whilst retaining or improving biological activity. Similar chemical modifications of resolvins are also discussed. The biological evaluation of these synthetic SPMs is also described in some detail. Original investigations into the biological activity of endogenous SPMs led to the pairing of these ligands with the FPR2/LX receptor, and these results have been challenged in more recent work, leading to conflicting results and views, which are again discussed.

Enantioselective Synthesis of Sterically Hindered α-Allyl-α-Aryl Lactams via Palladium-Catalysed Decarboxylative Asymmetric Allylic Alkylation

Declan J. Galvin, Patrick J. Guiry*
Centre for Synthesis and Chemical Biology, School of Chemistry, University College Dublin
European Journal of Organic Chemistry Volume27, Issue23
https://doi.org/10.1002/ejoc.202400314
Published 17 April 2024

Abstract

The Pd-catalysed decarboxylative asymmetric allylic alkylation (DAAA) of sterically hindered α-aryl,β-amido allyl ester lactams has been developed. The key step in the synthesis of a range of α-aryl lactam substrates for catalysis was a Pb-mediated α-arylation of a β-amido allyl ester affording 14 novel examples of α-aryl-β-amido allyl ester lactams in good yields (up to 80 %). The Pd-catalysed DAAA was optimised with the 2,4,6-trimethoxyphenyl-containing substrate. Using (*S*,*S*)-DACH-phenyl Trost as the optimal chiral ligand, enantioselectivities of up to 82 % ee were obtained. A substrate scope of 11 examples of α-aryl-β-amido allyl ester lactams showed that products containing

the di-*ortho*-methoxy-substituted phenyls and naphthyl groups gave rise to the highest ees, whereas products not bearing this substitution pattern showed lower enantioselectivities (<60 % *ee*). Transition states to rationalise the observed stereochemical outcome are proposed.

Graphical Abstract

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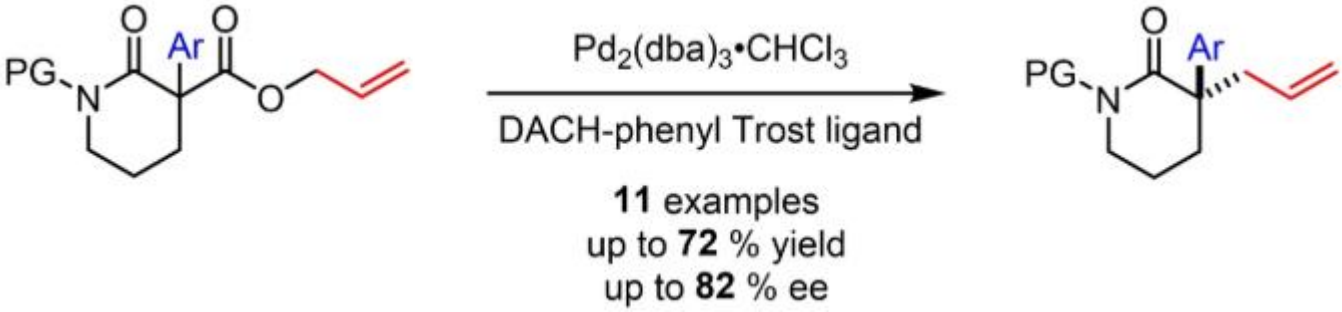


Synthesis of a Bicyclo[1.1.1]pentane-Containing Aromatic Lipoxin B4 Analogue and Heteroaromatic Congeners

Benjamin Owen, Patrick J. Guiry*

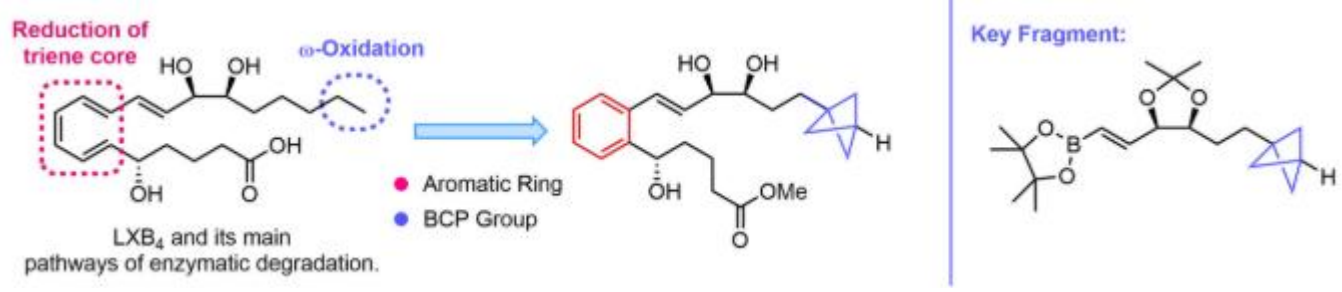
European Journal of Organic Chemistry, 27(23)
https://doi.org/10.1002/ejoc.202400256
Published 23 March 2024

Abstract

Lipoxins are pro-resolving mediators that play an important role in the resolution phase of the innate inflammatory response. However, because of their chemical and metabolic instability, the design of more stable synthetic analogues of lipoxin A_4 and lipoxin B_4 is an ongoing area of study. Herein we report the asymmetric synthesis of an aromatic lipoxin B_4 analogue containing a conformationally rigid and potentially more metabolically resistant bicyclo[1.1.1]pentane (BCP) ring incorporated into the upper alkyl chain. This was achieved by the development of a 9-step chiral-pool synthesis of a novel BCP-containing boronic ester coupling partner which could serve as a common precursor to the target analogue as well as other analogues with further modifications to the aromatic core.

Graphical Abstract

This work describes the asymmetric synthesis of an aromatic analogue of lipoxin B_4 containing a conformationally rigid and potentially more metabolically resistant bicyclo[1.1.1]pentane (BCP) ring incorporated into the upper alkyl chain. This was achieved via the design of a key BCP-containing fragment that could be used as a common intermediate in the synthesis of the target analogue as well as other heteroaromatic congeners.



Commercial Transaminases for the Asymmetric Synthesis of Bulky Amines

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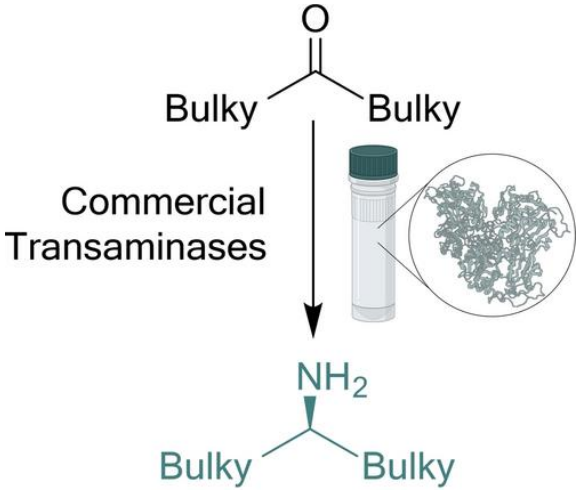
School of Chemistry, University College Dublin Belfield, Dublin
Asymmetric Synthesis of Bulky Amines.
European Journal of Organic Chemistry, 27(23)
https://doi.org/10.1002/ejoc.202400257
Published 24 March 2024

Abstract
Transaminase-catalysed asymmetric amination is a valuable transformation for the synthesis of chiral amines. However, its use in synthetic chemistry has been curtailed by a narrow substrate scope and limited information on commercially available catalysts. In this work we have explored the substrate scope of selected commercially available transaminases, focusing on prochiral ketones bearing two bulky substituents and their application in both enzyme-catalysed and enzyme-triggered reactions. (R)- and/or (S)-selective enzymes converted methyl-, isopropyl-, n-butyl-, and cyclohexyl-phenone substrates to the corresponding amines in the range of 6–>99 % ee. In some cases, a stereochemical switch was detected, in which (R)-enantioselectivity was observed with enzymes typically assigned as (S)-selective. Upscaling of selected biotransformations provided chiral amines, in >99 % ee and up to 40 % isolated yield. Furthermore, transaminase-triggered reactions, which were previously limited to methyl- and ethyl-derivatives, were expanded to phenyl-derivatives for the formation of a cis-2,6-disubstituted piperidine and 2,4-diphenyl pyrroline, and isolated in up to 67 % yield.
Graphical Abstract
Commercially available transaminases are valuable tools for the synthesis of chiral amine building blocks and are very accessible to the synthetic chemistry community. We demonstrate that selected commercially available enzymes from Codexis' transaminase collection can accept and aminate bulky-bulky ketones in up to 99 % ee.



Comparative Proton Coupled Electron Transfer at Glassy Carbon and Boron-Doped Diamond Electrodes

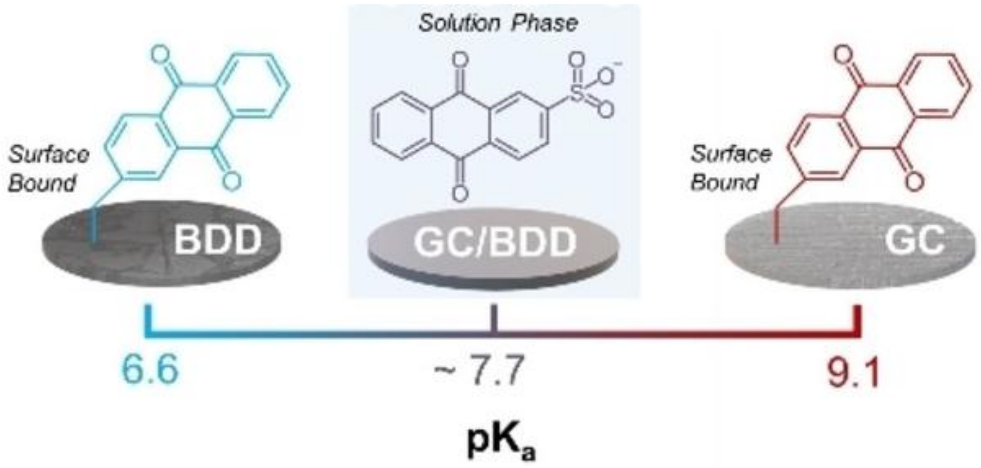
Shane P. O. Neill, Dr. Adrià Martínez-Aviñó, Charlie Keene, Sammi Hassan, Catriona Houston, Shekemi Denuga, Emer B. Farrell, Dr. Guzmán Gil-Ramírez, Dr. Robert P. Johnson
School of Chemistry, University College Dublin, Belfield, Dublin
***ChemElectroChem*, *11*(4)**
https://doi.org/10.1002/celc.202300470
Published 8 January 2024

Abstract
The surface modification of carbon electrodes is an area of great interest in both fundamental and applied electrochemistry. Herein we demonstrate a reliable route for the modification of sp3 boron-

doped diamond electrodes through a diazonium reduction and subsequent solid phase synthesis to produce a stable, immobilised layer of surface-bound anthraquinone. The electron transfer kinetics, surface coverage, and pKa of the immobilised anthraquinone were investigated and compared to those of anthraquinone immobilised via an identical synthetic route onto a glassy carbon sp2 interface. The pKa of anthraquinone was found to be 9.1 on glassy carbon but 6.6 on boron-doped diamond. Differences in pKa were observed despite the use of identical surface modification strategies and the achievement of comparable surface densities for both types of electrode, and are attributed to the differing dielectric properties of the surface-modified layers atop either an sp2 or sp3 interface. These results highlight how the underlying substrate can greatly influence the fundamental chemical and electrochemical properties of immobilised molecules, as well as the need for caution when applying well-established sp2 solid phase synthesis methodologies to sp3 substrates.

Graphical Abstract

The pK_a of anthraquinone in solution is circa 7.7, however when immobilised at an sp^2 glassy carbon interface the pK_a value shifts to 9.1, yet when immobilised at an sp^3 boron doped diamond interface the pK_a shifts to 6.6. This study highlights the need for caution when immobilising redox molecules to predominantly sp^3 surfaces using surface modification routes previously established for sp^2 interfaces.



Reproducibility and stability of silane layers in nanoconfined electrochemical systems

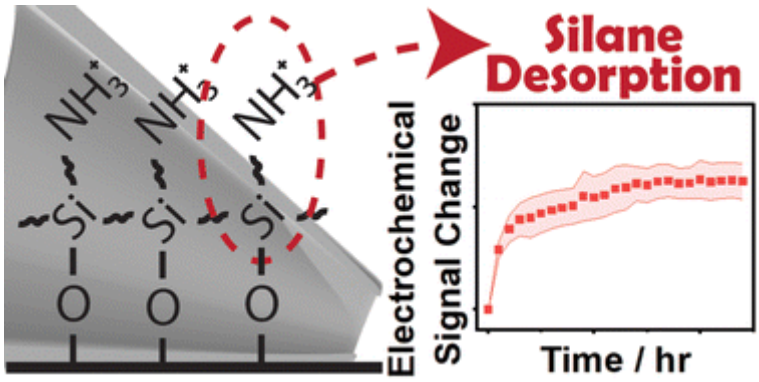
Dominik Duleba, [a] Shekemi Denuga [a] and Robert P. Johnson *[a]
University College Dublin
Phys. Chem. Chem. Phys., 2024,**26**, 15452-15460
DOI https://doi.org/10.1039/D4CP01181C

Abstract

Organosilanes are commonly utilized to attach bioreceptors to oxide surfaces. The deposition of such silane layers is especially challenging in nanoscale or nanoconfined devices, such as in nanopipettes, since rinsing off loosely bound silanes may not be possible due to geometric constrictions and because the thickness of multilayered silanes can cover or block nanoscale features. Furthermore, in electrochemical devices, the silane layers experience additional perturbations, such as electric migration and electroosmotic force. Despite its importance, there appears to be no consensus in the current literature on the optimal methodology for nanopipette silanization, with significant variations in reported conditions. Herein, we systematically investigate the reproducibility and stability of liquid- and vapor-phase deposited silane layers inside nanopipettes. Electrochemical monitoring of the changing internal silanized surface reveals that vapor-deposited APTES generates surface modifications with the highest reproducibility, while vapor-deposited APTMS generates surface modifications of the highest stability over a 24-hour time period. Practical issues of silanizing nanoconfined systems are highlighted, and the importance of carefully chosen silanization conditions

to yield stable and reproducible monolayers is emphasized as an underappreciated aspect in the development of novel nanoscale systems.

Graphical Abstract



Crystal structure and Hirshfeld surface of a penta-amine-copper(II) complex with urea and chloride

Olivia D. Breen[a] and Tony D. Keene[a]*
School of Chemistry, University College Dublin
Crystallographic Communications Volume 80| Part 6
https://doi.org/10.1107/S2056989024004298
Published June 2024

Chemical context (No Abstract)

Copper oxalate, Cu(ox), is primarily a synthetic compound that has been the subject of much research and can also be found naturally as the mineral moolooite (Clarke & Williams, 1986[Clarke, R. M. & Williams, I. R. (1986). Miner. Mag. 50, 295-298.]). It has been examined as a potential precursor to forming copper oxide particles with controlled morphologies (Rahimi-Nasrabadi et al., 2013[Rahimi-Nasrabadi, M., Pourmortazavi, S. M., Davoudi-Dehaghani, A. A., Hajimirsadeghi, S. S. & Zahedi, M. M. (2013). CrystEngComm, 15, 4077-4086.]) and has been the subject of thorough investigation of its structure (Fichtner-Schmittler, 1984[Fichtner-Schmittler, H. (1984). Cryst. Res. Technol. 19, 1225-1230.]; O'Connor et al., 2019[O'Connor, B. H., Clarke, R. M. & Kimpton, J. A. (2019). Powder Diffr. 34, 21-34.]; Kornyakov et al., 2023[Kornyakov, I. V., Gurzhiy, V. V., Kuz'mina, M. A., Krzhizhanovskaya, M. G., Chukanov, N. V., Chislov, M. V., Korneev, A. V. & Izatulina, A. R. (2023). Int. J. Mol. Sci. 24, 6786.]). Unlike other first row transition-metal oxalate compounds, which form mainly as dihydrates, copper oxalate forms as anhydrous chains with chemisorbed water on the particle's surface, with the amount of water being dependent on the reaction conditions. The amount of water present also contributes to disorder (O'Connor et al., 2019[O'Connor, B. H., Clarke, R. M. & Kimpton, J. A. (2019). Powder Diffr. 34, 21-34.]; Kornyakov et al., 2023[Kornyakov, I. V., Gurzhiy, V. V., Kuz'mina, M. A., Krzhizhanovskaya, M. G., Chukanov, N. V., Chislov, M. V., Korneev, A. V. & Izatulina, A. R. (2023). Int. J. Mol. Sci. 24, 6786.]). Copper oxalate forms as a microcrystalline powder so we were inter-ested in investigating the use of alternative solvents that could allow for the synthesis of single crystals of anhydrous copper oxalate compounds.

Enantioconvergent and Site-Selective Etherification of Carbohydrate Polyols through Chiral Copper Radical Catalysis

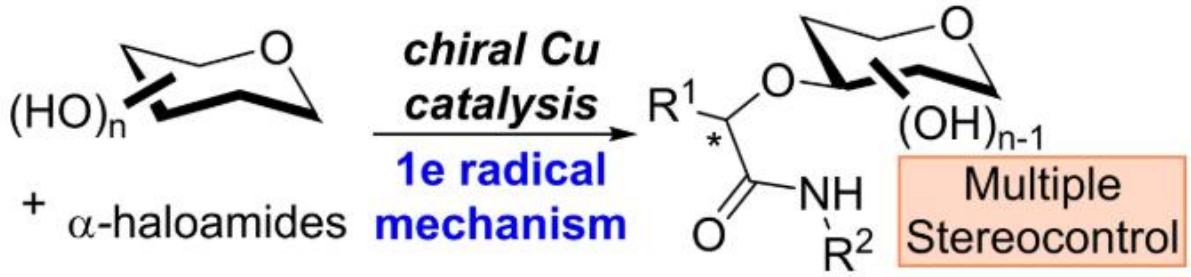
Dr. Hao Guo, Dilber Tan, Prof. Dr. Christian Merten, Dr. Charles C. J. Loh*
*School of Chemistry, University College Dublin
Angewandte Chemie - International Edition Volume63, Issue48 November 25, 2024 e202409530
https://doi.org/10.1002/anie.202409530
First Published 16 August 2024

Abstract

Going beyond currently reported two electron transformations that formed the core backdrop of asymmetric catalytic site-selective carbohydrate polyol functionalizations, we herein report a seminal demonstration of an enantioconvergent copper catalyzed site-selective etherification of minimally protected saccharides through a single-electron radical pathway. Further, this strategy paves a rare strategy, through which a carboxamide scaffold that is present in some glycomimetics of pharmacological relevance, can be selectively introduced. In light of the burgeoning interest in chiral radical catalysis, and the virtual absence of such stereocontrol broadly in carbohydrate synthesis, our strategy showcased the unknown capability of chiral radical copper catalysis as a contemporary tool to address the formidable site-selectivity challenge on a remarkable palette of naturally occurring saccharides. When reducing sugars were employed, a further dynamic kinetic resolution type glycosylation can be activated by the catalytic system to selectively generate the challenging β-*O*-glycosides.

Graphical Abstract

By harnessing a chiral radical copper catalytic system, the challenging enantioconvergent and site-selective etherification of carbohydrate polyols is achieved. Besides being broadly applicable over a considerable range of sugars, multiple dimensions of stereocontrol can be tackled simultaneously. Remarkably, when anomeric unprotected reducing sugars were employed, dynamic kinetic resolution is further activated to achieve β-O-glycosylation.



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First Published 16 August 2024

Abstract

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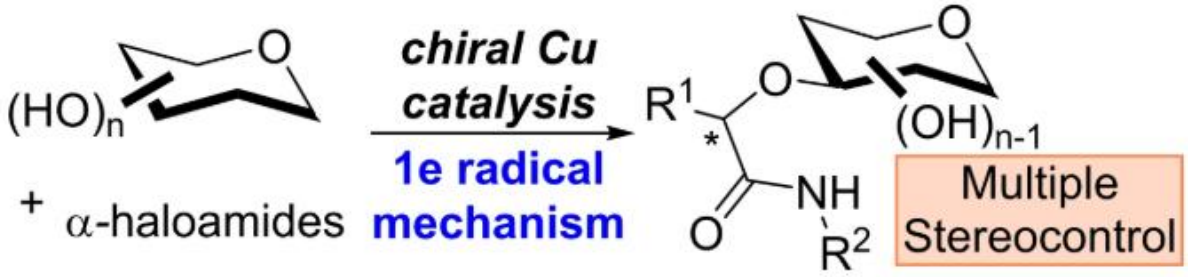


Organotransition Metal Chemistry of Terpenes: Syntheses, Structures, Reactivity and Molecular Rearrangements

Michael J. McGlinchey
School of Chemistry, University College Dublin
Molecules 2024, 29(6), 1409
https://doi.org/10.3390/molecules29061409
Published 21 March 2024

Abstract

The impact of organometallic chemistry on the terpene field only really blossomed in the 1960s and 1970s with the realisation that carbon–carbon bond formation under mild conditions could be achieved by using nickel or iron carbonyls as synthetic reagents. Concomitantly, the development of palladium derivatives capable of the controlled coupling of isoprene units attracted the attention of numerous highly talented researchers, including future Nobel laureates. We discuss briefly how early work on the syntheses of simple monoterpenes soon progressed to sesquiterpenes and diterpenes of increasing complexity, such as humulene, flexibilene, vitamin A, or pheromones of commercial value, in particular those used in perfumery (muscone, lavandulol), or grandisol and red scale pheromone as replacements for harmful pesticides. As the field progressed, there has been more emphasis on developing organometallic routes to enantiopure rather than racemic products, as well as gaining precise mechanistic data on the transformations, notably the course of metal-promoted molecular rearrangements that have long been a feature of terpene chemistry. We note the impact of the enormously enhanced analytical techniques, high-field NMR spectroscopy and X-ray crystallography, and their use to re-examine the originally proposed structures of terpenes and their organometallic derivatives. Finally, we highlight the very recent ground-breaking use of the crystalline sponge method to acquire structural data on low-melting or volatile terpenes. The literature cited herein covers the period 1959 to 2023.

Total synthesis of antifungal lipopeptide iturin A analogues and evaluation of their bioactivity against F. graminearum

Periklis Karamanis, Jimmy Muldoon, Cormac D. Murphy*, Marina Rubini*
BiOrbic Bioeconomy SFI Research Centre, UCD School of Chemistry, University College Dublin
Journal of Peptide Science Volume30, Issue6 June 2024 e3569
https://doi.org/10.1002/psc.3569
First published: 01 February 2024

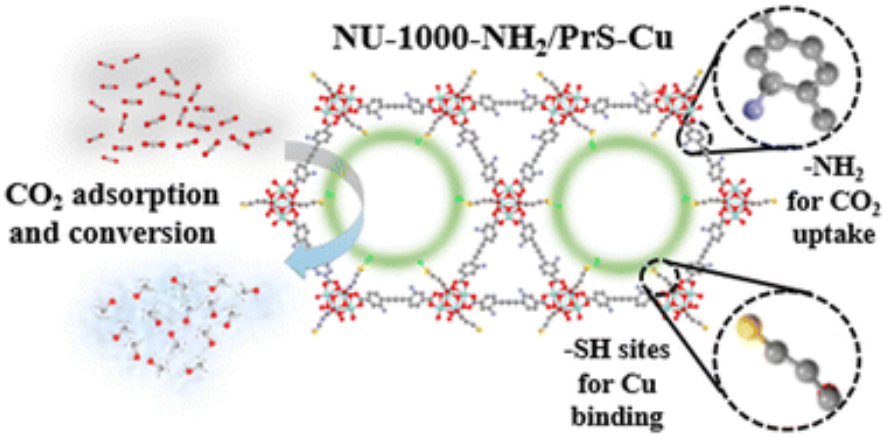
Abstract
The pursuit of novel antifungal agents is imperative to tackle the threat of antifungal resistance, which poses major risks to both human health and to food security. Iturin A is a cyclic lipopeptide, produced by *Bacillus* sp., with pronounced antifungal properties against several pathogens. Its challenging synthesis, mainly due to the laborious synthesis of the β-amino fatty acid present in its structure, has hindered the study of its mode of action and the development of more potent analogues. In this work, a facile synthesis of bioactive iturin A analogues containing an alkylated cysteine residue is presented. Two analogues with opposite configurations of the alkylated cysteine residue were synthesized, to evaluate the role of the stereochemistry of the newly introduced amino acid on the bioactivity. Antifungal assays, conducted against *F. graminearum*, showed that the novel analogues are bioactive and can be used as a synthetic model for the design of new analogues and in structure–activity relationship studies. The assays also highlight the importance of the β-amino acid in the natural structure and the role of the stereochemistry of the amino fatty acid, as the analogue with the D configuration showed stronger antifungal properties than the one with the L configuration.

Multifunctionalized zirconium-based MOF as a novel support for dispersed copper: application in CO_2 adsorption and catalytic conversion†

Albert Rosado, [a] Ioana-Maria Popa,[b] Ahmad Abo Markeb, [cd] Javier Moral-Vico,[c] Eva Maria Naughton, [f] Hans-Georg Eckhardt,[f] José A. Ayllón, [e] Ana M. López-Periago, [a] Concepción Domingo *[a] and Leila Negahdar *[f]
School of Chemistry, University College Dublin and others outside Ireland
J. Mater. Chem. A, 2024,**12**, 21758-21771
https://doi.org/10.1039/D4TA03268C
First Published 19 July 2024

Abstract
CO_2 conversion and utilization for global sustainability is an integral part of greenhouse gases management, typically for the production of fuels and specialty chemicals. Added value products, such as methanol, methane or formate, can be obtained by electrocatalysis and thermocatalysis, the two techniques addressed in this study. The main motivation of this study is to develop a copper based catalyst active in both processes, confronting the main concerns regarding typical metal catalysts related to nanoparticles aggregation and concomitant deactivation. For this, modified NU-1000, a water-stable mesoporous MOF, is used as a platform for the simultaneous coordination–stabilization of copper single atoms and CO_2 adsorption. NU-1000 is synthetized with primary amino groups (–NH_2 with affinity for CO_2) by modifying the ligand prior to MOF synthesis, while post-synthetic solvent-assisted ligand incorporation is applied to insert thiol functionalities (–SH with affinity for copper) within the framework. To make the functionalized MOF catalytically active, a Cu^{2+} salt is impregnated into the MOF channels, which is further reduced with H_2 to Cu^{+}/Cu^{0} before performance assessment in CO_2 conversion processes. The as-synthetized and spent catalysts were analysed regarding the structure (X-ray diffraction, infrared), bulk (mass spectrometry) and surface (X-ray photoelectron spectroscopy) composition, morphology (electronic microscopy and energy dispersive spectroscopy) and textural properties (N_2 physisorption). The electrocatalytic reduction of CO_2 was performed in the potential range of −0.8 to −1.8 V, indicating the formation of formic acid. Thermocatalytic experiments were carried out in an economically and energetically sustainable low-

pressure (1 MPa) hydrogenation process. Methanol was obtained with 100% selectivity at temperatures up to 280 °C, and a space-time yield of *ca.* 100 $mg_{MeOH}\ g_{cat}^{-1}\ h^{-1}$ which overcomes that of commercial CuZnO NPs designed for this purpose.



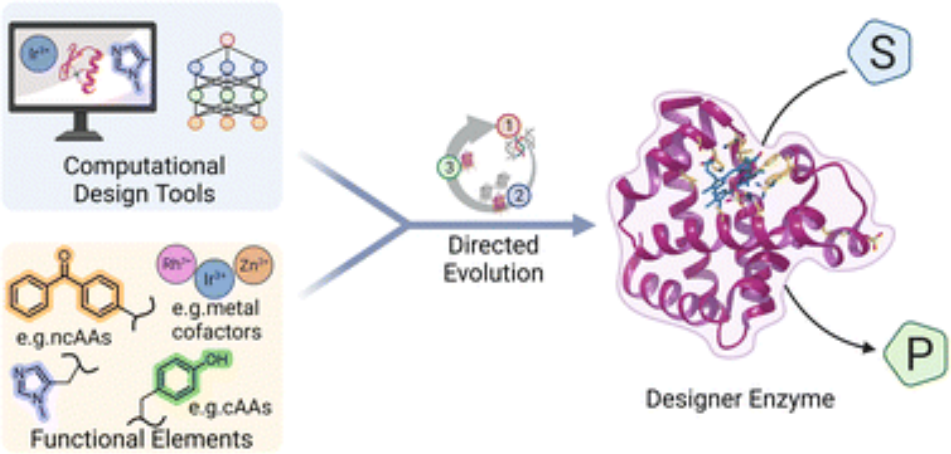
Strategies for designing biocatalysts with new functions

Elizabeth L. Bell, †[ab] Amy E. Hutton,†[b] Ashleigh J. Burke,†[bc] Adam O'Connell, [d] Amber Barry, [d] Elaine O'Reilly *[d] and Anthony P. Green *[b]
School of Chemistry, University College Dublin and others outside Ireland
Chem. Soc. Rev., 2024,**53**, 2851-2862
https://doi.org/10.1039/D3CS00972F
First published 14 Feb 2024

Abstract

The engineering of natural enzymes has led to the availability of a broad range of biocatalysts that can be used for the sustainable manufacturing of a variety of chemicals and pharmaceuticals. However, for many important chemical transformations there are no known enzymes that can serve as starting templates for biocatalyst development. These limitations have fuelled efforts to build entirely new catalytic sites into proteins in order to generate enzymes with functions beyond those found in Nature. This bottom-up approach to enzyme development can also reveal new fundamental insights into the molecular origins of efficient protein catalysis. In this tutorial review, we will survey the different strategies that have been explored for designing new protein catalysts. These methods will be illustrated through key selected examples, which demonstrate how highly proficient and selective biocatalysts can be developed through experimental protein engineering and/or computational design. Given the rapid pace of development in the field, we are optimistic that designer enzymes will begin to play an increasingly prominent role as industrial biocatalysts in the coming years.

Graphical Abstract



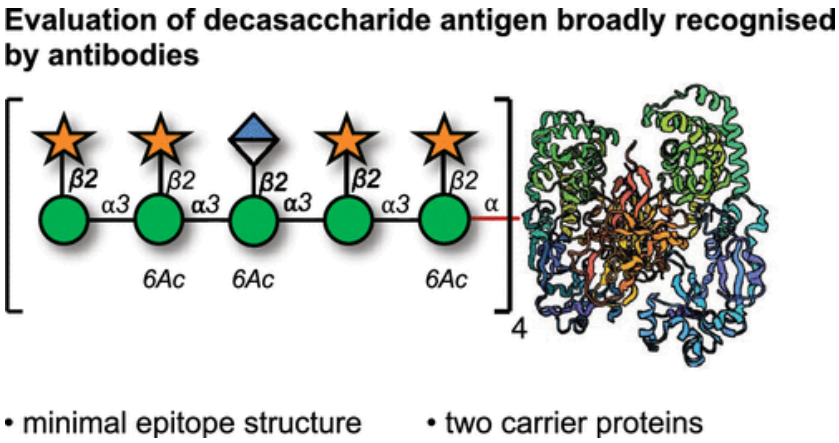
Semisynthetic Glycoconjugate Vaccine Candidates against Cryptococcus neoformans

Conor J. Crawford, Livia Liporagi-Lopes, Carolina Coelho, Samuel R. Santos Junior, André Moraes Nicola, Maggie P. Wear, Raghav Vij, Stefan Oscarson*, Arturo Casadevall*
Centre for Synthesis and Chemical Biology, University College Dublin, Department of Molecular Microbiology and Immunology, Johns Hopkins Bloomberg School of Public Health, Baltimore, Maryland, United States
ACS Infect. Dis. 2024, 10, 6, 2089–2100
https://doi.org/10.1021/acsinfecdis.4c00094
Published May 31, 2024

Abstract

Cryptococcus neoformans is a fungus classified by the World Health Organization as a critically important pathogen, which poses a significant threat to immunocompromised individuals. In this study, we present the chemical synthesis and evaluation of two semisynthetic vaccine candidates targeting the capsular polysaccharide glucuronoxylomannan (GXM) of *C. neoformans*. These semisynthetic glycoconjugate vaccines contain an identical synthetic decasaccharide (M2 motif) antigen. This antigen is present in serotype A strains, which constitute 95% of the clinical cryptococcosis cases. This synthetic oligosaccharide was conjugated to two proteins (CRM197 and Anthrax 63 kDa PA) and tested for immunogenicity in mice. The conjugates elicited a specific antibody response that bound to the M2 motif but also exhibited additional cross-reactivity toward M1 and M4 GXM motifs. Both glycoconjugates produced antibodies that bound to GXM in ELISA assays and to live fungal cells. Mice immunized with the CRM197 glycoconjugate produced weakly opsonic antibodies and displayed trends toward increased median survival relative to mice given a mock PBS injection (18 vs 15 days, $p = 0.06$). These findings indicate promise, achieving a successful vaccine demands further optimization of the glycoconjugate. This antigen could serve as a component in a multivalent GXM motif vaccine.

Graphical Abstract

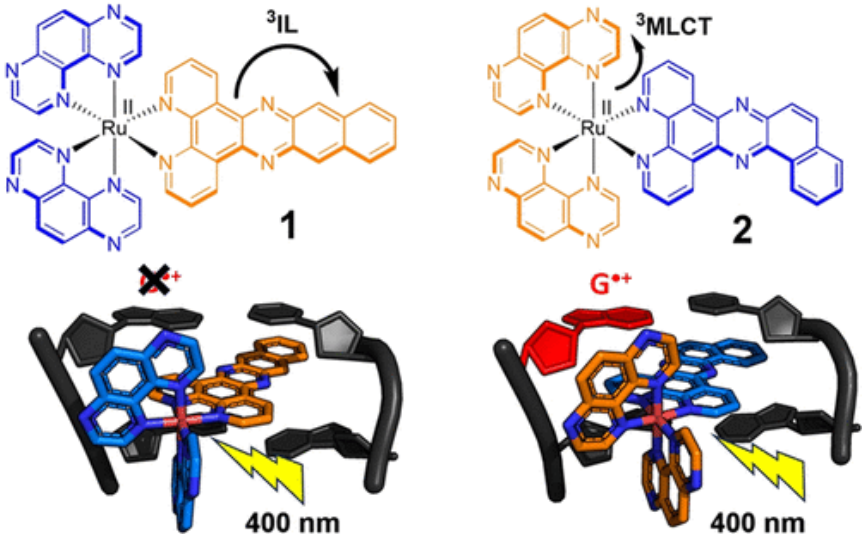


Contrasting Photosensitized Processes of Ru(II) Polypyridyl Structural Isomers Containing Linear and Hooked Intercalating Ligands Bound to Guanine-Rich DNA

Mark Stitch Rosie Sanders Igor V. Sazanovich Michael Towrie Stanley W. Botchway Susan J. Quinn*
Note Author links not active here. Active in the original paper.
School of Chemistry, University College Dublin, Dublin and Central Laser Facility, Research Complex at Harwell, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Oxfordshire

J. Phys. Chem. B 2024, 128, 32, 7803–7812
https://doi.org/10.1021/acs.jpcb.4c04129
Published August 6, 2024

Abstract with Graphical Abstract



The DNA binding and cellular uptake of the lambda enantiomer of two bis-tetraazaphenanthrene (TAP) Ru(II) polypyridyl complexes containing either a linear dppn (**1**) or a hooked bdppz (**2**) benzodipyridophenazine ligand are reported, and the role of different charge-transfer states of the structural isomers in the photo-oxidation of guanine is explored. Both complexes possess characteristic metal-to-ligand charge-transfer (MLCT) bands between 400 and 500 nm and emission at ca. 630 nm in an aerated aqueous solution. Transient visible absorption (TrA) spectroscopy reveals that 400 nm excitation of **1** yields a dppn-based metal-to-ligand charge-transfer (MLCT) state, which in turn populates a dppn intraligand (^{3}IL) state. In contrast, photoexcitation of **2** results in an MLCT state on the TAP ligand and not the intercalating bdppz ligand. Both **1** and **2** bind strongly to double-stranded guanine-rich DNA with a loss of emission. Combined TrA and time-resolved infrared (TRIR) spectroscopy confirms formation of the guanine radical cation when **2** is bound to the $d(G_5C_5)_2$ duplex, which is not the case when **1** is bound to the same duplex and indicates a different mechanism of action in DNA. Utilizing the long-lived triplet excited lifetime, we show good uptake and localization of **2** in live cells as well as isolated chromosomes. The observed shortening of the excited-state lifetime of **2** when internalized in cell chromosomes is consistent with DNA binding and luminescent quenching due to guanine photo-oxidation.

Volatile Memristive Devices with Analog Resistance Switching Based on Self-Assembled Squaraine Microtubes as Synaptic Emulators

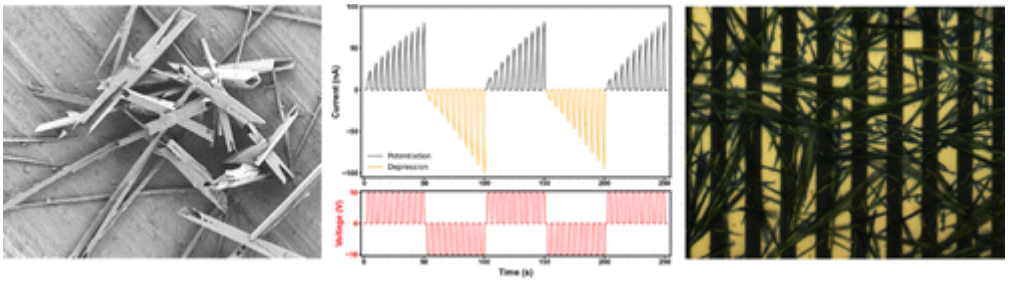
Karl Griffin, Gareth Redmond* Author links active in original paper
School of Chemistry, University College Dublin, Belfield, Dublin 4
ACS Appl. Mater. Interfaces 2024, 16, 2, 2539–2553
https://doi.org/10.1021/acsami.3c13735
Published January 4, 2024

Abstract

In this work, the discovery of volatile memristive devices that exhibit analog resistive switching (RS) and synaptic emulation based on squaraine materials is presented. Specifically, organic microtubes (MTs) based on 2,4-bis[(4-(*N*,*N*-diisobutyl)-2-6-hydroxyphenyl]squaraine (SQ) are prepared by evaporation-induced self-assembly (EISA). The MTs are ca. 2 μm in diameter (aspect ratio: 10–130). While powder X-ray diffraction data for MTs identify monoclinic and orthorhombic polymorphs, optical data report the monoclinic phase with energetic disorder. By favorable energetic alignment of the Au work function with the SQ HOMO energy, unipolar (hole-only) symmetric metal–insulator–metal devices are formed by EISA of MT meshes on interdigitated electrodes. The DC *I*–*V* characteristics acquired exhibit pinched hysteretic *I*–*V* loops, indicative of memristive behavior. Analysis indicates Ohmic transport at low bias with carrier extraction by thermionic emission. At high bias, space-charge-limited conduction in the presence of traps distributed in energy, enhanced by a

Poole-Frenkel effect and with carrier extraction by Fowler-Nordheim tunnelling, is observed. These data indicate purely electronic conduction. *I–V* hysteresis attenuates at smaller voltage windows, suggesting that carrier trapping/detrapping underpins the hysteresis. By applying triangular voltage waveforms, device conductance gradually increases sweep-on-sweep, with wait-time-erase or voltage-erase options. Using square waveforms, repeated erase-write-read of multiple distinct conductance states is achieved. Such analog RS behaviour is consistent with trap filling/emptying effects. By waveform design, volatile conductance states may also be written so that successive conductance states exhibit identical current levels, indicating forgetting of previously written states and mimicking the forgetting curve. Finally, advanced synaptic functions, i.e., excitatory postsynaptic current, paired-pulse facilitation, pulse-dependent plasticity, and a transition from short- to long-term memory driven by post-tetanic potentiation, are demonstrated.

Graphical Abstract



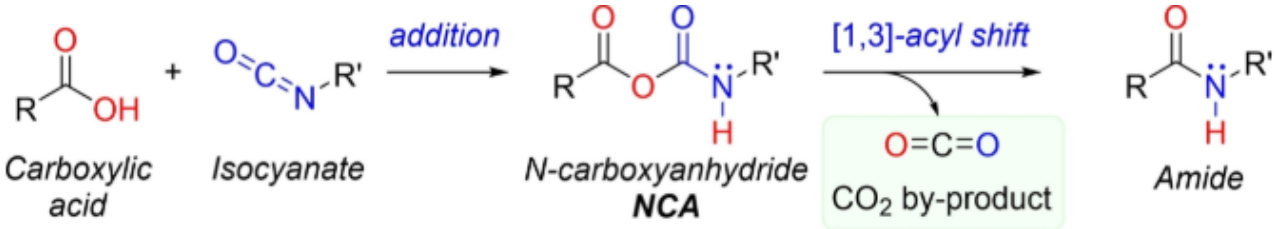
Trinity College Dublin, School of Chemistry, Publications 2024 Focus on of Journal Articles

N-Carboxyanhydrides (NCAs): Unorthodox and Useful Reagents for Amide Synthesis

Dr. Simon N. Smith, Prof. Stephen J. Connon*
School of Chemistry, Trinity Biomedical Sciences Institute, Trinity College Dublin
European Journal of Organic Chemistry: Volume 27, Issue 7
https://doi.org/10.1002/ejoc.202301032
First Published 19 January 19, 2024

Abstract
N-Carboxyanhydrides (NCAs) are compounds derived from the addition of a carboxylic acid to an isocyanate, and are known to form amides readily with the release of CO2 as a by-product. NCAs have been known for over 120 years, but despite their lengthy history, have remained so far overshadowed by more traditional approaches to amide bond formation. In this review, the potential utility of NCAs in the context of amide bond formation is reviewed and their preparation, reactivity and practical application are also discussed.

Graphical Abstract
N-Carboxyanhydrides are species derived from the addition of a carboxylic acid to an isocyanate, and are well-known to form amides products with release of CO_2. Although first reported over 120 years ago, their potential use as reagents for amide bond-forming reactions is currently underexplored. In this article, the properties, synthesis and current applications of NCAs are highlighted.



Chiral Pd2L4 Capsules from Readily Accessible Tröger's Base Ligands Inducing Circular Dichroism on Fullerenes C60 and C70

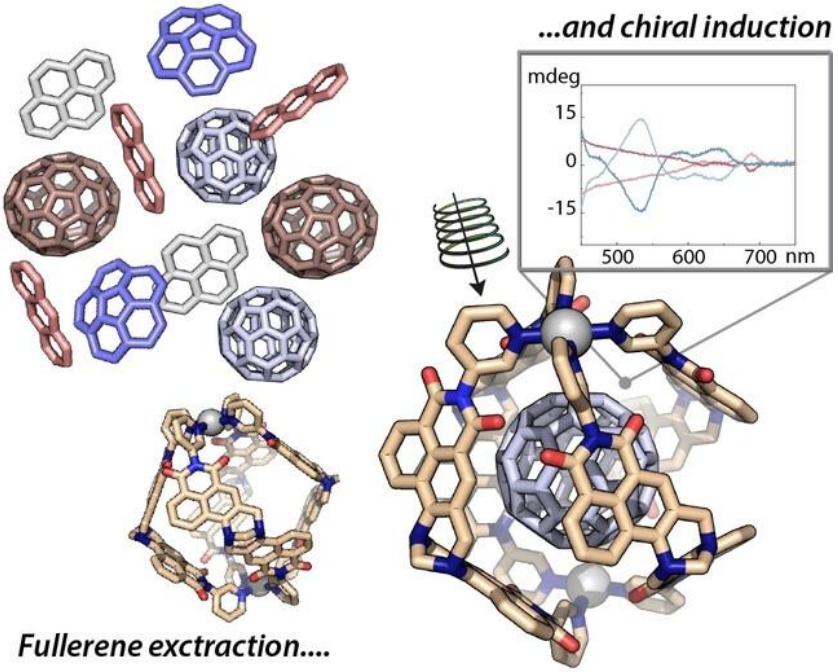
Dr. Elie Benchimol, Dr. Helen M. O'Connor, Björn Schmidt, Nicola Bogo, Dr. Julian J. Holstein, Dr. June I. Lovitt, Dr. Sankarasekaran Shanmugaraju, Prof. Dr. Christopher J. Stein, Prof. Dr. Thorfinnur Gunnlaugsson, Prof. Dr. Guido H. Clever
Supramolecular & Medicinal Chemistry Group, Chemistry Department, TCD
Angewandte Chemie Volume 64, Issue10 March 3, 2025 e202421137
https://doi.org/10.1002/anie.202421137
First published: 03 December 2024

Abstract
The induction of chirality on pristine fullerenes through non-covalent embedding in an asymmetric nano-confinement has only been rarely reported. Bringing molecules with such a unique electronic structure and broad application range into a chiral environment is particularly appealing for the development of chiroptical materials, enantioselective photoredox catalysts and systems showing chirality-induced spin selectivity (CISS). In this study, we report the formation of a chiral, configurationally stable Pd2L4 capsule assembled from a C2-symmetric, 'ribbon-shaped' ligand with a Tröger's base naphthalimide (TbNaps) backbone, easily synthesized in three steps from commercially available compounds. Embedding chirality directly into the ligand backbone ensures a relatively

lightweight receptor design whose aromatic panels create a strongly shielded inner cavity of about 700 Å3 volume. Fullerenes C60 and C70, as well as a pair of corannulenes, can be bound in acetonitrile (where unsubstituted fullerenes are insoluble) and X-ray structures of host-guest complexes were obtained. Tight interactions between the chiral host and the fullerene guests leads to the induction of a circular dichroism (CD) on the characteristic absorption bands of the forbidden π–π* transitions of the fullerenes, backed up by sTDA TD-DFT calculations and detailed investigation of the electronic excited states.

