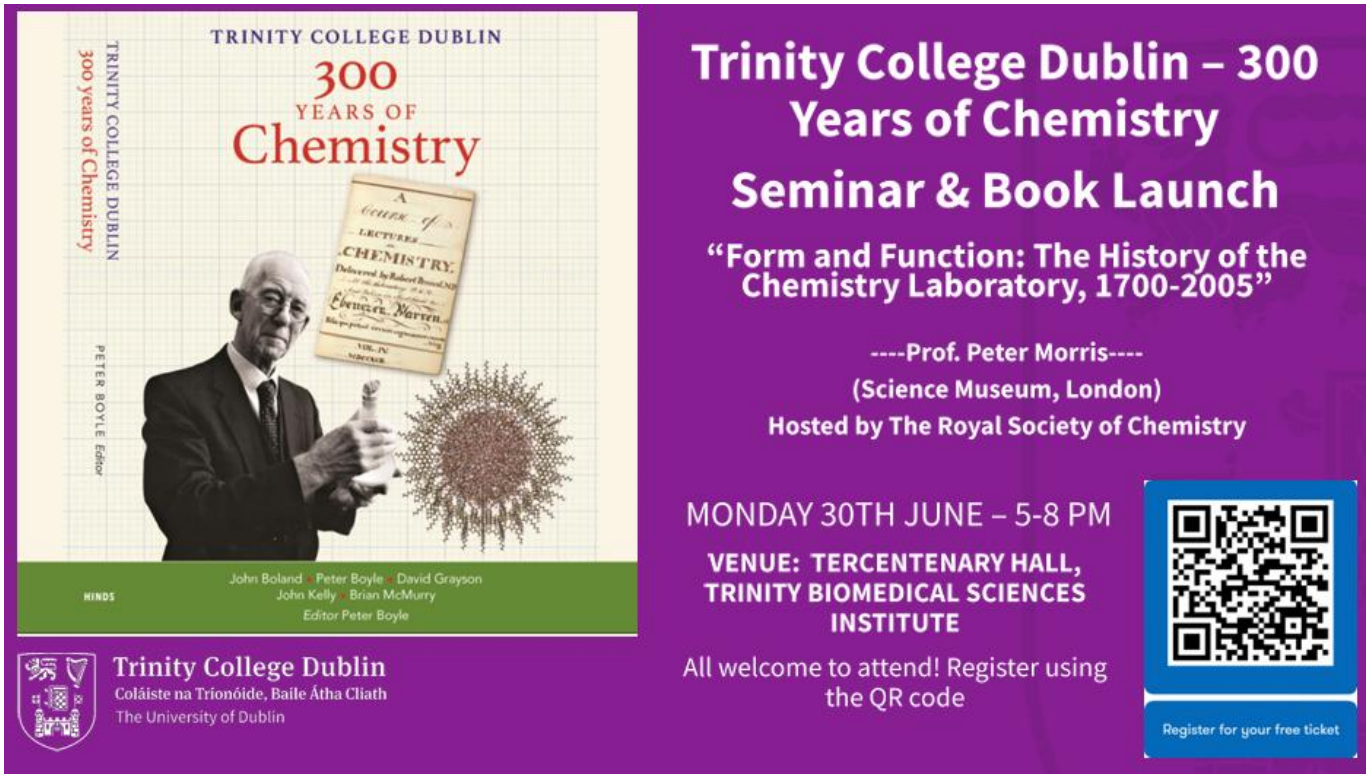
# Irish Chemical News

## A Journal of the Institute of Chemistry of Ireland




**Chemistry Building TDC**

**The Institute of Chemistry of Ireland**
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# Professional Body representing Chemists in Ireland

**Professor of Physical Chemistry,**
**School of Chemistry & Chemical Engineering, QUB**
**Queen's University,**
**Belfast BT9 5AG.**

# A Message from the President

Dear Fellows, Members, Graduates and Associates.

Welcome to this issue of ICN which carries reports on several notable ICI events and activities of the past months. Notable among these was the 76th Irish Universities Chemistry Research Colloquium which was hosted by Maynooth University and was an outstanding success. The Colloquium has been going from strength to strength in recent years and provides a tremendous opportunity for our younger researchers to present their work to large and well- informed audiences.

This is a daunting task since the standard of the presentations is now extremely high but the way which the speakers and poster presenters stepped up to the challenge reflects well of the health of PhD programmes across the Island. It was a difficult task to decide on award winners, but we did at least have the opportunity to recognise quite a few excellent contributions thanks to the generosity of our sponsors. We can now look forward to next year's Colloquium in Cork.

This issue also has a report on the ICI Annual Congress 2025 which was hosted by Prof Mike Lyons at TCD. Again, this was an event which showcased high quality science and, in this case, gave a real opportunity for the electrochemistry community to come together and to celebrate the strength in depth we have in this area.

I am glad to be able to point readers to the biography of Professor Kevin B. Nolan (RCSI) who was award an ICI Honorary Fellowship this year. This is the highest award to Institute can bestow and was awarded in recognition of Prof Nolan's commitment to excellence in teaching and research and service, and for his role in advancing the field of chemistry both nationally and internationally.

Finally, I am glad to welcome Dr Francesca Adami as the new Chair of the ICI-YCN (Young Chemistry Network) and two new members onto the ICI's Council. Dr Hannah Crory (QUB) with be joining as the Northern Ireland representative while Dr Davide Tiana (UCC) will represent the Southern Region. We expect the work of the council to expand over the coming year as we work along with the new Committees to discuss and possibly update aspects of the organisation and activities of the Institute. I would like to take this opportunity to thank all members who volunteered to sit on the new Committees which are now just

starting their work.

One of those Committees has been tasked at look at ways we might modify the format of ICN to reduce the burden which producing regular editions places on everyone involved but in particular our Editor, Pat Hobbs who invests a huge amount of time and effort in producing every issue of the ICN. I hope you will see that results of the process in the near future.

Steven

President, Institute of Chemistry of Ireland

Prof Stephen Bell FICI, FRSC

18/12/2025

## Editorial

This is Part 2 of Issue 3 covering June to December 2025. University Research Publications not covered in Part 1 are reported here. In order to keep the size to a reasonable number of pages none of the Technological Universities including TU Dublin are included. Instead, they will have an Issue devoted to them along with Research Ireland, IDA and Enterprise Ireland reports. This issue is currently in preparation. Thanks to Anita McGuire UCC and Paul Murphy UG for helping find some of the published papers.

The lead article here is the launch of a wonderful book on 300 years of chemistry at Trinity College Dublin. The book was edited by John Boland, and the five contributors were John Boland, Peter Boyle, David Grayson, John M. Kelly and Brian McMurry. It's a very high quality hard back with many photos and well worth having on your bookshelf. The book launch took place in the Trinity Biomedical Sciences Institute Pearse Street, Dublin on the 30th of June 2025.

The evening started with a talk by Professor Peter Morris (Science Museum London) entitled "Form and Function: The History of the Chemistry Laboratory, 1700-2005" who then launched to book. Introductions were made by Prof Sylvia Draper, Chair of the Local Section of the RSC. The event and launch were hosted by the Royal Society of Chemistry, along with a wine reception.

Three other significant symposia are reported, 9th Symposium of the Irish Biological Inorganic Chemistry Society, IV Medicinal & Biological Chemistry Ireland Conference and Inorganic Ireland Symposium 2025.

The Nobel Prize in Chemistry 2025 is covered and as there was a lot of commentary this year, clickable links are included to some of these articles. One winner is of special interest to ICI as one of our Plenary Speakers at ECC9 hosted by ICI in Dublin in July 2024 was **Omar Yaghi** first speaker on the Monday morning. He was one of three winners for their work on ***Metal–Organic Frameworks.***

The 2025 United Nations Climate Change Conference (COP30) is covered. Due to space and copyright considerations coverage is mainly via active links and some photos.

Finally, any researcher or group whose publications are not included here please contact the Editor and let's know where access to your papers is located or send you name and the DOI of the paper(s) to the Editors email 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**

20 January 2025

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

# TRINITY COLLEGE DUBLIN

## 300 YEARS OF CHEMISTRY

Edited by Peter Boyle,
contributors John Boland, Peter Boyle
David Grayson, John Kelly and Brian McMurry

This new book will be launched by Professor Peter Morris of the Science Museum, London, on Monday 30 June 2025 at 6.00 pm in the Tercententary Theatre, TBSI building.* The launch will be preceded by a lecture at 5 pm by Professor Morris, sponsored by the Royal Society of Chemistry, on *"Form and Function: The History of the Chemistry Laboratory, 1700-2005"*

All interested are welcome to attend

* 152-160 Pearse Street

The event will consist of a talk by Professor Peter Morris (Science Museum London) entitled "Form and Function: The History of the Chemistry Laboratory, 1700-2005" hosted by the Royal Society of Chemistry, followed by the official book launch and a wine reception.