Graphical Abstract

A chiral Pd2L4 capsule based on Tröger's base is reported and shown to bind several polyaromatic hydrocarbons (PAH). It shows strong affinity for fullerenes C70 and C60 and is able to extract the latter from complex mixtures. Host-to-guest chirality transfer onto the fullerenes is observed by circular dichroism spectroscopy and theoretically analyzed by sTDA time-dependent DFT methods.



Ligand Chirality Transfer from Solution State to the Crystalline Self-Assemblies in Circularly Polarized Luminescence (CPL) Active Lanthanide Systems

David F. Caffrey, Tumpa Gorai, Bláithín Rawson, Miguel Martínez-Calvo, Jonathan A. Kitchen, Niamh S. Murray, Oxana Kotova*, Steve Comby, Robert D. Peacock, Patrycja Stachelek, Robert Pal, Thorfinnur Gunnlaugsson*

Supramolecular & Medicinal Chemistry Group, Chemistry Department, TCD

Advances Science Volume11, Issue18 May 15, 2024 2307448
https://doi.org/10.1002/advs.202307448
First published: 06 March 2024

Abstract

The synthesis of a family of chiral and enantiomerically pure pyridyl-diamide (**pda**) ligands that upon complexation with europium [$Eu(CF_3SO_3)_3$] result in chiral complexes with metal centered luminescence is reported; the sets of enantiomers giving rise to both circular dichroism (CD) and circularly polarized luminescence (CPL) signatures. The solid-state structures of these chiral metallosupramolecular systems are determined using X-ray diffraction showing that the ligand chirality is transferred from solution to the solid state. This optically favorable helical packing arrangement is confirmed by recording the CPL spectra from the crystalline assembly by using steady state and enantioselective differential chiral contrast (EDCC) CPL Laser Scanning Confocal Microscopy (CPL-LSCM) where the two enantiomers can be clearly distinguished.

A Structural and Functional Mimic of P680+

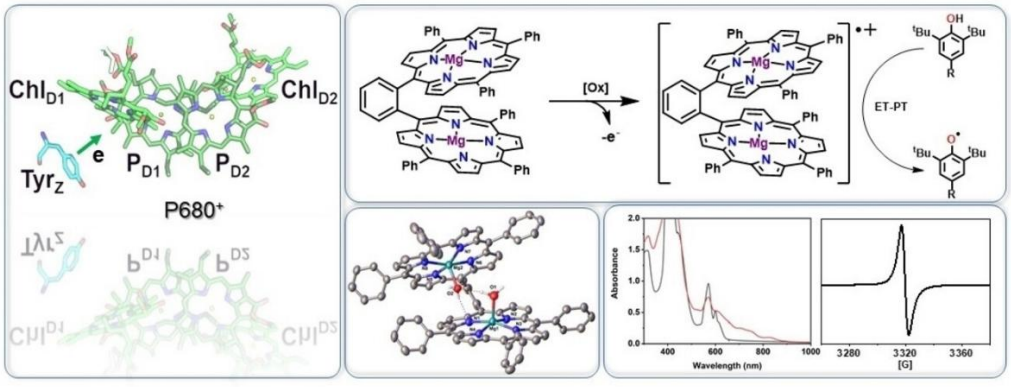
Sachidulal Biswas, Oscar Reid Kelly, Brendan Twamley, Aidan R. McDonald*
Bioinspired Inorganic Chemistry Group Chemistry Department TCD
Abgewandte Volume64, Issue 3 January 15, 2025 e202415688
https://doi.org/10.1002/anie.202415688
First Published 23 October 2024
Bioinspired Inorganic Chemistry Group Chemistry Department TCD

Abstract

One or multiple chlorophyll *a* molecules are employed in the reaction center of photosystem II′s main electron donor (defined as P680). We have a poor understanding of how the reaction center facilitates water oxidation in photosystem II and the roles that mono- and/or multimeric chlorophyll groups play when P680 oxidizes a neighboring tyrosine in order to drive water oxidation at the oxygen evolving complex. We have prepared a dimeric Mg^{II}-porphyrin complex [Mg_2(BTPP)] (**1**, H_4-BTPP=1,2-bis-(10,15,20-triphenylporphyrin-5-yl)-benzene) as a structural and functional mimic of the dimeric core of P680. **1** was oxidized by one-electron to the corresponding π-cation radical complex **2**. The radical cation was characterized by UV/Vis-NIR, FT-IR, and EPR spectroscopic techniques. **2** was shown to be reactive towards phenols to give the corresponding phenoxyl radicals, mimicking the reactivity of the P680 cation radical which oxidizes tyrosine to tyrosyl radical. Critically, the dimeric π-cation radical showed markedly higher rates of proton coupled electron transfer oxidation (PCET) of phenols when compared to its monomeric counterpart [Mg(TPP)] (TPP=5,10,15,20-tetraphenylporphyrin). Our findings demonstrate that Mg^{II}-porphyrin complexes are reliable mimics of photosynthetic PCET processes and suggest that photosynthetic reaction centers with multiple π-conjugated complexes likely lower the barrier to PCET oxidation by π-cation radical species.

Graphical Abstract

A dimeric Mg^{II}-porphyrin complex has been developed as a structural and functional mimic of the dimeric-chlorophyll reaction center found in photosystem II. The corresponding π-cation radical complex was prepared and characterized. The dimeric π-cation radical showed markedly higher rates of proton coupled electron transfer (PCET) oxidation of phenols compared to its monomeric counterpart indicating that photosynthetic reaction centers may employ multiple π-conjugated complexes in order to lower the barrier to PCET oxidation.



Reduction of exfoliated MoS2 nanosheets yields the semi-conducting 2H-polymorph rather than the metallic 1T-polymorph

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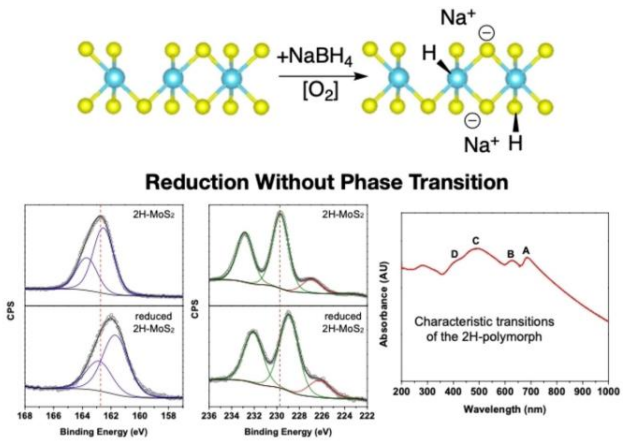
Bioinspired Inorganic Chemistry Group Chemistry Department TCD
Eur. J. Inorg. Chem. 2024, e202400292
https://doi.org/10.1002/ejic.202400292

Abstract

Delaminated two-dimensional (2D) transition metal dichalchogenides (TMDs) have attracted significant attention due to their potential application in electronics, catalysis, and biomedical devices. Chemical derivation of TMDs often relies on the generation of a metallic polymorph (1T) which is unsuitable for such applications. We explored the reactivity of the semi-conducting polymorph (2H) of pre-exfoliated MoS_2 nanosheets (as a model TMD). Pristine liquid exfoliated 2H-MoS_2 was reacted with $NaBH_4$. A novel reduced two-dimensional TMD, r-2H-MoS_2, was identified as evidenced by electronic absorption, XPS, photoluminescence, DRIFT, and Raman spectroscopies, and cyclic voltammetry. The material demonstrated a full preservation of the semi-conducting phase rather than conversion to the metallic 1T-nanomaterial that is commonly observed in the chemical derivation/exfoliation of TMDs.

Graphical Abstract

Delaminated two-dimensional (2D) transition metal dichalchogenides (TMDs) have attracted significant attention due to their potential application in electronics, catalysis, and biomedical devices. We demonstrate the preparation of a novel reduced two-dimensional form of MoS_2. UV-vis, XPS, photoluminescence, infra-red, and Raman spectroscopies alongside cyclic voltammetry confirmed electronic doping in the novel material, while showing a full preservation of the semi-conducting phase.



A Co^{II}-hydroxide complex that converts directly to a Co^{II}-acetamide during catalytic nitrile hydration.

Philipp Heim, Sachidulal Biswas, Hugo Lopez, Robert Gericke, Brendan Twamley, Aidan R. McDonald*

Bioinspired Inorganic Chemistry Group Chemistry Department TCD

Inorg. Chem. **2024**, *63*, 17, 7896-7902.

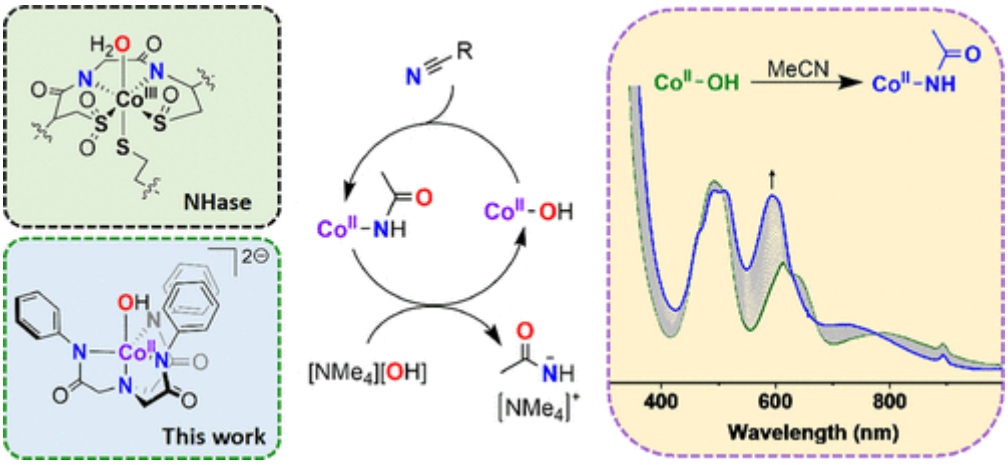
https://doi.org/10.1021/acs.inorgchem.4c00754

Abstract

In exploring structural and functional mimics of nitrile hydratases, we report the synthesis of the *pseudo*-trigonal bipyramidal Co^{II} complexes (K)[Co^{II}(DMF)(L^{Ph})] (**1(DMF)**), (NMe_4)$_2$[Co^{II}(OAc)(L^{Ph})] (**1(OAc)**), and (NMe_4)$_2$[Co^{II}(OH)(L^{Ph})] (**1(OH)**) (L^{Ph} = 2,2′,2”-nitrilo-*tris*-(*N*-phenylacetamide; DMF = *N*,*N*-dimethylformamide; $^{-}$OAc = acetate)). The complexes were characterized using NMR, FT-IR, ESI-MS, electronic absorption spectroscopy, and X-ray crystallography, showing the L^{Ph} ligand to bind in a tetradentate tripodal fashion alongside the respective ancillary donor. One of the complexes, **1(OH)**, is an unusual structural and functional mimic of the Co active site in Co nitrile hydratases. **1(OH)** reacted with acetonitrile to yield the Co^{II}-acetamide complex (NMe_4)$_2$[Co^{II}($NHC(O)CH_3$)(L^{Ph})], **2**, which was also thoroughly characterized. In the presence of excess hydroxide, **1(OH)** was found to catalyze quantitative conversion of the added hydroxide into acetamide. Despite the differences in Co oxidation state in nitrile hydratases

and **1(OH)** (Co^{III} versus Co^{II}, respectively), **1(OH)** was nonetheless an effective nitrile hydration catalyst, selectively producing acetamide over multiple turnovers.

Graphical Abstract



Synopsis

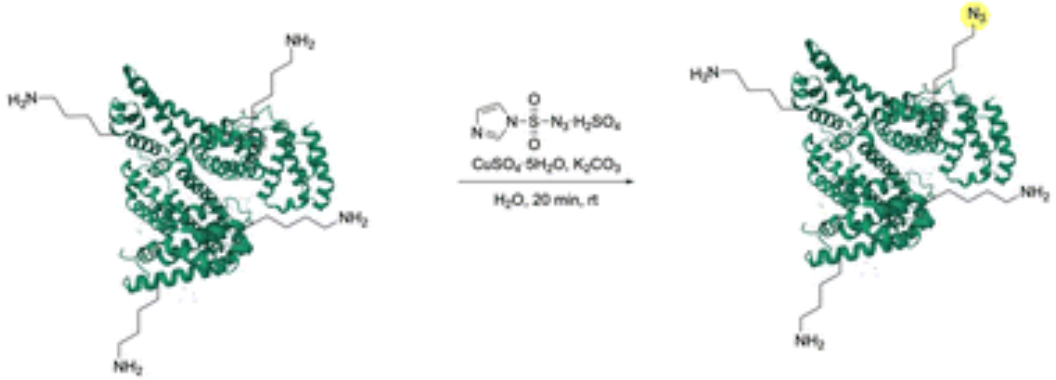
A Co^{II}-hydroxide complex reacted with acetonitrile to yield the corresponding Co^{II}-acetamide complex. In the presence of excess hydroxide, the reaction with acetonitrile was catalytic with the quantitative conversion of the added hydroxide into acetamide. Despite the difference in Co oxidation state in Co NHase (Co^{III}), the Co^{II} synthetic model was nonetheless an effective nitrile hydration catalyst.

Rapid diazotransfer for selective lysine labelling

Susannah H. Calvert, [ab] Tomasz Pawlak, [a] Gary Hessman [a] and Joanna F. McGouran *[ab]
Chemical Biology TCD
Org. Biomol. Chem., 2024,**22**, 7976-7981
https://doi.org/10.1039/D4OB01094A
First Published 116 Sep 2024

Abstract
Azide functionalization of protein and peptide lysine residues allows selective bioorthogonal labeling to introduce new, site selective functionaltiy into proteins. Optimised diazotransfer reactions under mild conditions allow aqueous diazotransfer to occur in just 20 min at pH 8.5 on amino acid, peptide and protein targets. In addition, conditons can be modified to selectively label a single lysine residue in both protein targets investigated. Finally, we demonstrate selective modification of proteins containing a single azidolysine using copper(I)-catalyzed triazole formation.

Graphical Abstract



Zinc-Binding Oligonucleotide Backbone Modifications for Targeting a DNA-Processing Metalloenzyme

Mark Berney, Ellen M. Fay, William Doherty, John J. Deering, Eva-Maria Dürr, Steven Ferguson, Joanna F. McGouran*
Chemical Biology TCD

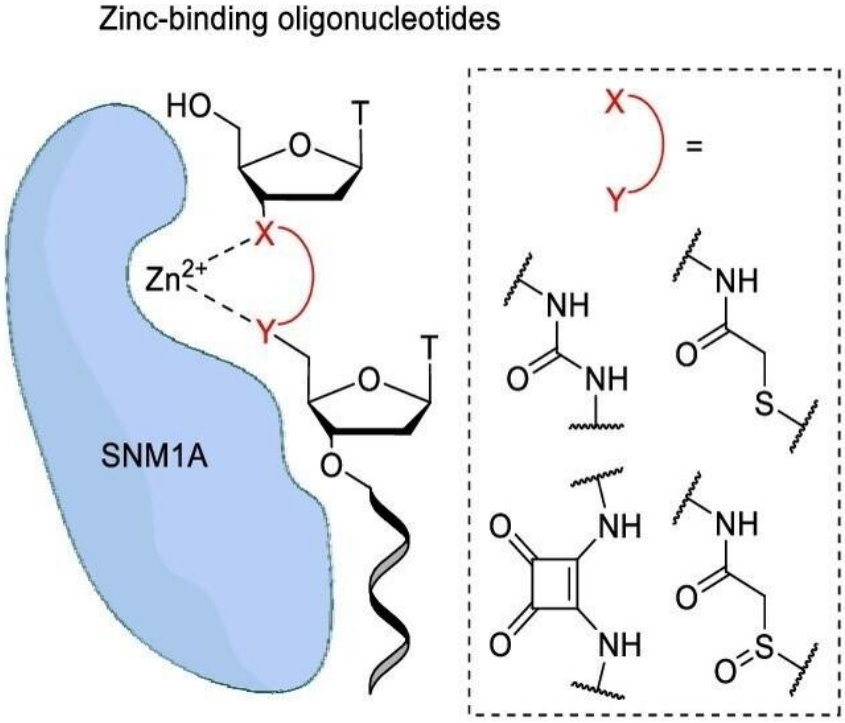
ChemBioChem Volume25, Issue21 November 4, 2024 e202400528
https://doi.org/10.1002/cbic.202400528
First published: 18 July 2024

Abstract

A series of chemically modified oligonucleotides for targeting the DNA repair nuclease SNM1A have been designed and synthesised. Each oligonucleotide contains a modified internucleotide linkage designed to both mimic the native phosphodiester backbone and chelate to the catalytic zinc ion(s) in the SNM1A active site. Dinucleoside phosphoramidites containing urea, squaramide, sulfanylacetamide, and sulfinylacetamide linkages were prepared and employed successfully in solid-phase oligonucleotide synthesis. All the modified oligonucleotides were found to interact with SNM1A in a gel electrophoresis-based assay, demonstrating the first examples of inhibition of DNA damage repair enzymes for many of these groups in oligonucleotides. One strand containing a sulfinylacetamide-linkage was found to have the strongest interaction with SNM1A and was further tested in a real-time fluorescence assay. This allowed an IC_{50} value of 231 nM to be determined, significantly lower than previously reported substrate-mimics targeting this enzyme. It is expected that these modified oligonucleotides will serve as a scaffold for the future development of fluorescent or biotin-labelled probes for the *in vivo* study of DNA repair processes.

Graphical Abstract

DNA oligonucleotides bearing a modified internucleotide linkage that enables chelation of zinc ions were synthesized. Modifications included urea, squaramide, sulfanylacetamide and sulfinylacetamide moieties. The interaction of the oligonucleotides with the zinc-dependent DNA repair enzyme SNM1A was studied. The oligonucleotides were capable of strong binding to SNM1A, and the most potent compound inhibited SNM1A activity with an IC_{50} of 231 nM.

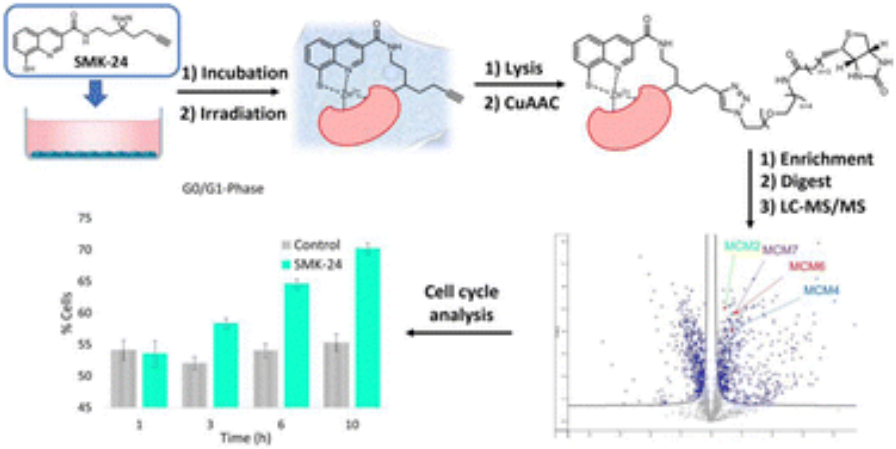


Probing the metalloproteome: an 8-mercaptoquinoline motif enriches minichromosome maintenance complex components as significant metalloprotein targets in live cells†

Sean M. McKenna,[ab] Bogdan I. Florea,[c] Daniela M. Zisterer,[d] Sander I. van Kasteren[c] and Joanna F. McGouran*[ab]
Chemical Biology TCD
ChemBioChem
RSC Chem. Biol., 2024,**5**, 776-786
https://doi.org/10.1039/D4CB00053F
First Published 25 Jun 2024

Abstract
Affinity-based probes are valuable tools for detecting binding interactions between small molecules and proteins in complex biological environments. Metalloproteins are a class of therapeutically significant biomolecules which bind metal ions as part of key structural or catalytic domains and are compelling targets for study. However, there is currently a limited range of chemical tools suitable for profiling the metalloproteome. Here, we describe the preparation and application of a novel, photoactivatable affinity-based probe for detection of a subset of previously challenging to engage metalloproteins. The probe, bearing an 8-mercaptoquinoline metal chelator, was anticipated to engage several zinc metalloproteins, including the 26S-proteasome subunit Rpn11. Upon translation of the labelling experiment to mammalian cell lysate and live cell experiments, proteomic analysis revealed that several metalloproteins were competitively enriched. The diazirine probe **SMK-24** was found to effectively enrich multiple components of the minichromosome maintenance complex, a zinc metalloprotein assembly with helicase activity essential to DNA replication. Cell cycle analysis experiments revealed that HEK293 cells treated with **SMK-24** experienced stalling in G0/G1 phase, consistent with inactivation of the DNA helicase complex. This work represents an important contribution to the library of cell-permeable chemical tools for studying a collection of metalloproteins for which no previous probe existed.

Graphical Extract



Single-Entity Electrochemistry of N-Doped Graphene Oxide Nanostructures for Improved Kinetics of Vanadyl Oxidation

Maida Aysla Costa de Oliveira, Marc Brunet Cabré, Christian Schröder, Hugo Nolan, Filippo Pota, James A. Behan, Frédéric Barrière, Kim McKelvey*, Paula E. Colavita*
Nanoscale Electrochemical Systems Group TCD
Nano.Micro small Volume21, Issue3 January 22, 2025 2405220
https://doi.org/10.1002/smll.202405220
First published: 16 November 2024

Abstract

N-doped graphene oxides (GO) are nanomaterials of interest as building blocks for 3D electrode architectures for vanadium redox flow battery applications. N- and O-functionalities have been reported to increase charge transfer rates for vanadium redox couples. However, GO synthesis typically yields heterogeneous nanomaterials, making it challenging to understand whether the electrochemical activity of conventional GO electrodes results from a sub-population of GO entities or sub-domains. Herein, single-entity voltammetry studies of vanadyl oxidation at N-doped GO using scanning electrochemical cell microscopy (SECCM) are reported. The electrochemical response is mapped at sub-domains within isolated flakes and found to display significant heterogeneity: small active sites are interspersed between relatively large inert sub-domains. Correlative Raman-SECCM analysis suggests that defect densities are not useful predictors of activity, while the specific chemical nature of defects might be a more important factor for understanding oxidation rates. Finite element simulations of the electrochemical response suggest that active sub-domains/sites are smaller than the mean inter-defect distance estimated from Raman spectra but can display very fast heterogeneous rate constants >1 cm s^{-1}. These results indicate that N-doped GO electrodes can deliver on intrinsic activity requirements set out for the viable performance of vanadium redox flow battery devices.

Metal–Organic Frameworks for Electrocatalytic CO2 Reduction: Developments and Prospects,

Shae Patel, Kim McKelvey*, Lujia Liu*

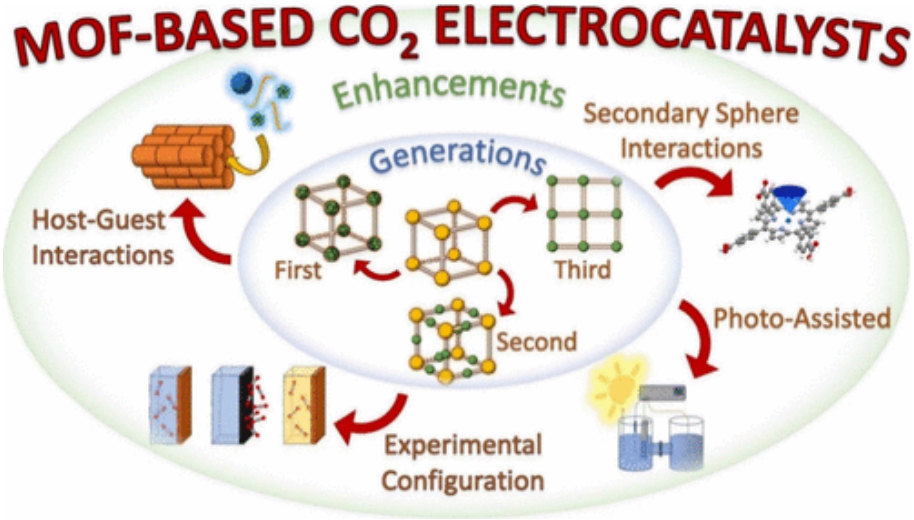
Nanoscale Electrochemical Systems Group TCD

Chem. Mater. 2024, 36, 20, 10054–10087

https://doi.org/10.1021/acs.chemmater.4c01137

First Published 4 October 2024

Abstract



The urgent need to reduce carbon emissions has intensified research into carbon dioxide (CO_2) conversion systems, with electrochemical reduction emerging as a promising approach. Efficient electrocatalysts are crucial for the challenging conversion of CO_2 into valuable products. Metal–organic frameworks (MOFs) have garnered significant attention as electrocatalysts for CO_2 electrolysis due to high surface areas, permanent porosity, modularity, and tunability. The exceptional tunability of MOFs enables precise engineering of the chemical environment surrounding the active site, facilitating a deeper understanding of structure–activity relationships for CO_2 reduction. This review catalogues diverse MOF-based electrocatalyst designs for CO_2 reduction, categorizing them into distinct generations based on active site structures. The first generation utilizes traditionally insulating metal node or linker components as the active site. The second generation uses a single atom active site embedded onto the organic linker. The third generation utilizes active sites within electrically conductive MOFs. Additionally, this review identifies specific enhancements that boost the electrocatalytic performance of MOF-based systems, including experimental setup optimization, host–guest interactions, secondary sphere interactions and photoassistance. Understanding how these enhancements overcome electrocatalytic limitations and improve performance will guide the development of high-performing MOF electrocatalyst systems for efficient CO_2 conversion.

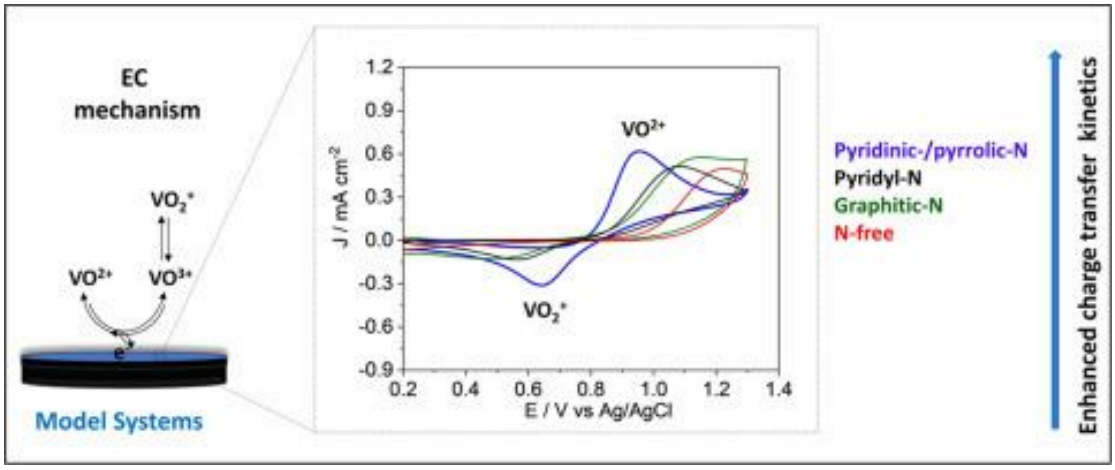
Effects of N-functional groups on the electron transfer kinetics of VO2+/VO2+ at carbon: Decoupling morphology from chemical effects using model systems

Maida A. Costa de Oliveira [a], Christian Schröder [a], Marc Brunet Cabré [a], Hugo Nolan [a b], Antoni Forner-Cuenca [c], Tatiana S. Perova [d], Kim McKelvey [a e], Paula E. Colavita [a b]
Nanoscale Electrochemical Systems Group TCD
Electrochimica Acta Volume 475, 20 January 2024, 143640
https://doi.org/10.1016/j.electacta.2023.143640
Version of Record 11 December 2023

Abstract

Carbons and nanocarbons are important electrode materials for vanadium redox flow battery applications, however, the kinetics of vanadium species are often sluggish at these surfaces, thus prompting interest in functionalization strategies to improve performance. Herein, we investigate the effect of N-functionalities on the VO^{2+}/VO_2^+ redox process at carbon electrodes. We fabricate thin film carbon disk electrodes that are metal-free, possess well-defined geometry and display smooth topography, while featuring different N-site distribution, thus enabling a mechanistic investigation of the intrinsic surface activity towards VO^{2+}/VO_2^+. Voltammetry and electrochemical impedance spectroscopy show that N-functionalities improve performance, with pyridinic/pyrrolic-N imparting the most significant improvements in charge transfer rates and reversibility, compared to graphitic-N. This was further supported by voltammetry studies on nitrogen-free electrodes modified via aryldiazonium chemistry with molecular pyridyl adlayers. Computational modeling using an electrochemical-chemical mechanism indicates that introduction of surface pyridinic/pyrrolic-N can increase the heterogeneous rate constants by approximately two orders of magnitude relative to those observed at nitrogen-free carbon ($k^0 = 1.29 \times 10^{-4}$ vs 9.34×10^{-7} cm/s). Simulations also suggest that these N-functionalities play a role in affecting reaction rates in the chemical step. Our results indicate that nitrogen incorporation via basic functional groups offers an interesting route to the design of advanced carbon electrodes for VRFB devices.

Graphical abstract



Searching for "Greener" Bioequivalents of CF3 to Lower its Environmental Impact

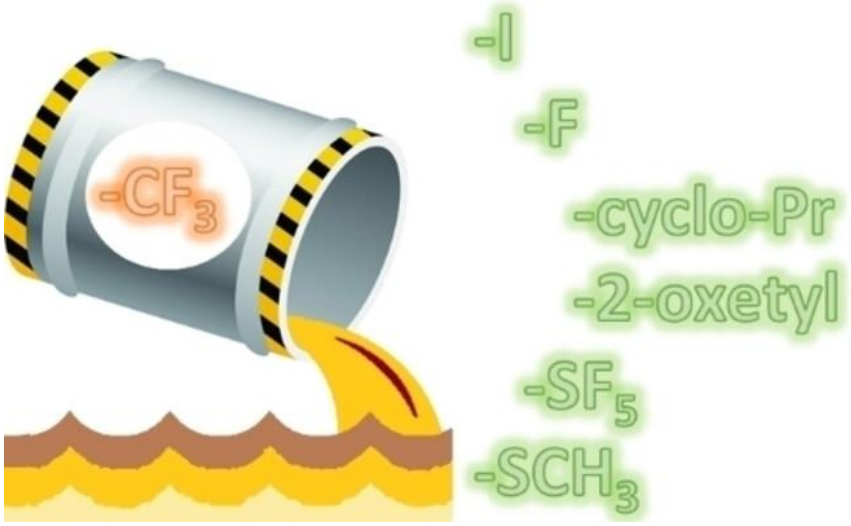
Marco Minneci, Matas Misevicius, Isabel Rozas*
Drug Discovery and Medicinal Chemistry TCD
Chemistry A European Journal Volume30, Issue 50 September 5, 2024 e202401954
https://doi.org/10.1002/chem.202401954
First published: 03 July 2024

Abstract

Considering the broad use of the trifluoromethyl functional group (−CF3) in medicinal chemistry and taking into account the recent concerns on the negative environmental effects of CF3 containing compounds, we are searching for “greener” alternatives. Thus, different chemical groups (i. e. iodide, fluoride, cyclopropyl, isopropyl, cyclobutyl, 3-oxetyl, 2-oxetyl, methylsulfide, pentafluorosulfide, methylsulfonyl and sulfonamide) have been considered as potential bioequivalents of −CF3 aiming to use them in compounds with therapeutic interest instead of the polyfluoride functionality. Different structural (molecular surface and volume) and physicochemical (electronic and lipophilic) aspects of the bioequivalent functionalities proposed have been theoretically calculated and compared to those of −CF3. Additionally, the corresponding phenyl derivatives carrying these functionalities have been purchased or prepared and their experimental lipophilicity (i. e. LogP) measured using shake-flask experiments and UV-vis spectroscopy.

Graphical Abstract

Considering concerns on the negative environmental effects of CF3 containing compounds, we searched for “greener” alternatives. We found −I as the best alternative since it is equivalent in all aspects studied, size, electronic and lipophilic, followed by −F, -cyclo-Pr, −2-oxetyl, −SF5 and −SCH3. We suggest using these functionalities as an alternative to −CF3 in the preparation of new therapies.



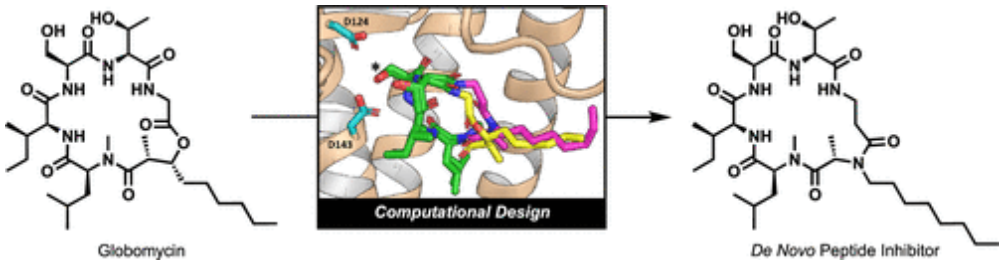
Computational Design of Cyclic Peptide Inhibitors of a Bacterial Membrane Lipoprotein Peptidase

Timothy W. Craven,¶ Mark D. Nolan,¶ Jonathan Bailey,¶ Samir Olatunji, Samantha J. Bann,Katherine Bowen, Nikita Ostrovitsa, Thaina M. Da Costa, Ross D. Ballantine, Dietmar Weichert,Paul M. Levine, Lance J. Stewart, Gaurav Bhardwaj, Joan A. Geoghegan,* Stephen A. Cochrane,*Eoin M. Scanlan,* Martin Caffrey,* and David Baker*

Biomolecular and Bioconjugate Synthesis Group TCD

ACS Chem. Biol. 2024, 19, 5, 1125–1130
https://doi.org/10.1021/acschembio.4c00076
Published 7 May 2024

Abstract

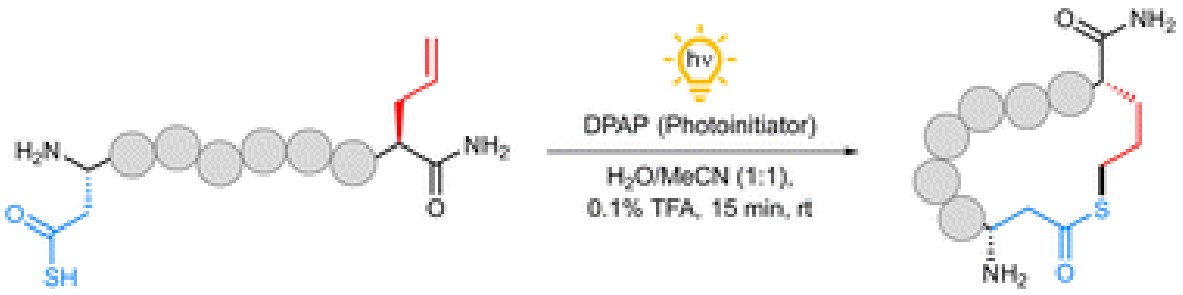


There remains a critical need for new antibiotics against multi-drug-resistant Gram-negative bacteria, a major global threat that continues to impact mortality rates. Lipoprotein signal peptidase II is an essential enzyme in the lipoprotein biosynthetic pathway of Gram-negative bacteria, making it an attractive target for antibacterial drug discovery. Although natural inhibitors of LspA have been identified, such as the cyclic depsipeptide globomycin, poor stability and production difficulties limit their use in a clinical setting. We harness computational design to generate stable *de novo* cyclic peptide analogues of globomycin. Only 12 peptides needed to be synthesized and tested to yield potent inhibitors, avoiding costly preparation of large libraries and screening campaigns. The most potent analogues showed comparable or better antimicrobial activity than globomycin in microdilution assays against ESKAPE-E pathogens. This work highlights computational design as a general strategy to combat antibiotic resistance.

Synthesis of macrocyclic thiolactone peptides via photochemical intramolecular radical acyl thiol–ene ligation†

Alby Benny [a] and Eoin M. Scanlan *[a]
Biomolecular and Bioconjugate Synthesis Group TCD
Chem. Commun., 2024,**60**, 7950-7953
https://doi.org/10.1039/D4CC02442G
First published 05 Jul 2024

Graphical Abstract
A photochemical acyl thiol–ene reaction can be used to rapidly cyclise fully unprotected peptides bearing both a thioacid and alkene to form peptide thiolactones. This strategy represents the first reported synthesis of peptide thiolactones under radical-mediated conditions.



Radical Mediated Decarboxylation of Amino Acids via Photochemical Carbonyl Sulfide (COS) Elimination

Alby Benny, Lorenzo Di Simo, Lorenzo Guazzelli, and Eoin M Scanlan
Biomolecular and Bioconjugate Synthesis Group TCD
Molecules, 2024, 29(7), 1465
https://doi.org/10.3390/molecules29071465
Published: 25 March 2024

Abstract
Herein, we present the first examples of amino acid decarboxylation via photochemically activated carbonyl sulfide (COS) elimination of the corresponding thioacids. This method offers a mild approach for the decarboxylation of amino acids, furnishing *N*-alkyl amino derivatives. The methodology was

compatible with amino acids displaying both polar and hydrophobic sidechains and was tolerant towards widely used amino acid-protecting groups. The compatibility of the reaction with continuous-flow conditions demonstrates the scalability of the process.

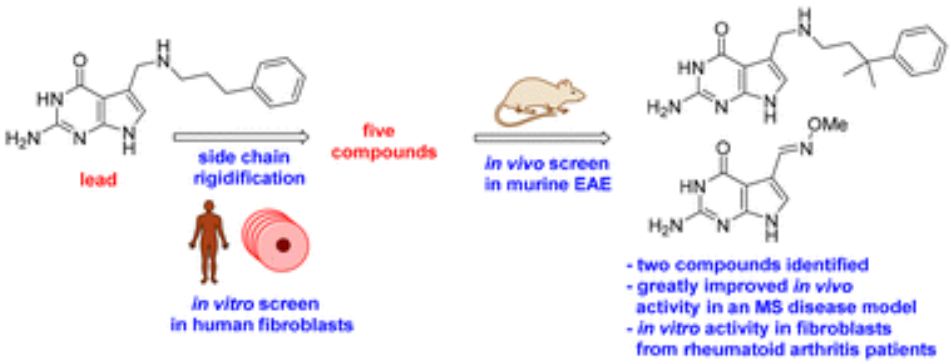
A new class of 7-deazaguanine agents targeting autoimmune diseases: dramatic reduction of synovial fibroblast IL-6 production from human rheumatoid arthritis patients and improved performance against murine experimental autoimmune encephalomyelitis†

Michelle Cotter,[a] Shauna M. Quinn,[b] Ursula Fearon,[c] Sharon Ansboro,[c] Tatsiana Rakovic,[c] John M. Southern, *[a] Vincent P. Kelly *[b] and Stephen J. Connon *[a]
Synthetic and Medicinal Chemistry TCD
RSC Med. Chem., 2024,**15**, 1556-1564
https://doi.org/10.1039/D4MD00028E
First Published 28 Mar 2024

Abstract

A simple *in vitro* assay involving the measurement of IL-6 production in human synovial fibroblasts from rheumatoid arthritis patients has been utilised to select candidates from a targeted library of queuine tRNA ribosyltransferase (QTRT) substrates for subsequent *in vivo* screening in murine experimental autoimmune encephalomyelitis (EAE – a model of multiple sclerosis). The *in vitro* activity assay discriminated between poor and excellent 7-deazaguanine QTRT substrates and allowed the identification of several structures which subsequently outperformed the previous lead in EAE. Two molecules were of significant promise: one rigidified analogue of the lead, and another considerably simpler structure incorporating an oxime motif which differs structurally from the lead to a considerable extent. These studies provide data from human cells for the first time and have expanded both the chemical space and current understanding of the structure–activity relationship underpinning the remarkable potential of 7-deazguanines in a Multiple Sclerosis disease model.

Graphical Abstract



University College Cork, School of Chemistry, Publications 2024 Focus on of Journal Articles

Deep-ultraviolet absorption cross sections of strongly absorbing atmospheric species

Meng Wang, Sean C. Connolly, Dean S. Venables*School of Chemistry and Environmental Research Institute UCC

Journal of Quantitative Spectroscopy and Radiative Transfer Volume 323, September 2024, 109050
https://doi.org/10.1016/j.jqsrt.2024.109050
Published Sep 2024

Abstract

Absorption of deep-ultraviolet photons gives rise to intense vibronic transitions in molecules and can be exploited for sensitive and selective quantification of trace gases. Accurate absorption cross sections at appropriate resolution are essential for such applications, but are not well characterised for even major atmospheric species like nitric oxide (NO) and key biogenic and anthropogenic volatile organic compounds (BVOCs and AVOCs). This study reports new absorption cross section spectra from 197 to 235 nm for NO at 1 atm and 293 K and important aromatic AVOCs (benzene, toluene, ethylbenzene, and o-, m-, and p-xylene) and BVOCs (α-pinene, β-pinene, limonene, 3-carene, and myrcene) at 1 atm across a temperature range of 293 K to 296 K.

Measurements were made with a xenon flashlamp spectrometer using a flow cell configuration for gas mixtures and a static cell arrangement for vapour-phase VOC samples. The resolution of the spectrum at 253.7 nm was approximately 0.3 nm. Both configurations showed excellent agreement in magnitude and spectral features with well-established literature cross sections. Flow cell measurements were validated against the absorption cross section of sulfur dioxide (SO_2) and static cell measurements against that of isoprene. Our absorption cross sections of NO and m-xylene reconcile large differences in the magnitude and spectral structure of previous cross sections. The deep-UV absorption cross sections of 3-carene, myrcene and ethylbenzene are reported for the first time, and confirmed for α-pinene, β-pinene, and limonene. We discuss the potential and challenges of using deep-UV absorption for quantifying these gases ambient air monitoring, emissions monitoring, and breath analysis.

Spatial analysis of PM2.5 using a concentration similarity index applied to air quality sensor networks

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School of Chemistry and Environmental Research Institute UCC

Atmos. Meas. Tech., 17, 5129–5146
https://doi.org/10.1016/j.atmosenv.2024.120794
Published 5 Sep 2024

Abstract

Air quality sensor (AQS) networks are useful for mapping $PM_{2.5}$ (particles with a diameter of 2.5 µm or smaller) in urban environments, but quantitative assessment of the observed spatial and temporal variation is currently underdeveloped. This study introduces a new metric – the concentration similarity index (CSI) – to facilitate a quantitative and time-averaged comparison of the concentration–time profiles of $PM_{2.5}$ measured by each sensor within an air quality sensor network. Following development on a dataset with minimal unexplained variation and robust tests, the CSI function is used to represent an unbiased and fair depiction of the air quality variation within an area covered by a monitoring network. The measurement data is used to derive a CSI value for every combination of sensor pairs in the network, yielding valuable information on spatial variation in $PM_{2.5}$. This new method is applied to two separate AQS networks, in Dungarvan and in the city of Cork, Ireland. In

Dungarvan there was a lower mean CSI value $(\bar{x}_{\text{CSI. Dungarvan}} = 0.61, \bar{x}_{\text{CSI. Cork}} = 0.71)$, indicating lower overall similarity between locations in the network. In both networks, the average diurnal plots for each sensor exhibit an evening peak in $PM_{2.5}$ concentration due to emissions from residential solid-fuel burning; however, there is considerable variation in the size of this peak. Clustering techniques applied to the CSI matrices identify two different location types in each network; locations in central or residential areas that experience more pollution from solid-fuel burning and locations on the edge of the urban areas that experience cleaner air. The difference in mean $PM_{2.5}$ between these two location types was 6 $\mu g\, m^{-3}$ in Dungarvan and 2 $\mu g\, m^{-3}$ in Cork. Furthermore, the examination of winter and summer months (January and May) indicates that higher $PM_{2.5}$ levels during periods of increased residential solid-fuel burning act as a major driver for greater differences (lower similarity indices) between locations in both networks, with differences in mean seasonal CSI values exceeding 0.25 and differences in mean seasonal $PM_{2.5}$ exceeding 7 $\mu g\, m^{-3}$. These findings underscore the importance of including wintertime PM data in analyses, as the differences between locations is enhanced during periods when solid-fuel burning activities are at a peak. Additionally, the CSI method facilitates the assessment of the representativeness of the $PM_{2.5}$ measured at regulatory air quality monitoring locations with respect to population exposure, showing here that location type is more important than physical proximity in terms of similarity and spatial representativeness assessments. Applying the CSI in this manner can allow for the placement of monitoring infrastructure to be optimised. The results indicate that the population exposure to $PM_{2.5}$ in Dungarvan is moderately represented () by the current regulatory monitoring location, and the regulatory monitoring location assessed in Cork represented the city-wide $PM_{2.5}$ levels well $(\bar{x}_{\text{CSI}} = 0.76)$.