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 handmaid 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.

1887 Chemistry building

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.

## Quote by book Editor Professor John Boland TCD

***"This book provides a historical perspective of the development of Chemistry at Trinity College Dublin, from its roots in medicine to how it became a fully-fledged independent discipline that ultimately led to the establishment in 1711 of one of the first departments of chemistry in Europe. In doing so it introduces the reader to the individuals who forged this history – teachers and researchers whose curiosity, passion and drive helped shape and secure the future of chemistry at Trinity for the generations that followed. It also lays bare the many challenges now facing Chemistry at Trinity in this era of multi-disciplinarity and record levels of participation in 3rd level education."***

**Biography of the Authors**

**John Boland,** who conceived the idea of this book, received a BSc in chemistry from University College Dublin in 1979 and a PhD from Caltech in 1984. He then joined the staff at IBM Research in New York and in 1994 was appointed Chair in Chemistry at the University of North Carolina at Chapel Hill. He returned to Ireland in 2002 as an SFI Research Professor in the School of Chemistry at Trinity. He was Director of the CRANN nanoscience institute from 2005 to 2013, appointed to a personal Chair in Chemistry in 2007 and served as Trinity's Dean of Research from 2015 to 2017. He is a Fellow of Trinity, the American Vacuum Society, and the American Association for the Advancement of Science. He received the 2011 ACSIN (Atomically Controlled Surfaces, Interfaces, and Nanostructures) international prize for nanoscience, the Outstanding Researcher Awards from IBM and Intel, and was named Science Foundation Ireland Researcher of the Year in 2018. Today, he continues his research on nanoscale materials and the properties of micro- and nano-plastics.

**Peter Boyle** graduated from Trinity in 1960 and obtained his PhD in 1965 under the direction of Professor Cocker. He joined the staff of the Trinity chemistry department in 1961 as a Junior Lecturer and then in 1966 worked in the Syntex Institute of Steroid Research in California. He was elected a Fellow of the College in 1972. In 1976 he was awarded an Alexander von Humboldt Fellowship at the University of Konstanz. As well as his teaching and research commitments, he was active in College affairs, serving on the Board, as a College tutor, as Senior Dean, as chairman of Trinity Week, and as treasurer of the Common Room. He was also chairman of the Quatercentenary Committee that organised the 1992 Trinity Quatercentenary Celebrations. He retired in 2003 and is now a Fellow Emeritus. He is the author of *Trinity College Dublin: The Provosts 1592 -1927* published in 2015.

**David Grayson** is a native of Limerick. He entered Trinity in 1964, graduating in Chemistry in 1968. He then completed a PhD with Professor Cocker and moved to Cambridge, England, in 1971 as a research fellow in the Battersby group where he worked on the biosynthesis of haem. He returned to Trinity in 1973 to take up a Government of Ireland research fellowship and was appointed to the academic staff in 1977. He became Associate Professor in 2001, and served as Head of School from 2008-2013, retiring in the same

year. He has been active in the Royal Society of Chemistry, being successively Chair of the Professional Affairs & Membership Board, of the Benevolent Fund and of the defined benefit Pension Scheme Trustees. Between 2013-2017 he was Honorary Treasurer and Chair of the Finance & Resources Board. He now lives in County Meath.

**John M. Kelly** studied for a BSc in chemistry at the University of Manchester before carrying out MSc research in organic photochemistry at McMaster University in Canada and a PhD in physical photochemistry at the Royal Institution/University College London. Between 1969 and 1971 he was a Leverhulme Teaching Fellow at the University of the West Indies and then carried out postdoctoral research at the Max Planck Institut für Strahlenchemie, Mülheim. He joined the staff at Trinity College Dublin in 1973, being elected a Fellow in 1978, appointed an Associate Professor in 1987, and to a personal Chair in Chemistry in 2007. He was Director of Science of Materials 1989-2002 and Head of the Chemistry Department 1994-2000. During his time in Trinity his research has been in photochemistry and ultrafast mechanistic and photophysical studies including those relevant to solar energy conversion and storage, DNA photochemistry and materials.

**Brian McMurry** graduated in Experimental Science from Trinity in 1953, and obtained his PhD for research in 1956, working under the supervision of Professor Cocker. He joined the staff of the Chemistry Department in Trinity in 1955. He spent one year in Harvard working with R.B. Woodward on the synthesis of vitamin B12, and another at the University of Lagos as its hirst Professor of Chemistry, under an exchange programme. He was elected a Member of the Royal Irish Academy and awarded a ScD by Trinity. A Senior Fellow of the College, over the years he served as Dean of Graduate Studies, Registrar of the College, and Treasurer and Trustee of the Trinity Association and Trust. He became interested in organic photochemistry, and then medicinal chemistry. He led a group that developed a drug against melanoma which reached Phase 2 clinical trials before it was dropped due to toxicity levels. He retired in 2001. Sadly, he died in 2023 before this book was published.

**AI Summary**

Trinity College Dublin (TCD) celebrated 300 years of chemistry with the launch of a book titled "**Trinity College Dublin – 300 Years of Chemistry**" in June 2025, chronicling its rich history from the first lecturer in 1711 to modern research, highlighting its impact on industry and education, and featuring contributions from current and emeritus professors. This anniversary marks the establishment of the first chemistry lectures in 1711, alongside medicine and botany, evolving into a leading research school.

**Key Aspects of TCD's Chemistry History:**

**Early Beginnings (1711):** The School's roots trace back to the appointment of the first chemistry lecturer, coinciding with posts in Medicine and Botany, initially focusing on medicinal plants for medical students.

**Evolution & Growth:** Over three centuries, the department grew from foundational teaching to a vibrant, modern institution involved in groundbreaking research.

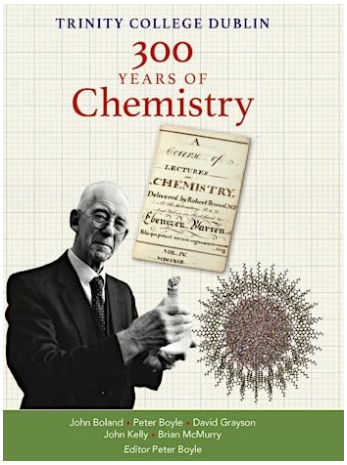
**Book Publication (2025):** A significant milestone was the book launch, detailing the school's legacy, significant figures, and contributions to pharmaceuticals and other sectors.

**Key Contributors:** Professors like Peter Boyle, John Kelly, David Grayson, John Boland, and the late Brian McMurry were instrumental in writing the history.

**Celebrating Milestones:** Events, including seminars with the Royal Society of Chemistry and alumni gatherings, marked these tercentenary celebrations, acknowledging a long-standing tradition in science.

This anniversary celebrates a journey from early lectures to a leading global research centre, emphasizing tradition, innovation, and future relevance

# A Review of the book by Prof Peter Childs (UL)




***Trinity College Dublin: 300 years of chemistry*, Dublin: Hinds, 2025, ed. Peter Boyle**
**ISBN-13 978-1-909442-09-2**

Trinity College Dublin (TCD) is the top-rated Irish university and its chemistry department is the top-rated chemistry department in Ireland, in the top 100 in the world. This is an achievement for a small country like Ireland, and for a small university in international terms. TCD can also claim to be one of the oldest chemistry departments in the world, having appointed a Professor of Chemistry in 1711. The tercentenary of this in 2011 and this book commemorates the 300 years of chemistry in Dublin. The book is dedicated to Dr Mary Carson, the first woman lecturer in the Department, who worked at TCD from 1967 to her retirement in 2000. She died in 2019 and left a legacy to the department which helped fund this book. Chemistry at TCD has a long and distinguished history and this detailed and profusely illustrated book is a worthy tribute to mark its long history. It consists of six chapters, each covering a period of its history and authored by past staff members. Sadly, Brian McMurry did not live to see its publication. The chapters are as follows:

1. Chemistry, the handmaid of medicine 1711-1844 (Peter Boyle)
2. A new era 1844-1903 (Peter Boyle)
3. Young and Werner 1903-1947 (Brian McMurry)
4. The Cocker years 1947-1978 (David Grayson)
5. The department in transition 1978-2000 (John Kelly)
6. The new millennium 2001-2022 (John Boland)
7.

Chemistry started off in TCD as an adjunct to medicine and all the early professors were doctors, until 1844, from which date it was headed by qualified chemists. Its history as a centre of chemical excellence, in teaching and research, can be summed up as BC – Before Cocker – and AC – after Cocker. Wesley Cocker was a Lancastrian, (1908-2007), and was recruited as Professor of Chemistry in 1947, in the aftermath of WW2. (Figure 1) Previously he was a lecturer in Chemistry at King's College, Newcastle on Tyne. He remained as head of department until he retired in 1978. Figure 1 shows the chemistry staff in 1978. Most of these have now retired or died and will be familiar to many TCD chemistry graduates.