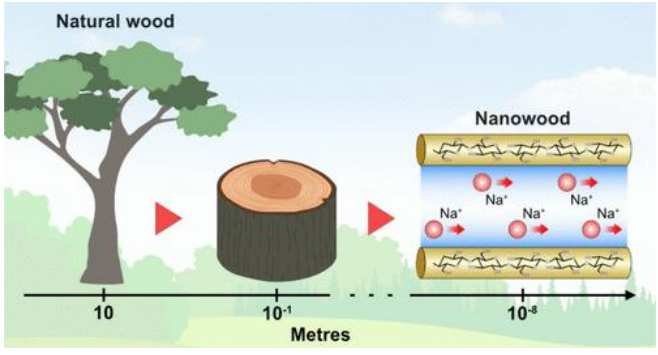
'Nanowood: A Unique Natural Nanomaterial That Can Be Obtained Using Household Chemicals'

Ievgen Nedrygailov*, Darragh O'Brien, Scott Monaghan, Paul Hurley,Subhajit Biswas, Justin D. Holmes*
School of Chemistry, University College Cork, Cork
J. Chem. Educ. 2024, 101, 11, 4931–4936
https://doi.org/10.1021/acs.jchemed.4c00166
Published October 10, 2024

Abstract

At the nanometer scale, electrolyte solutions behave differently compared to their bulk counterparts. This phenomenon forms the basis for the field of nanofluidics, which is dedicated to studying the transport of fluids within and around objects with dimensions of less than 100 nm. Despite the increasing importance of nanofluidics for a wide range of chemical and biochemical applications, the ability to study this field in undergraduate laboratories remains limited due to challenges associated with producing suitable nanoscale objects. This article outlines a straightforward procedure, using easily accessible materials and chemical reagents, to create nanofluidic membranes, called nanowood, containing channels with diameters less than 100 nm. We describe the fabrication process of nanofluidic channels in wood and demonstrate the presence of these nanochannels based on conductance measurements using electrochemical impedance spectroscopy.

Graphical Abstract



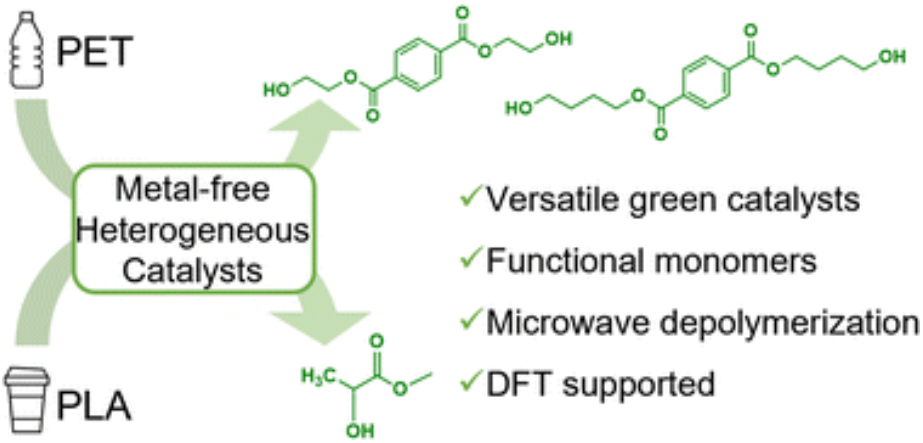
'Guanidine functionalized porous SiO2 as heterogeneous catalysts for microwave depolymerization of PET and PLA'

Éadaoin Casey,[ab] Rachel Breen,[ab] Gerard Pareras, [c] Albert Rimola, [c] Justin D. Holmes [ab] and Gillian Collins *[ab]
School of Chemistry, University College Cork, Cork
RSC Sustainability, 2024,**2**, 1040-1051
DOI
https://doi.org/10.1039/D3SU00425B
6 Mar 2024

Abstract

Chemical recycling is an important strategy to tackle the growing global problem of plastic waste pollution. The development of metal-free catalysts for depolymerization of plastics is attractive as it avoids the use of metal salts, which are potentially damaging to the environment. Here we report a metal-free heterogeneous catalyst for the glycolysis of polyethylene terephthalate (PET) and methanolysis of polylactic acid (PLA). The catalysts are synthesized by covalent surface modification of mesoporous silica (SiO_2) with guanidine ligands and evaluated under conventional thermal and microwave-assisted heating. A surface bound cyanoguanidine ligand was found to be the best catalyst leading to 100% PET conversion with 80% BHET yield. The nature of the catalyst support material influenced the catalytic performance of the guanidine ligands with porous SiO_2 supports outperforming activated carbon in conventional thermal glycolysis, while the opposite trend was observed with microwave assisted glycolysis. Dedicated density functional theory (DFT) computations were performed to simulate the depolymerization processes, obtain the free energy profiles of the reaction mechanisms, and identify the important role of hydrogen bonding in the reaction mechanism.

Graphical Abstract



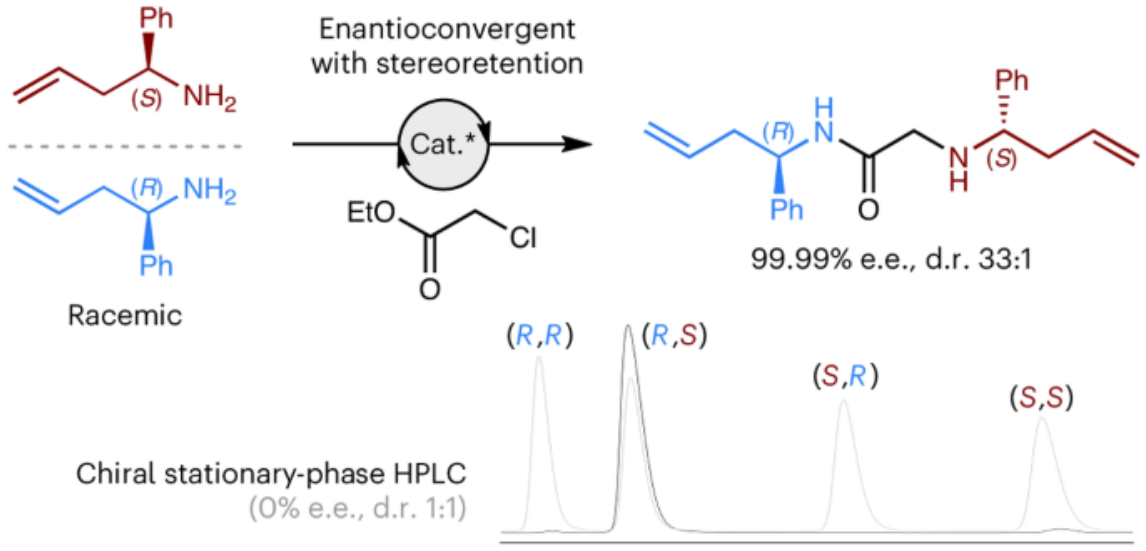
Stereoretentive enantioconvergent reactions

Steven H. Bennett, Jacob S. Bestwick, Vera P. Demertzidou, David J. Jones, Helen E. Jones, François Richard, Joshua A. Homer, Rosie Street-Jeakings, Andrew F. Tiberia & Andrew L. Lawrence*
University College Cork and others
Nature Chemistry **volume 16, pages1177–1183 (2024)**
https://doi.org/10.1038/s41557-024-01504-1
Published 17 April 2024

Abstract

Enantioconvergent reactions are pre-eminent in contemporary asymmetric synthesis as they convert both enantiomers of a racemic starting material into a single enantioenriched product, thus avoiding the maximum 50% yield associated with resolutions. All currently known enantioconvergent processes

necessitate the loss or partial loss of the racemic substrate's stereochemical information, thus limiting the potential substrate scope to molecules that contain labile stereogenic units. Here we present an alternative approach to enantioconvergent reactions that can proceed with full retention of the racemic substrate's configuration. This uniquely stereo-economic approach is possible if the two enantiomers of a racemic starting material are joined together to form one enantiomer of a non-*meso* product. Experimental validation of this concept is presented using two distinct strategies: (1) a direct asymmetric coupling approach, and (2) a multicomponent approach, which exhibits statistical amplification of enantiopurity. Thus, the established dogma that enantioconvergent reactions require substrates that contain labile stereogenic units is shown to be incorrect.



Regioselective Partial Hydrogenation and Deuteration of Tetracyclic (Hetero)aromatic Systems Using a Simple Heterogeneous Catalyst

Roberta Kehoe, Amy Lowry, Mark Light, David J. Jones, Peter A. Byrne, Gerard Patrick McGlacken*
University College Cork
Chemistry - A European Journal Volume 30, Issue 17, 20 March 2024 e202400102
https://doi.org/10.1002/chem.202400102
First Published 17 January 2024

Abstract

The introduction of added '3-dimensionality' through late-stage functionalisation of extended (hetero)aromatic systems is a powerful synthetic approach. The abundance of starting materials and cross-coupling methodologies to access the precursors allows for highly diverse products. Subsequent selective partial reduction can alter the core structure in a manner of interest to medicinal chemists. Herein, we describe the precise, partial reduction of multicyclic heteroaromatic systems using a simple heterogeneous catalyst. The approach can be extended to introduce deuterium (again at late-stage). Excellent yields can be obtained using simple reaction conditions.

Graphical Abstract

The introduction of added '3-dimensionality' through late-stage functionalisation is a powerful synthetic approach to biologically significant moieties. Herein, a hydrogenative, regioselective dearomatisation of extended (hetero)aromatic systems is described, using a simple Pd catalyst at atmospheric hydrogen pressure. Deuteration is also demonstrated, and some initial mechanistic insights are revealed.

Synthesis and Reactivity of α-Diazo-β-keto Sulfonamides

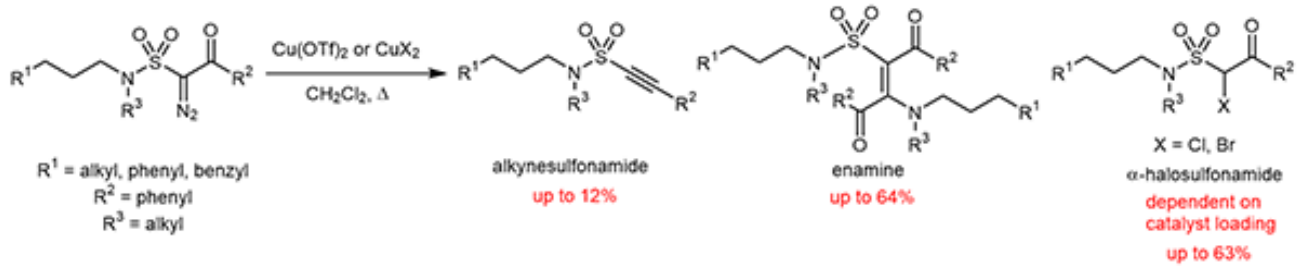
Evan R. Judge, Keith O'Shaughnessy, Simon E. Lawrence, Stuart G. Collins*, Anita R. Maguire*
School of Chemistry, Analytical & Biological Chemistry UCC

Synthesis 2024; 56(24): 3752-3768 (Special Issue Recent Advances in The Chemistry of Diazo Compounds)
DOI: 10.1055/a-2348-5631
Published on Line 24 May 2024

Abstract

Copper-mediated reactions of α-diazo-β-keto sulfonamides led to a range of products, including alkynesulfonamides, enamines, and α-halosulfonamides, with no evidence for intramolecular C–H insertion in any of the reactions, in contrast to the reactivity of the comparable α-diazo-β-oxo sulfones. Use of copper(II) triflate (5 mol%) led to the isolation of a series of alkynesulfonamides (up to 12% yield) and enamines (up to 64% yield). Use of copper(II) chloride (5 mol%) led to the formation, in addition, of α-halosulfonamides; use of stoichiometric amounts of copper(II) chloride/bromide enabled facile halogenation of the β-keto sulfonamide to form α-halosulfonamides (up to 63% yield).

Graphical Abstract



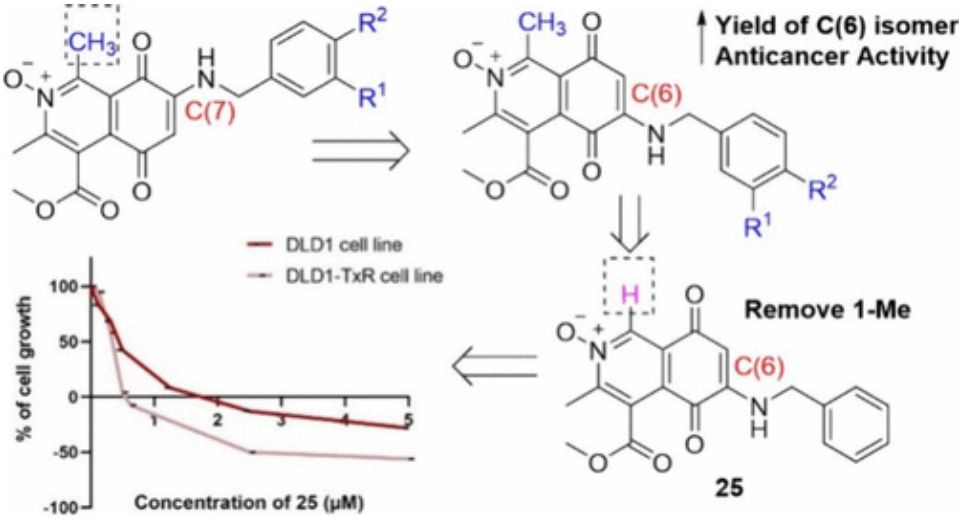
Discovery of Potent Isoquinolinequinone N-Oxides to Overcome Cancer Multidrug Resistance

Ryan D. Kruschel, Mélanie A. G. Barbosa, Maria João Almeida, Cristina P. R. Xavier, M. Helena Vasconcelos*, Florence O. McCarthy*
School of Chemistry, Analytical and Biological Chemistry Research Facility and others, UCC

J. Med. Chem. 2024, 67, 16, 13909–13924
https://doi.org/10.1021/acs.jmedchem.4c00705
Published 2 August 2024

Abstract

Multidrug resistance (MDR) of human tumors has resulted in an immediate need to develop appropriate new drugs. This work outlines the development of 20 potent IQQ *N*-oxide derivatives in two isomeric families, both exhibiting nanomolar GI_{50} against human tumor cell lines.



Preliminary NCI-60 tumor screening sees the C(6) isomers achieve a mean GI_{50} > 2 times lower than the corresponding C(7) isomers. MDR evaluation of nine selected compounds reveals that each presents lower GI_{50} concentrations in two MDR tumor cell lines. Four of the series display nanomolar GI_{50} values against MDR cells, having selectivity ratios up to 2.7 versus the sensitive (parental) cells. The most potent compound **25** inhibits the activity of drug efflux pumps in MDR cells, causes significant ROS accumulation, and potently inhibits cell proliferation, causing alterations in the cell cycle profile. Our findings are confirmed by 3D spheroid models, providing new candidates for studies against MDR cancers.

BDSF Analogues Inhibit Quorum Sensing-Regulated Biofilm Production in Xylella fastidiosa

by

Conor Horgan[1,2,3,†], Clelia Baccari[4,†], Michelle O'Driscoll[1,2,3], Steven E. Lindow[4,*] and Timothy P. O'Sullivan[1,2,3,*]

School of Chemistry, University College Cork and other.

Microorganisms **2024**, *12*(12), 2496

https://doi.org/10.3390/microorganisms12122496

Published: 4 December 2024

Abstract

Xylella fastidiosa is an aerobic, Gram-negative bacterium that is responsible for many plant diseases. The bacterium is the causal agent of Pierce's disease in grapes and is also responsible for citrus variegated chlorosis, peach phony disease, olive quick decline syndrome and leaf scorches of various species. The production of biofilm is intrinsically linked with persistence and transmission in X. fastidiosa. Biofilm formation is regulated by members of the Diffusible Signal Factor (DSF) quorum sensing signalling family which are comprised of a series of long chain cis-unsaturated fatty acids. This article describes the evaluation of a library of N-acyl sulfonamide bioisosteric analogues of BDSF, XfDSF1 and XfDSF2 for their ability to control biofilm production in X. fastidiosa. The compounds were screened against both the wild-type strain Temecula and an rpfF* mutant which can perceive but not produce XfDSF. Planktonic cell abundance was measured via OD600 while standard crystal violet assays were used to determine biofilm biomass. Several compounds were found to be effective biofilm inhibitors depending on the nature of the sulfonamide substituent. The findings reported here may provide future opportunities for biocontrol of this important plant pathogen.

Synthesis, evaluation and mechanistic insights of novel IMPDH inhibitors targeting ESKAPEE bacteria

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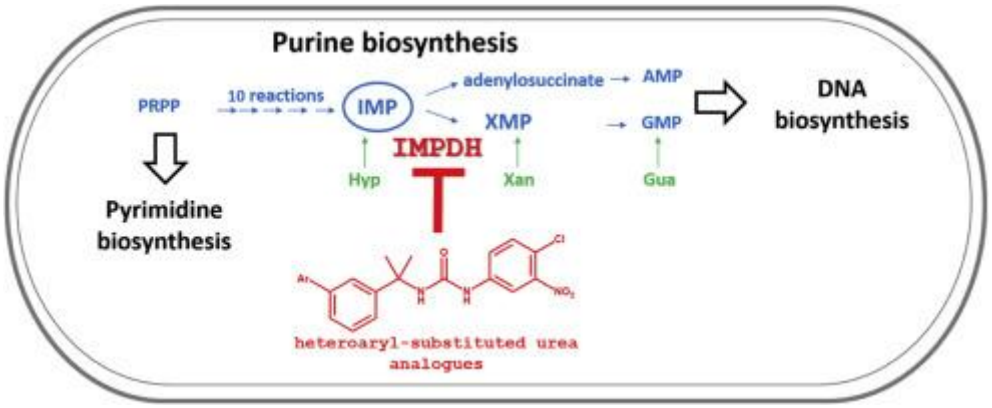
School of Chemistry, University College Cork, Cork
European Journal of Medicinal Chemistry Volume 280, 15 December 2024, 116920
https://doi.org/10.1016/j.ejmech.2024.116920
Published Version of Record 5 October 2024

Abstract
Antimicrobial resistance poses a significant threat to global health, necessitating the development of novel therapeutic agents with unique mechanisms of action. Inosine 5′-monophosphate dehydrogenase (IMPDH), an essential enzyme in guanine nucleotide biosynthesis, is a promising target for the discovery of new antimicrobial agents. High-throughput screening studies have previously identified several urea-based leads as potential inhibitors, although many of these are characterised by reduced chemical stability. In this work, we describe the design and synthesis of a series of heteroaryl-susbtituted analogues and the evaluation of their inhibitory potency against IMPDHs. Our screening targets ESKAPEE pathogens, including *Pseudomonas aeruginosa*, *Staphylococcus aureus* and *Escherichia coli.* Several analogues with submicromolar inhibitory potency are identified and show no inhibitory potency on human IMPDH nor cytotoxic effects on human cells. Kinetic studies revealed that these molecules act as noncompetitive inhibitors with respect to the substrates and ligand virtual docking simulations provided insights into the binding interactions at the interface of the NAD^+ and IMP binding sites on IMPDH.

Graphical abstract



Flow Chemistry and Continuous Processing: More Mainstream than Ever!

Kevin P. Cole*, Jonathan N. Jaworski, C. Oliver Kappe, Shu Kobayashi, Anita R. Maguir, Anne O'Kearney-McMullan, Jaan A. Pesti
School of Chemistry and School of Pharmacy, Analytical and Biological Chemistry Research Facility, UCC & Industry Partners
Org. Process Res. Dev. 2024, 28, 5, 1269–1271
https://doi.org/10.1021/acs.oprd.3c00483
Published 17 May 2024

Abstract
Abstract not available

The role of PAT in the development of telescoped continuous flow processes

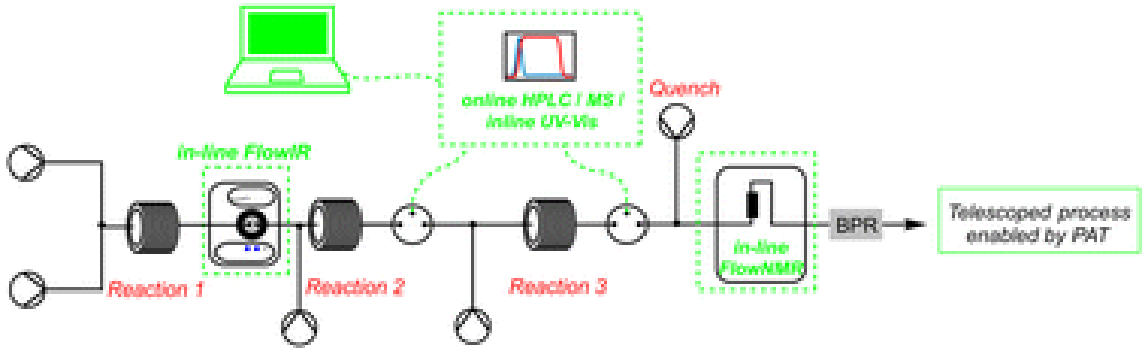
Aoife M. Kearney, [a] Stuart G. Collins *[b] and Anita R. Maguire *[c]
School of Chemistry and School of Pharmacy, Analytical and Biological Chemistry Research Facility, UCC

React. Chem. Eng., 2024,**9**, 990-1013
https://doi.org/10.1039/D3RE00678F

Abstract

This review highlights the advantages of incorporating Process Analytical Technologies into continuous flow processes, especially in the context of telescoped multistep flow sequences. Use of FlowIR, in-line UV-vis, online HPLC, online MS and Flow NMR are discussed within this review, with multiple PAT techniques used in conjunction with one another in some instances. PAT is key in ensuring as much information as possible can be gathered during a chemical transformation, with real-time analysis allowing for rapid reaction optimization.

Graphical Abstract



Elucidating the Degradation Pathways of Human Insulin in the Solid State

Andrew Fagan, Lorraine M. Bateman, Joseph P. O'Shea & Abina M. Crean*
SSPC, the SFI Centre for Pharmaceutical Research, School of Pharmacy, University College Cork

J. Anal. Test. **8**, 288–299 (2024)
https://doi.org/10.1007/s41664-024-00302-5
Published 6 May 2024

Abstract

While there have been significant advances in the development of peptide oral dosage forms in recent years, highlighted by the clinical and commercial success of approved peptides such as Rybelsus®, there remain several barriers in the way of broad range applicability of this approach to peptide delivery. One such barrier includes the poor physical and chemical stability inherent to their structures, which persists in the solid state although degradation typically occurs at different rates and via different pathways in comparison to the solution state. Using insulin as a model peptide, this work sought to contribute to the development of analytical techniques for investigating common insulin degradation pathways. Chemically denatured, deamidated and aggregated samples were prepared and used to benchmark circular dichroism spectroscopy, reverse phase HPLC and size exclusion chromatography methods for the investigation of unfolding, chemical modifications and covalent aggregation of the insulin molecule respectively. Solid state degraded samples were prepared by heating insulin powder at 60 °C and 75% relative humidity for 1, 3, 5 and 7 d, and the degradation profiles of the samples were evaluated and compared with those observed in solution. While no unfolding was observed to occur, significant deamidation and covalent aggregation were detected. Reductive disulfide bond cleavage using dithiothreitol allowed for separation of the insulin A- and B-

chains, offering a facile yet novel means of assessing the mechanisms of deamidation and covalent aggregation occurring in the solid state.

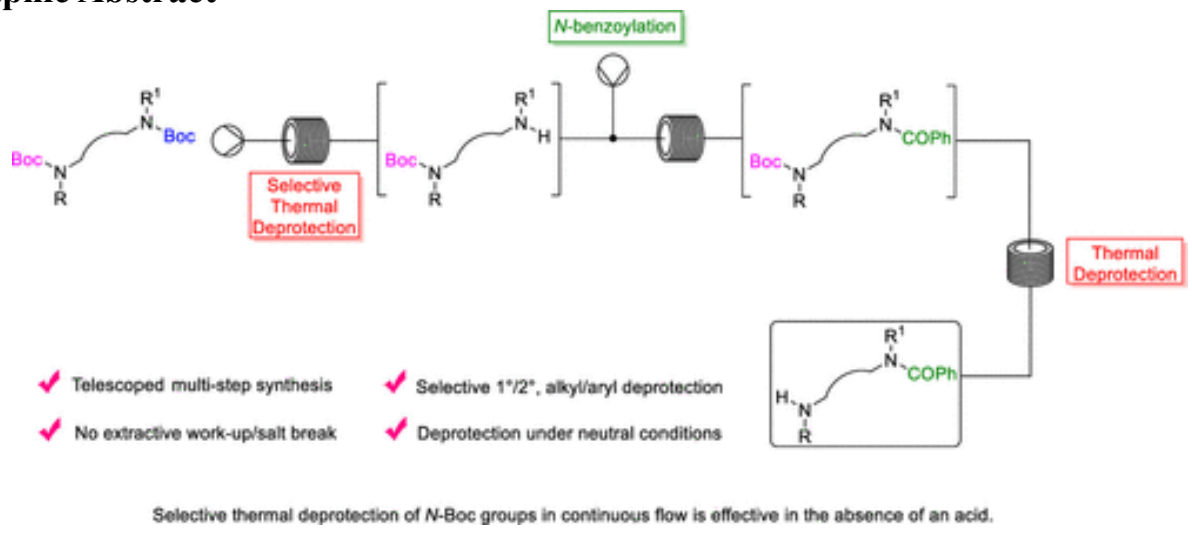
Selective Thermal Deprotection of N-Boc Protected Amines in Continuous Flow

Michelle-Rose Ryan, Denis Lynch, Stuart G. Collins*, Anita R. Maguire*
School of Chemistry, Analytical and Biological Chemistry Research Facility, UCC
Org. Process Res. Dev. 2024, 28, 5, 1946–1963
https://doi.org/10.1021/acs.oprd.3c00498
Published 25 April 2024

Abstract

Thermal *N*-Boc deprotection of a range of amines is readily effected in continuous flow, in the absence of an acid catalyst. While the optimum results were obtained in methanol or trifluoroethanol, deprotection can be effected in a range of solvents of different polarities. Sequential selective deprotection of *N*-Boc groups has been demonstrated through temperature control, as exemplified by effective removal of an aryl *N*-Boc group in the presence of an alkyl *N*-Boc group. As a proof of principle, a telescoped sequence involving selective deprotection of an aryl *N*-Boc group from **9h** followed by benzoylation and deprotection of the remaining alkyl *N*-Boc group to form amide **13** proved successful.

Graphic Abstract



Selective thermal deprotection of *N*-Boc groups in continuous flow is effective in the absence of an acid.

Susceptibility of the Different Oxygen-Sensing Probes to Interferences in Respirometric Bacterial Assays with Complex Media

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School of Biochemistry and Cell Biology, University College Cork & Others
Sensors 2024, 24(1), 267
https://doi.org/10.3390/s24010267
Published: 2 January 2024

Abstract

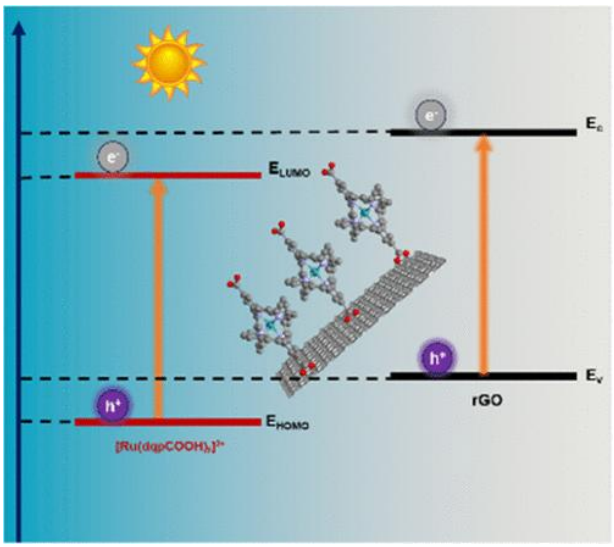
Respirometric microbial assays are gaining popularity, but their uptake is limited by the availability of optimal O_2 sensing materials and the challenge of validating assays with complex real samples. We conducted a comparative evaluation of four different O_2-sensing probes based on Pt-porphyrin phosphors in respirometric bacterial assays performed on standard time-resolved fluorescence reader. The macromolecular MitoXpress, nanoparticle NanO2 and small molecule $PtGlc_4$ and $PtPEG_4$ probes

were assessed with *E. coli* cells in five growth media: nutrient broth (NB), McConkey (MC), Rapid Coliform ChromoSelect (RCC), M-Lauryl lauryl sulfate (MLS), and Minerals-Modified Glutamate (MMG) media. Respiration profiles of the cells were recorded and analyzed, along with densitometry profiles and quenching studies of individual media components. This revealed several limiting factors and interferences impacting assay performance, which include probe quenched lifetime, instrument temporal resolution, inner filter effects (mainly by indicator dyes), probe binding to lipophilic components, and dynamic and static quenching by media components. The study allowed for the ranking of the probes based on their ruggedness, resilience to interferences and overall performance in respirometric bacterial assays. The 'shielded' probe NanO2 outperformed the established MitoXpress probe and the small molecule probes $PtGlc_4$ and $PtPEG_4$.

Enhanced Photostability and Photoactivity of Ruthenium Polypyridyl-Based Photocatalysts by Covalently Anchoring Onto Reduced Graphene Oxid

Seán Hennessey, Roberto González-Gómez*, Kathryn McCarthy, Christopher S. Burke, Camille Le Houérou, Nirod Kumar Sarangi, Patrick McArdle, Tia E. Keyes, Fabio Cucinotta, Pau Farràs*
School of Biological and Chemical Sciences, Energy Research Centre, Ryan Institute, University of Galway,
UCC, DCU, Newcastle University, UK.
ACS Omega 2024, 9, 12, 13872–13882
https://doi.org/10.1021/acsomega.3c08800
Published March 14, 2024

Abstract



Recentstudies toward finding more efficient ruthenium metalloligands for photocatalysis applications have shown that the derivatives of the linear $[Ru(dqp)_2]^{2+}$ (dqp: 2,6-di(quinolin-8-yl)-pyridine) complexes hold significant promise due to their extended emission lifetime in the μs time scale while retaining comparable redox potential, extinction coefficients, and absorption profile in the visible region to $[Ru(bpy)_3]^{2+}$ (bpy: 2,2′-bipyridine) and $[Ru(tpy)_2]^{2+}$ (tpy: 2,2′:6′,2″-terpyridine) complexes. Nevertheless, its photostability in aqueous solution needs to be improved for its widespread use in photocatalysis. Carbon-based supports have arisen as potential solutions for improving photostability and photocatalytic activity, yet their effect greatly depends on the interaction of the metal complex with the support. Herein, we present a strategy for obtaining Ru–polypyridyl complexes covalently linked to aminated reduced graphene oxide (rGO) to generate novel materials with long-term photostability and increased photoactivity. Specifically, the hybrid Ru(dqp)@rGO system has shown excellent photostable behavior during 24 h of continual irradiation, with an enhancement of 10 and 15% of photocatalytic dye degradation in comparison with $[Ru(dqp)_2]^{2+}$ and Ru(tpy)@rGO, respectively, as well as remarkable recyclability. The presented strategy corroborates the potential of $[Ru(dqp)_2]^{2+}$ as an interesting photoactive molecule to produce more advantageous light-active materials by covalent attachment onto carbon-based supports.

Colyophilized Sugar–Polymer Dispersions for Enhanced Processing and Storage Stability

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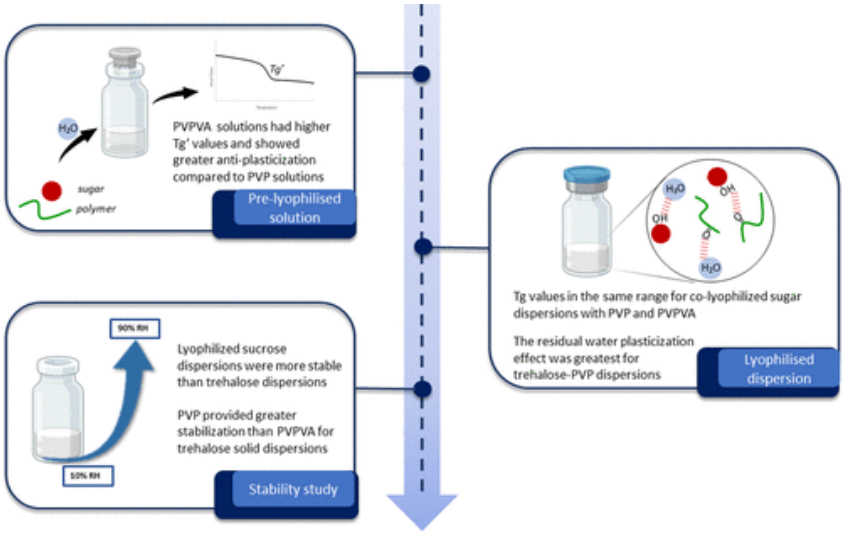
Mol. Pharmaceutics 2024, 21, 6, 3017–3026
https://doi.org/10.1021/acs.molpharmaceut.4c00187
Published May 17, 2024

Abstract

Sucrose and trehalose pharmaceutical excipients are employed to stabilize protein therapeutics in a dried state. The mechanism of therapeutic protein stabilization is dependent on the sugars being present in an amorphous solid-state. Colyophilization of sugars with high glass transition polymers, polyvinylpyrrolidone (PVP), and poly(vinylpyrrolidone vinyl acetate) (PVPVA), enhances amorphous sugar stability. This study investigates the stability of colyophilized sugar–polymer systems in the frozen solution state, dried state postlyophilization, and upon exposure to elevated humidity. Binary systems of sucrose or trehalose with PVP or PVPVA were lyophilized with sugar/polymer ratios ranging from 2:8 to 8:2. Frozen sugar–PVPVA solutions exhibited a higher glass transition temperature of the maximally freeze-concentrated amorphous phase (T_g') compared to sugar–PVP solutions, despite the glass transition temperature (T_g) of PVPVA being lower than PVP. T_g values of all colyophilized systems were in a similar temperature range irrespective of polymer type. Greater hydrogen bonding between sugars and PVP and the lower hygroscopicity of PVPVA influenced polymer antiplasticization effects and the plasticization effects of residual water. Plasticization due to water sorption was investigated in a dynamic vapor sorption humidity ramping experiment.

Lyophilized sucrose systems exhibited increased amorphous stability compared to trehalose upon exposure to the humidity. Recrystallization of trehalose was observed and stabilized by polymer addition. Lower concentrations of PVP inhibited trehalose recrystallization compared to PVPVA. These stabilizing effects were attributed to the increased hydrogen bonding between trehalose and PVP compared to trehalose and PVPVA. Overall, the study demonstrated how differences in polymer hygroscopicity and hydrogen bonding with sugars influence the stability of colyophilized amorphous dispersions. These insights into excipient solid-state stability are relevant to the development of stabilized biopharmaceutical solid-state formulations.

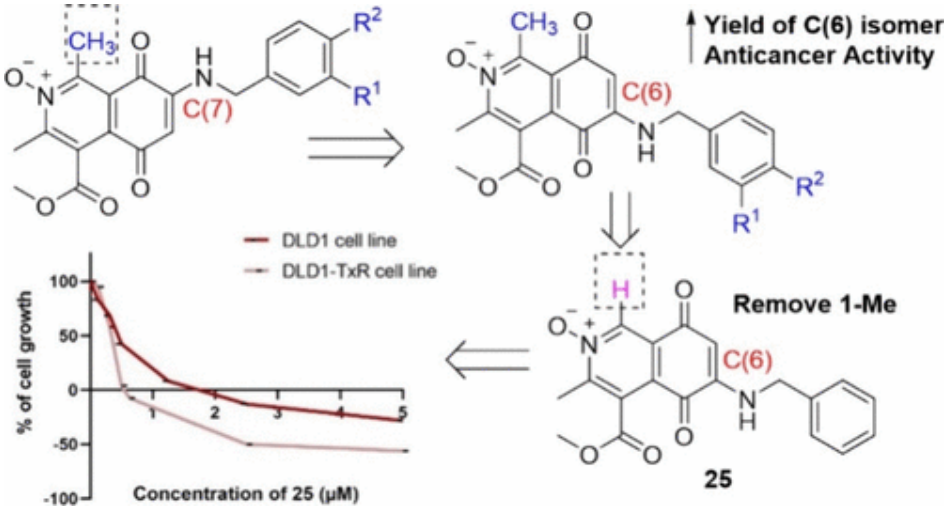


Discovery of Potent Isoquinolinequinone N-Oxides to Overcome Cancer Multidrug Resistance

Ryan D. Kruschel, Mélanie A. G. Barbosa, Maria João Almeida, Cristina P. R. Xavier, M. Helena Vasconcelos, Florence O. McCarthy
School of Chemistry, Analytical and Biological Chemistry Research Facility, University College Cork & others
J. Med. Chem. 2024, 67, 16, 13909–13924
https://doi.org/10.1021/acs.jmedchem.4c00705
Published August 2, 2024

Abstract

Multidrug resistance (MDR) of human tumors has resulted in an immediate need to develop appropriate new drugs. This work outlines the development of 20 potent IQQ *N*-oxide derivatives in two isomeric families, both exhibiting nanomolar GI_{50} against human tumor cell lines. Preliminary NCI-60 tumor screening sees the C(6) isomers achieve a mean $GI_{50} > 2$ times lower than the corresponding C(7) isomers. MDR evaluation of nine selected compounds reveals that each presents lower GI_{50} concentrations in two MDR tumor cell lines. Four of the series display nanomolar GI_{50} values against MDR cells, having selectivity ratios up to 2.7 versus the sensitive (parental) cells. The most potent compound **25** inhibits the activity of drug efflux pumps in MDR cells, causes significant ROS accumulation, and potently inhibits cell proliferation, causing alterations in the cell cycle profile. Our findings are confirmed by 3D spheroid models, providing new candidates for studies against MDR cancers.



Regioselective Partial Hydrogenation and Deuteration of Tetracyclic (Hetero)aromatic Systems Using a Simple Heterogeneous Catalyst

Roberta A. Kehoe, Dr. Amy Lowry, Dr. Mark E. Light, Dr. David J. Jones, Dr. Peter A. Byrne, Dr. Gerard P. McGlacken

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Chemistry A European Journal Volume30, Issue17 March 20, 2024 e202400102

https://doi.org/10.1002/chem.202400102

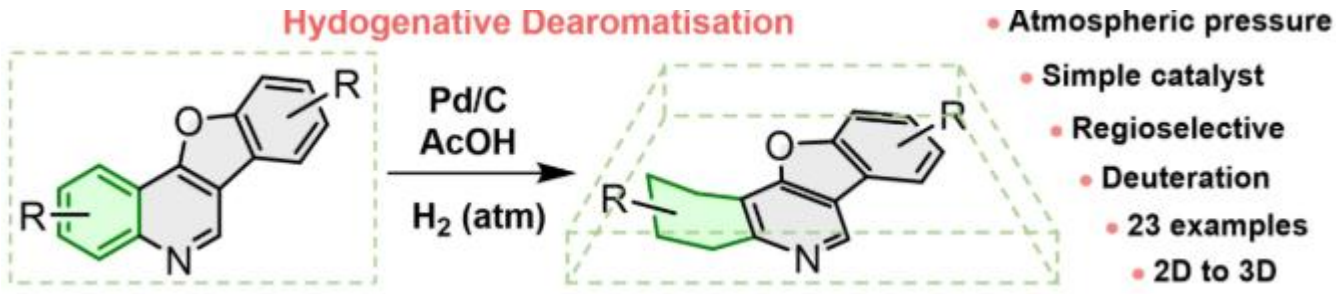
First published: 12 January 2024

Abstract

The introduction of added '3-dimensionality' through late-stage functionalisation of extended (hetero)aromatic systems is a powerful synthetic approach. The abundance of starting materials and cross-coupling methodologies to access the precursors allows for highly diverse products. Subsequent selective partial reduction can alter the core structure in a manner of interest to medicinal chemists. Herein, we describe the precise, partial reduction of multicyclic heteroaromatic systems using a simple heterogeneous catalyst. The approach can be extended to introduce deuterium (again at late-stage). Excellent yields can be obtained using simple reaction conditions.

Graphical Abstract

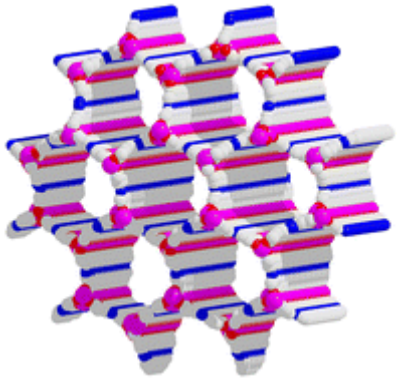
The introduction of added '3-dimensionality' through late-stage functionalisation is a powerful synthetic approach to biologically significant moieties. Herein, a hydrogenative, regioselective dearomatisation of extended (hetero)aromatic systems is described, using a simple Pd catalyst at atmospheric hydrogen pressure. Deuteration is also demonstrated, and some initial mechanistic insights are revealed.



Synthesis and characterisation of antimicrobial metal–organic frameworks as multi-drug carriers

Ahmed Ahmed; Aileen Kelly; Dayle Leonard; Waleed Saleem; Andrey Bezrukov; Constantinos G. Efthymiou; Michael J. Zaworotko; Davide Tiana; Aoife Boyd; Constantina Papatriantafyllopoulou
UCC, University of Galway UL and SSPC
Dalton Trans., 2024,**53**, 11867-11875
https://doi.org/10.1039/D4DT01100G
First published 21 Jun 2024

Abstract
Antibiotic resistance is a significant global concern, necessitating the development of either new antibiotics or advanced delivery methods. With this in mind, we report on the synthesis and characterisation of a new family of Metal–Organic Frameworks (MOFs), **OnG6** MOFs, designed to act as multi-drug carriers for bacterial infection treatment. **OnG6** is based on the pro-drug 4,4′-azodisalicylic acid ($AZDH_4$), which *in vivo* produces two equivalents of *para*-aminosalicylic acid (ASA), a crucial drug for *M. tuberculosis* treatment. X-ray and computational studies revealed that **OnG6** MOFs are mesoporous MOFs with **etb** topology and an $[M_2(AZD)]$ formula (M = Zn, **OnG6-Zn**; Mg, **OnG6-Mg**; Cu, **OnG6-Cu**; and Co, **OnG6-Co**), featuring 1-dimensional channel type pores of 25 Å diameter. **OnG6** MOFs are the first reported MOFs bearing the ligand $AZDH_4$, joining the family of mesoporous MOFs arranged in a honeycomb pattern. They absorb isoniazid (INH) and ciprofloxacin (CIPRO) with the former being a specific antibiotic for *M. tuberculosis*, and the latter being a broader-spectrum antibiotic. The stability of the MOFs and their capacity for antibiotic uptake depend on the nature of the metal ion, with **OnG6-Mg** demonstrating the highest drug absorption. The antimicrobial activity of these species was assessed against *S. aureus* and *E. coli*, revealing that the carriers containing CIPRO displayed optimal efficacy.



Dublin City University, School of Chemistry Publications 2024 Focus on Journal Articles

Gene Editing with Artificial DNA Scissors

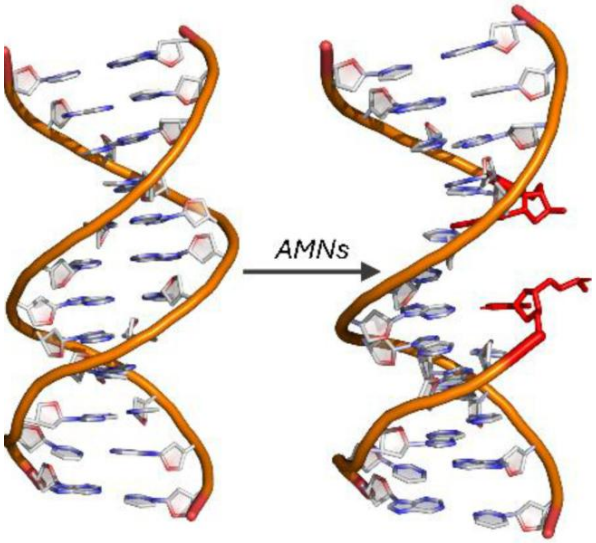
Dr. Alex Gibney, Prof. Dr. Andrew Kellett*
SSPC, The Science Foundation Ireland Research Centre for Pharmaceuticals, School of Chemical Sciences, Dublin City University
Chemistry – A European Journal: Volume 30, Issue 57 e202401621 11 October 2024
https://doi.org/10.1002/chem.202401621
First published: 10 July 2024

Abstract

Artificial metallo-nucleases (AMNs) are small molecule DNA cleavage agents, also known as DNA molecular scissors, and represent an important class of chemotherapeutic with high clinical potential. This review provides a primary level of exploration on the concepts key to this area including an introduction to DNA structure, function, recognition, along with damage and repair mechanisms. Building on this foundation, we describe hybrid molecules where AMNs are covalently attached to directing groups that provide molecular scissors with enhanced or sequence specific DNA damaging capabilities. As this research field continues to evolve, understanding the applications of AMNs along with synthetic conjugation strategies can provide the basis for future innovations, particularly for designing new artificial gene editing systems.

Graphical Abstract

Artificial metallonucleases (AMNs) are small molecule DNA cleavage agents, also known as molecular scissors, and represent an important class of chemotherapeutic agent. This review introduces concepts core to this area such as DNA structure, AMN design, and cleavage mechanisms. We also describe hybrid molecules where AMNs are covalently attached to directing groups that provide sequence specific DNA damaging capabilities.



Asymmetric synthesis of enantioenriched α-allyl esters through Pd(BINAPHANE)-catalysed allylation of disubstituted ketenes†

Ahmad A. Ibrahim [b], Stephen C. J. O'Reilly [a], Margot Bottarel[a] and Nessan J. Kerrigan *[a]
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Chem. Commun., 2024, **60**, 3283-3286
DOI: 10.1039/D4CC00057A
First published 26 February 2024

Abstract
$Pd_2dba_3 \cdot CHCl_3$ (2.5 mol%)-BINAPHANE (5 mol%) was used to promote the first catalytic enantioselective allylation of disubstituted ketenes to give α-allyl esters. The ester products were formed in good to excellent yields (61–93% yield for 13 examples, 16 examples in all), with moderate to good enantioselectivity (68–80% ee for 7 examples).

Wirefree Electrochemistry for Enhanced Detection and Treatment of Disease

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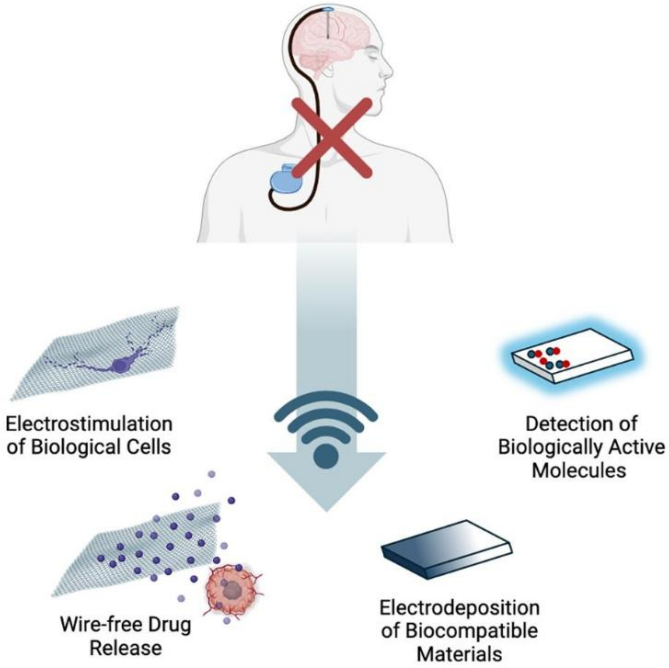
School of Chemical Sciences, DCU, FutureNeuro, SFI Research Centre for Chronic and Rare Neurological Diseases
Electrochemistry Communications Volume 169, December 2024, 107832
https://doi.org/10.1016/j.elecom.2024.107832
Version of Record 9 November 2024

Abstract
Wirefree, or bipolar electrochemistry, BPE, has the potential to transform patient outcomes through early diagnosis using ultrasensitive sensors for multiple biomarkers and personalised treatments such as enhanced cell growth, differentiation and destruction as well as local delivery of therapeutics. We highlight the emerging field of wirefree electroceuticals and show how BPE could enable precise modulation of neural circuits, non-pharmaceutical therapies for conditions like Parkinson's disease and chronic pain management, as well as on-demand drug delivery with high spatial and temporal precision. Moreover, it explores the integration of advanced nanomaterials illustrating their pivotal role in enhancing electrode performance and biocompatibility, thereby maximising their potential diagnostic and therapeutic efficacy especially *in vivo*.

Graphical abstract



Prebiotic membrane structures mimic the morphology of alleged early traces of life on Earth

Seán F. Jordan*, Mark A. van Zuilen, Joti Rouillard, Zita Martins & Nick Lane
Life Sciences Institute, School of Chemical Sciences, Dublin City University
Commun Earth Environ **5**, 234 (2024)
https://doi.org/10.1038/s43247-024-01372-0

Published: 10 May 2024

Abstract
Elucidating compositions of the first cell membranes requires experiments with molecules and chemical conditions representative of early Earth. The molecules used are described as 'prebiotically plausible', i.e., they could have formed through abiotic reactions before the emergence of biology. Similarly, the chemical properties of solutions in which these membranes are formed (e.g., pH, temperature, ionic strength) must represent early Earth environments. Here, using confocal and transmission electron microscopy combined with population morphometry, we show that prebiotically plausible molecules, in solutions representative of Hadean submarine alkaline hydrothermal vents, form microstructures with substantial morphological diversity. The microstructures hold the potential for use as analogues of prebiotic processes in the rock record. Additionally, many of the structures are morphologically similar to purported early microfossils, highlighting limitations of morphological interpretation in these studies. Detailed analyses of abiotic microstructures are essential for understanding the earliest life on Earth, and for interpretation of potential biosignatures from extra-terrestrial bodies.

Spectroscopic detection of bioaerosols with the wibs-4+: Anthropogenic and meteorological impacts

Emma Markey [a], Jerry Hourihane Clancy [a], Moisés Martínez-Bracero [a], Roland Sarda-Estève [b], Dominique Baisnée [b], Eoin J. McGillicuddy [c], Gavin Sewell [c], Carsten Ambelas Skjøth [d], David J. O'Connor [a]
School of Chemical Sciences, Dublin City University, TU Dublin and Another
Science of The Total Environment Volume 943, 15 September 2024, 173649
https://doi.org/10.1016/j.scitotenv.2024.173649
Version of Record 12 June 2024

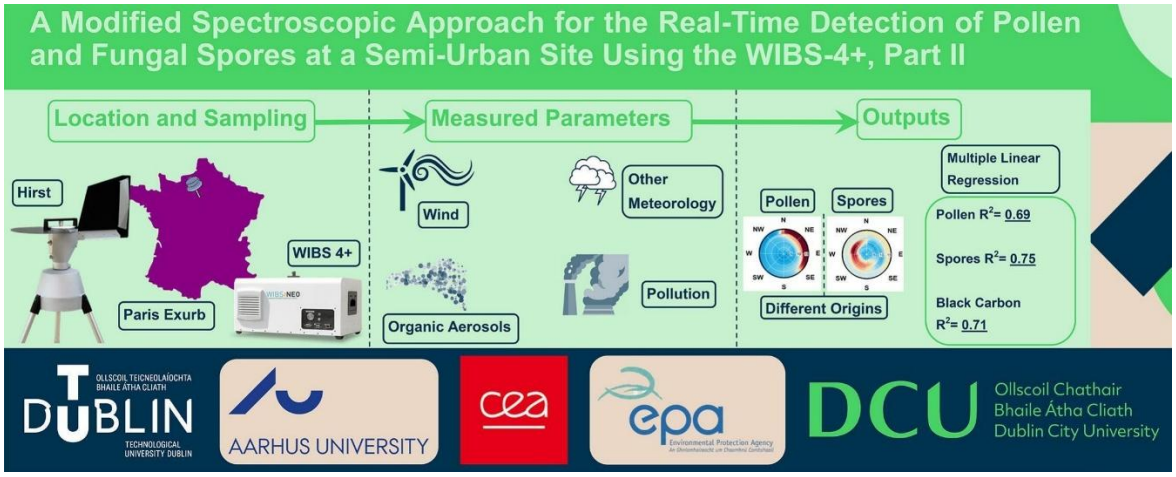
Abstract

This research builds upon a previous study that explored the potential of the modified WIBS-4+ to selectively differentiate and detect different bioaerosol classes. The current work evaluates the influence of meteorological and air quality parameters on bioaerosol concentrations, specifically pollen and fungal spore dynamics.
Temperature was found to be the most influential parameter in terms of pollen production and release, showing a strong positive correlation. Wind data analysis provided insights into the potential geographic origins of pollen and fungal spore concentrations. Fungal spores were primarily shown to originate from a westerly direction, corresponding to agricultural land use, whereas pollen largely originated from a North-easterly direction, corresponding to several forests.

The influence of air quality was also analysed to understand its potential impact on the WIBS fluorescent parameters investigated. Most parameters had a negative association with fungal spore concentrations, whereas several anthropogenic influences showed notable positive correlations with daily pollen concentrations. This is attributed to similar driving forces (meteorological parameters) and geographical origins. In addition, the WIBS showed a significant correlation with anthropogenic pollutants originating from combustion sources, suggesting the potential for such modified spectroscopic instruments to be utilized as air quality monitors.

By combining all meteorological and pollution data along with WIBS-4+ channel data, a set of Multiple Linear Regression (MLR) analyses were completed. Successful results with R^2 values ranging from 0.6 to 0.8 were recorded. The inclusion of meteorological parameters was dependent on the spore or pollen type being examined.

Graphical abstract



Pyrolysis, a recovery solution to reduce landfilling of residual organic waste generated from mixed municipal waste

Jessica Graça, Marzena Kwapinska*, Brian Murphy, Tim Duggan, James J. Leahy & Brian Kelleher
DCU, Department of Chemical Sciences, University of Limerick & Others
Environ Sci Pollut Res **31**, 30676–30687 (2024)
https://doi.org/10.1007/s11356-024-33282-1
Published13 April 2024

Abstract

Despite policies to restrict the mixing of organic waste with other general waste and improve its separation at source, municipal solid waste still contains a high proportion of organic waste. The residual organic waste is generated as a by-product of the mechanical treatment of municipal solid waste (MSW) and is mainly disposed in landfills after composting. Its reuse and recovery status varies across European countries. Most countries restrict the use of biostabilised residual waste (BSRW) to landfill cover, whereas others have regulated it as marketable compost. Crucially, BSRW is set to lose its "recycled" status under the revised European Union waste framework, with probably tighter restrictions and increased costs imposed for the landfilling of organic waste. Our research aimed to investigate pyrolysis as an alternative technology to treat the 10–40 mm fraction of BSRW (representing 50% of BSRW generated). Pyrolysis at 700 °C was carried out and feedstock and pyrolysis products were characterized. Mass and energy balances showed that pyrolysis produced hot vapour/gas whose combustion may render the pyrolysis process energetically sustainable. Biochar comprises 30–50% of BRSW mass after removal of glass, metal and stones. Our results indicate that pyrolysis has the potential to create options for contributing to reduce the landfilling of BSRW; however, the presence of residual impurities may limit biochar applications.

Enhancing Phototoxicity in BODIPY-Perylene Charge Transfer Dyads by Combined Iodination and Mesylation

Rhianne C. Curley, Ruben Arturo Arellano-Reyes, James N. McPherson, Vickie McKee, Tia E. Keyes*
Chemistry Europe A European Journal Volume30, Issue71 December 18, 2024 e202403149
https://doi.org/10.1002/chem.202403149
First published: 07 October 2024

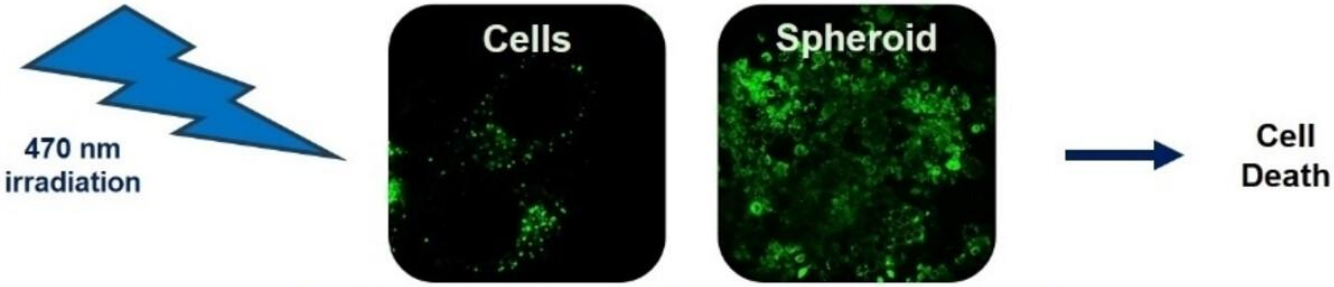
Abstract

The uptake and phototoxicity of a family of BODIPY-perylene charge transfer dyads are compared in live cancer and non-cancer cell lines to evaluate their performance in imaging and photodynamic therapy (PDT). The impact of iodination and mesylation of the meso position of the compounds on

their optical properties, cell uptake and toxicity are compared. Notably, across all derivatives the probes were minimally dark toxic up to 50 μM, (the maximum concentration tested), but exhibited outstanding phototoxicity with nanomolar IC50 values and impressive phototoxic indices (PI, ratio of dark IC50 to light IC50), with best performance for the mesylated iodinated derivative MB2PI, which had a PI of >218 and >8.9 in MCF-7 cells and tumour spheroids respectively. This is significantly higher than non-iodinated analogue MB2P in MCF-7 cells with an observed PI of >109 and slightly higher than MB2PI in spheroids with a PI of >8. This compound also showed interesting emission spectral variation with localisation that responded to stimulation of inflammation. Additional studies confirmed efficient singlet oxygen generation by the BODIPYs, suggesting a Type II mechanism of phototoxicity. Overall, the data indicates that combining charge transfer and iodination is an effective strategy for enhancing phototherapeutic capacity of BODIPY PS.

Graphic Abstract

We report a family of BODIPY-perylene charge transfer compounds with and without iodination and/or a mesityl group. The BODIPY derivatives reported show high phototoxicity in both 2D cell cultures and multicellular tumour spheroids, where MB2PI (iodinated BODIPY-perylene with a mesityl group) was the most phototoxic derivative, indicating that combining strategies to enhance phototoxicity can yield positive results.



MCF-7 cells and tumour spheroids with BODIPY-perylene

Integrating soil phosphorus sorption capacity with agronomic indices to improve sustainable P use in agriculture

Sifan Yang, Blánaid White, Fiona Regan, Nigel Kent, Rebecca L. Hall & Karen Daly*
Environment, Soils and Land Use Department Teagasc, Johnstown Castle Research Centre, Wexford, DCU Water Institute
J Soils Sediments **24**, 3396–3406 (2024)
https://doi.org/10.1007/s11368-024-03900-z
Published 13 September 2024

Abstract

Purpose

Phosphorus (P) sorption processes in soils can influence P plant-availability and influence ‘build-up’ and ‘draw-down’ P cycles. Current fertiliser recommendations do not take these processes into account. This study aimed to integrate soil P sorption behaviour and P agronomic-indices to strengthen P management recommendations.

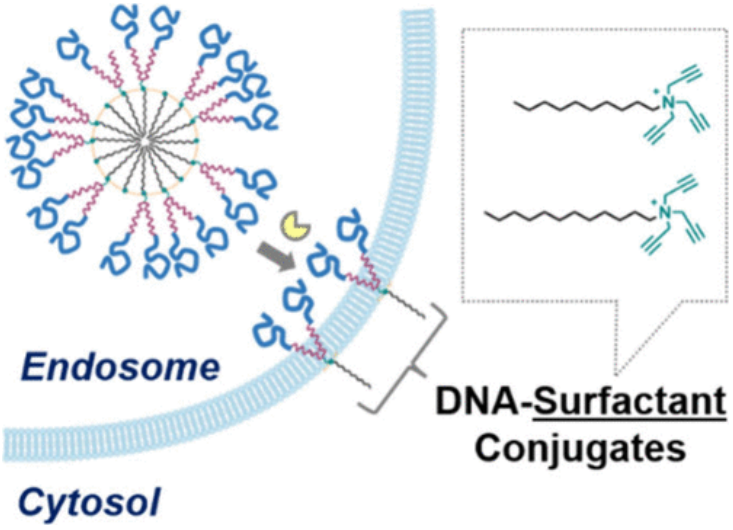
Methods

Mineral soil covering 35,716-km^2 of Ireland was characterised by P status (Morgan’s P and Mehlich-3 P), and Langmuir sorption parameters of P sorption maximum capacity (Smax, mg·kg^{-1}) and binding energy (k, L·mg^{-1}).

Determining the Role of Surfactant on the Cytosolic Delivery of DNA Cross-Linked Micelles

Ina F. de la Fuente, Shraddha S. Sawant, Kiang W. Kho, Nirod K. Sarangi, Rachelle C. Canete, Suman Pal. Lisa H. Liang, Tia E. Keyes, Jessica L. Rouge
National Centre for Sensor Research, DCU, Department of Chemistry, University of Connecticut, Storrs, US
ACS Appl. Mater. Interfaces 2024, 16, 33, 43400–43415
https://doi.org/10.1021/acsami.4c09894
Published in issue 21 August 2024

Abstract



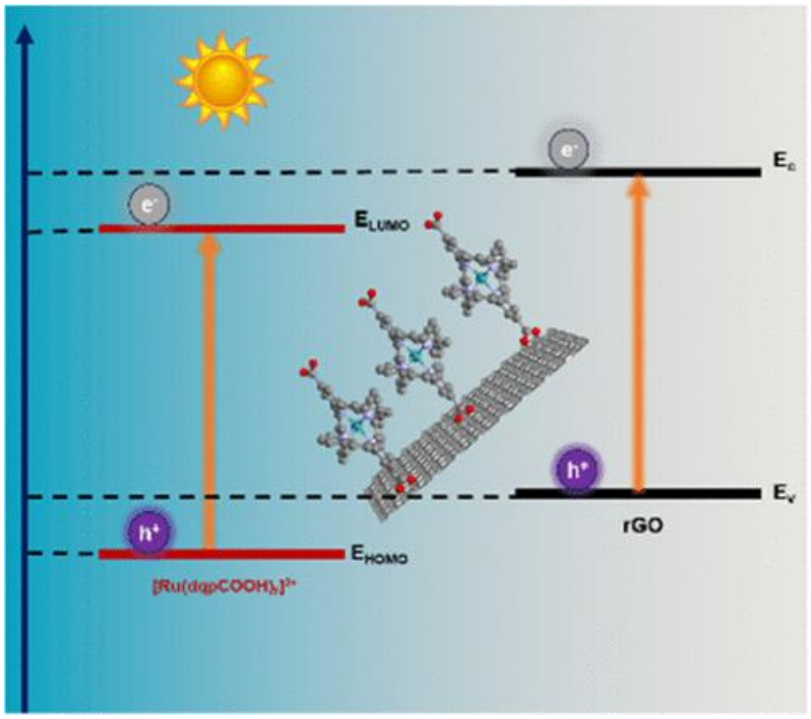
Nucleic Acid Nanocapsules (NANs) are nucleic acid nanostructures that radially display oligonucleotides on the surface of cross-linked surfactant micelles. Their chemical makeup affords the stimuli-responsive release of therapeutically active DNA–surfactant conjugates into the cells. While NANs have so far demonstrated the effective cytosolic delivery of their nucleic acid cargo, as seen indirectly by their gene regulation capabilities, there remain gaps in the molecular understanding of how this process happens. Herein, we examine the enzymatic degradation of NANs and confirm the identity of the DNA–surfactant conjugates formed by using mass spectrometry (MS). With surface enhanced (resonance) Raman spectroscopy (SE(R)RS), we also provide evidence that the energy-independent translocation of such DNA–surfactant conjugates is contingent upon their release from the NAN structure, which, when intact, otherwise buries the hydrophobic surfactant tail in its interior. Such information suggests a critical role of the surfactant in the lipid disruption capability of the DNA surfactant conjugates generated from degradation of the NANs. Using NANs made with different tail lengths (C_{12} and C_{10}), we show that this mechanism likely holds true despite significant differences in the physical properties (i.e., critical micelle concentration (CMC), surfactants per micelle, N_{agg}) of the resultant particles (C_{12} and C_{10} NANs). While the total cellular uptake efficiencies of C_{12} and C_{10} NANs are similar, there were differences observed in their cellular distribution and localized trafficking, even after ensuring that the total concentration of DNA was the same for both particles. Ultimately, C_{10} NANs appeared less diffuse within cells and colocalized less with lysosomes over time, achieving more significant knockdown of the target gene investigated, suggesting more effective endosomal escape. These differences indicate that the surfactant assembly and disassembly properties, including the number of surfactants per particle and the CMC can have important implications for the cellular delivery efficacy of DNA micelles and surfactant conjugates.

Enhanced Photostability and Photoactivity of Ruthenium Polypyridyl-Based Photocatalysts by Covalently Anchoring Onto Reduced Graphene Oxide

Seán Hennessey, Roberto González-Gómez*, Kathryn McCarthy, Christopher S. Burke, Camille Le Houérou, Nirod Kumar Sarangi, Patrick McArdle, Tia E. Keyes, Fabio Cucinotta, Pau Farràs*
DCU, School of Biological and Chemical Sciences, Energy Research Centre, Ryan Institute, University of Galway, UCC & Other
ACS Omega 2024, 9, 12, 13872–13882
https://doi.org/10.1021/acsomega.3c08800
Published 26 March 2024

Abstract

Recentstudies toward finding more efficient ruthenium metalloligands for photocatalysis applications have shown that the derivatives of the linear $[Ru(dqp)_2]^{2+}$ (dqp: 2,6-di(quinolin-8-yl)-pyridine) complexes hold significant promise due to their extended emission lifetime in the μs time scale while retaining comparable redox potential, extinction coefficients, and absorption profile in the visible region to $[Ru(bpy)_3]^{2+}$ (bpy: 2,2′-bipyridine) and $[Ru(tpy)_2]^{2+}$ (tpy: 2,2′:6′,2″-terpyridine) complexes. Nevertheless, its photostability in aqueous solution needs to be improved for its widespread use in photocatalysis. Carbon-based supports have arisen as potential solutions for improving photostability and photocatalytic activity, yet their effect greatly depends on the interaction of the metal complex with the support. Herein, we present a strategy for obtaining Ru–polypyridyl complexes covalently linked to aminated reduced graphene oxide (rGO)



to generate novel materials with long-term photostability and increased photoactivity. Specifically, the hybrid Ru(dqp)@rGO system has shown excellent photostable behavior during 24 h of continual irradiation, with an enhancement of 10 and 15% of photocatalytic dye degradation in comparison with $[Ru(dqp)_2]^{2+}$ and Ru(tpy)@rGO, respectively, as well as remarkable recyclability. The presented strategy corroborates the potential of $[Ru(dqp)_2]^{2+}$ as an interesting photoactive molecule to produce more advantageous light-active materials by covalent attachment onto carbon-based supports.

Deposition of high-quality, nanoscale SiO2 films and 3D structures

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DCU: School of Physical Sciences, National Centre for Plasma Science & Technology, School of Biotechnology, Nano Research Facility (NRF)

Applied Materials Today, Volume 38, June 2024, 102175

https://doi.org/10.1016/j.apmt.2024.102175

Version of Record 29 March 2024

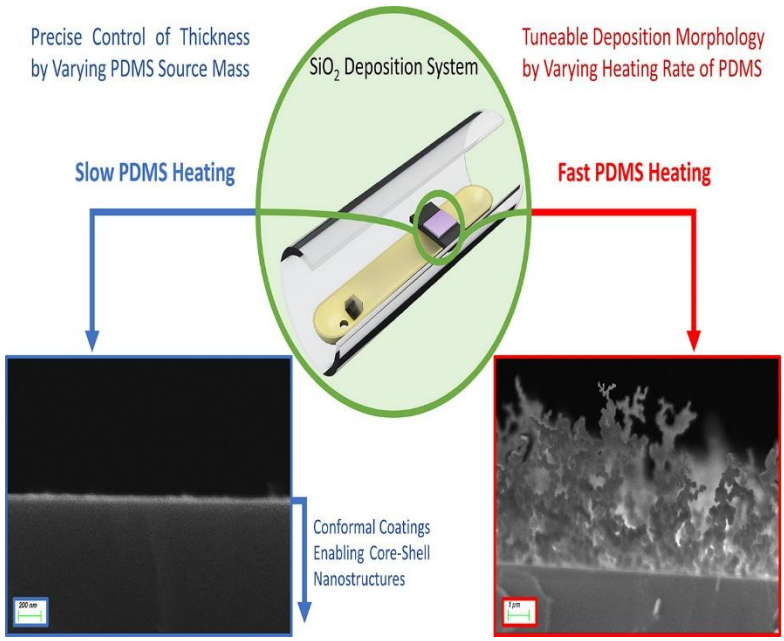
Abstract

Silicon dioxide (SiO_2) is ubiquitous in biomedical diagnostics and other applications as a capture medium for nucleic acids and proteins. Diagnostic devices have seen rapid miniaturisation in recent years, due to the increased demand for portable point-of-care diagnostics. However, there are increasing challenges with incorporating SiO_2 nanostructures into diagnostic devices, due to the complexity of nanostructured SiO_2 synthesis, often involving etching and chemical vapour deposition under high vacuum conditions.

We report a novel and straightforward method for deposition of high-quality, nanoscale SiO_2 films and 3D SiO_2 structures using thermal decomposition of polydimethylsiloxane (PDMS), in a furnace at atmospheric pressure at 500 °C. This method allows individual nanometre controllability of conformal pinhole-free layers on a variety of materials and morphologies. The temperature ramp rate is a key factor in determining the SiO_2 deposit morphology, with slower ramp rates leading to highly conformal 2D films and faster ones yielding 3D nanodentrite structures. For the 2D films, the film thickness, as

determined by spectroscopic ellipsometry and confirmed by SEM data, is shown to correlate excellently with initial PDMS source material mass in the thickness range 0.8–18 nm. Fits to ellipsometry models confirm that the refractive index of the deposited film matches the expected value for SiO_2, while electrical breakdown measurements confirm that the breakdown strength of the films is comparable to that of high-quality thermal oxides. Depositions on high aspect ratio ZnO nanostructures are shown to be highly conformal, leading to core-shell ZnO-SiO_2 nanostructures whose shell thickness is in excellent agreement with the expected values from deposition on planar substrates. At faster ramp rates an abrupt morphological transition is seen to a deposit which displays a 3D nanodentrite morphology. The possibilities for applications of both morphologies (and core-shell combinations with other nanostructured materials) in biosensing and related areas are briefly discussed, and the DNA capture capabilities of each nanostructure are measured. The high aspect ratio nanodendrite structures allow for significant DNA capture within microfluidic devices in the presence of low DNA concentrations, with a maximum average capture efficiency of 43.4 % achieved in the presence of 10 ng/mL of DNA, which is an improvement by a factor of ~ 3 over planar Si surfaces. Improvements by factors of >10 over planar surfaces were achieved at higher DNA concentrations of 100 and 1000 ng/mL.

Graphical Abstract



Enhancing pancreatic ductal adenocarcinoma (PDAC) therapy with targeted carbon nano-onion (CNO)-mediated delivery of gemcitabine (GEM)-derived prodrugs

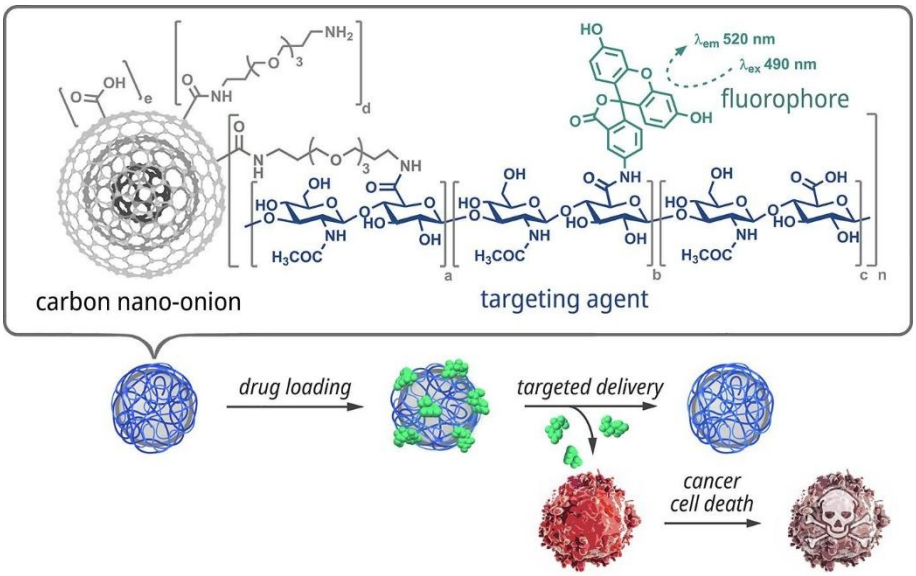
Michał Bartkowski, Valeria Bincoletto, Iris Chiara Salaroglio, Giacomo Ceccone, Raul Arenal, Sara Nervo, Barbara Rolando, Chiara Riganti, Silvia Arpicco, Silvia Giordani*
School of Chemical Sciences DCU, University of Torino, Italy and Others
Journal of Colloid and Interface Science Volume 659, April 2024, Pages 339-354
https://doi.org/10.1016/j.jcis.2023.12.166 (paid Subscription or
April 2024

Abstract

Nanotechnology's potential in revolutionising cancer treatments is evident in targeted drug delivery systems (DDSs) engineered to optimise therapeutic efficacy and minimise toxicity. This study examines a novel nanocarrier constructed with carbon nano-onions (CNOs), engineered and evaluated for its ability to selectively target cancer cells overexpressing the hyaluronic acid receptor; CD44. Our results highlighted that the CNO-based nanocarrier coupled with hyaluronic acid as the targeting agent demonstrated effective uptake by CD44+ PANC-1 and MIA PaCa-2 cells, while avoiding CD44- Capan-

1 cells. The CNO-based nanocarrier also exhibited excellent biocompatibility in all tested pancreatic ductal adenocarcinoma (PDAC) cells, as well as healthy cells. Notably, the CNO-based nanocarrier was successfully loaded with chemotherapeutic 4-(*N*)-acyl- sidechain-containing prodrugs derived from gemcitabine (GEM). These prodrugs alone exhibited remarkable efficacy in killing PDAC cells which are known to be GEM resistant, and their efficacy was amplified when combined with the CNO-based nanocarrier, particularly in targeting GEM-resistant CD44+ PDAC cells. These findings demonstrate the potential of CNOs as promising scaffolds in advancing targeted DDSs, signifying the translational potential of carbon nanoparticles for cancer therapy.

Graphical abstract



CARBON DOTS: Bioimaging and Anticancer Drug Delivery

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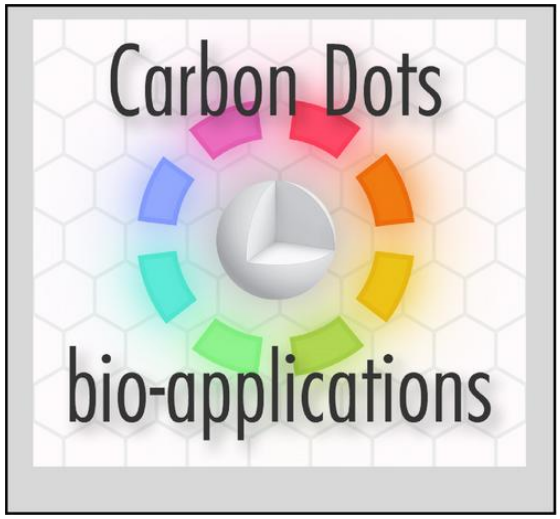
Chemistry – A European Journal, Volume30, Issue19 April 2, 2024 e202303982
https://doi.org/10.1002/chem.202303982
First published: 11 January 2024

Abstract

Cancer, responsible for approximately 10 million lives annually, urgently requires innovative treatments, as well as solutions to mitigate the limitations of traditional chemotherapy, such as long-term adverse side effects and multidrug resistance. This review focuses on Carbon Dots (CDs), an emergent class of nanoparticles (NPs) with remarkable physicochemical and biological properties, and their burgeoning applications in bioimaging and as nanocarriers in drug delivery systems for cancer treatment. The review initiates with an overview of NPs as nanocarriers, followed by an in-depth look into the biological barriers that could affect their distribution, from barriers to administration, to intracellular trafficking. It further explores CDs′ synthesis, including both bottom-up and top-down approaches, and their notable biocompatibility, supported by a selection of *in vitro, in vivo*, and *ex vivo* studies. Special attention is given to CDs′ role in bioimaging, highlighting their optical properties. The discussion extends to their emerging significance as drug carriers, particularly in the delivery of doxorubicin and other anticancer agents, underscoring recent advancements and challenges in this field. Finally, we showcase examples of other promising bioapplications of CDs, emergent owing to the NPs flexible design. As research on CDs evolves, we envisage key challenges, as well as the potential of CD-based systems in bioimaging and cancer therapy.

Graphical Abstract

This review explores Carbon Dots (CDs) in cancer treatment, highlighting their synthesis, bioimaging applications, and role in drug delivery. The review details potential barriers to drug delivery, and details recent studies and developments, with a focus on the use of CDs as nanocarriers in drug delivery systems designed for the delivery of doxorubicin.



Royal College of Surgeons in Ireland, School of Chemistry Publications 2024, Focus on Journal Articles

Time-resolved fluorescence imaging with color-changing, "turn-on/turn-on" AIE nanoparticles

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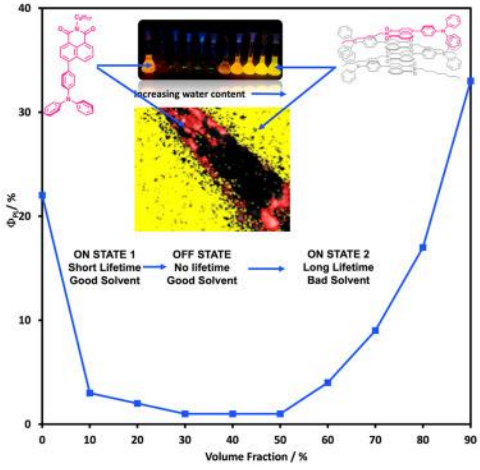
Department of Chemistry, RCSI, Department of Chemistry, RCSI-TCD, AMBER, SSPC and Others
Chem, Volume 10, Issue 2 p578-599
DOI: 10.1016/j.chempr.2023.10.001
Published 08 February 2024

Summary

Two aggregation-induced emission (AIE) 1,8-naphthalimides (**1** and **2**) exhibiting "turn-on/turn-on" emission behavior are reported. They are emissive in good solvents of low/intermediate polarity (THF/hexane) but undergo drastic quenching in polar solvents (DMSO/MeOH) due to solvatochromic and energy gap law effects. Water also quenches the emission up to a critical volume (<50% water in THF), after which hydrophobicity drives them to aggregate into nanoparticles, restoring their emission. The mechanisms are revealed through spectroscopy and theory with distinct excited-state decay kinetics observed between the two turn-on/turn-on states. Self-assembly of **2** with the biocompatible poloxamer P188 generates luminescent particles that are taken up into MDA-MB 231 human breast cancer cells, at which point they disassemble, releasing **2**, which then localizes in the lipid droplets. Time-resolved fluorescence lifetime imaging (FLIM) distinguishes extracellular **2**-P188 particles emitting from the "aggregated on-state" and intracellular, free molecules of **2** emitting from the "disaggregated on-state" within the lipid droplets.

Graphical abstract



Review of Clinically Assessed Molecular Fluorophores for Intraoperative Image Guided Surgery

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Department of Chemistry, RCSI, University of Medicine and Health Sciences, Dublin
Molecules 2024, *29*(24), 5964
https://doi.org/10.3390/molecules29245964
Published: 18 December 2024

Abstract

The term “fluorescence” was first proposed nearly two centuries ago, yet its application in clinical medicine has a relatively brief history coming to the fore in the past decade. Nowadays, as fluorescence is gradually expanding into more medical applications, fluorescence image-guided surgery has become the new arena for this technology. It allows surgical teams to real-time visualize target tissues or anatomies intraoperatively to increase the precision of resection or preserve vital structures during open or laparoscopic surgeries. In this review, we introduce the concept of near-infrared fluorescence guided surgery, discuss the recent and ongoing clinical trials of molecular fluorophores (indocyanine green, 5-aminolevulinic acid, methylene blue, IR-dye 800CW, pafolacianine) and their surgical goals, highlight key chemical and medical factors for imaging agent optimization, deliberate challenges and potential advantages, and propose a framework for integrating this technology into routine surgical care in the near future. The notable clinical achievements of these fluorophores over the past decade strongly indicates that the future of fluorescence in surgery is bright with many more patient benefits to come.

Investigation of the Effectiveness of Photo Deprotection of Polypeptides in Solution and within the Core of Miniemulsion-Derived Nanoparticles

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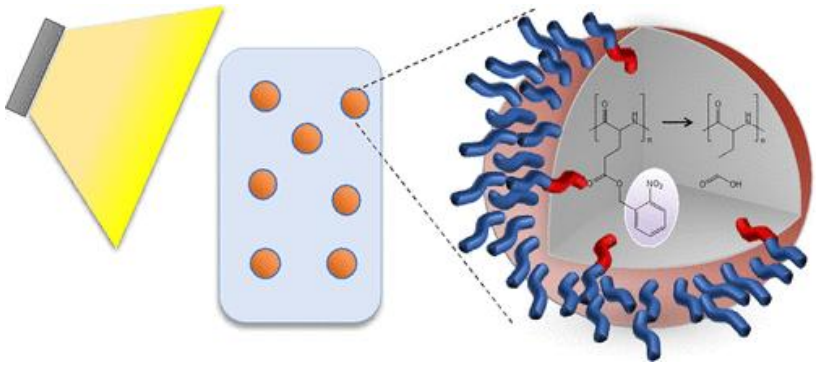
Macromolecules 2024, 57, 5, 1979–1987
https://doi.org/10.1021/acs.macromol.3c02538
27 February 2024

Abstract



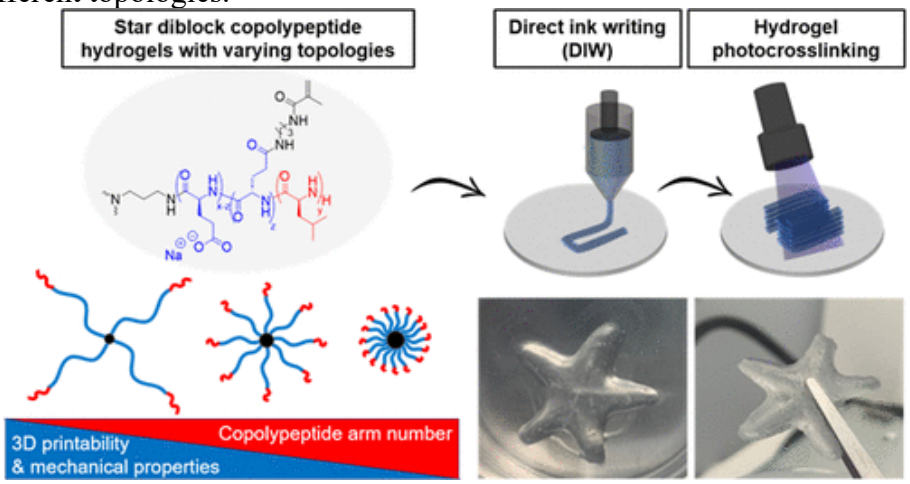
Homopolymerization of ortho-nitrobenzyl (*o*NB)-protected l-cysteine and l-glutamic acid was systematically studied in different solvents and at different monomer to initiator ratios, revealing the best reaction control in dimethylformamide (DMF) across a range of degrees of polymerization. In the subsequent ultraviolet (UV)-cleavage studies, it was found that quantitative deprotection upon UV exposure at 365 nm was not achievable for either of the homopolypeptides as confirmed by ^{1}H NMR and UV/visible (UV/vis) analyses. While the poly(*o*NB-l-cysteine) deprotected more readily with no effect of the polypeptide molecular weight, lower molecular weight poly(*o*NB-l-glutamate) reached maximum deprotection faster than high molecular weight samples. This was further confirmed by the pH changes of the solution. When incorporated into the core of miniemulsion-derived nanoparticles, both *o*NB-protected copolypeptides were successfully deprotected as evident from a color change and a pH change in the case of poly(*o*NB-l-glutamate). However, the removal of the deprotection byproduct nitrosobenzaldehyde proved unsuccessful, which indicates a diffusion barrier caused by the nanoparticle’s surfactant. The study provides insights and guidelines for the UV deprotection of polypeptides and demonstrates the ability to selectively UV-deprotect polypeptides in the confined space of a nanoparticle dispersion.

Tuning Star Polymer Architecture to Tailor Secondary Structures and Mechanical Properties of Diblock Polypeptide Hydrogels for Direct Ink Writing

Department of Chemistry, RCSI University of Medicine and Health Sciences, Dublin and Another
Muireann Cosgrave, Kulwinder Kaur, Christopher Simpson, Łukasz Mielańczyk, Ciara Murphy, Robert D. Murphy*, Andreas Heise*
Biomacromolecules 2025, 26, 1, 670–678

https://doi.org/10.1021/acs.biomac.4c01500
Published December 19, 2024

Abstract
Hydrogel three-dimensional (3D) printing has emerged as a highly valuable fabrication tool for applications ranging from electronics and biomedicine. While conventional hydrogels such as gelatin, alginate, and hyaluronic acid satisfy biocompatibility requirements, they distinctly lack reproducibility in terms of mechanical properties and 3D printability. Aiming to offer a high-performance alternative, here we present a range of amphiphilic star-shaped diblock copolypeptides of l-glutamate and l-leucine residues with different topologies.



Hydrophobic side chains of the l-leucine polymer block drive conformational self-assembly in water, spontaneously forming hydrogels with tunable mechanical properties, through variation of star topology. Their amenable shear-thinning and self-recovery properties render them suitable as hydrogel inks for direct ink writing. Well-defined 3D-printed structures can be readily generated and rapidly photo-cross-linked using visible light (405 nm) after methacrylamide functionalization, while hydrogel inks demonstrate good biocompatibility with top-seeded and encapsulated MC3T3 cells.

Ciprofloxacin as a tryptophan mimic within an antimicrobial peptide†

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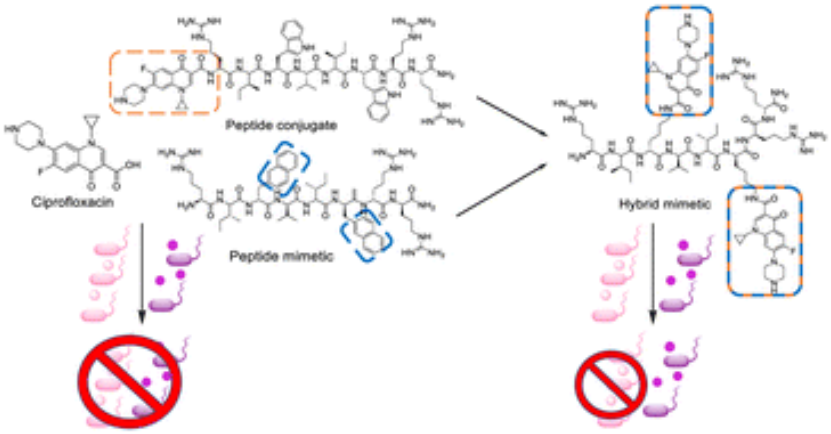
Department of Chemistry, RCSI University of Medicine and Health Sciences, Dublin and Others
New J. Chem., 2024,**48**, 15722-15725
https://doi.org/10.1039/D4NJ01445F
First published 13 Aug 2024

Abstract
Ciprofloxacin has been used to replace tryptophan at positions 3 and 6 in the antimicrobial peptide (AMP) Bac8c. Bac8c(Cip^{3,6}) showed comparable antimicrobial activity but increased selectivity toward some Gram-negative bacteria with MIC values of ≤6.25 μM. Bac8c(Cip^{3,6}) was also non-cytotoxic to cultured HepG2 cells at antimicrobial concentrations, with a CC_{50} >300 μM.