**Figure 1: Professor Cocker at his laboratory bench**

**Figure 2:** The chemistry staff at TCD in 1978, the year of Professor Cocker's retirement. (Fig. 5.1, p. 182 in the book)
*Front row: L to R George A. Lonergan, W.J. (Bill) Davis, T. Brian H. McMurry, Wesley Cocker, David C. Pepper, E.R. (Eddie) Stuart, Peter H. Boyle.*
*Back row: L to R John M. Kelly, G. Roy Brown, Mary S. Carson, D.A. (Tony) Morton-Blake, David H. Grayson, David J. Cardin, Christine J. Cardin, Kevin J. Crowley*

When Cocker took over there were 4 members of staff and the department was mainly concerned with service teaching, with little or no research, and poor physical facilities. It is not too much to say that Professor Cocker transformed the department and laid the foundation for its future growth and commitment to top-level research. He started the process to turn the department into am modern, research-focused centre with an international reputation. An appendix lists the PhDs awarded from 1950 to 2021: in 1950 there was 1 PhD; in 2021, 25. Initially most PhDs were in organic chemistry but now they reflect a wide range of modern topics in all branches of chemistry. Chemistry moderatorship rose from 6 in 1978 to 18 in 2000, though these numbers are now greatly increased with the addition of other chemistry-based degrees. Professor Cocker continued to be active in research and publication long after his retirement. He is commemorated by the Cocker Prize (1950-), funded by his relative Sr William Cocker who ran a chemical company; the Cocker Teaching Laboratory (1996); the SOCI Welsey Cocker Award (2008-); and the TCD Cocker Lecture (2021-). Professor Cocker wrote his own detailed account of chemistry at TCD in an article when he retired (Cocker, 1978).

Scientific research in Ireland was poorly funded until 2000 but since then the vastly increased support for Irish universities, for their facilities, equipment and student scholarships, has transformed the research scene in Ireland. A rising tide lifts all boats, and all the Irish Chemistry departments have benefited from the increased funding, probably TCD and UCD most of all. Ireland's international reputation as a location for biopharma companies, providing well-paid jobs for chemistry graduates, has also helped to promote the training of chemists and chemical research. For a small country Ireland is punching well above its weight,

thanks to support from SFI and the EC. The number of chemistry staff in TCD has grown from 4 in 1947, to 14 in 1978, to 24 today, with a concomitant growth in the number of research students. The last two chapters give a good overview of the development of research in the Department, especially since 2000. It is noteworthy that the majority of staff seems to have been imported, recruited from many countries, and this is also reflected in the composition of the postgraduate students. The chemistry department has long since expanded out from the 1887 building (Figure 3), familiar to generations of chemistry students, and its staff are now located in six different sites. TCD chemistry graduates have gone on to distinguished careers in academia, industry, business and teaching.

**Figure 3: The old chemistry building TCD**

This book will be of particular interest to TCD chemistry graduates and postgraduates and present and past staff. It should also be of interest to anyone interested in the history of chemistry in Ireland and TCD's important role in that history. It is well worth reading and is a bargain at €30. It is worth reading for the wealth of photos it contains. Randal Henly has written an interesting article online about his time at TCD. Popular (Henly, 2023). One of the staff, Dr. Roy Brown, was a great friend of the ISTA and a frequent speaker to chemistry teachers. He taught chemistry to premed students from 1962 to his retirement in 1995. In more recent years the Chemistry department has hosted the RSC Education Officer, and Dr. John O'Donoghue has made TCD an important centre for chemical education and outreach. It is clear from the final chapter that the Chemistry Department at TCD has a bright future in chemical education and research, building on its 300-year history.

## References

Cocker, W., (1978), 'A history of the university chemical laboratory, Trinity College, Dublin, 1711-1946,' *Hermathena*, CXXIV, pp 58-76

Henly, R., (2023), 'Memories of my undergraduate years, 1958-1962, Trinity News, Nov. 2023 Online at Randal Henly, Author at Trinity News Accessed 23/7/25

The book is available from:

Hinds Publishing Ltd, 13 Carlisle Avenue,
Donnybrook, Dublin 4, Ireland
Phone +353 1 667 4864 or within Ireland 01 667 4864
Mobile +353 87 114 5537 or within Ireland 087 114 5537
ross.hinds@hinds.ie
The price is 30 euro and is post free for Irish addresses.