Graphical Abstract



Novel Peptide–Drug Conjugates with Dual Anticancer Activity

Siobhán O'Flaherty [1,2,*], Olga A. Luzina [3], Nadezhda S. Dyrkheeva [4], Ysaline Krier [5], Jérôme Leprince [6,7],
Alexandra L. Zakharenko [4], Mikhail A. Pokrovsky [8], Andrey G. Pokrovsky [8], Olga I. Lavrik [4], Nariman F. Salakhutdinov [3], Mihayl Varbanov [5], Marc Devocelle [1,2,†] and Konstantin P. VolchoKonstantin P. Volcho [3,8,†]
[†]These authors contributed equally to this work.

Department of Chemistry, RCSI University of Medicine and Health Sciences Dublin
Int. J. Mol. Sci. **2024**, *25*(22), 12411
https://doi.org/10.3390/ijms252212411
Published: 19 November 2024

Abstract

Cationic antimicrobial peptides (AMPs), also called host defence peptides, have established antimicrobial and anticancer activities. Conjugation of an AMP to a bioactive molecule with complementary activity can address some of the clinical limitations of the peptide candidate. This approach has been particularly applied in antimicrobial applications of AMPs, but it remains relatively less explored in the generation of anticancer candidates. In this study, two usnic acid derivatives, based on hydrazinothiazole and benzylidenefuranone pharmacophore moieties, respectively, were conjugated to L-K6, a lysine/leucine-rich AMP, through a new pyrazole ligation intrinsically driven by the cargo molecule. Both components, the usnic acid derivative and the peptide, are selectively active against cancer cells, by targeting the human DNA repair enzyme tyrosyl-DNA phosphodiesterase 1 (TDP1) and through DNA damage, respectively. The two conjugates, based on a hydrazone linkage, exhibited pleiotropic effects, ranging from reduction in the activity of the parent drugs to their conservation or even enhancement. Notably, the conjugates retained some anti-TDP1 activity and displayed intermediate, or even higher, cytotoxicities against glioblastoma cells, compared to their individual components.

Synthesis and anti-leishmanial activities of uniflorol analogues

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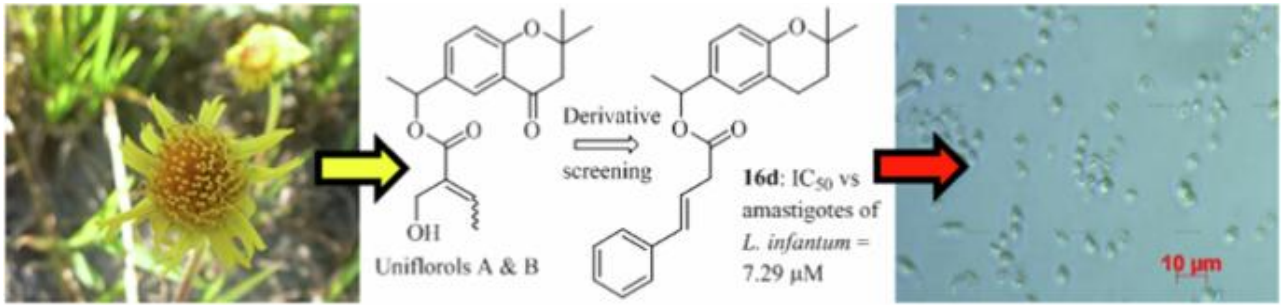
Department of Chemistry, RCSI University of Medicine and Health Sciences and Others
Med Chem Res 33, 1657–1670 (2024)
https://doi.org/10.1007/s00044-024-03275-3
Published 08 July 2024

Abstract

Chromanones are a subset of the benzopyran family, and display diverse biological activities, both as natural products and synthetic derivatives. Among these, we selected the natural product uniflorol, a 4-chromanone with an α,β-unsaturated ketone side chain, as a lead compound due to its reported anti-leishmanial properties. We designed and synthesised four series of novel compounds, varying the substitution patterns around the benzopyran core, and evaluated the compounds for anti-leishmanial activity against amastigotes of *L. infantum*. We prepared and characterised 24 novel compounds; upon screening, 12 compounds demonstrated activity values of <50 μM, with the most potent compound, **16d**, having an IC_{50} of 7.29 μM. Activity was favoured in compounds bearing a phenylalkenyl motif, such as cinnamyl, styryl or a more lipophilic extension, and amide analogues retained activity. Uniflorol analogues display promise as novel architectures towards the development of potential anti-leishmanial agents.

Graphical Abstract



The activity of a Ga(III) catecholate complex against Aspergillus fumigatus in conditions mimicking cystic fibrosis lung and inhaled formulations for its pulmonary administration

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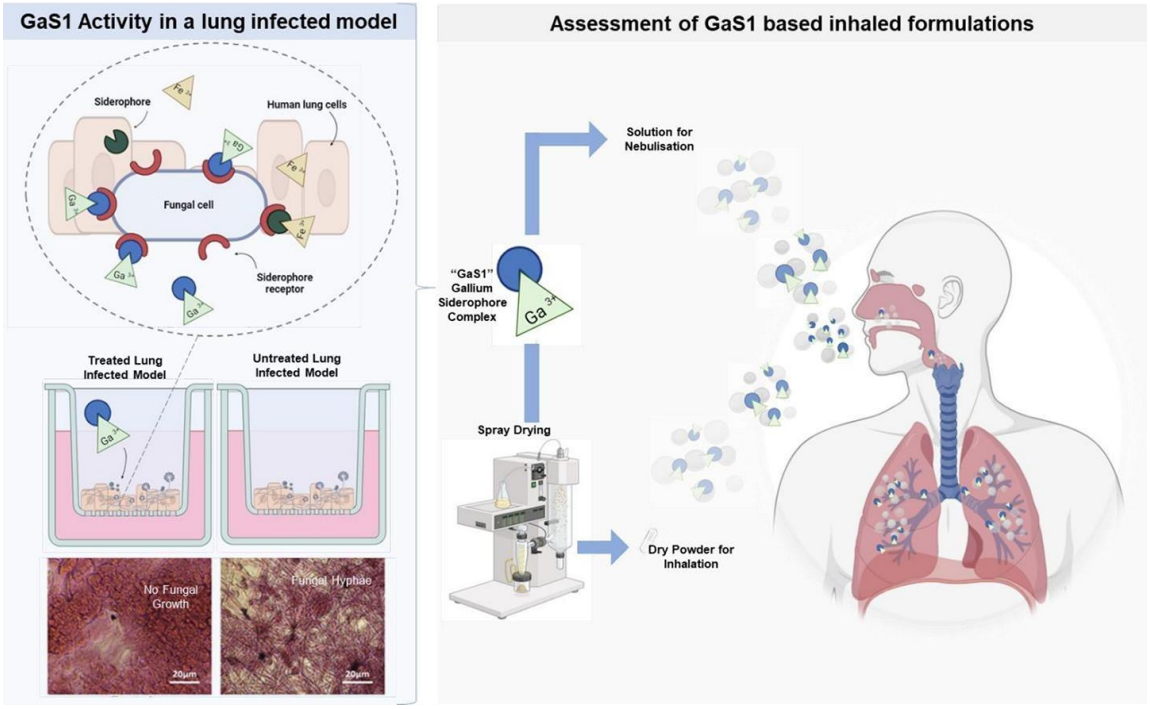
RCSI, MU, SSPC, TUD, University of Pisa, Italy
International Journal of Pharmaceutics Volume 667, Part A,
https://doi.org/10.1016/j.ijpharm.2024.124871
25 December 2024, 124871

Abstract

Azole-resistant *Aspergillus fumigatus* (*A. fumigatus)* is an emerging worldwide pathogen. Pulmonary *aspergillosis* primarily affects severely immunocompromised patients and is also a particularly critical condition for cystic fibrosis (CF) patients. A recently designed gallium polypyridyl catecholate complex, GaS1, has previously demonstrated *in vitro* and *in vivo* antimicrobial activity against Gram-negative bacteria. In the present work GaS1 activity was assessed against *A. fumigatus* clinical isolates in a novel air–liquid-interface lung infection model, mimicking the conditions found in the CF airways. Furthermore, in this study both a solution for nebulisation and dry powders for inhalation were developed with a view to optimising GaS1 delivery to the lung. The solution for nebulisation was characterised for its osmolality and pH, while the dry powders were characterised by scanning electron microscopy, powder X-ray diffraction, thermal analysis and laser light scattering particle size analysis. The aerodynamic deposition profiles of all formulations were determined using a next generation impactor. GaS1, tested in a concentration range of 0.016–0.5 mg/mL, inhibited the growth of *A. fumigatus* lung isolates in a complex host-environment-mimicking medium at the non-toxic concentration of 0.063 mg/mL. A marked dose-dependent antifungal activity of GaS1 was also observed in the presence of differentiated human distal lung epithelial cells (NCI-H441) at the air liquid interface, with nearly no fungal growth detected at the macroscopic and microscopic level. A solution for nebulisation and three different dry powder inhaler

formulations, prepared by spray-drying GaS1 with different concentrations of L-leucine, displayed suitable aerodynamic characteristics for GaS1 delivery to the lungs, while maintaining excellent antifungal activity. Overall, the results obtained highlight the potential of gallium-polypyridyl catecholate complexes for the management of difficult-to-treat *A. fumigatus* pulmonary infections.

Graphical abstract



Development of a fast and simple method for the isolation of superparamagnetic iron oxide nanoparticles protein corona from protein-rich matrices

Mahmoud G. Soliman[a] [b]*, Duong N. Trinh[a], Costanza Ravagli[c], Paula Meleady[d], Michael Henry[d], Dania Movia[e] [f], Saer Doumett[c], Laura Cappiello[c], Adriele Prina-Mello[e] [g], Giovanni Baldi[c], Marco P. Monopoli[a]*

Chemistry Department, RCSI, Dublin, DCU Dublin, TCD, and Others

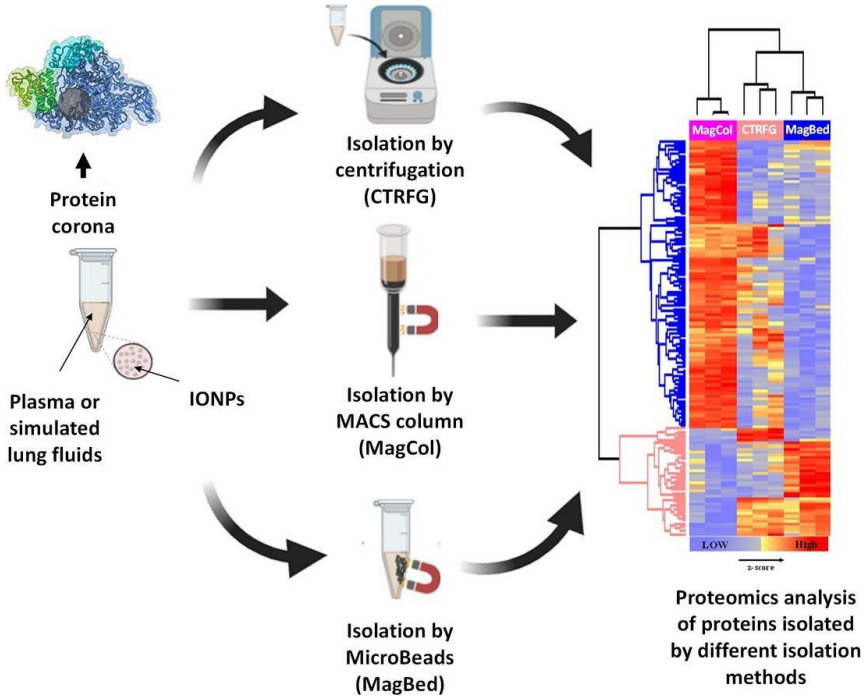
Journal of Colloid and Interface Science Volume 659 April 2024, Pages 503-519
https://doi.org/10.1016/j.jcis.2023.11.177
Version of Record 6 January 2024

Abstract

The adsorption of proteins onto the surface of nanoparticle (NP) leads to the formation of the so-called "protein corona" as consisting of both loosely and tightly bound proteins. It is well established that the biological identity of NPs that may be acquired after exposure to a biological matrix is mostly provided by the components of the hard corona as the pristine surface is generally less accessible for binding. For that reason, the isolation and the characterisation of the NP-corona complexes and identification of the associated biomolecules can help in understanding its biological behaviour. Established methods for the isolation of the NP-HC complexes are time-demanding and can lead to different results based on the isolation method applied. Herein, we have developed a fast and simple method using ferromagnetic beads isolated from commercial MACS column and used for the isolation of superparamagnetic NP following exposure to different types of biological milieu. We first demonstrated the ability to easily isolate superparamagnetic iron oxide NPs (IONPs) from different concentrations of human blood plasma and also tested the method on the corona isolation using more complex biological matrices, such as culture medium containing pulmonary mucus where the ordinary corona methods cannot be applied. Our developed method showed less than 20% difference in plasma

corona composition when compared with centrifugation. It also showed effective isolation of NP-HC complexes from mucus-containing culture media upon comparing with centrifugation and MACS columns, which failed to wash out the unbound proteins. Our study was supported with a full characterisation profile including dynamic light scattering, nanoparticle tracking analysis, analytical disk centrifuge, and zeta potentials. The biomolecules/ proteins composing the HC were separated by vertical gel electrophoresis and subsequently analysed by liquid chromatography-tandem mass spectrometry. In addition to our achievements in comparing different isolation methods to separate IONPs with corona from human plasma, this is the first study that provides a complete characterisation profile of particle protein corona after exposure in vitro to pulmonary mucus-containing culture media.

Graphical abstract



Understanding the role of biomolecular coronas in human exposure to nanomaterials

Mahmoud Soliman, Alberto Martinez Serra, Giulia Antonello, Marko Dobricic, Terence Wilkins, Tommaso Serchi, Ivana Fenoglio, Marco Monopoli
Chemistry Department, RCSI (Royal College of Surgeons in Ireland) & Others
Environ. Sci: nano
https://doi.org/10.1039/d4en00488d
Publication 20 December 2024

Summary
Nanomaterials (NMs) are increasingly used in medical treatments, electronics, and food additives. However, nanosafety—the possible adverse effects of NMs on human health—is an area of active research. This review provides an overview of the influence of biomolecular coronas on NM transformation following various exposure routes. We discuss potential exposure pathways, including inhalation and ingestion, describing the physiology of exposure routes and emphasising the relevance of coronas in these environments. Additionally, we review other routes to NM exposure, such as synovial fluid, blood (translocation and injection), dermal and ocular exposure, as well as the dose and medium impact on NM interactions. We emphasize the need for an in-depth characterisation of coronas in different biological media, highlighting the need and opportunity to study lung and gastric fluids to understand NM behaviour and potential toxicity. Future research aims to predict better in vivo outcomes and address the complexities of NM interactions with biological systems.

Technological University Dublin, School of Chemistry Publications 2024, Focus on Journal Articles

Influence of deep eutectic solvents on redox biocatalysis involving alcohol dehydrogenases

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School of Food Science and Environmental Health, Technological University Dublin, Grangegorman Lower, Dublin, School of Chemical Sciences, Dublin City University
Heliyon, Volume 10, Issue 12, e32550
DOI: 10.1016/j.heliyon.2024.e32550
https://www.cell.com/heliyon/fulltext/S2405-8440(24)08581-5
June 30, 2024

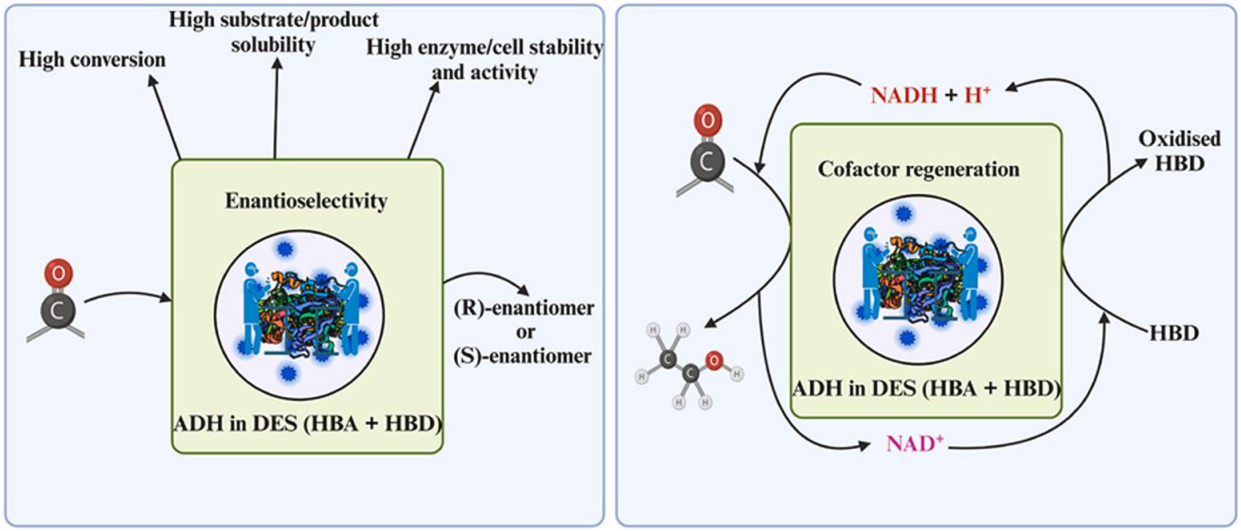
Abstract

Redox biocatalysis plays an increasingly important role in modern organic synthesis. The recent integration of novel media such as deep eutectic solvents (DESs) has significantly impacted this field of chemical biology. Alcohol dehydrogenases (ADHs) are important biocatalysts where their unique specificity is used for enantioselective synthesis.

This review explores aspects of redox biocatalysis in the presence of DES both with whole cells and with isolated ADHs. In both cases, the presence of DES has a significant influence on the outcome of reactions albeit via different mechanisms. For whole cells, DES was shown to be a useful tool to direct product formation or configuration - a process of solvent engineering. Whole cells can tolerate DES as media components for the solubilization of hydrophobic substrates. In some cases, DES in the growth medium altered the enantioselectivity of whole cell transformations by solvent control. For isolated enzymes, on the other hand, the presence of DES promotes substrate solubility as well as enhancing enzyme stability and activity. DES can be employed as a smart solvent or smart cosubstrate particularly for cofactor regeneration purposes.

From the literatures examined, it is suggested that DES based on choline chloride (ChCl) such as ChCl:Glycerol (Gly), ChCl:Glucose (Glu), and ChCl:1,4-butanediol (1,4-BD) are useful starting points for ADH-based redox biocatalysis. However, each specific reaction will require optimisation due to the influence of several factors on biocatalysis in DES. These include solvent composition, enzyme source, temperature, pH and ionic strength as well as the substrates and products under investigation.

Graphical abstract



Microbial and Enzymatic Biodegradation of Plastic Waste for a Circular Economy

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***Appl. Sci.* 2024**, *14*(24), 11942;
DOI: **https://doi.org/10.3390/app142411942**

Abstract

Plastics play a crucial role in modern life, but their accumulation poses a serious threat to both the environment and human health. Due to their effects on the terrestrial and aquatic environment, it is essential to develop sustainable approaches to dispose of waste plastics. Traditional methods of plastic disposal, such as burning and landfilling, are problematic since they produce hazardous byproducts. Biodegradation is a potentially effective, eco-friendly approach which uses microbial consortia or isolated enzymes to break down plastic waste. Enzymes interact with plastic surfaces and hydrolyse the large polymer chains into smaller units. These byproducts can then be utilised as carbon sources by microbes, which are eventually converted into CO_2 and water. This review explores the principal approaches to plastic degradation, with a focus on existing and emerging polymers made to be readily biodegradable. In addition, sustainable valorisation methods for converting plastic waste into valuable byproducts are considered. The implementation of a circular plastic economy is expected to lead to further development, including scaling up of efficient plastic bio-upcycling processes, which can serve to stimulate environmental waste removal and value-added use of post-consumer plastic streams.

Hybrid silver(I) coumarin-carbene and coumarin-triphenylphosphine complexes: Towards more effective antimicrobial therapies

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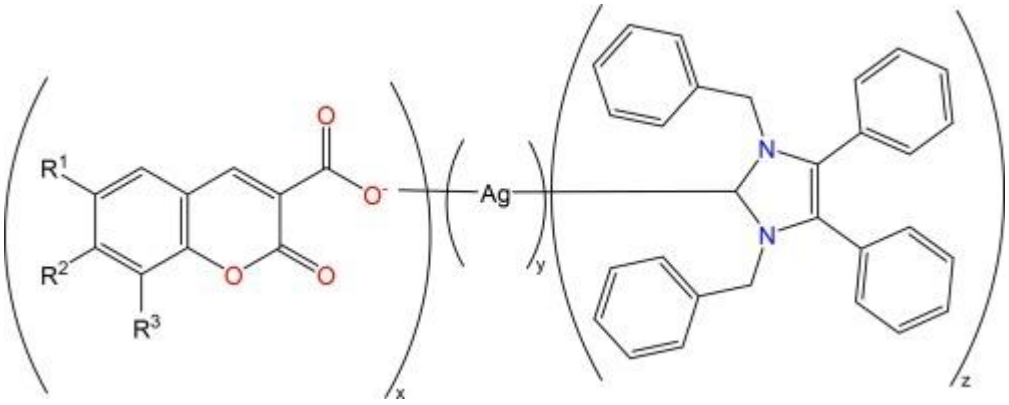
Version of Record 20 July 2024.

Abstract

The rise of antimicrobial resistance and the resulting societal burden has highlighted the need for the development of novel therapeutics. Towards that end, a series of hybrid silver(I) coumarin-carbene and coumarin-triphenylphosphine complexes were synthesised and characterised by spectroscopic analysis including IR, ^{1}H and ^{13}C NMR spectroscopy, elemental analysis, and X-ray crystallography. Isolation of coumarin-carbene hybrid complexes was achieved using two methods, with isolation via firstly the in-situ generation of a free carbene under Schlenk conditions, followed by reaction with a coumarin silver(I) complex resulting in the formation of a hybrid complex with two silver ions forming a strong argentophilic Ag(I)–Ag(I) interaction. In this hybrid complex one silver(I) ion was bound to two coumarin carboxylate ligands with the other ion bound to two carbene ligands. Isolation via an ionic carbene route led to more complex aggregates but both types of complexes had good solubility and photostability as did the triphenylphosphine hybrid complexes. All the hybrid complexes showed therapeutic potential as antimicrobial agents against MRSA with the carbene hybrid complexes exhibiting an increased antimicrobial activity against both *E. coli* and MRSA when compared to the initial silver(I) complexes.

Graphical abstract

Structure of hybrid silver(I) coumarin carbene complexes, with enhanced antimicrobial activity, is dependent on synthetic protocol used.



Heteroleptic Coumarin-Based Silver(I) Complexes: Possible New Antimicrobial Agents

Erika Mooney [1,2]*, Brendan Twamley [3], Gordon Cooke [1,2]*, Emma Caraher [1,2], Matthias Tacke[4*], Fintan Kelleher [1,2] and Bernadette S. Creaven[2,5,*]

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Molecules **2024**, *29*(24), 5917
DOI: https://doi.org/10.3390/molecules29245917
Published: 15 December 2024

Abstract

Heteroleptic coumarin-based silver(I) complexes with improved solubility profiles were synthesised using either triphenylphosphine or an *N*-heterocyclic carbene as adduct ligands, and were fully characterised using IR and NMR spectroscopy, elemental analysis, and, where possible, X-ray crystallography. The triphenylphosphine adducts formed well-resolved structures, where the oxyacetate ligands asymmetrically chelated the silver(I) ion in a bidentate chelating mode, and the silver(I) ion was also bound to two triphenylphosphine ligands. The solubility profile and photostability of the adducts were considerably improved compared to those of previously isolated simple coumarin silver(I) complexes. Analysis of the coumarin *N*-heterocyclic carbene(NHC) silver(I) adduct indicated that it likely formed as a complex aggregate species with an overall stoichiometry of 1:1:1 coumarin:Ag(I):NHC. The Kirby Bauer assay and broth microdilution assays were used to assess the silver(I) complexes' and adducts' antimicrobial activity against pathogenic strains of *Pseudomonas aeruginosa*, *Escherichia coli*, and MRSA. Interestingly, the formation of more soluble complexes did not increase the activity of the silver(I) complexes and, in effect, made them less effective antimicrobial agents, particularly against *Escherichia coli* and *Pseudomonas aeruginosa*, although they retained their activity against MRSA.

Coffee: Lighting Its Complex Ground Truth and Percolating Its Molecular Brew

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Beverages **2024**, *10*(4), 119
DOI: https://doi.org/10.3390/beverages10040119
Published: 2 December 2024

Abstract

Coffee is one of the most widely traded commodities worldwide and its popularity is only increasing. The International Coffee Organisation (ICO) reported a 6% increase in global production in 2020 to 10.5 million tonnes. Coffee production is quite involved (from sowing to harvesting, processing, packaging, and storage); consequently, the industry faces major challenges in terms of the assessment of its quality, flavour, and the components which contribute to coffee's characterisation, as well as the sustainability of coffee production and global trade. This has prompted multiple studies on the nature of the aroma and taste of the many varieties of coffee around the world, which has resulted in the identification of approximately 1000 volatile compounds and the development and implementation of upwards of 100 lexicons to describe the specific sensory characteristics of coffee. The complex nature of coffee has necessitated the development and incorporation of new analytical methodologies, such as multidimensional separation technologies and spectroscopy coupled with multivariant analysis, to qualify the essential characteristics of coffee's flavour. This work aims to review the research on coffee's flavour, covering the roasting process of coffee beans, the volatile and non-volatile components generated by this process, and the chemical reactions responsible for their formation, as well as coffee's sustainability, the coffee value chain, and various forms of regulation, particularly the current emphasis on 'fair trade'.

Monitoring the curing, degradation and moisture ingress into alkyl 2-cyanoacrylate adhesives using electrochemical impedance spectroscopy

Kevin Raheem, John Cassidy*, Bernard Ryan & Anthony Betts
Journal of Solid State Electrochemistry, Volume 28, pages 4029–4040, (2024)
DOI: https://doi.org/10.1007/s10008-024-06003-4
Published: 15 July 2024

Abstract

Electrochemical impedance spectroscopy (EIS) was employed in an attempt to gain insight into the mechanisms of ethyl 2-cyanoacrylate (ECA) curing (polymerisation) and bonding on aluminium alloy 2024 metal. EIS can detect ionic movement, adsorption processes, charge transfer and storage occurring at an adhesive/substrate interface and/or in a bulk bond line during curing. Low-frequency capacitance measurements demonstrated sensitivity to surface polymerisation reactions and were modelled using an equivalent circuit model with two time constants in series. At a frequency of 1 kHz, changes in the dielectric polymer could be readily followed with time, confirmed by employing a crown ether to accelerate the polymerisation process. Hydrolytic degradation of poly-ECA bonds at a stainless steel interface was also investigated. An equivalent circuit model containing a number of circuit components comprising pore, charge transfer and diffusional impedances, along with polymer film, double layer and diffusional capacitances (represented by constant phase elements), was developed. Three regions were identified in the frequency domain and ascribed to processes taking place at the polymer/electrolyte and polymer/metal oxide interfaces. In short, EIS can be employed to

follow the rate of polymerisation of ethyl-2-cyanoacrylate and also the degradation of the resulting polymer in saline solution.

In situ tuning and investigating the growth process of size controllable gold nanoparticles and statistical size prediction analysis

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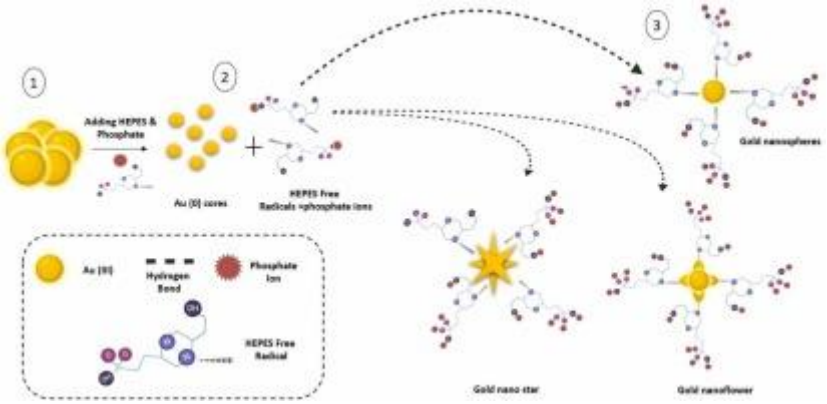
[b] Nanolab, FOCAS Research Institute, Technological University Dublin, Dublin, Ireland
[c] RELX, Risk Solutions Group, D18 X6N2, Dublin, Ireland
Colloids and Surfaces A: Physicochemical and Engineering Aspects Volume 681, 132733
DOI: https://doi.org/10.1016/j.colsurfa.2023.132733
Published 20 January 2024

Abstract

A critical understanding of the formation and growth process of gold nanoparticles (GNPs) is crucial, in order to synthesize monodisperse gold nanocrystals of controllable size and shape in a predictable way. GNPs of different shapes and sizes can be produced by altering different physicochemical reaction conditions, such as pH, temperature, and the ratio of reactants. The significant variations in the morphological features of GNPs can be monitored in situ in a time-dependent manner by using UV–visible spectroscopy. In this study, we have synthesized seedless GNPs by reduction of $HAuCl_4$ by using various molar ratios of HEPES and Na_2HPO_4. The shape and the geometry of the gold nanostructures were optimized by varying the pH (5, 7, and 9) of the HEPES, molar concentrations of disodium phosphate to $HAuCl_4$, and reaction temperatures (20 °C, 40 °C, and 60 °C). The changes in the color of the reaction mixtures over time were recorded in situ in terms of the absorbance of the UV–visible light to tune and investigate the growth process of gold nanostructures. Transmission electron microscopic (TEM) images indicated that the gold nanostructures are anisotropic, stable, and exist in the size range of < 1–100 nm. The present study also confirms that the change in the color of nanostructure reaction mixtures is a function of the surface plasmon resonance bands under the influence of physicochemical reaction conditions and corroborates with the size and shape of nano-gold. Physicochemical parameters such as temperature, pH, and the molar concentration of the reactants act synergistically to influence the growth, molecular mechanics, and reaction thermodynamics that aid to affect the particle size, shape, and surface corona of the GNPs. By tracking the growth process, we can confirm that the nucleation, growth process, size, and shape of the gold nanostructures depend on the HEPES free radicals and phosphate ions which cluster to form polymeric chains on the gold nanocore. The present study's findings explain the growth process of the GNPs of various colors that can be observed by the naked eye and have promising applications, for example in the development of the biosensing rapid lateral flow immunoassays (LFIA) for the detection of mycotoxins in food samples.

Graphical Abstract



University of Galway, School of Chemistry Publications 2024, Focus on Journal Articles

Small lectin ligands as a basis for applications in glycoscience and glycomedicine†

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Chem. Soc. Rev., 2024,**53**, 9428-9445
DOI: https://doi.org/10.1039/D4CS00642A
First published 20 Aug 2024

Abstract

Glycan recognition by lectins mediates important biological events. This Tutorial Review aims to introduce lectin–ligand interactions and show how these molecular recognition events inspire innovations such as: (i) glycomimetic ligands; (ii) multivalent ligand agonists/antagonists; (iii) ligands for precision delivery of therapies to cells, where therapies include vaccines, siRNA and LYTACs (iv) development of diagnostics. A small number of case studies are selected to demonstrate principles for development of new ligands for applications inspired by knowledge of natural glycan ligand structure and function.

Graphical Abstract

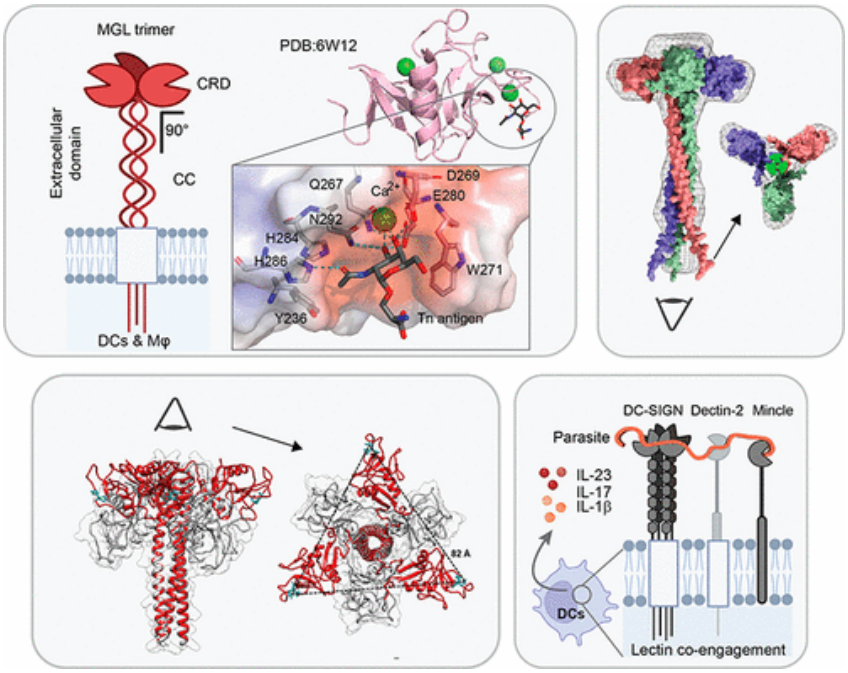
Beyond the Crystal Structure of Human Macrophage C-Type Lectin

Adele Gabba*, Paul V. Murphy, Laura L. Kiessling, Gabriel Birrane
Massachusetts Institute of Technology, University of Galway, Harvard Medical School
Biochemistry 2024, 63, 2, 191–193
DOI: https://doi.org/10.1021/acs.biochem.3c00642
Published January 2, 2024

Abstract

Antigen presenting cells (APCs) such as dendritic cells (DCs) and macrophages (Mϕs) employ cell-surface lectins to recognize carbohydrates on other cells and determine if they are encountering friend or foe. A long-standing goal has been to modulate lectins to induce immune responses that protect from infectious agents, cancer, and various other threats.

Graphical Abstract



Multivalent Calixarene Complexation of a Designed Pentameric Lectin

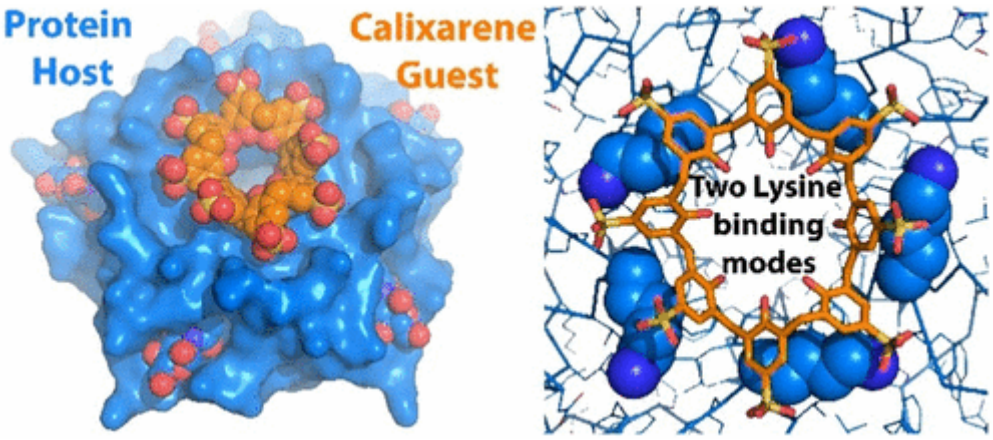
Ronan J. Flood, Linda Cerofolini, Marco Fragai, Peter B. Crowley*
University of Galway, University of Florence, Consorzio Interuniversitario Risonanze Magnetiche di Metallo Proteine (CIRMMP)

Biomacromolecules 2024, 25, 2, 1303–1309
DOI: https://doi.org/10.1021/acs.biomac.3c01280
Published January 16, 2024

Abstract

We describe complex formation between a designed pentameric β-propeller and the anionic macrocycle sulfonato-calix[8]arene ($sclx_8$), as characterized by X-ray crystallography and NMR spectroscopy. Two crystal structures and ^{15}N HSQC experiments reveal a single calixarene binding site in the concave pocket of the β-propeller toroid. Despite the symmetry mismatch between the pentameric protein and the octameric macrocycle, they form a high affinity multivalent complex, with the largest protein-calixarene interface observed to date. This system provides a platform for investigating multivalency.

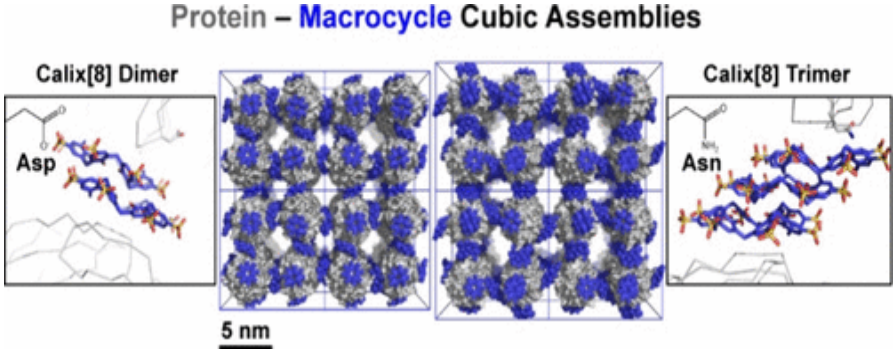
Graphical Abstract



Supramolecular Synthons in Protein-Ligand Frameworks

Ronan J. Flood, Niamh M. Mockler, Aurélien Thureau, Maura Malinska, Peter B. Crowley*
University of GalwayBeamline ANATOMIXUniversity of Warsaw
Cryst. Growth Des. 2024, 24, 5, 2149–2156
DOI: https://doi.org/10.1021/acs.cgd.3c01480
Published February 19, 2024

Abstract



Supramolecular synthons, defined as reproducible intermolecular structural units, have greatly aided small molecule crystal engineering. In this paper, we propose that supramolecular synthons guide ligand-mediated protein crystallization. The protein RSL and the macrocycle sulfonato-calix[8]arene cocrystallize in at least four ways. One of these cocrystals is a highly porous cube comprising protein nodes connected by calixarene dimers. We show that mutating an aspartic acid to an asparagine results in two new cubic assemblies that depend also on the crystallization method. One of the new cubic arrangements is mediated by calixarene trimers and has a ∼30% increased cell volume relative to the original crystal with calixarene dimers. Crystals of the sulfonato-calix[8]arene sodium salt were obtained from buffered conditions similar to those used to grow the protein–calix[8]arene cocrystals. X-ray analysis reveals a coordination polymer of the anionic calix[8]arene and sodium cation in which the macrocycle is arranged as staggered stacks of the pleated loop conformation. Remarkably, the calixarene packing arrangement is the same in the simple salt as in the protein cocrystal. With the pleated loop conformation, the calixarene presents an extended surface for binding other calixarenes (oligomerization) as well as binding to a protein patch (biomolecular complexation). Small-angle X-ray scattering data suggest pH-dependent calixarene assembly in solution. Therefore, the calix[8]arene–calix[8]arene structural unit may be regarded as a supramolecular synthon that directs at least two types of protein assembly, suggesting applications in protein crystal engineering.

The combustion chemistry of ammonia and ammonia/hydrogen mixtures: A comprehensive chemical kinetic modelling study

Yuxiang Zhu, Henry J. Curran*, Sanket Girhe, Yuki Murakami, Heinz Pitsch, Kelly Senecal, Lijun Yang, Chong Wen Zhou*
Yuxiang Zhu [a] [b], Henry J. Curran [a], Sanket Girhe [c], Yuki Murakami [a], Heinz Pitsch [c], Kelly Senecal [d], Lijun Yang [e], Chong-Wen Zhou [a] [b]
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[b] School of Energy and Power Engineering, Beihang University, Beijing 102206, PR China
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[e] School of Astronautics, Beihang University, Beijing 102206, PR China
Combustion and Flame, Volume 260, February 2024, 113239
DOI: https://doi.org/10.1016/j.combustflame.2023.113239
Publication February 2024 (16 December 2023)

Abstract

Ammonia (NH_3) is relatively less reactive compared to hydrocarbon fuels. Therefore, ammonia mixtures blended with hydrogen (H_2) have been shown to be a promising fuel for internal combustion engines. In this study, a detailed NH_3/H_2 chemical kinetic model is developed over a wide range of engine-relevant conditions and comprehensively validated to describe the combustion of NH_3/H_2 mixtures using available experimental literature data, including ignition delay times, laminar flame speeds and species concentration profiles. The new model captures very well the combustion properties of pure NH_3 and NH_3/H_2 mixtures at most conditions. By performing sensitivity and reaction path flux analyses the key reactions controlling fuel reactivity at high-temperature ($\geq$ 1500 K) and low-to-intermediate temperature (1000 $\leq T \leq$ 1500 K) regimes are identified. Moreover, the formation and consumption pathways of nitrogen oxides (NO_x) in NH_3/H_2 combustion at different conditions have also been investigated, which are found to be highly coupled to the underlying chemical reactions that dictate fuel reactivity. The kinetic data for the important reactions and species thermochemistry data used in our model are rigorously evaluated and are discussed in detail.

A theoretical and kinetic study of key reactions between ammonia and fuel molecules, part III: H-atom abstraction from esters by ṄH2 radicals

Jingwu Sun, Lijun Yang, Dongsheng Wen, Henry J. Curran, Chong Wen Zhou
Beihang UniversityTechnical, University Munich, University of Galway

Combustion and Flame Volume 270, December 2024, 113738
DOI: https://doi.org/10.1016/j.combustflame.2024.113738
Publication December 2024

Abstract

Hydrogen atom abstraction reactions by $\dot{N}H_2$ radicals play a crucial role in determining the reactivity of ammonia/fuel binary blends. Esters are a typical component of environmentally friendly and economically promising biofuels. The feasibility of the ammonia/biofuel dual-fuel approach has been proven in practical engines. [Energy and Fuels 22 (2008) 2963] and [Int. J. Energy Res. 2023 (2023) 9920670]. $\dot{N}H_2$ radicals play a critical role in the combustion and pyrolysis chemistry of ammonia and N-containing-rich fuels. In ammonia/biofuels hybrid combustion, $\dot{N}H_2$ radicals can react with biofuel molecules in a reaction class that is particularly important especially when sufficient ammonia is blended in order to eliminate NO_x emissions. To help unravel the chemistry of ammonia/biofuel blends, a systematic theoretical kinetic study of H-atom abstraction from eleven alky esters of $C_nH_{2n+1}COOCH_3$ (n = 1–4), $CH_3COOC_mH_{2m+1}$ (m = 1–4), and $C_2H_5COOC_2H_5$, by $\dot{N}H_2$ radicals is performed in this work. The geometry optimization, frequency, and zero-point energy calculations for all related species, as well as the hindrance potential energy surface for low frequency torsional modes in the reactants and transition states, were performed at the M06–2X/6–311++G(d,p) level of theory. Intrinsic reaction coordinate calculations were performed to validate the connections between the transition states and expected minima energy species. The energies of all of the species involved were calculated at the QCISD(T)/cc-pVXZ (X = D, T, Q) and MP2/cc-pVYZ (Y = T, Q) levels of theory and then extrapolated to the complete basis set. Rate constants of 39 reactions were calculated using the Master Equation System Solver (MESS) program in the temperature range of 500 – 2000 K. These rate constants for different H-atom abstraction sites are provided and can be extrapolated to larger esters. The kinetic effects from the functional group are also illustrated by performing detailed comparisons with the previous studies of $\dot{N}H_2$ radical reactions with alkanes, alcohols and ethers.