P. E. Childs

# Competition for choosing the Irish representative at the 13th EFMC Young Medicinal Chemists' Symposium (September 10-11, 2026, Basel, Switzerland)

**CALL FOR ABSTRACTS**

The 13th edition of the EFMC Young Medicinal Chemists' Symposium will be held in Basel, Switzerland on September 10-11, 2026. The symposium is jointly organised by the European Federation for Medicinal Chemistry and Chemical Biology (EFMC) and the EFMC Young Scientists Network (YSN). The EFMC Young Scientists meeting will take place after the EFMC International Symposium on Medicinal Chemistry (ISMC-EFMC, 2026, https://www.efmc-ismc.or), for details see

**https://www.efmc-ymcs.org**

This year, the Irish representative will be chosen through submission of a scientific abstract and an online oral presentation competition.

The committee of the ICI Division for Medicinal and Biological Chemistry will select up to 10 young researchers in the fields of Medicinal Chemistry and/or Chemical Biology for an oral presentation from the submitted abstracts. The winner of the competition for the best oral presentation will be the Irish representative at the Symposium.

The selected representative will receive a support for their travel to Basel from the ICI (€200) and can apply for extra support from the EFMC (details to be given later).

**Eligibility**: Final year and recently graduated PhD students (up to 12 months since graduation) in the fields of Medicinal Chemistry and/or Chemical Biology.

**Deadlines:**
26th of January: call for abstracts opens
13th of February: deadline for abstracts submission
23rd of February: notification to the presenters
2nd of March: oral presentation competition (10 a.m.-1 p.m.)
3rd of March: notification of the winner

## Abstracts should be sent to Dr Marina Rubini

marina.rubini@ucd.ie

EuChemS
European Chemical Society

ECC10


# Final Extension: Abstract submission deadline extended to 10 February 2026

**Submit now!**

Dear Colleague,

We are pleased to announce a **final extension** of the abstract submission deadline for the **10th EuChemS Chemistry Congress (ECC10).**

**Final Deadline: 10 February 2026, 23:59 CET**
This is the last and final opportunity to submit your abstract. No further extension will be granted.

If you are planning to contribute to ECC10, now is the time to finalize and submit your work. We warmly invite you to submit an abstract for an **oral or poster presentation** across the **8 scientific themes and Industry Day**, and to join us for five days of cutting-edge science and networking in Antwerp.


## International Carbohydrate Organization Young Researcher Award 2026 – *Call For Applications*

The International Carbohydrate Organization invites applications for the ICO Young Researcher Award. This award was established in 2012 to encourage carbohydrate research by young investigators and shall be given to a researcher working on a project focused on any aspect of glycochemistry and/or glycobiology. The recipient of this award will be invited to present their work orally at the XXXII International Carbohydrate Symposium, Bratislava, Slovakia (July 5th - 9th, 2026). The award covers registration expenses and a cash prize of 5000 USD.

### Conditions for award eligibility

The award can be given to a fulltime graduate student or researcher who is 35 years old or younger as of July 9th, 2026, and working within the first 7 years after Ph.D. completion. Career breaks due to parental or personal circumstances will be taken into account when fully justified.

### Application details

To apply for the award, nominators should provide a one page cover letter, an abstract of one page describing the candidate's work, and a complete CV of no more than 3 pages (all 12 point font), including date of birth and date of granting of PhD.

### Please send nominations as a single PDF file to:

Prof M. Carmen Galan (m.c.galan@bris.ac.uk)
Secretary, International Carbohydrate Organization

***Deadline:*** *27th of February 2026.*

# Institute of Chemistry of Ireland as a Co-Owner Benefits when you publish in PCCP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***Phys. Chem. Chem. Phys.***,
15 August 2025, Volume **27**, Issue 37
Pages 19642-19650
https://doi.org/10.1039/D5CP02321A

## 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

IBICS

Irish Biological Inorganic Chemistry Society

Advancing Inorganic Chemistry in Life Sciences and Health

IBICS-9

**The Irish Biological Inorganic Chemistry Society will host its 9th Symposium (IBICS-9) in Maynooth University, on**

**Friday, 31st October 2025**

Maynooth University
National University of Ireland Maynooth

**The symposium will include 2 plenary lectures from international experts:**

***Prof. Sylvestre Bonnett***

*Department of Chemistry, University of Leiden, Netherlands*

***Prof. Kevin Kavanagh***

*Department Biology, Maynooth University, Ireland*

**The symposium will include the presentation of the IBICS Postgraduate Gold Medal 2025**
**Nominations are open**: https://ibics.ie/ibics-awards/