Application of Sublimation in the Synthesis and Crystal Growth of Organosulfones

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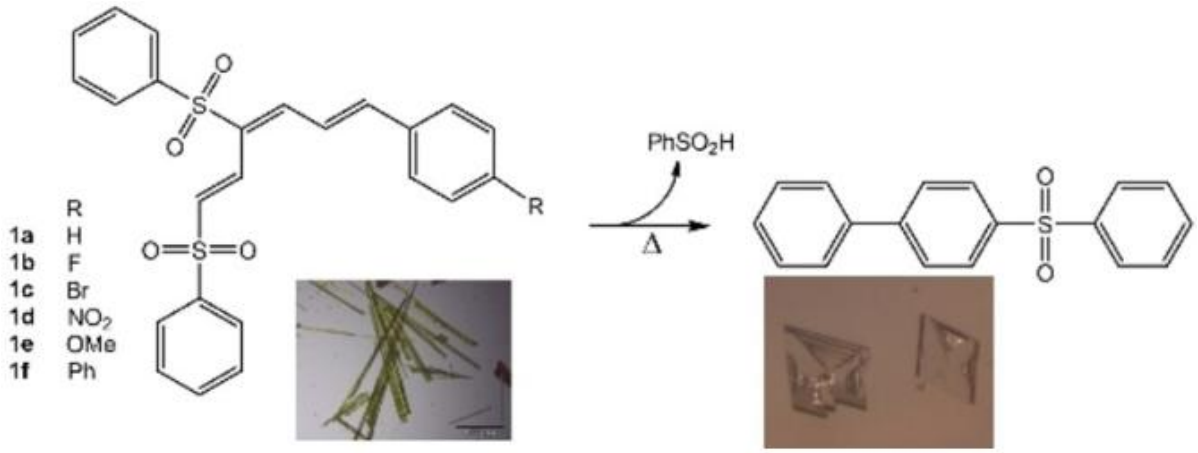
School of Biological and Chemical Sciences, University of Galway, Synthesis and Solid State Pharmaceutical Centre (SSPC), Limerick, Ireland.
Chemistry in Europe, Volume30, Issue 36 e202400672
DOI: https://doi.org/10.1002/chem.202400672
Published June 25, 2024.

Abstract

The solvent-free elimination of sulfinic acid and aromatization of 1,6-trans-substituted bis(arylsulfone) trienes is reported. It is shown that sublimation can be used as a 'green' method to combine the thermal transformation of six trienes and the crystal growth of the resulting 4-(phenylsulfonyl)biphenyls. When the sublimation conditions are carefully controlled, high quality single crystals of the 4-(phenylsulfonyl)biphenyls are obtained. Theoretical modelling of the reaction using the simplified triene Ph-$(CH)_6$-SO_2H showed that the cyclization is energetically feasible and that the complete conversion is possible during the timescale of the sublimation. At temperatures slightly higher than the optimum sublimation temperature two of the trienes transformed into 1,4-cyclohexadienes that did not eliminate phenylsulfinic acid. A reaction mechanism involving a 1,3-hydrogen shift induced by free PhS• radicals is proposed for the formation of the 1,4-cyclohexadienes.

Graphical Abstract

1,6-trans-substituted bis(arylsulfone) trienes undergo aromatization and elimination of phenylsulfinic acid during sublimation leading to the growth of high quality, pure single crystals of the resulting (4-phenylsulfonyl)biphenyls in the desublimation area.



Unravelling the Atomic Structure of a Metal-Covalent Organic Framework Assembled from Ruthenium Metalloligands

Seán Hennessey, Roberto González-Gómez*, Nicolás Arisnabarreta, Anna Ciotti, Jing Hou, Nadezda V. Tarakina, Andrey Bezrukov, Kunal S. Mali, Michael Zaworotko, Steven De Feyter, Max García-Melchor*, Pau Farràs *
University of Galway, KU Leuven, Trinity College Dublin, Research Campus Golm,University of Limerick, Basque Research and Technology Alliance (BRTA), Basque Foundation for Sciences
Advanced Materials, Volume37, Issue13, 2502155
DOI: https://doi.org/10.1002/adma.202502155
Published April 2, 2025

Abstract

Covalent and metal-organic frameworks (COFs and MOFs) have shown great promise in light-driven processes mainly due to their ligand-to-metal charge-separation properties, as well as having access to a diverse range of photoactive metalloligands and organic linkers. However, both frameworks present individual drawbacks that can potentially be avoided by combining both systems (metal and covalent) to produce metal-covalent organic frameworks (MCOFs), exhibiting the advantages of both material types. Yet, due to their poor crystallinity, the understanding of the structure-properties relation of MCOFs remains unclear. Herein, we report photoactive linkers in the form of a $[Ru(tpy)_2]^{2+}$ (tpy: 2,2′,6,2″-terpyridine) complex which covalently binds to a luminescent pyrene core to yield a new, photoactive Schiff-base MCOF. The structure, thermal, electronic, and optical properties of this novel material have been exhaustively characterized by a wide range of microscopy, spectroscopic, and computational methods. This combined experimental and computational work represents a significant step toward the fundamental understanding of the photoactive units within the framework, their hierarchical arrangement and interactions with substrates, which is essential for the future design of efficient photocatalytic materials.

A split herbicide application strategy reduces surface runoff

Shane Scannell, Mark G. Healy, Gustavo Sambrano, John McGinley, Paraic C. Ryan, Per-Erik Mellander, Liam Morrison, Jenny Harmon O'Driscoll, Alma Siggins*
Civil EngineeringSchool of Biological and Chemical Sciences, University of GalwayUniversity College CorkTeagasc - Irish Agriculture and Food Development AuthorityEarth and Ocean Sciences.
Soil Use and Management, Volume40, Issue3, e13086
DOI: https://doi.org/10.1111/sum.13086
Published 17 July 2024

Abstract

Herbicides, such as MCPA and clopyralid, may be transported to surface waters via runoff, which can have unintended environmental consequences. A split herbicide application strategy, wherein applications are spread across a season, may improve herbicide effectiveness, although impacts of this strategy on runoff mitigation have not been investigated. Therefore, this study aimed to (1) quantify the impact of split-dose applications of MCPA and clopyralid on herbicide losses in surface runoff and (2) assess the impact of split-dose applications of MCPA on the quantity and classification of MCPA-degrading soil bacteria. Intact grassed soil sods were placed in 1 m-long × 0.25 m-wide × 0.1 m-deep laboratory flumes, onto which either MCPA or clopyralid were applied in one full-dose (13.5 kg MCPA ha^{-1}; 2 kg clopyralid ha^{-1}) or two split-doses (each 6.75 kg MCPA ha^{-1}; 1 kg clopyralid ha^{-1}) 42 days apart. On days 2, 7 and 21 following herbicide applications, flumes were subjected to controlled rainfall simulations at an intensity of 11 mm h^{-1}, and the herbicides in the runoff were quantified. MCPA and clopyralid concentrations in the runoff were highest immediately after the initial application. Both herbicides were below the limit of detection (0.1 μg l^{-1} for MCPA and 0.45 μg l^{-1} for clopyralid) by 44 days. No herbicides were detected in the runoff following the second split-dose application. For MCPA, this was attributed to an adaptation in the microbial community with the emergence of bacteria possessing the *tfdA* class III gene in the soil. These results support split-dose herbicide application as a strategy for agricultural management.

Synthesis and characterisation of antimicrobial metal-organic frameworks as multi-drug carriers

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DOI: https://doi.org/10.1039/D4DT01100G
First Published 21 June 2024

Abstract
Antibiotic resistance is a significant global concern, necessitating the development of either new antibiotics or advanced delivery methods. With this in mind, we report on the synthesis and characterisation of a new family of Metal–Organic Frameworks (MOFs), OnG6 MOFs, designed to act as multi-drug carriers for bacterial infection treatment. OnG6 is based on the pro-drug 4,4′-azodisalicylic acid (AZDH4), which in vivo produces two equivalents of para-aminosalicylic acid (ASA), a crucial drug for M. tuberculosis treatment. X-ray and computational studies revealed that OnG6 MOFs are mesoporous MOFs with etb topology and an [M2(AZD)] formula (M = Zn, OnG6-Zn; Mg, OnG6-Mg; Cu, OnG6-Cu; and Co, OnG6-Co), featuring 1-dimensional channel type pores of 25 Å diameter. OnG6 MOFs are the first reported MOFs bearing the ligand AZDH4, joining the family of mesoporous MOFs arranged in a honeycomb pattern. They absorb isoniazid (INH) and ciprofloxacin (CIPRO) with the former being a specific antibiotic for M. tuberculosis, and the latter being a broader-spectrum antibiotic. The stability of the MOFs and their capacity for antibiotic uptake depend on the nature of the metal ion, with OnG6-Mg demonstrating the highest drug absorption. The antimicrobial activity of these species was assessed against S. aureus and E. coli, revealing that the carriers containing CIPRO displayed optimal efficacy.

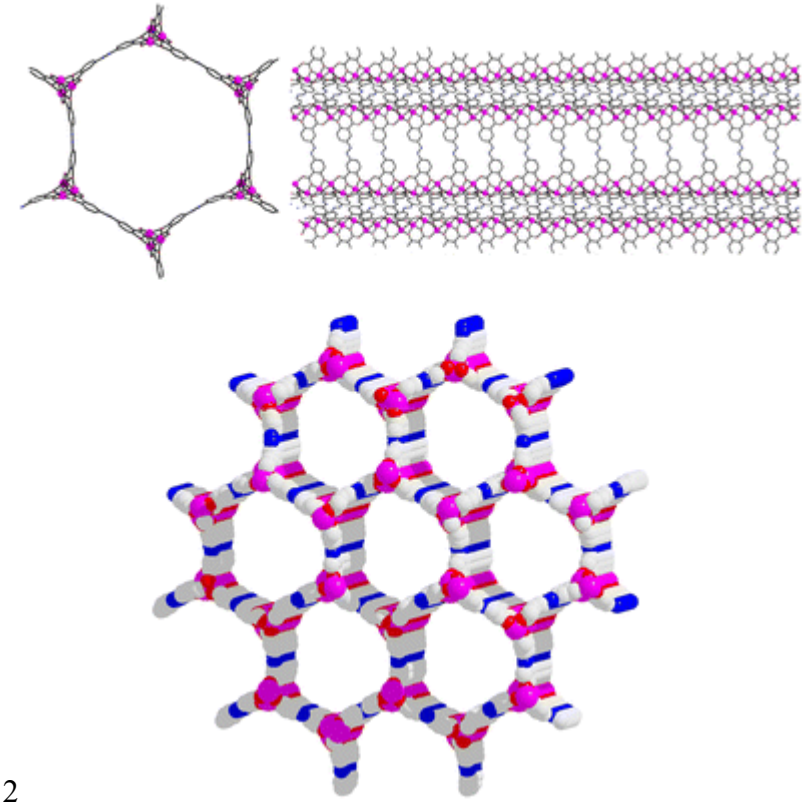

Fig 2

Nanoplatforms for Magnetic-Photo-Heating of Thermo-Resistant Tumor Cells: Singular Synergic Therapeutic Effects at Mild Temperature

Binh T. Mai, Tamara Fernandez-Cabada, John S. Conteh, Giulia E.P. Nucci, Sergio Fiorito, Helena Gavilán, Doriana Debellis, Lorenci Gjurgjaj, Teresa Pellegrino
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Small, *20*(51), Article 2310522.
DOI: https://doi.org/10.1002/smll.202310522
Published 19 December 2024

Abstract
A self-assemble amphiphilic diblock copolymer that can incorporate iron oxide nanocubes (IONCs) in chain-like assemblies as heat mediators for magnetic hyperthermia (MHT) and tuneable amounts of IR780 dye as agent for photothermal therapy (PTT) is developed. MHT-heating performance of photobeads in viscous media have the same heat performances in water at magnetic field conditions of clinical use. Thanks to IR780, the photobeads are activated by infrared laser light within the first biological window (808 nm) with a significant enhancement of photo-stability of IR780 enabling the raise of the temperature at therapeutic values during multiple PTT cycles and showing unchanged optical features up to 8 days. Moreover, the photobeads fluorescent signal is preserved once internalized by glioblastoma multiforme (GBM) cells. Peculiarly, the photobeads are used as toxic agents to eradicate thermo-resistant GBM cells at mild heat, as low as 41 °C, with MHT and PTT both of clinical use. Indeed, a high U87 GBM cell mortality percentage is obtained only with dual MHT/PTT while each single treatment dose not provide the same cytotoxic effects. Only for the combined treatment, the cell death mechanism is assigned to clear sign of apoptosis as observed by structural/morphological cell studies and enhanced lysosome permeability.

Synthesis and Application of a New Class of Planar and Centrally Chiral Ferrocenyl Amino Alcohol Ligands

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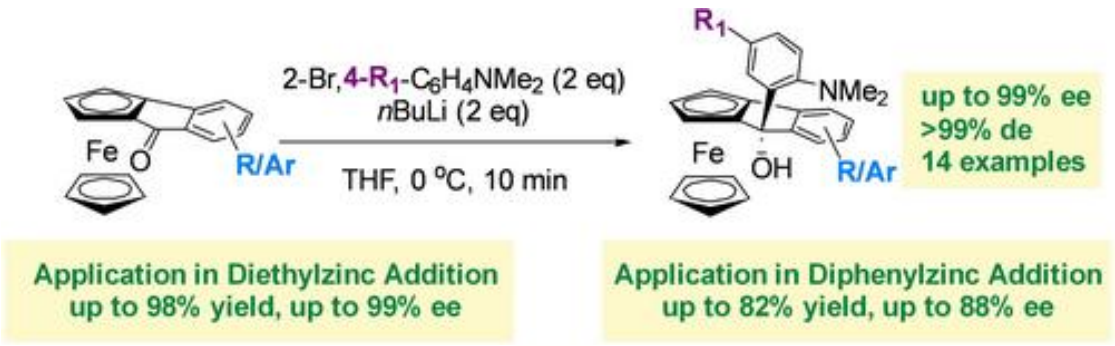
University College Dublin, University of Galway

EurJOC, Volume27, Issue18 May 13, 2024 e202300951
DOI: https://doi.org/10.1002/ejoc.202300951
First published: 18 February 2024

Abstract
A family of ferrocenyl amino alcohols (14 examples) has been prepared from the corresponding planar chiral ketones and evaluated as a new class of chiral ligands for asymmetric ethyl- and phenylzinc additions to aldehydes. The highly enantioselective synthesis of these ligands is facile, scalable, robust and relies on the use of cheaply available starting materials. Asymmetric ethyl additions proceeded smoothly at ambient temperature, with reaction times as short as 1 hour furnishing the desired products in up to 90 % yield and 99 % ee. The corresponding phenyl additions afforded products in up to 81 % yield and 88 % ee. The observed stereochemical outcome for the addition of diethylzinc was rationalized and the key proposed transition state was supported by an analysis of the X-ray structures of a series of amino alcohol ligands.

Graphical Abstract
The highly enantioselective, facile, scalable, and robust synthesis of a new family (14 examples) of amino alcohol ligands possessing planar and central chirality that is described. They were applied to the diethylzinc and diphenylzinc additions to aldehydes with up to 98 % yield and 99 % ee and 82 % yield and 88 % ee, respectively.



Atlantic Technological University (ATU) Chemistry, Publications 2024, Focus on Journal Articles

Unravelling the impact of lower vacuum activation temperature on Fe2+/Fe3+ mixed-valence unsaturated iron centres in MIL-101(Fe) and its impact on Fenton degradation of acetaminophen

Keerthi
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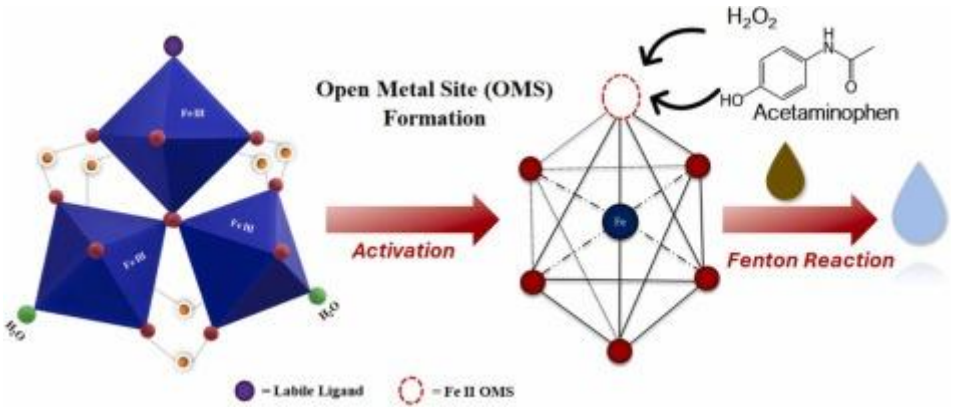
Journal of Environmental Chemical Engineering, Volume 12, Issue 5, 113615
DOI: https://doi.org/10.1016/j.jece.2024.113615
Published October 2024

Abstract

The impact of varying activation temperatures under vacuum on the Metal-Organic Framework (MOF), MIL-101(Fe), and its consequential effects on H2O2 activation and Fenton degradation of one of the contaminants of emerging concerns, acetaminophen (ACT) is investigated in this work. MIL-101(Fe) underwent vacuum activation at temperatures ranging from 60 °C to 150 °C, and an in-depth analysis of the resulting samples' physical and chemical properties were conducted. XRD, FTIR and microscopic studies revealed that the structure and crystallinity of the samples were preserved irrespective of the activation temperature. MIL-101(Fe) activated at 120 °C (MIL-101–120) demonstrated the highest degradation kinetics when examined for Fenton degradation of ACT. XPS analysis revealed that MIL-101–120 exhibited the highest Fe2+: Fe3+ ratio and a complete degradation of ACT was attained within 60 minutes of the reaction. This indicated a direct correlation between increased Fe2+ content and the rate of Fenton degradation. A possible catalytic mechanism for the ACT degradation by MIL-101(Fe) was further proposed, indicating the influence of different active sites and radicals in the reaction. Overall, the study provides insight into the significance of optimizing various activation conditions to improve the catalytic efficiency of MIL-101(Fe).

Graphical Abstract



Impact of Au on the transition temperature and photocatalytic activity of TiO2

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Journal of Photochemistry and Photobiology A: Chemistry, Volume 456, 115848
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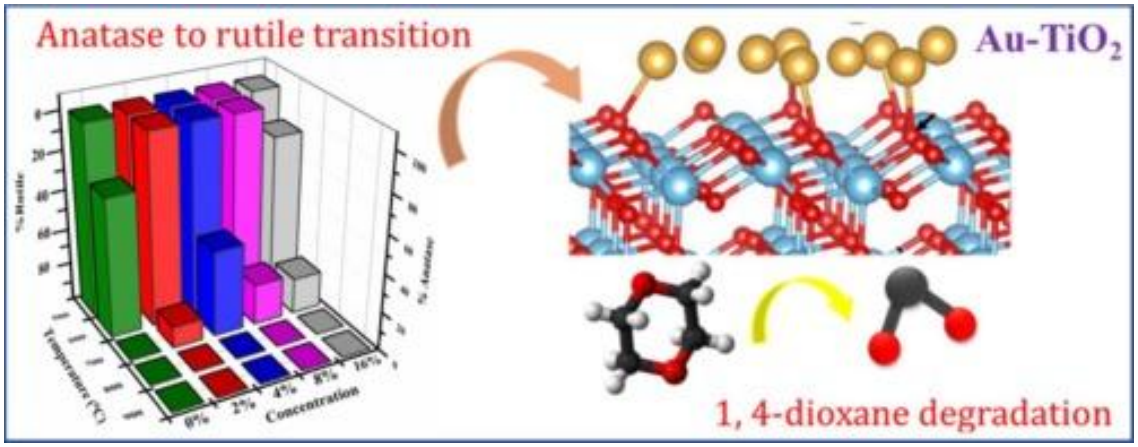
Published 1 November 2024

Abstract

The effect of gold (Au) addition on the anatase to rutile transition temperature (ART) of titanium dioxide (TiO_2) was investigated. Concentrations of 2, 4, 8 and 16 mol. % of Au have been synthesised *via* a sol–gel technique and calcined at various temperatures (500–900 °C). The inclusion of gold improves the ART at 700 °C, maintaining 44.5 % anatase content for 4 % Au. Density functional theory studies indicated that the addition of Au in the anatase phase results in considerable lattice distortions, while Au 4*d* states and occupied Ti 3*d* orbitals contribute to the valence-conduction band energy gap upon doping. However, no sign of lattice substitution was observed in the experimental analysis. Instead, we demonstrate that the actual structure is well described by gold nanoparticles deposited on anatase and present a detailed DFT description of gold-modified anatase (1 0 1). All Au-TiO_2 samples exhibit reduced photocatalytic degradation properties compared to the control TiO_2 at 500 °C. However, after calcining at 600 °C the addition of Au increases the photocatalytic activity of TiO_2 from 49 % to 61 %, at an optimal concentration of 2 % Au-TiO_2. The modification of titania with gold does push the transition temperature higher. However, this comes at the cost of reduced activity for 1,4-dioxane degradation, with the unmodified titania sample having better overall photocatalytic activity.

Graphical abstract



Sustainable energy harvesting and breath sensing with electrospun triboelectric nylon-6

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Journal of Physics: Energy, Volume 6, Number 2 025010
DOI https://doi.org/10.1088/2515-7655/ad29fe
Published28 February 2024

Abstract

A high-performance triboelectric nanogenerator (TENG) has been developed for breath sensing applications, utilizing tribopositive electrospun nylon-6 nanofibers and tribonegative fluorinated ethylene propylene (FEP). The optimization toward the development of electrospun nylon-6-based TENG includes a range of factors such as the applied force and frequency on tribo responses, the thickness of the fiber mat, the concentration of nylon-6 in the fiber mats, and the selection of the tribonegative material for pairing with nylon-6 nanofiber. Among these parameters, the nanofiber prepared with 18 wt% nylon-6, characterized by a uniform fiber distribution, the highest surface area of 55.69 $m^2 g^{-1}$, and an optimal thickness of 0.169 mm, demonstrated excellent TENG performance, among others. The TENG module constructed using nanofiber in a 4 cm^2 area showed the TENG responses of more than 30 μA short-circuit current, 200 V open-circuit voltage, and 90 nC charge when hand-pressed. It achieved a substantial power density of 890 mW m^{-2} at 20 MΩ by applying a constant force of 10 N at a 10 Hz frequency. Charging a 1 μF capacitor to approximately 30.1 V in just 30 s highlights the potential of electrospun nylon-6 as a promising material for nanogenerator energy harvesting and sensing applications. The TENG device was found to be sufficient to power small, portable electronics such as LEDs and digital watch displays. A wearable belt was fabricated to showcase its breath-sensing capabilities by pairing it with FEP. The microcontroller connected to the TENG in the wearable belt is used to analyze the output produced through breathing patterns, subsequently activating a buzzer and LED by the nature of the breathing.

"Parametric optimisation of PDMS/PMMA nanofibers prepared using emulsion electrospinning technique."

Ryan Walden [a b], Irthasa Aazem [a b], Steven Hinder [d], Barry Brennan [a], Amit Goswami [a c], Gerard McG ranaghan [a c], Suresh C. Pillai [a b] ∗

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[b] Health and Biomedical (HEAL) Research Centre, Atlantic Technological University, ATU Sligo, Ash Lane, Sligo, F91YW50, Ireland
[c] Department of Mechanical and Manufacturing Engineering, Atlantic Technological University, ATU Sligo, Ash Lane, Sligo, F91YW50, Ireland
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Results in Materials 22 (2024) 100576
DOI: https://doi.org/10.1016/j.rinma.2024.100576
Published June 2024, 100576

Abstract

With the massive potential for nanofiber applications within the expanding field of functional materials and green energy materials, electrospinning has become an increasingly interesting method of fabrication, generating many different methods to fabricate different nanofiber types. However, due to limitations, either chemical or instrumental, some polymeric nanofibers can only be synthesised using co-axial or emulsion electrospinning methods. To date fabrication of poly (dimethylsiloxane) (PDMS)/poly (methyl methacrylate) (PMMA) nanofibers via electrospinning have been limited to coaxial method. These nanofibers have found use in medical fields as well as environmental remediation efforts as membranes and filters and also in new age wearable electronics. In addition, there have been no systematic studies documented on the parametric optimisation of PDMS/PMMA nanofibers using electrospinning, particularly concerning applied voltage, flow rate, and collector distance. In this work, a PDMS/PMMA co-polymer nanofiber, synthesised through an optimised emulsion electrospinning method, was fabricated and characterised. A systematic examination of electrospinning parameters was conducted and optimised parameters of 18.5 kV supplied voltage, 10 cm tip-collector distance and a flow rate of 0.2 mL/h resulted in the fabrication of nanofibers with an average diameter of ~199 nm and super-hydrophobicity, with a contact angle of ~162°, is reported on.

Limerick University/SSPC Chemistry, Publications 2024, Focus on Journal Articles

Evaluating experimental, knowledge-based and computational cocrystal screening methods to advance drug-drug cocrystal fixed-dose combination development

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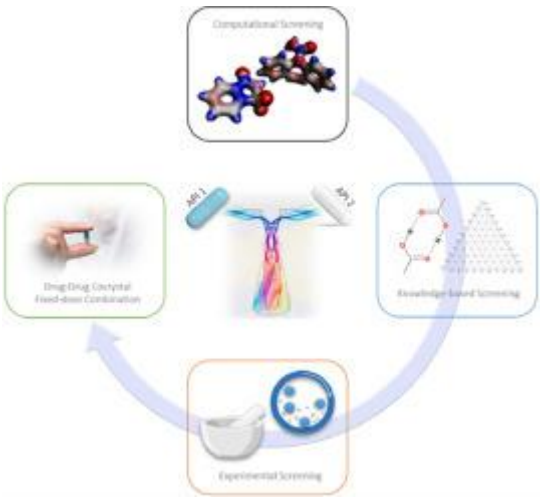
[b] Cook Medical, Castletroy, Limerick, Ireland
European Journal of Pharmaceutical Sciences, 203, 106931.
DOI: https://doi.org/10.1016/j.ejps.2024.106931
Published 1 December 2024

Abstract
Fixed-dose combinations (FDCs) offer significant advantages to patients and the pharmaceutical industry alike through improved dissolution profiles, synergistic effects and extended patent lifetimes. Identifying whether two active pharmaceutical ingredients have the potential to form a drug-drug cocrystal (DDC) or interact is an essential step in determining the most suitable type of FDC to formulate. The lack of coherent strategies to determine if two active pharmaceutical ingredients that can be co-administered can form a cocrystal, has significantly impacted DDC commercialisation. This review aims to accelerate the development of FDCs and DDCs by evaluating existing experimental, knowledge-based and computational cocrystal screening methods; the background of their development, their application in screening for cocrystals and DDCs, and their limitations are discussed. The evaluation provided in this review will act as a guide for selecting suitable screening methods to accelerate FDC development.

Graphical Abstract



High Entropy Oxides: Mapping the Landscape from Fundamentals to Future Vistas

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ACS Energy Letters, Vol 9/Issue 8, 3694–3718
DOI: https://doi.org/10.1021/acsenergylett.4c01129
Published July 5, 2024

Abstract

High-entropy materials (HEMs) are typically crystalline, phase-pure and configurationally disordered materials that contain at least five elements evenly blended into a solid-solution framework. The discovery of high-entropy alloys (HEAs) and high-entropy oxides (HEOs) disrupted traditional notions in materials science, providing avenues for the exploration of new materials, property optimization, and the pursuit of advanced applications. While there has been significant research on HEAs, the creative breakthroughs in HEOs are still being revealed. This focus review aims at developing a structured framework for expressing the concept of HEM, with special emphasis on the crystal structure and functional properties of HEOs. Insights into the recent synthetic advances, which foster prospective outcomes and their current applications in electrocatalysis, and battery, are comprehensively discussed. Further, it sheds light on the existing constraints in HEOs, highlights the adoption of theoretical and experimental tools to tackle challenges, while delineates potential directions for exploration in energy application.

Graphical Abstract

Lignin and its carbon derivatives: Synthesis techniques and their energy storage applications

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Materials Today Sustainability, Volume 28, 100990

DOI: https://doi.org/10.1016/j.mtsust.2024.100990

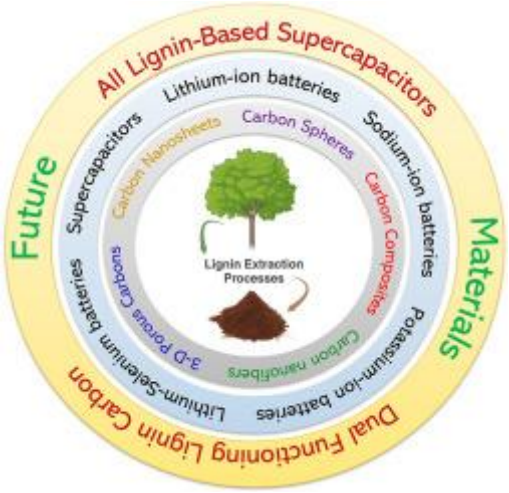
Published December 2024.

Abstract

Lignin, a complex phenolic polymer abundantly present in the papermaking and biofuel industries, stands out as a cost-effective, plentiful, and non-toxic material. In recent years, there has been significant interest in utilizing this green biopolymer for energy storage devices. This review thoroughly examines lignin structure, chemistry, and classification based on separation techniques. It then explores the most recent breakthroughs in creating carbon materials (nanosheets, nanofibers, spheres, composites, and 3D hierarchical porous carbon) from lignin, discussing its versatility in supercapacitors and batteries. Finally, this study highlights future materials and their prospects, the critical challenges which must be addressed while suggesting future research avenues for lignin-derived carbon materials in energy storage. By combining insights from different studies, this review

aims to offer readers a thorough understanding of how lignin-derived carbon materials could play a crucial role in promoting sustainable energy solutions.

Graphical abstract



Porphyrin-based MOFs for sensing environmental pollutants

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Chemical Engineering Journal Volume 492, 152377

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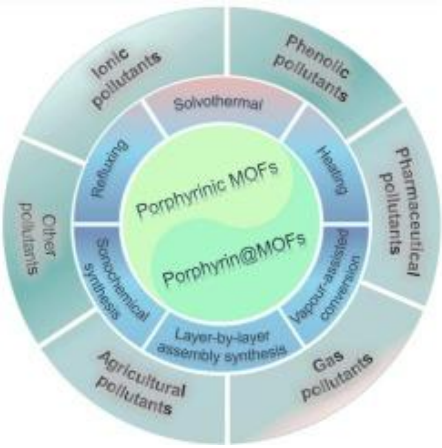
Published 15 July 2024

Abstract

Utilizing porphyrin molecules as the building blocks (ligands) of metal–organic frameworks (MOFs) leads to porphyrinic MOFs (including incorporation of functional materials into porphyrinic MOFs), whereas the immobilization of porphyrin molecules into porous MOFs afford porphyrin@MOFs. These two kinds, collectively regarded as porphyrin-based MOFs (PP-MOFs), are known to feature distinct photophysical and electrochemical properties lending towards several applications. This is because PP-MOFs can overcome the instability and self-quenching issues oft-encountered in porphyrins. Thanks to the ordered immobilization of porphyrins and electron-hopping mobility, this relatively new class of MOFs has received a surge of attention in sensing environmental pollutants. This review will explore the strengths and weaknesses of PP-MOFs in this context, as well as the influence of various sensory mechanisms associated with them. Libraries of porphyrinic MOFs and porphyrin@MOFs are reviewed herein, a number of them featuring the optimal selectivity and sensitivity for device fabrication. Finally, the challenges and prospects of PP-MOFs for environmental monitoring are critically interrogated.

Graphical abstract



Si Nanowires: From Model System to Practical Li-Ion Anode Material and Beyond

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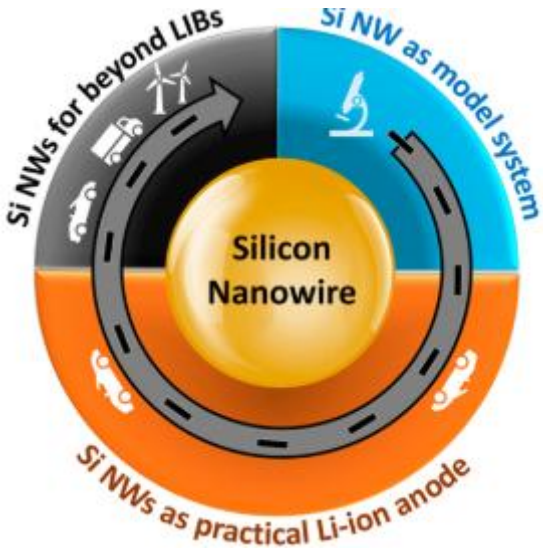
Department of Chemical Sciences, University of Limerick, Limerick V94 T9PX, Ireland
Bernal Institute, University of Limerick, Limerick V94 T9PX, Ireland
ACS Energy Lett. 2024, 9, 4, 1548–1561
DOI: https://doi.org/10.1021/acsenergylett.4c00262
Published March 17, 2024

Abstract

Nanowire (NW)-based anodes for Li-ion batteries (LIBs) have been under investigation for more than a decade, with their unique one-dimensional (1D) morphologies and ability to transform into interconnected active material networks offering potential for enhanced cycling stability with high capacity. This is particularly true for silicon (Si)-based anodes, where issues related to large volumetric expansion can be partially mitigated and the cycle life can be enhanced. In this Perspective, we highlight the trajectory of Si NWs from a model system to practical Li-ion battery anode material and future prospects for extension to beyond Li-ion batteries. The study examines key research areas related to Si NW-based anodes, including state-of-the-art (SoA) characterization approaches followed by practical anode design considerations, including NW composite anode formation and upscaling/full-cell considerations. An outlook on the practical prospects of NW-based anodes and some future directions for study are detailed.

Graphical abstract



State of the art, challenges and prospects in metal–organic frameworks for the separation of binary propylene/propane mixtures

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e Basic Research Center for Energy Interdisciplinary, China University of Petroleum-Beijing, Beijing 102249, China
Coordination Chemistry Reviews Volume 506, 215697
DOI: https://doi.org/10.1016/j.ccr.2024.215697
Published 1 May 2024

Abstract

Propylene (C_3H_6) as one of the most crucial raw chemical materials has been widely used in the chemical industry. The high-purity C_3H_6 (higher than 99.5 %) is in great demand for producing polypropylene or other chemical products. C_3H_6 is nevertheless mostly produced by steam cracking naphtha or dry gas refining and is invariably blended with minor impurity gases like propane (C_3H_8). At present, the petrochemical industry depends almost exclusively on the heat-driven cryogenic distillation process for C_3H_6 purification. However, both C_3H_6 and C_3H_8 molecules have very similar physical properties (such as kinetic diameter, boiling point, polarity, etc.), which makes conventional cryogenic distillation inefficient and energy-intensive. To decrease energy consumption, cost-efficient, and tend to be environmentally friendly, adsorptive-based separation using porous materials is expected to accomplish C_3H_6 purification from C_3H_6/C_3H_8 mixtures under ambient conditions. In particular, metal–organic frameworks (MOFs) with high porosity, regular adjustable pore shape and pore environment have promising advantages as porous adsorbents for C_3H_6 purification. This thesis provides an in-depth review of the present MOF materials that show promise for the separation of C_3H_6/C_3H_8 mixtures using adsorptive technology. It focuses particularly on recent developments in the usage of MOFs to achieve reversed C_3H_6/C_3H_8 separation. Meanwhile, we interpret the separation mechanism and further classify the relevant mechanisms of flexible materials, then we also summarize the separation research methods, and related techniques. Ultimately, we propose a bold conjecture regarding the future perspectives and urgent problems in the exploitation of MOFs for C_3H_6 purification in industry and the academic community and give possible development directions.

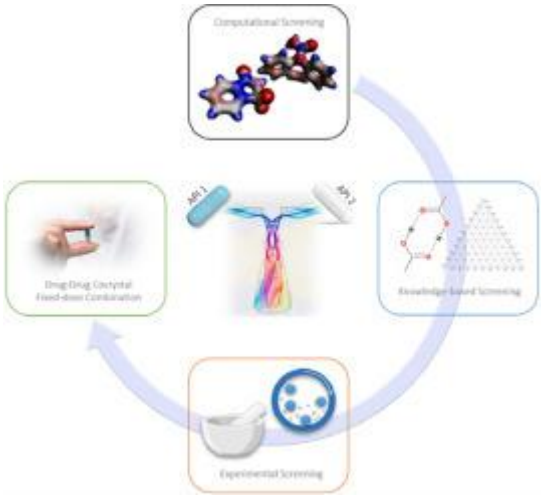
SSPC Publications 2024 (Listed under SSPC Publications)

Evaluating experimental, knowledge-based and computational cocrystal screening methods to advance drug-drug cocrystal fixed-dose combination development

Alice Parkes [a], Ahmad Ziaee [b], Emmet O'Reilly [a*]
[a] Department of Chemical Sciences, SSPC the SFI Research Centre for Pharmaceuticals, Bernal Institute, University of Limerick, Limerick, Ireland
[b] Cook Medical, Castletroy, Limerick, Ireland
European Journal of Pharmaceutical Sciences Volume 203, 1 December 2024, 106931
DOI: https://doi.org/10.1016/j.ejps.2024.106931
Published 1 December 2024

Abstract
Fixed-dose combinations (FDCs) offer significant advantages to patients and the pharmaceutical industry alike through improved dissolution profiles, synergistic effects and extended patent lifetimes. Identifying whether two active pharmaceutical ingredients have the potential to form a drug-drug cocrystal (DDC) or interact is an essential step in determining the most suitable type of FDC to formulate. The lack of coherent strategies to determine if two active pharmaceutical ingredients that can be co-administered can form a cocrystal, has significantly impacted DDC commercialisation. This review aims to accelerate the development of FDCs and DDCs by evaluating existing experimental, knowledge-based and computational cocrystal screening methods; the background of their development, their application in screening for cocrystals and DDCs, and their limitations are discussed. The evaluation provided in this review will act as a guide for selecting suitable screening methods to accelerate FDC development.

Graphical Abstract



Recent Advances in Mapping Protein Self-Assembly and Aggregation for Common Proteinopathies

S. Bhattacharya D. Thompson

Acta Phys. Pol. A, vol. 145, no. 3, p. S37
DOI: doi: 10.12693/APhysPolA.145.S37
18 April 2024
Vol. 145 No. 3 (2024): The Special Issue of Acta Physica Polonica A, pp. S1-S70
The Special Issue in Memory of Professor Marek Cieplak (1950–2021)

Abstract
The accumulation of abnormal conformation by brain peptides and proteins followed by their aberrant self-assembly into insoluble aggregates is the hallmark of "proteinopathies", common across many neurodegenerative disorders. Experiments suggest that soluble low-molecular-weight oligomers formed in the early stages of assembly are neurotoxic, and hence, drug targets. However, the inherent polymorphic nature of these short-lived oligomers restricts their experimental characterisation in pathological protein self-assembly pathways. Here, we shed light on the latest contributions from atomic-level modelling techniques, such as computer-based molecular dynamics simulations in bulk solution and on surfaces, which are guiding experimental efforts to map early stages of protein self-assembly in common proteinopathies, including Alzheimer's and Parkinson's diseases, which could potentially aid in molecular-level understanding of disease pathologies. Predictive computational modelling of amyloid-β and tau protein assemblies in Alzheimer's disease and α-synuclein protein assemblies in Parkinson's disease highlights the potential for identification and characterisation of new therapeutic targets for currently incurable neurodegeneration.

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Physical Chemistry Chemical Physics
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21 February 2025, Issue 7,
Page 3513 to 4008
DOI:10.1039/D4CP03468F

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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

https://www.researchireland.ie

Research Ireland Infrastructure Programme

The Research Ireland Infrastructure Programme is now open.
This Programme seeks to fund equipment, facilities, and resources that will enable Ireland to address major societal challenges, advance knowledge creation, and maintain competitiveness in a global research environment. The call will run in collaboration with the Sustainable Energy Authority of Ireland (SEAI).

The deadline for the Expression of Interest is **23rd June 2025, 13:00 Dublin local time.** The Full Proposal deadline is **31st July 2025, 13:00 Dublin local time.**
An Information webinar will be hosted by Research Ireland on **11th June 2025.**
For further information on this call, and to register for the webinar, visit our website:
Research Ireland Infrastructure Programme

Contact Us
Email: info@researchireland.ie **/ Website:** researchireland.ie

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Research Ireland - Gas Networks Ireland Innovation Challenge

The **Research Ireland - Gas Networks Ireland Innovation Challenge** is now open for applications.

This pilot initiative aims to incentivise and support research projects that will explore STEM-based solutions for utilisation of renewable gases by the energy industry in Ireland.

The full proposal deadline is **26th September 2025, 13:00 Dublin local time.**

An information webinar will take place on 12th June 2025, 14:00 Dublin local time.

For more information on the Challenge, webinar, and how to apply, visit our website:

Research Ireland – Gas Networks Ireland Innovation Challenge

Contact Us
Email: info@researchireland.ie **/ Website:** researchireland.ie

Taighde Éireann
Research Ireland

Research Ireland Enterprise Fellowships

Prior to their amalgamation to form Research Ireland, both SFI and the IRC offered a suite of enterprise-facing fellowship programmes to support collaboration with enterprise.
As Research Ireland works towards developing a new consolidated fellowship programme, the original SFI Industry RD&I Fellowship programme will run one last time under the **Placement Stream** and the IRC Enterprise Fellowship Scheme (Postdoctoral) will run one final time under the **Partnership Stream** of the Research Ireland Enterprise Fellowship Programme.

- The **Placement Stream** supports academic researchers (at faculty, postdoctoral and late-stage PhD level) wishing to spend time based in industry worldwide.
- The **Partnership Stream** supports suitably qualified postdoctoral fellows or late-stage PhD students pursuing, or intending to pursue, full-time research based in an eligible research body while partnering with enterprise.

Both streams are now open for application with a deadline date of **15th July 2025**.
Research Ireland will host an information webinar, covering both streams**,** on 14th May at 10:00 (Irish local time).

For more information on the Research Ireland Enterprise Fellowships and how to apply, visit our website:

Research Ireland Enterprise Fellowships

Contact Us

Email: info@researchireland.ie **I Website:** researchireland.ie

Taighde Éireann
Research Ireland

Research Ireland Infrastructure Programme 2025

The Research Ireland Infrastructure Programme 2025 Call will open this month. This call represents a pivotal initiative under Research Ireland's broad remit and will fund state-of-the-art infrastructure to enable high-quality, impactful research across Ireland.

Key details for the 2025 Call

- **Expanded remit**: The programme will support research infrastructure that underpins all disciplines.
- **Application process**: A two-step application process consisting of an Expression of Interest, followed by the submission of a full proposal.
- **Application cap**: Maximum of 6 applications per Research Body.
- **Budget threshold**: Minimum budget request of €500,000 with no maximum budget cap; a minimum, additional 10% cash cost share is required.
- **Lead applicant eligibility**: Independent researcher with a PhD (or equivalent) for at least 3 years, who either holds or has held a significant, internationally peer-reviewed research grant.
- **Emphasis**: Strong focus on inter-institutional sharing and interdisciplinary collaboration.

Further information on the 2025 Call, including eligibility and submission deadlines, will be available on the **Research Ireland website** when the Call formally opens. We encourage you to begin planning for the 2025 Call now, particularly when considering strategic inter-institutional collaborations.

For queries, please contact: **infrastructure@researchireland.ie**

Taighde Éireann
Research Ireland

Research Ireland New Foundations 2025

The Research Ireland New Foundations 2025 Call will open **5th June 2025**.
This scheme supports eligible researchers who intend to pursue research, networking and/or dissemination activities within and across the diversity of disciplines. Eligible applicants must, on the call deadline hold a contract of sufficient duration with an Eligible Research Body to carry out the proposed research from the project start date until the project end date.

Deadline for applicants is **17th July 2025, 16:00 Dublin local time**.
For further information on this Call, visit our website:

New Foundations

Contact Us

Email: info@researchireland.ie / Website: researchireland.ie

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Research Ireland Discover Programme

The **Research Ireland Discover Programme** 2025 Call is now open.
Research Ireland welcomes applications from a wide range of organisations to develop and deliver STEM education and public engagement projects that aim to broaden participation and engagement of the public with STEM.

The deadline for applications is 24th June **2025, 13:00 Dublin local time**.

This Programme is running in collaboration with the Department of Education.

For further information on this Call, visit our website:
Research Ireland Discover Programme

Contact Us
Email: info@researchireland.ie I Website: researchireland.ie

Research Ireland Discover Programme
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Deadline
24th June 2025 (13:00 local Irish time)

Duration
Up to 2 years

The **Research Ireland Discover Programme** is part of Research Ireland's role to promote and support an awareness and understanding of the value of research and innovation to society and to facilitate engagement of members of the public with those engaged in research and innovation activities.

The Programme aims to empower participation, grow talent and inspire deep public engagement in STEM. The Programme addresses critical areas such as broadening participation and ensuring equity of access, promoting climate action and sustainability, and encouraging co-creation with stakeholder groups.

This Programme will be run in collaboration with the Department of Education. Research Ireland is open to forging new co-funding partnerships with agencies and organisations.

Research Ireland Discover Programme Call Document

Download 2025-Discover-Programme-Call-2.pdf

Eligibility	https://www.researchireland.ie/funding/discover
Downloads	https://www.researchireland.ie/funding/discover
How to apply	https://www.researchireland.ie/funding/discover
Information webinar	https://www.researchireland.ie/funding/discover

Tips and useful information
https://www.researchireland.ie/funding/discover

For Programme related queries, please contact discover.programme@researchireland.ie

Taighde Éireann
Research Ireland

Minister Lawless welcomes the appointment by the Board of Taighde Éireann – Research Ireland of Dr Diarmuid O'Brien as new CEO

Dr Diarmuid O'Brien, CEO of Taighde Éireann – Research Ireland

The Minister for Further and Higher Education, Research, Innovation and Science has today welcomed the appointment by the Board of Taighde Éireann – Research Ireland, the state agency responsible for supporting research and innovation, of Dr Diarmuid O'Brien as its new Chief Executive Officer (CEO). Dr O'Brien will take up the role in September 2025.

Welcoming the decision by the Board, **Minister Lawless** said:

"I congratulate Diarmuid on his appointment as CEO of Taighde Éireann. I look forward to working with him and the Board, to realise the ambition and opportunity for research and innovation in Ireland created through the establishment of the agency.

"Taighde Éireann is central to the delivery of the Government's research and innovation strategy – Impact 2030. At this time, it is crucial that Ireland capitalises on all available opportunities. We must leverage our strengths in people, connectivity, and curiosity by continuing to support the development of new knowledge, talented researchers, and innovators. This focus will enable us to address the challenges facing our society and economy and seize emerging opportunities across all areas of research and innovation."

Commenting on the appointment, **Michael Horgan, Chairperson of Research Ireland,** said: "On behalf of the Board, I am delighted to welcome Diarmuid as CEO. Diarmuid has a wealth of experience and an outstanding track record. He brings a deep understanding of the public research ecosystem across all disciplines, and of the wider national and international research and innovation environment. Together with the Board, I look forward to working with Diarmuid to develop and deliver our strategic priorities over time and wish him every success as CEO of Research Ireland."

Concluding, Michael Horgan said, "On behalf of the Board, I want to sincerely thank Celine Fitzgerald, who stepped into the role of Interim CEO last September, for her excellent leadership and outstanding contribution to Research Ireland during the establishment phase of the organisation."

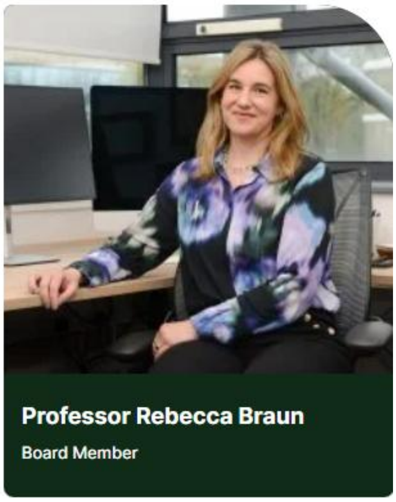
Commenting on his appointment by the Board, **Dr O'Brien** said:

"It is a great privilege to have been appointed to this position. The formation of Research Ireland creates a huge opportunity for Ireland, and I am excited to play a central role in its development. I look forward to working with the Board, my new colleagues, and partners across the wider research and innovation system, as well as with the Minister and the Department. By working collaboratively, we will build Research Ireland into an agency that supports talented researchers, shapes Ireland's research and innovation landscape, and delivers outcomes that contribute to a sustainable and prosperous future for Ireland's economy and society."

Dr O'Brien's appointment follows an open competition run by the Public Appointments Service. Dr Diarmuid O'Brien has a strong track record and brings 20 years of senior experience. He is a highly accomplished senior leader with a deep commitment to research and innovation. He joins from the role of Pro-Vice-Chancellor for Innovation at the University of Cambridge in the UK and was previously Chief Executive of Cambridge Enterprise. Prior to that, he worked in a range of roles in Trinity College Dublin over fifteen years including being Trinity's first Chief Innovation & Enterprise Officer.

Dr O'Brien brings extensive experience in leading a variety of research, innovation and cultural activities in partnership with universities, global companies, investors, high-potential start-ups, cultural organisations and government. This includes managing research institutes, developing new university campuses, creating accelerator programmes, forming large-scale industry research partnerships, creating cultural centres, implementing new translational research infrastructure, raising venture capital funds, licensing intellectual property and scaling new company creation.

Board Members



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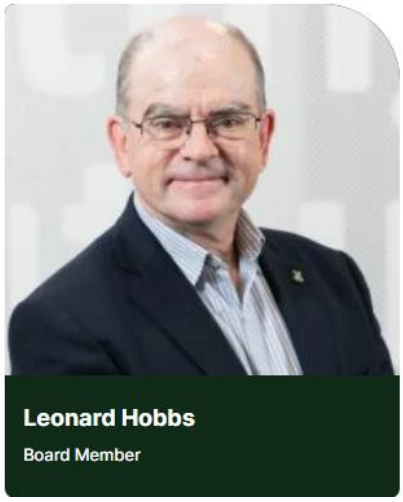

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Ministers Lawless and McEntee announce €6.5 million funding for 40 initiatives to inspire STEM public engagement

4 April 2025

Minister for Further and Higher Education, Research, Innovation and Science, James Lawless TD, and Minister for Education and Youth, Helen McEntee TD, have announced a €6.5 million investment in 40 projects designed to enhance public engagement in science, technology, engineering, and mathematics (STEM).

The Research Ireland Discover Programme focusses on creating meaningful public engagement with STEM, emphasising collaboration with communities. The programme seeks to drive innovation in STEM education and public engagement, contributing to Ireland's industry, enterprise, and societal progress.

Announcing the funding, Minister Lawless highlighted the importance of the initiatives:

These Discover-funded projects are crucial for triggering curiosity and encouraging greater participation in STEM across all education levels and within our communities. In particular, this investment will help foster a deeper understanding of STEM among underrepresented voices and inspire many of them to potentially become more involved in studies and careers in these fields. This will empower future generations to tackle societal challenges and share innovative solutions.

Welcoming her department's co-funding of eight Discover projects, **Minister for Education and Youth Helen McEntee** said:

In today's world, STEM stretches far beyond the classroom and lecture halls, and the projects we are supporting today will help bring the learnings and theories students are working on to real-world application.

Promoting awareness and appreciation of STEM in all communities is vital in inspiring students of all ages. I am proud that the Department of Education will partner again with the Department of Further and Higher Education, Research, Innovation and Science through this Research Ireland Discover Programme.

Celine Fitzgerald, Interim CEO at Research Ireland, welcomed the announcement, stating:

The Research Ireland Discover Programme is a cornerstone of our education and public engagement strategy. We are so pleased to be supporting these 40 projects and look forward to seeing them strengthen STEM engagement across Ireland and encourage more inclusive participation in shaping the future of science and innovation in Ireland.

Among the 40 projects supported through the Research Ireland Discover Programme are:

- All-Ireland STEM Passport for Inclusion 2025-2027, which partners with universities and industry to support 5,350 students through university-accredited qualifications, industry mentoring, and industry work experience to explore STEM education and employment opportunities.
- A Brush with Climate, which develops workshops and training material which empowers hairdressers to steer conversations toward climate action, using small talk as a tool for change.
- Rooted: Building Connections to Nature in our Communities through Theatre, which brings together scientists, dancers, theatre-makers, students, and rural communities through public performances, expert talks, and an evening-length dance theatre production to explore our connection to nature and inspire action against the climate crisis.
- Inclusive Artificial Intelligence for the next generation of innovators. The goal of this project is to embed AI knowledge and skills in the learning approach of schools and youth services. It is inclusion focused and aims to enhance the capacity of teachers and youth workers to support young people in marginalised communities, raise their awareness of AI, develop an understanding of AI skills, spark further learning and career pathways to address diversity gaps in AI development.
-

Among the institutions and organisations involved are: Maynooth University, Trinity College Dublin, Kinia, University of Galway, Teen-Turn, University College Dublin, Munster Technological University, University of Limerick, National College of Ireland, Dublin City University, National Concert Hall, Cork City Council, Technological University Dublin, National Youth Council of Ireland and Teagasc.

Research Ireland Discover Programme Awards
Download here

Three Ireland-based researchers awarded prestigious Royal Society Fellowships

15 April 2025

Left-right: Dr Laura Hayes (Dublin Institute for Advanced Studies), Dr Boris Galkin (Tyndall National Institute) and Dr Anthony Redmond (University College Dublin).

Funding boost for researchers based at Tyndall National Institute, Dublin Institute for Advanced Studies and UCD

The Royal Society has announced prestigious University Research Fellowships (URFs) to three researchers in Ireland.
The funding, totalling €5.25 million, will enable the following early-career researchers to establish independent research programs at their higher education institutions, advancing knowledge in diverse and impactful scientific fields over the next eight years:

- **Dr Laura Hayes (Dublin Institute for Advanced Studies)** will lead the project titled: *'FLASH: FLare Acceleration Studies with High-energy observations'.* Dr. Hayes will explore how the Sun accelerates high-energy particles during solar flares, a key process in astrophysics that also affects satellite technology and Earth's magnetic field. Using data from the Solar Orbiter mission, the project aims to reveal new insights into the physics of particle acceleration in space.
- **Dr Anthony Redmond (University College Dublin)** will lead the project titled: *'Immunity in the Fast Lane: Reconstructing the Evolution of the Animal Immune System and Prospecting for Novel Antimicrobials'*. Dr. Redmond's research will uncover the origins of animal immune systems by studying unique marine invertebrates. The work has the potential to identify novel antimicrobial compounds, which could lead to new treatments in the fight against antibiotic resistance.
- **Dr Boris Galkin (Tyndall National Institute)** will lead the project titled: *'SONGBIRD: Sensing Operations in Networks of Ground-and-Air Devices'.* Dr. Galkin's project will harness radio signal reflections to develop AI-powered mapping technology for drones. This could revolutionize emergency response, air traffic control, and urban planning, enabling drones to generate highly detailed environmental maps without expensive cameras or sensors.

Sir Adrian Smith, President of The Royal Society, said:

"Long-term funding for early career researchers to pursue novel and exciting scientific questions is vital to attracting talent and ensuring we are developing the next generation of word-leading scientists. It is gratifying to see the Royal Society – Research Ireland University Research Fellowships supporting such an array of outstanding research and researchers."

Celine Fitzgerald, Interim CEO of Research Ireland, added:

"Ireland has a strong track record of scientific excellence, and investing in our researchers is key to maintaining this position on the global stage. The Royal Society – Research Ireland University Research Fellowship is a vital initiative that provides talented scientists with the freedom and stability they need to pursue innovative research. Research Ireland is delighted to support this year's awardees, whose projects in space science, immunology, and AI-driven sensing demonstrate the depth and diversity of Irish research talent."

The Royal Society – Research Ireland University Research Fellowship supports exceptional early-career scientists in building independent research careers, offering long-term flexible funding, and fostering the next generation of global research leaders. The awards provide eight years of support, with a mid-term assessment ensuring continued excellence and impact.

The full list of 2024 University Research Fellows can be found **here**.

Research Ireland and National Science Foundation sign new partnership

13 March 2025

Pictured today in Washington D.C. signing a new, five-year bilateral partnership between Research Ireland and the National Science Foundation were Deputy CEO of Research Ireland, Dr Ciarán Seoighe, and Director of the National Science Foundation, Dr Sethuraman 'Panch' Panchanathan.Image Credit: John Harrington Photography 2025.

- Bilateral partnership to foster a culture of innovation and entrepreneurship, enhancing transatlantic enterprise engagement between academia and industry
- Training programmes and early-career researcher supports to help deliver a diverse talent pipeline and a more connected research ecosystem between the two jurisdictions

Research Ireland and the National Science Foundation have today signed a new, five-year bilateral partnership that will create a unique international government-academia-enterprise partnership delivering world-leading research and strengthening industry-academic collaboration on both sides of the Atlantic.

Among the guiding principles of the partnership are that the NSF and Research Ireland will focus on the facilitation of excellent research and training activities; cooperate in the approach to design and implementation of merit (peer) review; avoid additional burden on proposers, reviewers, and funders; and carry out transparent proposal and review processes.

Signing the new partnership, **Dr Sethuraman 'Panch' Panchanathan, Director of the National Science Foundation**, commented:

"NSF is delighted to sign a partnership with Research Ireland, formalizing and fortifying a research bond that stretches back over two decades," said NSF Director Sethuraman Panchanathan. "We look forward to the partnership promoting knowledge transfer, innovation, and research and enterprise opportunities for both our countries across a range of priority sectors."

Signing the partnership on behalf of Research Ireland, **Deputy CEO, Dr Ciarán Seoighe**, said:

"Ireland and the US have a long-standing and deep collaboration in research, development and innovation – one that is greatly valued. This new partnership signed here today builds upon that, and paves the way for the development of specific funding opportunities, coordinated peer review processes, joint conferences and workshops, staff exchanges to facilitate shared learning and develop dialogues, and alignment of larger investments, including collaboration on facilities."

The new partnership follows an intensive series of workshops involving academics from US universities and Irish research institutions in October 2024.

Photo caption: *Pictured today in Washington D.C. signing a new, five-year bilateral partnership between Research Ireland and the National Science Foundation were Deputy CEO of Research Ireland, Dr Ciarán Seoighe, and Director of the National Science Foundation, Dr Sethuraman 'Panch' Panchanathan.Image credit: John Harrington Photography 2025.*

The Following Section is for Advertising

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Commercial enterprises can have paid advertising placed in this section

Commercial entities and service providers play an important role in supporting and facilitating chemical research. These organisations supply the chemicals and reagents both routine and novel, along with instruments and new laboratories technologies researchers need for discovery.
Often a given laboratory needs to reach outside to another scientific provider for a service not available in their own laboratory.

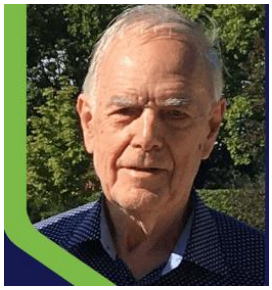
These providers should have a voice and a place to showcase their wares and services.

Here is a place to do just that!

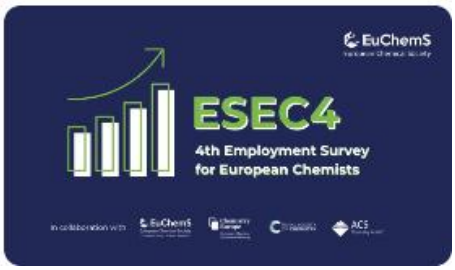
EuChemS News & Updates

European Chemical Society

EuChemS magazine



Editorial by Reiner Salzer



Invitation to the 4th Employment Survey for European Chemists (ESEC4)

EuChemS invites all members of the chemical workforce to participate in the 4th Employment Surveys for European Chemists.

Reiner Salzer,
TU Dresden, Germany
March 14, 2025

EuChemS conducted three employment surveys (ESEC1 – ESEC3) between 2013 and 2020. The responses provided unique data. For example, the data showed that chemists have always been very satisfied with their jobs, that 54% of the respondents had never experienced gender pay inequality in their workplace and that 78% had never experienced sexual harassment at work (https://doi.org/10.1002/chem.202401222).

ESEC questionnaires are multiple choice. These questionnaires allow convenient backtracking of the conditions surveyed. They end with the request: "Is there anything else you would like to let us know?" There are no restrictions on the topic or length of the free- text response, as we want to get individual thoughts from the members of the chemical workforce and to learn about issues that might otherwise be neglected. In the case of ESEC3, the free-text responses together were over 6000 words, a clear indication of the issues that needed to be addressed.

The ESEC3 free-text responses covered a wide range of topics. Many of these responses touched on very different points within a single answer. It was a challenge to analyse them all in a systematic way. Several attempted to categorise the responses by conventional means. Their results looked very different and it was almost impossible to combine them into a coherent picture. Later, we analysed the mix of topics in the responses using different AI algorithms. Similar to human analysis, different AI results look different, but only at first glance. On closer inspection, different AI algorithms simply split the responses into more categories or used alternative terms for the categories. The AI results could easily be grouped into five categories.

"Discrimination and Harassment" is the main topic in the free-text responses. 33% of all responses relate to this topic. Within this group, most refer to gender discrimination. Sexual harassment plays a minor role. The conclusion is that sexual harassment does not occur often in the chemical workforce, but when it does, it is a serious problem.

"Equality and Career" is the second biggest concern in the free-text responses. Within this category, 50% of the responses relate to pay and career progression. This corresponds well with the responses in the multiple-choice part of the questionnaire (see above). Balancing work and family life as well as problems with support programmes are the main issues in this category. It is very concerning that these issues disproportionately affect the female workforce in chemistry.

"Health and Safety issues" are mentioned in many entries under "Work Environment and Conditions". "Personal Opinions and Survey Feedback" contain a number of suggestions for improving the questionnaire. The main topic under "Academic challenges" refers to deficiencies in the supervision of PhD students and postdocs. There are also concerns about research funding, academic hierarchy and even academic corruption.

Based on feedback from previous surveys, the ESEC4 questionnaire has been revised to include questions about your expectations for the future development of your workplace. Your responses will provide a sound basis for decision-makers. A large number of participants will give great weight to the results so please support the efforts of EuChemS and participate in ESEC4, which is prepared in collaboration with EYCN, Chemistry Europe, Royal Society of Chemistry and the American Chemical Society.

EuChemS supports reform of research assessment through CoARA

EuChemS has been actively supporting the Coalition for Advancing Research Assessment (CoARA), a collective initiative aimed at reforming research evaluation frameworks. As an early signatory and member, EuChemS is committed to creating more inclusive, transparent, and responsible assessment methods, working alongside a wide range of stakeholders to improve how research is evaluated.

Chiara Capodacqua,
EuChemS
May 12, 2025

The European Chemical Society (EuChemS) has formally joined efforts to improve how research is assessed by endorsing the principles laid out by the Coalition for Advancing Research Assessment (CoARA). In October 2022, EuChemS signed the agreement that defines a shared direction for reforming current evaluation practices in the research landscape.

This commitment reflects EuChemS's dedication to fostering responsible and inclusive research environments. By aligning with CoARA, EuChemS adds its voice to a broad coalition of over 700 organisations, including research institutions, funders, assessment bodies, and professional societies, who support a shift toward fairer, more nuanced assessment methods.

At the heart of the reform is a desire to move beyond traditional metrics, such as publication counts and citation scores, which often dominate the evaluation of research and researchers. CoARA promotes an approach that balances quantitative indicators with qualitative judgement, such as peer review, and encourages greater transparency and responsibility in how research impact is assessed.

To further advance this initiative, CoARA's Working Group on Responsible Metrics and Indicators (RMI WG) recently launched a survey to gather insights on current uses of metrics in research evaluation. The responses will help develop a more integrated framework that reflects both quantitative and qualitative dimensions. Institutions and individuals involved in research assessment are invited to share their practices and perspectives.

By taking part in this effort, contributors help shape a more equitable and transparent research assessment system. EuChemS encourages wide participation, underscoring that collective input is vital to achieving meaningful and lasting change in how research is valued.

EuChemS engages in European Commission's efforts on PFAS regulation

EuChemS continues to engage with the European Commission on measures aimed at addressing the environmental and health risks posed by per- and polyfluoroalkyl substances (PFAS). The Commission's planned actions, including restrictions on PFAS in firefighting foams and other key regulations, are part of ongoing efforts to mitigate their impact.

Chiara Capodacqua,
EuChemS
May 12, 2025

EuChemS continues to closely follow developments regarding the European Commission's actions on per- and polyfluoroalkyl substances (PFAS). These substances, often referred to as "forever chemicals," have raised significant environmental and public health concerns due to their persistence in the environment and potential toxic effects. EuChemS, with its focus on sustainable chemistry, is engaging with the ongoing regulatory actions and exchanges that aim to mitigate the risks posed by PFAS while supporting informed and effective solutions.

The European Commission has been progressively strengthening its regulatory framework to address the risks associated with PFAS. This includes a combination of existing and new policies, regulations, and directives targeting the reduction of pollutants at their source. These measures range from the POPs Regulation and REACH restrictions to updates in the Industrial Emissions Directive and the Industrial Emissions Portal Regulation, all working to limit emissions across various sectors. Furthermore, the Commission has integrated PFAS concerns into other key regulations, such as the Drinking Water Directive, the Urban Wastewater Treatment Directive, and the Soil Monitoring Law, which are designed to track and limit environmental contamination.

The Commission's step-by-step approach toward managing PFAS focuses on carefully assessing the need for restrictions and alternative solutions. Notably, the Commission has already implemented REACH restrictions on certain PFAS chemicals, such as perfluorocarboxylic acids (PFCAs) and perfluorohexanoic acid (PFHxA). The next significant step is a proposed restriction on PFAS in

firefighting foams, with a vote scheduled for the near future. However, the European Commission has acknowledged the challenges in replacing PFAS in some industrial applications, where alternatives are not yet viable. In these cases, the use of PFAS will continue until sustainable alternatives are developed, as a full ban could significantly impact industries and the economy.

EuChemS, as part of the broader scientific community, supports the Commission's focus on a gradual and evidence-based approach to PFAS regulation. While the urgency to address PFAS contamination, particularly in water resources and human health, is clear, the European Commission has stressed the importance of relying on thorough scientific research and data from agencies such as the European Chemicals Agency. Premature regulatory actions without adequate data could lead to unintended consequences, and the Commission's commitment to an evidence-based path remains central to its regulatory actions.

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EuChemS President Angela Agostiano named Professor Emeritus by the University of Bari

Angela Agostiano, President of EuChemS, has been appointed Professor Emeritus by the University of Bari, recognising her contributions to teaching and academic leadership in the field of chemistry.

Chiara Capodacqua,
EuChemS
April 14, 2025

Angela Agostiano, President of the European Chemical Society, has been honoured with the prestigious title of Professor Emeritus by the University of Bari, recognising her career in academia and her role in advancing the chemical sciences.

This recognition highlights Professor Agostiano's contributions to the field of chemistry, both in terms of her academic work and her role in the development of the scientific community. It is a tribute to her commitment to teaching and research, and her dedicated service to the university over the years.

A continued commitment to science and education
Angela Agostiano's recognition as Professor Emeritus reflects her impact on the chemistry community at both national and international levels. Her leadership in EuChemS continues to contribute to meaningful dialogue across scientific disciplines and to the promotion of chemistry's role in addressing societal challenges.
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Bringing science and policy: EuChemS Rare Earth Elements event

May 30, 2025

On 14 May 2025, the European Chemical Society (EuChemS) held an event on Rare Earth Elements (REEs), a topic of growing strategic importance for Europe. The event included a morning session at the European Parliament and an afternoon session at the EuChemS office, bringing together scientists, policymakers, and industry experts to address REE availability, criticality, and sustainability.

This event was part of EuChemS' ongoing series dedicated to individual chemical elements, from the EuChemS Table of Chemical Elements, which highlights each element's availability and sustainability challenges.

Science-policy focused morning session at the European Parliament

Hosted by MEP Annalisa Corrado, the session began with opening remarks from EuChemS President Angela Agostiano. She reaffirmed EuChemS' mission to promote evidence-based policymaking and sustainable chemical practices, highlighting its European network of over 140,000 chemists. Angela Agostiano underscored the relevant role of chemistry in tackling climate and digital challenges, supporting young scientists, and bridging the gap between science and policy.

Peter Roesky (Karlsruhe Institute of Technology), Scientific Chair of the event, introduced REEs as critical to Europe's sustainability and autonomy. Nicola Armaroli (CNR and EuChemS) followed, presenting the EuChemS Table of Chemical Elements and stressing the urgency of circular material flows to mitigate resource scarcity.

These introductory talks which set the scene were followed by presentations on geopolitics, recycling, and policy.

Andrea Dini (CNR, Pisa) examined REE extraction, focusing on Europe's dependence on external sources, particularly China. Marie Perrin (ETH Zürich & REEcover) highlighted advancements in REE recycling from waste streams, essential for a European circular economy. Milan Grohol (European Commission, DG GROW) provided an institutional update on the Critical Raw Materials Act and EU strategies to strengthen supply chain resilience and innovation.

A dynamic Q&A followed, covering EU recycling incentives and global cooperation. The session closed with remarks from MEP Corrado, affirming the Parliament's support for research-led sustainability efforts.

Science focused afternoon session

The afternoon shifted to scientific applications of REEs in energy, materials, and catalysis. Talks included:

- *Andries Meijerink* (Utrecht University) on REEs' optical properties in lighting and sensors
- *Mario Ruben* (KIT) on their magnetic role in wind turbines and EV motors
- *Evgueni Kirillov* (University of Rennes) on catalytic uses in pollution control and hydrogen production
- *Jürgen Gassmann* (Fraunhofer IWKS) on REEs in energy transition and future battery and hydrogen technologies

A final panel discussion, moderated by Angela Agostiano, continued the exploration of REEs, with speakers reflecting on the scientific insights shared throughout the day and their implications for future research and innovation.
The recording of the event will be available soon on the EuChemS Youtube channel.
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EuChemS at the EYCN Delegate Assembly 2025

Mar 26, 2025

From 20–22 March 2025, the European Young Chemists' Network (EYCN) Delegate Assembly took place in Prague, bringing together young chemists from across Europe. As the younger division of EuChemS, EYCN provides a valuable platform for early-career chemists to exchange ideas, develop skills, and connect with the broader scientific community.

This year's Delegate Assembly featured a rich and diverse agenda, showcasing EYCN's ongoing and future initiatives while fostering discussions on leadership, collaboration, and science policy.
The event opened with a welcome address from EYCN Chair Claudia Bonfio, Organising Committee Chair Petr Leinweber, and EuChemS President Angela Agostiano, who highlighted the importance of supporting young chemists and fostering collaboration to advance chemistry across Europe. A key moment of the assembly was the introduction of candidates for the next EYCN Board, who shared their visions for the future of the network.

Another highlight was the presentation of EYCN's collaboration with Elsevier, which featured two interactive workshops focused on leadership skills and teamwork. Discussions also addressed preparations for the upcoming EuChemS Chemistry Congress 2026 (ECC10), ensuring young chemists play an active role in this major event. Additionally, a session led by Angela Agostiano and EuChemS Science Communication and Policy Officer Chiara Capodacqua explored the 10th Framework Programme for Research and Innovation.

To conclude the first day, EuChemS presented its latest survey on employability, providing valuable insights into the challenges faced by chemists entering the workforce.
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Looking to the Future
The Assembly concluded with the election of a new EYCN Board the following day. EuChemS warmly congratulates the newly elected board members and looks forward to continuing its strong collaboration with EYCN in the years ahead.

EuChemS stands with ALLEA in defending academic freedom and global research cooperation

EuChemS has endorsed ALLEA's 2025 statement addressing threats to academic freedom and global research collaboration.

Chiara Capodacqua,
EuChemS
April 14, 2025

In response to recent policy shifts in the United States, the European Chemical Society (EuChemS) has formally endorsed a statement by ALLEA addressing growing concerns over threats to academic freedom and international scientific collaboration.

ALLEA's warning
In February 2025, ALLEA released a statement condemning a series of executive actions introduced by the new U.S. Administration. These directives include halting substantial federal research funding and restricting academic inquiry into critical topics such as climate science and gender studies. The resulting disruption has affected the functioning of major U.S. research institutions and government science agencies, causing delays, uncertainty, and in some cases, the suspension of ongoing projects.

According to ALLEA, these developments have consequences far beyond U.S. borders. The increasingly interconnected nature of the global research landscape means that political constraints in one country can significantly impact the international scientific community. Suppressing academic freedom and limiting research scope undermines the integrity and advancement of science on a global scale.

EuChemS reaffirms its commitment
EuChemS has consistently promoted academic freedom, institutional autonomy, and international cooperation as foundational values of scientific progress.

By publicly supporting ALLEA's 2025 statement, EuChemS reinforces its dedication to upholding these principles and expresses solidarity with scholars and researchers affected by restrictive measures.
To read the full ALLEA statement click here.

https://www.idaireland.com

IDA Updates & Reports

IDA Ireland launches new five year strategy Adapt Intelligently: A Strategy for Sustainable Growth and Innovation, 2025-29

19/02/2025

New strategy will:

- Focus on winning, strengthening and maintaining long term investment with existing and new client base
- Secure 1,000 new investments will deliver €250bn to the Irish economy and further embed FDI clients in Ireland.
- Scale RD&I investment to €7bn to position Ireland at the centre of cutting-edge global technological innovation in next 5 years
- Enable upskilling of 40,000 people within IDA Ireland client base
- Support the creation of 75,000 new jobs across priority sectors of growth and opportunity
- Enhance balanced regional development through securing 550 investments into regional locations
- Support 35% reduction of carbon emissions by IDA Ireland clients and attract new green and digitally enabled investments

IDA Ireland today unveiled its new five-year strategy, Adapt Intelligently: A Strategy for Sustainable Growth and Innovation, 2025-29, building on its previous success in helping to transform the Irish economy. The strategy has been developed from a position of strength evidenced by the significant economic impact delivered to Ireland and the global economy through the investments from IDA Ireland's client base.

The FDI sector, established and embedded in Ireland, is a national asset which has been transformative for the economy and the people of Ireland, accounting for 11% of total national employment and expenditure of over €38bn in the Irish economy annually. Ireland is viewed internationally as a centre for value and knowledge creation, exporting over €420bn in goods and services globally on an annual basis.

The new strategy, which is aligned with the Programme for Government and the White Paper on Enterprise, sets out IDA Ireland's ambition for continued growth through four key strategic objectives;

- Strengthen long term investment
- Scale cutting-edge innovation
- Drive sustainable change
- Maximise regional opportunities

While recognising the challenges ahead for FDI investment including increased competition, geopolitical uncertainty, and rapid technological change, IDA Ireland has identified four key growth drivers – **digitalisation and AI; semiconductors; health; and sustainability** which will lead to a range of intersecting and connected opportunities across IDA Ireland's core sectors of focus – Life Sciences, International Financial Services (IFS), High Value Manufacturing, Engineering, and Technology and Content & Consumer Services.

STRATEGIC OBJECTIVES

Strengthen long term investment

IDA Ireland will prioritise retaining and renewing the 1,800 client companies based in Ireland,

acknowledging their vital role in the Irish economy. We will partner with them as they aim to enhance their competitiveness and productivity through transformative talent development initiatives and assist them in navigating challenges and seizing opportunities in a changing global economy.

Scale cutting-edge innovation
Ireland's FDI base has helped position the country as a central hub for global technological innovation. The new strategy aims to build on the existing innovation ecosystem, enhance pan-European and global innovation linkages, and increase the scale and impact of innovation by supporting next-generation and collaborative research, development, and innovation (RD&I).

Drive sustainable change
IDA Ireland client companies are instrumental in shaping a green and digital global economy. Ireland has the potential to be a prime location for green-powered and digitally enabled enterprises. IDA Ireland will collaborate with clients to enhance their digital maturity and sustainability, while attracting a new wave of green and digitally enabled investments.

Maximise regional opportunities
Maintaining the strength of Dublin as a key global hub remains a strategic priority. The significance of our capital city enables the attractiveness of Ireland and supports our ambition for balanced regional development. IDA Ireland client companies employ over 165,000 people in regional locations across Ireland, benefiting from the local ecosystem, infrastructure, and talent to drive investments. The regional strategy has proven to be successful, and IDA Ireland is committed to further enhancing regional opportunities for clients by providing next-generation sites and building solutions.

TARGETS
In pursuit of these objectives, IDA Ireland will win **1,000** investments to:

- Secure €7bn in new RD&I investment
- Deliver 550 regional investments
- Reduce IDA Ireland client carbon emissions by 35%
- Create 75,000 jobs
- Upskill 40,000 people

In turn, this will support IDA Ireland client spending in Ireland of €250bn over the lifetime of the strategy on wages, Irish goods and services, and capital investment, providing further opportunity and economic impact across local supply chains. By 2030, the strategy aims for a more competitive, innovative and sustainable FDI environment in Ireland. The ambitious plan underscores Ireland's commitment to fostering a resilient economy, adapting intelligently, and seizing new growth opportunities in an era of change and evolvement.

Minister Peter Burke, Minister for Enterprise Tourism & Employment said: "I very much welcome the publication of IDA Ireland's new strategy today and recognise the importance of ensuring we work together to protect FDI's position as a cornerstone of Irish economic success. Ireland remains committed to foreign direct investment (FDI) as one of the key components of the Irish economy. We have proven adept in the past at anticipating and responding to shifts in the global landscape, realising growth opportunities as sectors evolved and new technologies emerged. In a period of marked global change and uncertainty, this strategy will direct the focus of IDA Ireland as it partners with client companies to enhance the resilience, productivity, and innovation of Ireland's FDI base.

In a world of uncertainty, companies can be certain that Ireland remains determined to remain a leading location in which to grow, innovate and succeed. Through decades-long partnership across the public and private sector, Ireland has won investment and built up an FDI base in high value, cutting edge services and manufacturing sectors. Protecting this existing base, positioning it for further success and securing the next generation of investment is of critical importance. This strategy will ensure IDA adapts to a changed global landscape to achieve these ambitious objectives."

Feargal O'Rourke, Chair IDA Ireland said: "Our new strategy is designed to keep the FDI pipeline strong but also to recognise the importance of holding on to what we have. FDI companies in Ireland tell us of their need to constantly show relevance back at corporate HQ whether it is upskilling their employees with digital and AI skills, having a sustainable operation, or maximising their effectiveness and efficiency. Our role is to help our client companies in these areas and our strategy will underpin this. If we can lead, and play our part in delivering on our strategy, it will have a positive societal and economic impact for Ireland. While today marks the launch of our strategy, it also represents an opportunity for Ireland to recommit to a strong FDI strategy and to, in a sense, "renew our vows" to make Ireland the best, most sustainable and most welcoming country in the world for FDI."

Michael Lohan, CEO IDA Ireland said, "Innovation, competitiveness, resilience and ambition are at the core of our new strategy that is designed to further propel FDI in Ireland. I am extremely proud of the performance by the IDA team who, in partnership with our 1,800 clients and stakeholders, have achieved exceptional results against the objectives set out in our previous strategy. The impact of FDI is reflected in every facet of the Irish economy from our employment numbers to our enterprise base, integrated supply chains and the development of critical infrastructure.

We are now ready to rise to the challenges of today. Our new strategy recognises the scope and scale of our clients' activities, their transformational journeys, as well as the complexities of the global landscape in which IDA Ireland and our clients now operate. It identifies Ireland's areas of strength and the opportunities for continued FDI growth. It is now absolutely crucial that we build on the solid foundation we have laid and focus on continued partnerships with the strong FDI base in every region in Ireland, to drive sustainable growth through capital investment, innovation and talent development that will strengthen, maintain and deepen our position as a location of choice for continued foreign direct investment.

Download Adapt Intelligently: A Strategy for Sustainable Growth and Innovation **here**

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Cook Medical and IDA announce €3 million investment in renewable and energy-saving technologies

10/04/2025

- Advanced technologies, including 1 megawatt of solar panels, a heat pump upgrade, and electronically commutated fans, will be installed.
- The combined results will offset approximately 50% of carbon emissions from the manufacturing facility in Castletroy.
- The project, which is subject to planning approval from Limerick City and County Council, is part of Cook's Social Impact & Sustainability programme that commits to making sustainable and inventive choices across the organisation to protect the environment by reducing its carbon footprint and achieving impactful environmental goals.

Cook Medical has announced a €3 million investment in renewable and energy-saving technologies.

The project consists of a new 1 megawatt ground-mounted solar PV array on the grounds of the Limerick site, along with 1.2 megawatts of heat pumps to replace the existing chillers, an upgrade of electronically commutated fans, and a new energy management system.

The investment is part of the company's carbon reduction goals, with the new technologies helping to increase the operational efficiency of the facility in Castletroy and eventually offsetting approximately 50% of carbon emissions.

This project is expected to offset up to 269 tonnes of carbon annually, and over its 25-year life cycle it
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will remove a total of 6,725 tonnes of carbon. Coupled with the procurement of additional green energy technologies, this will result in the removal of 60% of the carbon from the Cook Ireland site.

This project is supported by the Irish Government through IDA Ireland. **Minister for Enterprise Tourism & Employment Peter Burke said,** "For almost 30 years, Cook Medical has been present in Ireland and today's announcement of a €3 million investment in renewable and energy-saving technologies is fantastic news. The combined plans are expected to offset 50% of their carbon emissions, which is in line with the Climate Action Plan to halve Ireland's emissions by 2030. It is really encouraging to see initiatives being taken by companies focused on carbon reduction measures, sustainability and protecting the environment for future generations. I wish Cook Medical success with these plans and all their future endeavours."

Commenting on the project, **Bill Doherty, executive vice president and managing director of Cook Medical Europe, said,** ''We are committed to making sustainable choices across our business and reducing our impact on the environment. By integrating solar panels into our operations, we're able to enhance our efficiency while also reducing our carbon footprint."

The company is committed to enhancing and maintaining the biodiversity of its site and will continue to safeguard the environment in its plans. In addition to reseeding native wildflowers in all areas under construction, the company will also preserve walking tracks and spaces for wildlife.

CEO of IDA Ireland Michael Lohan said: "This proposed project will position Cook's Irish operations as an exemplar with its global network, and as a key location of subject matter expertise around energy management systems. Strongly aligned to the National Climate Action Plan's Enterprise Pillar and IDA Ireland's sustainability targets, we wish Cook Medical every success with this initiative which has far reaching potential."

Upon completion of this project, Cook Ireland will reduce its annual import of electricity by 19% and release that capacity back to the grid. A 70% reduction in the annual use of natural gas consumption is expected from the installation of the heat pumps.

A planning application has been submitted to Limerick City and County Council. If successful, construction on this project is expected to begin in due course.

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How Ireland plans to make an impact in advanced therapies

08/05/2025

Ireland's advantage: coordinating multiple stakeholders

Compared with traditional pharmaceuticals, cell and gene therapy requires a coordinated effort between researchers, drug development and pharmaceutical companies, outsourced manufacturers, healthcare providers, investors, regulators and data scientists. Professor Athanasios (Sakis) Mantalaris believes this factor gives Ireland a crucial edge in this field.
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"For cell and gene therapy you need a complex network of multiple providers," says the world-renowned researcher, who was attracted to work in Ireland at the end of 2022 after prior posts at Georgia Tech in the USA and Imperial College London.
Prof Mantalaris contends that the need for interdisciplinary teams can help to make Ireland a "destination of choice" for the biomanufacturing industry and also for carrying out clinical trials. "Ireland is a small country. People see it as a weakness but we see it as a strength... It can achieve things that are harder to achieve in other countries," he contends.

Tackling complexity in the process

"Because Ireland is small, we intend to put together interdisciplinary, integrated teams and draw expertise – let's say from the appropriate immunologist or the manufacturing expert to the clinical expert or patient advocacy groups. We think that by creating this environment and because of the size, being small, will have a multiplying effect. We want to create a sustainable ecosystem in Ireland," he says.

Prof Mantalaris' work, together with his colleague Professor Nicki Panoskaltsis, is being undertaken by Trinity College Dublin's Trinity Translational Medicine Institute (TTMI), and The National Institute for Bioprocessing Research and Training (NIBRT), in conjunction with Research Ireland and St James's Hospital. It focuses on developing precision biomanufacturing to generate high-quality cellular therapy products.

Their work also feeds into the IMPACT centre, a consortium co-led by Trinity College Dublin and the University of Galway. All told, it includes seven Irish universities, five hospitals, four organisations including NIBRT and the Irish Blood Transfusion Service, and more than 60 principal investigators. The name stands for Irish Medicines – Centre for Personalised Advanced Cellular Therapeutics.

Professor Aideen Long, principal investigator and director of TTMI, adds her voice to the debate. "In Ireland, we have a very fluid relationship between industry, academia and other governmental and non-governmental bodies, working together, right through to the patient. Our research at TTMI is very patient-focused and we're close to patient research from the basic level right through to clinical trials and patients coming to clinics. There is quite a push forward in bringing all these people together," she says.

Challenges in manufacturing advanced therapies

There are lots of potential areas worth investigating for IMPACT. Every stage of the cell therapy production process presents multiple challenges from sourcing the cells through to modifying them, manufacturing and testing the therapy, distribution and delivery, through to clinical application. Along that complex chain, developers also need to check for donor variability of the cells; test to make sure there is no immune response in the patient; the therapy must be reproducible from one batch to the next; it has to be sterile, potent and pure. There are considerations around logistics and delivery times, and above all, the therapies need long-term monitoring for safety and efficacy of response.

> **The model for developing advanced therapies either involves a pharmaceutical company or a private biotech firm sponsoring their development, or it starts life in an academic centre and is subsequently commercialised by a pharma company. As ASU president Michael Crow recently pointed out, technological breakthroughs and innovations in any field often build on the "invisible" work of many academic researchers.**

This all helps to explain why IMPACT's work is already attracting the industry's attention. According to Prof Mantalaris, large pharmaceutical companies are responding positively to the proposal because of its potential to help them with manufacturing challenges.

"We go right from the design – the basic biology – all the way to the making and manufacture of the drug, putting the patient at the centre which ensures the patient's voice is heard and affordability takes

front and centre. We are not just trying to address research challenges but also clinical challenges and create a manufacturing industry for Ireland. We want to be able to attract biomanufacturers because of the great tradition in manufacturing that Ireland has," he says.

Another advantage for Ireland is its diverse demographics which can offer fresh perspectives from clinical trials. These take on oversized importance in cell and gene therapy because of how unique a treatment is to each patient. Thanks to much inward migration in recent years, Ireland's population provides an effective testbed for researchers who need to understand differences between various ethnic groups and people from different parts of the world. This diversity also helps to correct potential biases such as testing too many people with similar genetic backgrounds.

Healthcare and treatment benefits

The potential benefits could not be clearer: these advanced immune cell therapies offer the potential to treat different types of cancers, autoimmune conditions, as well as other inflammatory and degenerative diseases. This field has seen significant developments over the past decade, with a form of immune therapy that uses a patient's own immune cells to target otherwise incurable cancers.

As an example, in the seven years since the first clinically approved CAR-T cell therapy in 2017, there have been 9 FDA approved immune cell therapies. In comparison, there were four approved biologics in the seven years following the first clinically approved monoclonal antibody in 1986.

And as greater understanding and focused research leads to more breakthroughs in cell therapies, it's hoped this will lead to better outcomes for patients. Prof. Mantalaris' research, and the work of IMPACT, also aims to address both the availability and affordability of treatments, saving patients from needing to travel to other countries to get the therapies they need. "We have an ambitious vision for Ireland by 2034 to treat over 1,000 patients per year for multiple diseases using cell therapeutics, so there won't be a need to send patients outside Ireland," he says.

Analysis from Precision Research estimates that advanced therapies including cell and gene therapy research will account for approximately 20% of the size of the total pharmaceuticals market. In 2023, it valued this area at US$14.52 billion and is forecasting this will have more than doubled by 2027 and estimates the market for cell and gene therapy to be worth US$97 billion by 2033.

That's the scale of the opportunity awaiting Ireland, Prof Mantalaris believes. "We want Ireland to grow its own homegrown industry. We want to create 3,000+ jobs leveraging the biomanufacturing expertise that is in Ireland with the development of clinical trials and a clinical pathway. This is achievable."

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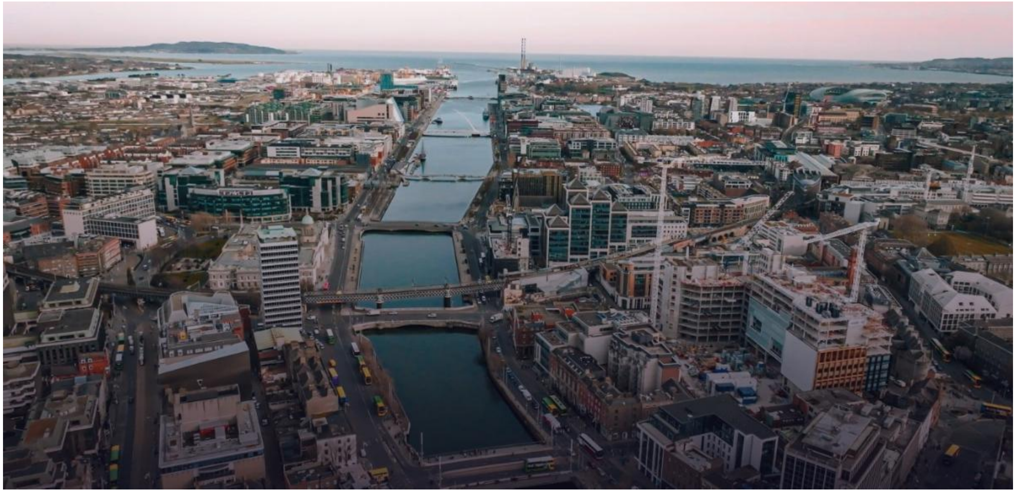
Why Ireland: Stable, resilient and reliable

08/05/2025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In tumultuous times, stability has never been more valuable, especially for businesses looking to plan for the long term and grow in new markets.

In Ireland, stability is what we do.