Institute of Chemistry of Ireland

ROYAL SOCIETY OF CHEMISTRY

**DETAILS**

**IBICS AGM:** During lunchtime of the symposium

**IBICS-9 Registration:** https://forms.office.com/e/BX23MVwKsc

IBICS members: Free

IBICS non-members: €30 via EFT

**Call for abstracts now open (Oral, poster, flash) Abstract deadline:** Friday 10th October 2025 **Registration deadline:** Friday 24th October

Further details on our website: https://ibics.ie/ or using the QR code

## Irish Chemical Events

# 9th Irish Biological Inorganic Chemistry Society Symposium (IBICS-9)

Report by: Diego Montagner

Event Date: 31/10/2025

Venue: JHL4, John Hume Building, Maynooth University

Event Type: Symposium

Report received: 17/11/2025

DOI: 10.5281/zenodo.17660333

http://zenodo.org/communities/ice/

Organising Committee: Dr. Diego Montagner* (Chair), Prof. Kevin Kavanagh (Co-Chair), Giulia Ferrari, Daryl Reidy, Esther Akingbagbohun

Maynooth University, Maynooth, Co. Kildare; *For further information on the event, contact: diego.montagner@mu.ie

Organisation: Irish Biological Inorganic Chemistry Society (IBICS).

***Event Sponsors***

Maynooth University, Anton Paar, Clinisciences, Frontiers in Molecular Biosciences, GPE, Scientific Laboratory Supplies (SLS), Royal Society of Chemistry Republic of Ireland Local Section, Institute of Chemistry of Ireland.

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## *Summary*

The 9th Symposium of the Irish Biological Inorganic Chemistry Society (IBICS-9) was held at Maynooth University on Friday, 31st October 2025. The annual IBICS symposia showcase recent work from researchers who work at the interface of inorganic chemistry and the life sciences and provides an opportunity for networking between society members and industry representatives (www.ibics.ie). At IBICS-9, over 80 attendees were present, including academics at all levels, from early career researchers to principal investigators, and industry sponsors and exhibitors. Two plenary speakers headed the scientific programme: Prof. Sylvestre Bonnet (University of Leiden, NL) and Prof. Kevin Kavanagh (Maynooth University). Three invited lectures were presented by Dr. Darren Griffith (RCSI), Prof. Angela Scala (University of Messina, IT) and Dr. Francesca Novara, (Wiley-VCH). Aligned with the spirit of IBICS, the remaining contributions to the symposium came from early career researchers with several excellent presentations, three flash presentations, and 21 poster presentations. The event was a huge success, thanks to the strong engagement from our Irish biological inorganic community and the fantastic financial support from industry sponsors. The short programme is shown below.

## *Attendees*

Postgraduate and postdoctoral researchers, academics, and industry exhibitors/representatives made up most of the 80+ attendees at IBICS-9, working diversely across fields of inorganic chemistry and its interface with the life sciences. There was an excellent balance of female and male representation, from across different Irish institutions and beyond, and this was reflected in our symposium programme (Table 1).

Target audience: academics, postgraduate researchers, postdoctoral researchers, early career (academia).