Since the beginning of this decade alone, there has been a global pandemic, geopolitical upheaval due to conflict, trade tension and supply chain disruptions. Yet Ireland's economy has remained strong; the fundamentals are robust and we count on a pro-enterprise policy that has been in place for several decades.

More than 1,800 businesses have availed of Ireland's reputation for reliability as a proven, stable location that supports international markets. As a small open economy, within the European Union, Ireland offers investors the track record and trusted relationships built up over decades, says IDA Ireland CEO Michael Lohan.

> **Ireland is ideally placed from a geographical perspective to serve as a gateway to the extensive European marketplace, offering companies access to a broad customer base and numerous business opportunities.**

"I fundamentally believe that for economies to continue to prosper, for companies to continue to invest internationally, they need locations like Ireland, they need to be able to go to locations that are proven, that are trusted, that are strong partners. Ireland is a real hub for international access whether into Europe or to the rest of the world. We're very confident in what we offer," he says.

What Ireland offers is founded on three pillars: stability and support; people and place; and ecosystem and environment.

Stability and support

Multinationals are drawn to Ireland due to its predictable and stable business environment, which facilitates ease of operations and long-term planning. "In my experience, what investors across the world are looking for is policy certainty and stability: a proven location with good talent that supports international business. Uncertainty leads to lack of decisions and lack of investment, and we're very conscious of that from an Ireland perspective," Michael Lohan adds.

> **Often, companies that set up operations go on to re-invest in Ireland, expanding their sites far beyond their original mandate. IDA Ireland's consistently positive annual results reaffirm the country's resilience and continued attractiveness for investment.**

That feeling is borne out by research from EY, which found that Ireland's attractiveness as a location for FDI remains strong. The 2024 latest EY Attractiveness Survey Ireland found that 66% of key investment decision makers expect that Ireland's attractiveness as a location for foreign direct investment will improve in the coming three years.

Ireland offers a mix of competitive taxes and incentives, allied to a business-friendly environment that's geared towards helping enterprises flourish.

People and place

Ireland's education system and emphasis on innovation have cultivated a highly skilled workforce attractive to foreign investors. Our emerging talent spans technical, business and creative disciplines. We benefit from having Europe's second youngest population. It is also one of the most educated and diverse workforces in the world, where 34% of the population is aged 25 or less, while our rate of completion for third level education is higher than the EU average (62.7% compared to 43.1%).

Many of our universities and higher education institutions work closely with multinationals,

developing courses and modules that closely match industry needs. And our workforce is internationally focused: there are 200 different nationalities represented in Ireland, and 22% of employees at FDI companies in Ireland – nearly one in four people – come from beyond these shores.

> **And our past success in attracting leading names has been a net positive. It might seem counterintuitive, but the presence of some of the industry's leading names in close proximity is a benefit, not a barrier, to more recent arrivals, believes Jon Ross, Zendesk's VP of Product, Messaging.**

"Dublin is such a hub for big tech companies that you might think 'if we come to Dublin, we're going to be competing with all of them, we won't be able to get good staff'. But I think the opposite is true. Because we've got such a base of well recognised brands in Dublin, that actually brings qualified people from all over Europe here," he says.

Our partnership approach also extends to the business relationships we cultivate with companies. Ruairi Conroy, VP of sales development with the software company Diligent, speaks about how IDA Ireland was at its side during various "sprint moments" as the business expanded its operations in Galway. "It genuinely does feel like a partnership rather than a one-and-done, and the after-sales experience is excellent too," he says.

Ecosystem and environment

Ireland offers the means and opportunity for companies to innovate. R&D investment by IDA client companies were at record levels, in the agency's most recent annual results. IDA Ireland remains committed to continuing this progress by enhancing supports for R&D activity.

One example of how Ireland is pushing boundaries is the announcement in March 2025 by the university spinout, Equal1, of a breakthrough in developing the world's first silicon-based quantum server which consumes less power than other quantum machines. The company also owes its origins to the presence of multinationals in Ireland. Jason Lynch, Equal1's CEO, began his career at Analog Devices, which first set up operations in Ireland in the 1970s.

> **"Quantum computing will be the next wave of growth for the semiconductor industry here in Ireland," says Lynch. "For me, it's the idea that Ireland is a small enough community that we can get together and do something meaningful with impact on the global stage."**

That compact size is also benefiting teams of researchers across academia and healthcare who are exploring new cell and gene therapies which have the potential to treat previously incurable illnesses.

Conclusion

Business craves certainty, as any wise investor knows. And in times of upheaval, removing risk from the equation is a good strategy. It's what makes Ireland a safe harbour and why, for IDA Ireland, sustainability has a second meaning: it stands for both a commitment to climate goals and decarbonisation, but also making businesses more resilient against external shocks and risk.

That's why sustainability is not just a key pillar of IDA Ireland's strategy; it's also an illustration of how we do business here in Ireland. When a company chooses to set up operations here, it is not the closing of the deal but the opening of a dialogue; an ongoing partnership that benefits all.

Download IDA Ireland's value proposition infographic **here**

AbbVie in Ireland

8 diverse sites across Ireland employing 2,500+ people

- 8 diverse sites across Ireland employing 2,500+ people
- 8 diverse sites across Ireland employing 2,500+ people

“Ireland plays a critical role in supporting AbbVie's international operations. Our new AbbVie North Dublin (AND) facility will be a key node in AbbVie's global Operations network, serving as a European hub bringing together our Dublin-based supply chain, engineering, quality assurance and manufacturing teams for the first time.”

Azita Saleki-Gerhardt
AbbVie EVP, Chief Operations Officer

AbbVie

AbbVie was founded in 2013 when it became a separate company from Abbott Laboratories. Headquartered in Chicago, AbbVie are one of the largest biopharmaceutucal companies in the world. Its products treat more than 62 million people every year, affected by over 60 conditions. The company is present in over 70 countries, and its total headcount is close to 50,000 people.

AbbVie in Ireland

AbbVie’s presence in Ireland dates back to 1974, combining the company’s own investment with facilities acquired through buyouts. It has eight sites in Ireland that, together, employ more than 2,600 people. Its site at Carrigtwohill near Cork celebrated its 20th anniversary in 2022, and the company has plants and office hubs in Dublin, as well as manufacturing medicines for global supply at locations on the west coast of Ireland, at Westport in County Mayo and in Sligo.

Ongoing investment

Recent expansion at its site on the outskirts of Cork involves a new €63 million facility using new technologies to support AbbVie’s aesthetics business. The site will employ 70 people in roles including sterile manufacturing, quality control and engineering. The site is due to be operational from 2025.

In 2020, when AbbVie completed its buyout of Allergan, the companies opened a second facility in Westport for producing Botox, in a $176 million investment. The 750,000 sq ft site employs 1,400 people.

In 2018, AbbVie spent $139 million on expanding one of its two plants in Sligo, to increase capacity to produce cancer drugs. That followed a $115 million investment four years previously to produce oral hepatitis C drugs in Sligo.

How Ireland Helps AbbVie

- Company presence in Ireland dates back five decades
- Close to 2,600 people employed at AbbVie in Ireland
- Activities in Ireland span commercial and manufacturing
- AbbVie continues to invest in its eight Irish sites spanning the country

WuXi Biologics: Pioneering Asian company locates first overseas factory in Ireland

- **Ireland chosen for Chinese pioneer's first international site**
- **€325 million invested in biologics drug substance manufacturing facility**

"We are committed to Ireland and will work with all local partners to build this state-of-art next generation biomanufacturing facility as a showcase to the global biotech community"

Dr Chris Chen
CEO, WuXi Biologics

Why Ireland for WuXi Biologics
Headquartered in Wuxi City, China, WuXi Biologics has pioneered the commercial biomanufacturing of biologics-based medicines, which uses cells rather than chemicals to develop innovative diagnostics and therapies to change how diseases are prevented and treated. The Hong Kong-listed global company offers multinational pharma and biotech companies services designed to help shorten the discovery and development time and lower the cost of biologics.

Greenfield site, ready to go
In 2018, WuXi Biologics invested €325 million in a new biologics drug substance manufacturing facility on a 26-hectare greenfield site in Dundalk, County Louth, supported by the Irish Government through IDA Ireland.

Part of the reason the company chose Ireland as its international base is because the country already hosts many of the leading global names in the pharmaceutical industry, many of which are WuXi Biologics customers. Another key factor in securing the investment was the existence of an IDA-owned site near Dundalk which had already secured planning permission for a biotechnology campus, saving 12 months in the planning process.

The Irish facility also happens to be geographically well placed, as the North American market is just five hours behind, central Europe is one hour ahead, and mainland China is seven hours ahead.

Ireland chosen as first site outside China

This 'factory of the future' facility is based on WuXi Biologics' pioneering multiple single-use bioreactors. The site is designed to manufacture around the clock using continuous bioprocessing, a next-generation manufacturing technology to be first implemented globally in this campus. The site is also able to change product lines rapidly in response to customer needs. It is the company's first site outside of China. Over the following five years as the site geared up to enter full production, it created 400 new jobs.

A year after that announcement, WuXi Vaccines, a subsidiary company, revealed plans for a $240 million vaccine production facility on the same campus, creating 200 additional new jobs over five years.

How Ireland helps WuXi Biologics

- Ireland chosen for Chinese pioneer's first international site
- €325 million invested in biologics drug substance manufacturing facility
- 12 months saved in planning process thanks to existing IDA Ireland site
- Irish location is geographically suited to global operations

Regeneron: Biologics leader scales rapidly across two strategic sites in Ireland

- Ireland chosen as the company's first manufacturing facility outside the U.S.
- Total investment at its Limerick biologics site exceeds $1 billion.

"In order to make space in our New York facilities to accommodate our COVID-19 efforts, we needed to ramp-up capacity here in Limerick. Despite ramping up commercial production sooner than planned, my team hasn't missed a beat. You can only perform like this if you have good people, and Ireland has lots of good people, so we are excited to be hiring 400 more".

Dan Van Plew
Executive Vice President & General Manager of IOPS, Regeneron

Regeneron
Founded by physician-scientists in New York 1988, Regeneron is a leading science and technology company delivering life-transforming treatments for serious diseases. The company has nine FDA-approved medicines, eight EMA-approved medicines and numerous product candidates in a range of diseases, including asthma, cancer and infectious diseases. Its revenues in 2022 were over $12 billion and it employs more than 12,000 people worldwide.

Rapid scale in Ireland
In 2013, Regeneron opened its European business office in Dublin and began hiring its first employees there. The same year, it chose Limerick to be the site of its first industrial operations and product supply (IOPS) site outside the United States. The following year, manufacturing commenced at its state-of-the-art facility in Limerick. By the end of 2016, the company had already beaten its initial projected headcount in Ireland with the hiring of its 350th employee.

At the same time, building began on a new quality control labs and process sciences building at the IOPS Limerick site, which in 2017 received a further $100 million investment, with the addition of 300 jobs. By then, the site was the largest bulk biologics production facility in Ireland.

Regeneron also received its first FDA and EMA approvals to manufacture medicine in Ireland for sale in the U.S. and EU. In 2019, construction got underway on a new laboratory and administrative building in Limerick, while a year later, the site reached the milestone of its 1,000th employee in Limerick. Also in 2020, the company announced 400 additional jobs.

The Limerick operation involves high-end specialist jobs in commercial manufacturing, process sciences, quality assurance/control, supply chain as well as various support functions for scientists, chemists and technicians.

How Ireland helps Regeneron
- Ireland chosen as the company's first manufacturing facility outside the U.S.
- Limerick site produces a number of Regeneron's portfolio of medicines.
- Total investment at its Limerick biologics site exceeds $1 billion.
- Employment at Limerick stands at over 1,400 people.

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Physical Chemistry Chemical Physics
28 May 2025, Volume 27, Number 20
Page 10529 to 2525210898
https://doi.org/10.1039/D4CP04781H

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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

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News & Reports

Enterprise Ireland launches new five-year strategy, Delivering for Ireland, Leading Globally (2025-2029)

06th March 2025

Pictured (l-r) Michael Carey, Chair, Enterprise Ireland, Peter Burke, Minister for Enterprise, Tourism and Employment, Charlene Flanagan, Co-Founder of Ella & Jo, Kevin Sherry, Interim CEO, Enterprise Ireland

- New strategy sets out ambitious targets to increase jobs in companies supported by Enterprise Ireland to 275,000 and to increase exports to €50bn by 2029
- Enterprise Ireland's ambition is that exporting Irish companies will become primary driver of the Irish economy
- Focus on strengthening skills and talent, funding ambition, embracing sustainability, with aim to see 1,700 new Irish-owned exporters and to support 1,000 new start-ups
-

Enterprise Ireland is today publishing its new five-year strategy *'Delivering for Ireland, Leading Globally (2025-2029)'*, which outlines the organisation's aims and ambitions for the Irish enterprise base and its purpose to 'Accelerate Sustainable Irish Business'.

Enterprise Ireland is the Irish Government organisation responsible for the development and growth of Irish enterprises in world markets, and it works with over 4,000 Irish-owned businesses to support them to start, compete, innovate and scale, and create jobs in towns and communities across Ireland. It's ambition over the next five years is to support Irish exporting companies to make an even greater contribution to the Irish economy through international growth and nationwide employment, with the long-term ambition that exporting Irish companies become the primary driver of the Irish economy.

This new strategy- which is aligned with the Programme for Government and the White Paper on Enterprise- sets out our four strategic objectives for the Irish enterprise base; Start, Compete, Scale and Connect.

- **Start** – Enhance the pipeline of innovative and scalable start-ups by supporting them with their long-term, sustainable growth ambitions. The target is to support 1,000 new start-ups over the five-year period, from 2025 to 2029

- **Compete –** Support companies to be more productive, founded on sustainability, innovation, digitalisation, operational efficiency, and strong leadership and capabilities. Key targets include a 35% reduction of CO2 emissions by 2030, a 3% annual average increase in productivity, 1,700 additional Irish-owned exporters and €2.2 billion spend on RD&I
- **Scale -** Increase the number of world-leading Irish companies, with targets of 275,000 employed in Enterprise Ireland supported companies by the end of 2029, €50 billion in export sales and 150 large Irish exporting companies of more than 250 employees supported by Enterprise Ireland by 2029
- **Connect -** To see an enhanced, internationally competitive, and interconnected enterprise and innovation ecosystem that fosters start-ups, drives enterprise growth and investment. Key targets include €55 billion spend within the domestic Irish economy, and the delivery of 10,000 enterprise engagements with Irish businesses through our research infrastructure and programmes

To advance these areas of focus, Enterprise Ireland will utilise six separate levers to achieve its goals; Funding Ambition, Igniting Innovation, Embracing Sustainability, Strengthening Skills and Talent, Maximising Global Opportunity and Driving Performance.

Peter Burke TD, Minister for Enterprise, Tourism and Employment, said: "*I welcome the publication of Enterprise Ireland's new strategy today and recognise the importance of working together to ensure that Ireland provides a supportive environment for Irish businesses to scale and grow. I am confident that the initiatives and actions outlined in this strategy will support this ambition and position Ireland ahead of emerging economic trends.*

"Irish exporters are a critical component of the Irish economy, and the Government is committed to supporting this sector to scale to further heights in the years ahead. I'm pleased to see Enterprise Ireland's ambitions under this strategy include increasing the number of internationally successfully Irish owned companies of scale, diversifying our exports and increasing the productivity of our SME sector. These efforts will all add to the resilience of Irish businesses, allowing them to continue to succeed in an increasingly competitive global market."

Alan Dillon TD, Minister of State for Small Business and Retail and Circular Economy, said: "*I'm pleased to see Enterprise Ireland's ambitions under this strategy include increasing the productivity and competitiveness of our SME sector. Enterprise Ireland will continue to prioritise collaboration with the Local Enterprise Offices to ensure that Irish businesses of all sizes are supported throughout their development. We are making progress in key areas such as decarbonisation, digitalisation, and innovation and it is important that we support Enterprise Ireland in delivering on our ambitions for a resilient, sustainable and regionally balanced economy in the White Paper on Enterprise."*

Niamh Smyth TD, Minister of State for Trade Promotion, Artificial Intelligence and Digital Transformation, said: *"Enterprise Ireland's Strategy "Delivering for Ireland, Leading Globally" aligns closely with the objectives of the new Programme for Government. It focuses on enterprise competitiveness and productivity, enhancement of supports for start-ups, and assisting companies to scale globally. I welcome efforts being made to diversify our export markets with a target to reach €50 billion in export sales by Enterprise Ireland supported companies by 2029. I also welcome Enterprise Ireland's commitment to continue to provide and enhance the level of targeted support, training and advice to businesses to drive the adoption of digitalisation and deployment of AI."*

Kevin Sherry, Interim CEO, Enterprise Ireland, said: *"Enterprise Ireland is committed to working with Irish businesses to help them grow and succeed in international markets. Our objective in our new five-year strategy 'Delivering for Ireland, Leading Globally', is to Accelerate Sustainable Irish Business, now and into the future. With companies supported by Enterprise Ireland now employing 234,454 people and over €34 billion in exports, this gives Enterprise Ireland a strong platform to*

launch our strategy, with ambitious targets for the Irish enterprise base which aims to support more Irish companies to achieve greater scale through international growth. It is our long-term ambition that exporting Irish companies will become the primary driver of the Irish economy."

Michael Carey, Chair, Enterprise Ireland, said:*"Enterprise Ireland's ambitious and exciting new strategy aims to increase client company export sales to €50 billion by the end of 2029, with a target to grow jobs numbers to 275,000. Despite the global economic challenges that lie ahead, we have every confidence in the resilience and agility of the Irish enterprise base who, with our support, have proven their ability to adapt, diversify and succeed, and we look forward to continuing to work closely with our client base to deliver for the benefit of the Irish economy over the next five years"*
A full copy of the strategy document, 'Delivering for Ireland, Leading Globally (2025-2029)' can be found here.

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SEAM Research Centre celebrates 15th year milestone with landmark launch

21st February 2025

- **The launch of the €2.2 million high-power (450kV) CT scanner cements SEAM Research Centre as the centre of excellence in Industrial CT applications in Ireland and beyond.**
- **SEAM's €1.6m Materials Sustainable will help companies on their green transition leading to reduced waste, reduced pollution and lowered CO_2 emissions.**

The South Eastern Applied Materials (SEAM) Research Centre has marked its 15th anniversary with the launch of Ireland's largest Industrial CT and X-ray Imaging Solutions Centre and the opening of the Materials Sustainability Laboratory at South East Technological University (SETU).

The milestone celebrations took place on Friday, 21 February during SEAM's Industry Day, which welcomed industry and academic delegates from across the country to SETU's Cork Road Campus in Waterford.

SEAM, Ireland's leading Technology Gateway Centre, based at SETU's Applied Technology Campus, plays a pivotal role in providing materials engineering solutions to a wide range of industrial sectors.
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The newly unveiled €2.2 million, high-power (450kV) CT scanner, funded under a Research Ireland Infrastructural Call Programme, strengthens SEAM's analytical capabilities, particularly for large and dense samples such as EV batteries. This advancement enables SEAM to rebrand its CT division as the 'Industrial CT & X-ray Imaging Centre of Ireland'.

In tandem, the €1.6 million Materials Sustainability Laboratory, funded through Enterprise Ireland's Capital Infrastructural and Innovation Partnership Programme, will support companies to adopt sustainable manufacturing practices. The facility aims to help companies reduce waste, pollution, and CO2 emissions, aligning with Ireland's sustainability and green transition goals as outlined in the Government's 'Project Ireland 2040' strategy.

Minister James Lawless, TD, Minister for Further and Higher Education, Research, Innovation and Science, officially unveiled the new facilities, stating, *"Today is the culmination of several years of planning and execution and, also, the start of a new phase in SEAM's journey, as its services and capabilities increase.*
"Today, in many respects, is a call to action to industry and other partners to consider the impact that SEAM can have on your operations and the help that it can provide through these great new facilities.
"SEAM has been blazing a trail for this region over the past 15 years, providing assistance to industries in the South and South-East region and beyond – supporting over 325 Irish based companies, including both multinationals and SMEs and executing over 4,000 directly-funded projects over that time.
"What we see here today is an excellent example of work that is progressing across Government, with different Departments and agencies progressing the initiatives for which they are ultimately responsible and accountable for but working to a common agenda to further our national interest."

Minister Mary Butler TD, Government Chief Whip and Minister of State at the Department of Health with responsibility for Mental Health, and Minister John Cummins TD, Minister of State at the Department of Housing, Local Government and Heritage, were among the invited guests.

Professor Veronica Campbell, President of SETU, in delivering the welcome address, remarked, *"Today's launch marks a key milestone for SETU and the SEAM Research Centre. The state-of-the-art Industrial CT and X-ray Imaging Centre and the Materials Sustainability Laboratory advances both cutting-edge imaging capabilities and sustainable innovation.*
"For the past 15 years, SEAM has been at the forefront of applied research and industry collaboration. As Ireland's top Technology Gateway Centre, SEAM provides advanced materials engineering solutions across multiple sectors."
"Aligned with SETU's Connecting for Impact strategy, SEAM Research Centre serves as a bridge between academia and industry, fostering partnerships, and delivering solutions that drive economic and societal progress. Today's launch celebrates SEAM and reflects the invaluable support of Enterprise Ireland, Research Ireland, the European Union and our industry partners," Prof. Campbell continued.

Dr Ramesh Raghavendra, SEAM Research Centre Director, expressed pride in SEAM's growth and continued impact, stating, *"Our ongoing commitment to create materials characterisation infrastructure of excellence at SETU has been further strengthened by today's launch. The Industrial CT X-ray imaging centre's comprehensive capabilities is expected to play a pivotal role in fostering innovation across industries ranging from manufacturing to material science.*
"Meanwhile, the opening of materials sustainability laboratory will support companies in their green transition initiatives. This infrastructure will not only benefit industries across diverse sectors but also provide a significant boost for postgraduate and post-doctoral researchers in advanced manufacturing and materials sustainability."

Dr Ciarán Seoighe, Deputy CEO, Research Ireland, added: *"Today is a major milestone in terms of industrial research and development in this country. The launch of these large-scale facilities is*

testament to the potential impact of research for economic progress and societal well-being. Some of our greatest successes come from collaborations – universities, industry partners, and government – working together to solve real-world challenges. I want to commend SEAM, SETU, and all industrial and other partners involved in bringing these facilities to life."

Marina Donohoe, Head of Research, Innovation and Infrastructure, Enterprise Ireland, also commended SEAM's contributions, stating, *"Enterprise Ireland is delighted to support the Materials Sustainability Laboratory at the SEAM. Enterprise Ireland is committed to supporting businesses in the transition towards a low-carbon economy and it is encouraging to see more and more businesses coming onboard to address sustainability challenges by working with SEAM to develop low carbon materials solutions.*
"Over the past 15 years the SEAM has made a huge contribution to innovation in sustainable and durable manufacturing practices. That work will become even more important over the coming years, and I am delighted that SEAM will be leading research in this vital area."

SEAM Research Centre is co-financed by the Government of Ireland and the European Union through the ERDF Southern, Eastern, and Midland Regional Programme 2021-27.

Media contact: Claire Quinn, Communications and PR Officer, +353 (0)87 710 5148,
email claire.quinn@setu.ie

Captions:
1: The South Eastern Applied Materials (SEAM) Research Centre has marked its 15th anniversary with the launch of Ireland's largest Industrial CT and X-ray Imaging Solutions Centre and the opening of the Materials Sustainability Laboratory at South East Technological University (SETU). Pictured at the launch event on Friday, 21 February were (front row L-R): Minister Mary Butler TD, Government Chief Whip and Minister of State at the Department of Health with responsibility for Mental Health, Professor Veronica Campbell, President, SETU, Minister James Lawless TD, Minister for Further and Higher Education, Research, Innovation and Science, and Dr Ramesh Raghavendra, SEAM Research Centre Director. (Back row l-r), Agnieszka Furman, SEAM, Professor Patrick Prendergast, Chairperson of the SETU Governing Body and Chancellor of the University, Marina Donohoe, Divisional Manager-Research & Innovation, Enterprise Ireland, Dr Ciarán Seoighe, Deputy CEO, Research Ireland, Minister John Cummins TD, Minister of State at the Department of Housing, Local Government and Heritage and Dr Ken Thomas, Head (Waterford) Faculty of Engineering & Built Environment at SETU. Picture: Patrick Browne, Brownes Photography.

2: South Eastern Applied Materials (SEAM) Research Centre has marked its 15th anniversary with the launch of Ireland's largest Industrial CT and X-ray Imaging Solutions Centre and the opening of the Materials Sustainability Laboratory at South East Technological University (SETU) Pictured at the launch event on Friday, 21 February were Marina Donohoe, Divisional Manager-Research & Innovation, Enterprise Ireland Professor Veronica Campbell, President, SETU, Minister James Lawless TD, Minister for Further and Higher Education, Research, Innovation and Science, Dr Ciarán Seoighe, Deputy CEO, Research Ireland and Dr Ramesh Raghavendra, SEAM Research Centre Director.

About:
SEAM Research Centre:
- SEAM Research Centre is the Leading Technology Gateway Centre in Ireland providing Materials Engineering solutions for wide ranging industrial sectors (Medical, Pharma, Precision Engineering, Electronics, Construction, Food, etc).
- SEAM has executed over 50 long duration projects arising from Innovation Partnership/DTIF/EU programmes.

- SEAM represents SETU as partner member of I-Form (Research Ireland's Advanced Manufacturing Research Centre).
- As part of academic research, SEAM supervises master and PhD students in the field of Additive Manufacturing (3D printing) of medical device components, development of sustainable Cement and Concrete materials, engineering simulations for optimisation of product components and process improvements.

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GreenTech HQ lands €1 million Enterprise Ireland Investment to deliver 300 new jobs in the South East

11th April 2025

Pictured (l-r) Ed Murphy, CEO of GreenTechHQ, Minister James Browne TD and Kevin Sherry, Interim CEO, Enterprise Ireland

Returning Wexford entrepreneur set up GreenTechHQ Business & Innovation Centre to drive growth, jobs and sustainability in the South East

Greentech HQ's new business accelerator programme, B.A.S.S.E. (Business Advantage & Sustainability South East), is set to drive transformational growth across the South East, providing ambitious SMEs with the tools, mentorship and strategic frameworks required to scale successfully and sustainably.

This programme isn’t just about business support — it’s about transformation. It’s about helping ambitious SMEs build real resilience, scale smart, and integrate sustainability in a way that strengthens not just their bottom line, but their long-term impact.

Serial entrepreneur Ed Murphy, who has created over 6,000 jobs across his career to date, returned to his native Wexford after 40 years and set up the not-for-profit GreenTechHQ. At the core of his passion project is to create worthwhile jobs that allow young people to continue to live and work in the region and to create a centre of excellence for renewable energy and sustainability in the South East. B.A.S.S.E. is the first initiative of its kind in Ireland. It is funded through Enterprise Ireland’s Smart Regions Stream 3 — a key national strategy for driving innovation and economic resilience through regional enterprise development.
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The €1million programme has been designed for growth-oriented companies across the South East seeking to double revenues, embed ESG at the heart of their operations, build long-term resilience, and prepare for next level growth profitability, investment or exit. It brings together some of the country's most successful entrepreneurs and business leaders to support participant companies through one-to-one mentoring, structured transformation sessions, peer networks and a tailored SaaS platform.

Participants will benefit from exclusive access to high-profile mentors and EY Entrepreneur of the Year alumni including Jamie Heaslip, Norman Crowley, Anne Herathy, David Walsh, John Purdy, Annmarie Hennessy, Padraig O'Ceidigh, and Michael Kearney. These experts offer real-world experience and insights that go beyond theory, empowering businesses to achieve meaningful and measurable growth.

Minister James Browne TD commented:

"This investment in GreenTech HQ and the B.A.S.S.E. programme marks a major step forward for the South East. It demonstrates our commitment to building regional resilience and ensuring that innovation and opportunity are not confined to urban centres. This initiative will help foster the kind of sustainable, high-quality jobs our communities need to thrive."

Kevin Sherry, Interim CEO of Enterprise Ireland, added:

"The B.A.S.S.E. programme is a prime example of how Enterprise Ireland's Smart Regions funding is enabling high-impact regional initiatives that drive innovation and enterprise. By supporting GreenTech HQ, we are backing a model that connects SMEs to world-class expertise, accelerates growth, and strengthens the South East's position as a vibrant hub for sustainable business."

The B.A.S.S.E. programme is deeply aligned with GreenTech HQ's ethos of embedding sustainability, innovation and resilience into business strategy. The initiative combines ESG integration, strategic scaling, leadership development, and board-level advisory support, creating a transformative pathway for SMEs determined to thrive in today's rapidly evolving economy.

Commenting on the launch, **Ed Murphy, CEO of GreenTechHQ**, said: *"B.A.S.S.E. is about more than growth — it's about preparing South East businesses to lead in a sustainable, resilient and future-focused economy. With the support of Enterprise Ireland and our exceptional mentors, we're proud to offer a programme that's truly tailored to the challenges and opportunities faced by ambitious SMEs."*

GreenTechHQ is co-funded by the Government of Ireland and the European Union through the ERDF Southern, Eastern & Midland Regional Programme 2021-2027.'

For media enquiries, please contact: liz.mcgonigal@greentechhq.com
Contact number 00 353 87 3777335

Enterprise Ireland Launches Proof-of-Concept Funding to Accelerate Commercialisation of Academic Research

17th April 2025

Enterprise Ireland has announced a new stream of support under its Commercialisation Fund: Proof of Concept Funding. Designed to be accessible, it will support the development of research and technology in its first steps towards market readiness.

The new funding offers up to €100,000 over a 12-month period, providing a vital bridge between initial research and the commercial market. This initiative supports a range of activities including customer discovery, prototype development, and early-stage human-use studies, helping researchers validate both the technical feasibility and market need for their innovations.

Marina Donohoe, Head of Research, Innovation and Infrastructure at Enterprise Ireland, said:
"At Enterprise Ireland, we recognise the critical importance of bridging the gap between groundbreaking research and market-ready solutions. The Proof-of-Concept Funding is designed to empower third-level researchers in Ireland by providing the necessary resources to validate their innovations. By supporting activities such as customer discovery and prototype development, this initiative aims to de-risk early-stage technologies and accelerate their journey towards commercialisation, ultimately contributing to Ireland's position as a leader in global innovation."

This new initiative is part of Enterprise Ireland's continued commitment to bridging the gap between research and industry, supporting the creation of high-potential start-ups and ensuring that Irish research delivers real-world impact.

The Proof-of-Concept Funding complements existing supports under the Commercialisation Fund, including the Feasibility Grant and the Commercialisation Fund Award. All researchers in the third-level sector and non-profit research agencies and organisations in the Republic of Ireland including staff on contract (e.g. post-doctoral scientists) can apply. Non-financial supports such as mentoring, networking and team development are also available.

Reflecting on the importance of early-stage support, **Dr. Cormac Farrelly, Chief Medical Officer and co-founder of LaNua Medical**, said:
"Securing early-stage support through Enterprise Ireland was a pivotal moment for our company. It enabled us to validate our innovative embolisation medical device, the ECORE, with real-world users and begin translating a clinically inspired concept into a commercial product with the potential to improve patient outcomes globally. This type of funding is essential for turning promising innovative ideas into high-impact solutions."

Enterprise Ireland is actively encouraging researchers across Ireland to get in touch and explore how this new funding can support their innovation journey. If you have a promising idea and are seeking support to accelerate its path to market, we want to hear from you.

How to apply:
1. Review eligibility on the Enterprise Ireland website: Commercialisation Fund | Business Support | Enterprise Ireland
2. Contact a member of Enterprise Ireland's Commercialisation Specialist Team
3. Submit your application through the online system - Apply here

Media queries: press@enterprise-ireland.com

Official Opening of Galway Biomedical Design & Manufacturing Facility

23rd April 2025

Caption: Pictured (from left): Conan Campbell, CEO and Founder of Galway Biomedical; Dara Calleary, Minister for Rural and Community Development & the Gaeltacht; Gillian Buckley, Head of Investment, The Western Development Commission; and Tom Cusack, Divisional Manager, Industrial & Life Sciences, Enterprise Ireland.

Galway, Ireland - Galway Biomedical Limited ("Galway Biomedical"), a trusted partner in the development and contract manufacturing of medical devices, today announced the opening of their new facility at Ballybrit Business Park, located in the centre of Galway's medical device ecosystem.

Speaking at the opening, **Dara Calleary, Minister for Rural and Community Development & the Gaeltacht,** who officially carried out the ribbon cutting ceremony said: "*This announcement from Galway Biomedical is a great boost to Galway and Ireland. This is particularly good news for the west of Ireland where we are now well established as leaders in the life sciences sector and have a reputation for excellence and innovation. However, we will never take this for granted and will continue to work hard to bring the best investment to all parts of the country. Galway Biomedical's plans to invest is fantastic. I am confident the team will find top talent to fill the new jobs planned. Congratulations to the entire team. I wish you all many years of continued success and growth.*"

Welcoming the announcement, **Minister for Enterprise, Tourism and Employment, Peter Burke T.D** *highlighted the government's commitment to technological innovation and employment growth. "Galway Biomedical is at the forefront of innovation, developing best in class solutions to meet the needs of the global healthcare sector. I'd like to congratulate Conan and the team on today's new state-of-the-art facility opening and the plans to create high quality jobs here in Galway. Today's announcement paves the way for this innovative medtech company to grow and scale. The Government, through Enterprise Ireland, looks forward to continued engagement with Galway Biomedical to support the growth of the business into the future."*

Galway Biomedical will develop and manufacture medical device components for use in the Vascular, Dental, Orthopaedic, Urology and General Surgery clinical fields. The company intends to build a global reputation as a dependable and responsive partner for the development and commercialization of cutting edge implantable medical devices.

"Today's official opening of the new facility marks a significant milestone in achieving our vision. We now plan to accelerate our growth momentum by significantly expanding our team, capacity, and capability. We look forward to serving new customers and welcoming new team members to our world-class facility." said **Conan Campbell, CEO and Founder of Galway Biomedical.** *"We chose the name Galway Biomedical for this new venture because of the reputation Galway has in the medical device industry. It is recognised as a centre of excellence along with other global regions such as the Bay Area in California, Minneapolis and Boston metropolitan areas. Our aim is to bolster that reputation by making the name of the city we proudly carry in our name even more synonymous with medical device excellence. We will do this by creating a first class facility with a highly skilled workforce from an exceptional pool of talent in Galway"*

The company recently closed an oversubscribed Series A investment round, with backers including the Western Development Commission (WDC), Enterprise Ireland (EI) and private medical device veteran investors. "*We are delighted to have completed our Series A financing round with such reputable medical device investors and the Irish State through The Western Development Commission and Enterprise Ireland and look forward to working together to accelerate the growth and value of Galway Biomedical*," said Campbell. "*We appreciate the trust put in us and intend to repay it by ensuring that our shareholders receive a significant return on their investment, but also by ensuring that Galway Biomedical strives relentlessly to enhance the reputation of Ireland as a world class centre for medical device excellence in innovation and manufacturing*."

The current year will be a landmark year for the company as it continues its extensive fit out of the Ballybrit facility. Within the 13,000 square foot facility Galway Biomedical are constructing a 4,000 square foot ISO Class 7/8 cleanroom which will ensure it stands above its global competitors in terms of facility design and capability. The company also plans to add new technologies to support its manufacturing capabilities, enabling customers to pioneer advancements in medicine.

Commenting on the funding announcement and the plans for Galway Biomedical, **Allan Mulrooney, CEO at The Western Development Commission** said: "*Galway Biomedical is an excellent Irish company delivering cutting-edge solutions that will enable its customers to pioneer advancements in biomaterial based medical device implants. At The Western Development Commission, we are proud to have supported the company's growth momentum and global ambition since it was established in 2024. Strengthening regional enterprise development is a central focus for The Western Development Commission, and we warmly welcome the ambitious expansion plans announced by Galway Biomedical following the close of the Series A funding round which will create high value new jobs in Galway*."

Tom Cusack, Divisional Manager for Industrial and Lifesciences at Enterprise Ireland said, "*I wish to congratulate Galway Biomedical on their new state-of-the-art facility here in Galway and commend the ambition of this indigenous company to compete at the highest level, through their design, development and manufacturing capabilities in the US, Asia and Europe. Enterprise Ireland is committed to supporting companies like Galway Biomedical to increase their level of innovation, improve their competitiveness and expand their global footprint, with the ultimate goal of delivering export growth and jobs in Ireland and we look forward to continuing to work with the company in the future"*.

For Media Interviews contact Conan Campbell, CEO at Galway Biomedical. 087 778 7720

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€27.6 Million Invested Start-Ups in 2024

07th May 2025

Pictured (L-R) Carol Gibbons, Enterprise Ireland, Minister Peter Burke, Aisling Browne, Founder, Glitch Ads, Jill Keogh, CEO, Sadie's Secrets

- **157 start-ups supported by Enterprise Ireland in 2024**
- **New five-year strategy aims to support 1,000 new start-ups**

Enterprise Ireland, the government agency responsible for the development and growth of Irish companies in global markets, invested €27.6 million in Irish start-ups and supported a total of 157 start-up companies in 2024. Investment was provided through Enterprise Ireland's High Potential Start-Up (HPSU) and Pre-Seed Start Fund (PSSF) programmes.

The results were announced today at Enterprise Ireland's annual Start-Up Day Conference in Dublin with over 600 delegates in attendance to include the 'Class of 2024' Enterprise Ireland supported Start-Up companies and the wider Start-Up ecosystem including investors, state agencies and start-up accelerators.

Start-ups supported by Enterprise Ireland in 2024 include:

- 90 High Potential Start-Up's (HPSU) with high growth potential - start-up businesses with the potential to create 10 jobs and €1 million in sales within three years of starting up
- 69 Pre-Seed Start Fund (PSSF) investments which inject critical early-stage funding into new businesses
- 63 of the companies supported were based outside of Dublin
- 45 women-led start-up companies were approved investment
- 13 HPSUs emerged from academic research
- 25 companies were spun out of third level institutions
- 34 companies were supported through the Enterprise Ireland Commercialisation Fund Programme.

2024 marked the final year of Enterprise Ireland's three-year strategy 'Leading in a Changing World 2022 -2024' and in that period there were a total of 266 HPSUs and 213 Pre-Seed Start Fund approvals with half of the companies based outside of Dublin. During that time period over €78 million was invested in these start-up companies.

Enterprise Ireland's Start-Up Day also includes a pitching element, featuring top university (pre) spin-out ventures emerging from Enterprise Ireland's Commercialisation Fund. These teams will pitch their

visionary concepts, competing for an award and the prestigious opportunity to participate in UC Berkeley's Venture Connectivity Program.

Opening Enterprise Ireland's Start-Up Day in Dublin today, **Minister for Enterprise, Tourism and Employment Peter Burke TD,** said: "*Today is about celebrating the spirit of Irish entrepreneurship. The strong pipeline of innovative start-ups emerging over the last three years demonstrates the extraordinary resilience and business ambition of Irish-founded start-up teams, particularly against the backdrop of a challenging global economic period.*

This government, through Enterprise Ireland, will continue to provide funding, mentorship, market access and tailored programmes as the stepping stones for success. Start-ups are critical to our economic future, our global reputation and our societal progress and we remain fully committed to fostering an environment where innovation flourishes, and where every entrepreneur has the tools needed to thrive and succeed."

Looking forward, enhancing the pipeline of innovative and scalable start-ups is a key objective of Enterprise Irelands new strategy, 'Delivering for Ireland, Leading Globally, with a target set to support 1,000 new start-ups over the five-year period, from 2025 to 2029.

Kevin Sherry, Interim CEO, Enterprise Ireland said, "*Start-up Day 2025 is a celebration of Ireland's strong and dynamic start-up community and the Start-Up class of 2024 have and will continue to play a significant role in contributing to the vibrancy of Ireland's start-up ecosystem. A key objective in our new strategy is to Accelerate Sustainable Irish Business so that in time exporting Irish companies will become the primary driver of the Irish economy. As part of our plan, Enterprise Ireland is undertaking a dedicated consultation process by engaging with the start-up ecosystem on the supports available for early-stage companies in Ireland. This aims to strengthen our pipeline of early-stage companies with the potential to scale internationally, furthering Ireland's position as a global leader in entrepreneurship and innovation."*

The Start-Up Day 2025 Directory is available to download here.

For information, please contact:
press@enterprise-ireland.com

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University of Limerick spin-out Oscil wins Big Ideas Award at Enterprise Ireland's Start-Up Day 2025

08th May 2025

Patrick Cronin of University of Limerick spin-out Oscil, was presented with the Big Idea's Award at Enterprise Ireland's Start-Up Day 2025 in the Aviva Stadium.

Oscil was one of six investor-ready potential spinouts that had three minutes to pitch their new technology solutions to a 600 strong audience made up of representatives from the Irish Start-up ecosystem including VCs and other funders, State support agencies & professional and financial services.

The award was presented to Patrick Cronin, for the outstanding pitch of the day. Oscil which is an Enterprise Ireland commercialisation funded project approaching spin-out, is an innovative deep tech technology operating at the intersection of Edge-AI and powder processing, initially targeting the pharmaceutical and dairy sectors. They have developed a proprietary, ATEX-compliant sensor and edge-AI solution that enables real-time, in-line analysis of powder flow—addressing critical issues like sensor fouling, yield loss, and process downtime.

As part of the Big Ideas award, Oscil will travel to the US to participate in UC Berkeley's Venture Connectivity Program.

Tara Dalton of University of Limerick spin-out TANGO received the Big Ideas runner-up award on the day.

Start-Up Day 2025 hosted the 'Class of 2024' High Potential Start-Up companies that Enterprise Ireland invested in during 2024. The event also played host to technology-based companies with origins deep rooted in groundbreaking research. In 2024, 34 companies were supported through the Enterprise Ireland Commercialisation Fund Programme with 25 companies spun out of third level institutions.

Presenting the award, Michael Carey, Chairman, Enterprise Ireland said, *"The Big Ideas pitching element and awards at Start-Up Day provides a platform to showcase Enterprise Ireland's commercialisation funded research approaching start-up status, with significant potential for success. The event also highlights the accomplishments of our national technology transfer system, the high calibre of research commercialisation activity within Ireland, and the significant impact these companies will have to help solve huge global challenges. I wish to congratulate both Oscil and TANGO on their achievements to date and wish them every success for the future."*

For more information:

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Notes to editor:

Commercialisation funded projects pitching include:

HyperPath - Tyndall National Institute and University College Cork
HyperPath is a SaaS solution focused on delivering fibre like connectivity to businesses, transportation and places where the deployment of fibre infrastructure is impractical or cost prohibitive. Using its patent pending Peer 2 Peer multi-connectivity architecture, it bonds multiple wireless/wired links into a single high-speed, high reliability low-latency connection.
Promotor: Ger McNamara

StarMAT - RCSI
StarMAT aims to revolutionize the formulation of Gene Therapies to enable more patients to avail of life-changing medicines by exploiting the inherent biocompatibility, power and flexibility of polyaminoacid chemistry for more effective, safer targeted delivery'
Promotor: Sarinj Fattahagha

Oscil (PowFreq) – University of Limerick
PowFreq is an innovative deep tech technology operating at the intersection of Edge-AI and powder processing, initially targeting the pharmaceutical and dairy sectors. The team are led by chemical and process engineer, with a deep understanding of powder engineering. They have developed a proprietary, ATEX-compliant sensor and edge-AI solution that enables real-time, in-line analysis of powder flow—addressing critical issues like sensor fouling, yield loss, and process downtime.
Promotor: Patrick Cronin

IntegrityIQ – Trinity College Dublin
IntegrityIQ is strategically positioned as a pioneer in the governance, risk, and compliance (GRC) sector, particularly in ethics and integrity management. Leveraging the power of AI, IntegrityIQ empowers ethics and compliance officers worldwide through two innovative platforms: personalised and immersive ethics and compliance training, supported by a dynamic data management solution.
Promotor: Daniel Malan

TANGO – University of Limerick
T-cells protect us against infections and diseases such as cancer, and genetically modified T-cells are now being used to treat these disorders. Currently we cannot routinely measure how well T-cells work, for example in people receiving vaccines or T cell therapies. Using novel microfluidics and chemistry, we have designed an instrument (TANGO) that can automate assays to measure T-cell function. TANGO will allow clinicians and researchers for the first time to routinely assess how well T-cells work, enabling us to fully realise the potential of T-cells in combatting diseases, more effectively monitor vaccine efficacy and better understand our immune system.
Promotor: Tara Dalton

Contenseo – Trinity College Dublin
Contenseo is a system that connects people who want to license (sell) their content with people who are looking to license (buy) high-quality content. Contenseo is a copyright exchange, assisted by AI, where copyright holders and those seeking to reuse their content can easily connect and license their material. By connecting buyers and sellers of copyrighted material, Contenseo makes licensing simple and transactional, unlocking new revenue for copyright holders.
Promotor: Stephen Conmy

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