| Time | Speaker and title of presentation | Code |
|---|---|---|
| 10:00 | Registration and poster setup | |
| 10:30 | Opening remarks – Dr. Luca Ronconi, IBICS President | |
| | **Session 1** - Chair: Prof. Michael Devereux | |
| 10:40 | **Plenary: Prof. Sylvestre Bonnet** (University of Leiden), *sponsored by Anton-Paar*<br>*Ruthenium-based photoactivated chemotherapy for the treatment of cancer: recent developments* | PL1 |
| 11:20 | Dr. Darragh McHugh (University of Galway) | O1 |
| 11:35 | Giulia Ferrari (Maynooth University) | O2 |
| 11:50 | **Invited: Prof. Darren Griffith** (Royal College of Surgeon in Ireland), *sponsored by CliniSciences Group*<br>*Exploiting Click and IEDDA Chemistry in the Development of Pt(II) Anticancer Probes* | IL1 |
| 12:20 | **Flash Presentation Session** – Chair Dr. Orla Howe<br>Amani Al Riyami, Tara McInerney, Wanyujin Wang | F1-F3 |
| 12:35 | Lunch (provided) | |
| 12:35 | **Poster Session**<br>*Sponsored by RSC Republic of Ireland Local Section and ICI Institute of Chemistry of Ireland* | P |
| 13:40 | IBICS Annual General Meeting | |
| | **Session 2** - Chair: Prof. Tia Keys | |
| 14:00 | **Invited: Dr. Francesca Novara** (Wiley-VCH)<br>*Opening the Editor's Black Box: Insider Tips for Successful Submissions* | IL2 |
| 14:30 | Daniel Graczyk (University College of Dublin) | O3 |
| 14:40 | Nidhi Singh (University of Galway) | O4 |
| 14:55 | **Invited: Prof. Angela Scala** (University of Messina), *sponsored by GPE scientific*<br>*Metals in hybrid drug delivery nanosystems: role, applications and perspectives* | IL3 |
| 15:25 | **Coffee Break** | F4-F6 |
| | **Session 3** - Chair: Prof. Deirdre Fitzgerald Hughes | |
| 15:45 | Federica Brescia (University of Galway) | O5 |
| 16:00 | Dr. Judith Fodor (Trinity College Dublin) | O6 |
| 16:15 | **Plenary: Prof. Kevin Kavanagh** (Maynooth University), *sponsored by Anton-Paar*<br>*A tale of two metals; Uncovering the mode of action of novel Silver and Gallium complexes* | PL2 |
| | **Session 4** – Chair: Dr. Luca Ronconi | |
| 16:55 | **IBICS Postgraduate Gold Medal Award** *Sponsored by Frontiers in Molecular Bioscience*<br>Dr. Darren Fergal Beirne (Dublin City University)<br>*Pt(IV) – Sunitinib dual action pro-drugs display enhanceed activity against Renal cancer types* | GM |
| 17:15 | Prize-giving and closing remarks – Dr. Luca Ronconi | |
| 17:30 | Wine reception | |

*Table 1. IBICS-9 Programme*

## Programme

IBICS-9 was a full one-day event, running from welcome and registration at 10am to closing remarks and reception at 5.30pm. Across four sessions, the scientific programme comprised twelve oral presentations contributed by two plenary speakers, three invited Ireland-based speakers, the IBICS Gold Medal Award winner, and six early career researchers. In addition, three flash presentations showcased a sample of the twenty-one poster presentations that were displayed at the designated poster sessions sponsored by the RSC Republic of Ireland Local Section and ICI. Each session was chaired by a leading academic in the field of bioinorganic chemistry. The IBICS AGM was held during the lunch break of the symposium.

## Proceedings

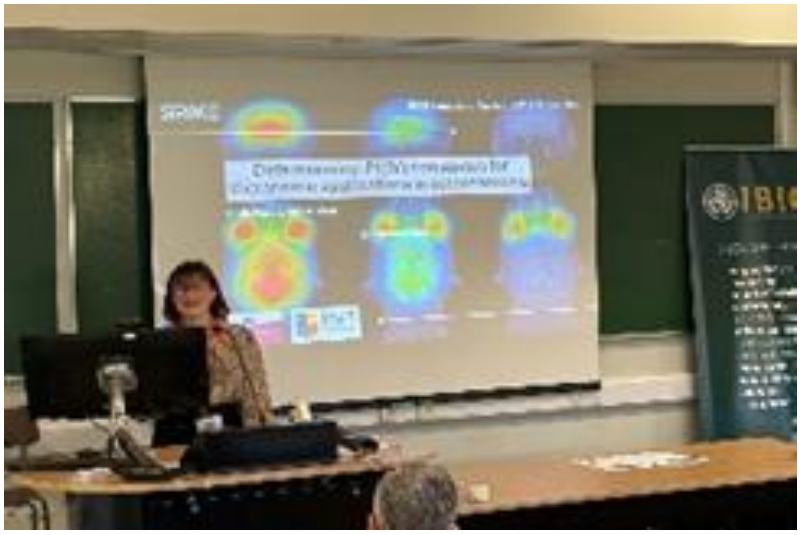
The IBICS president, **Dr. Luca Ronconi** (University of Galway), officially opened the symposium giving an overview of the history of IBICS symposia and the scientific programme to follow.


**Session 1 – Chair : Prof. Michael Devereux (TUD)**

Our first international *plenary speaker*, **Prof. Sylvestre Bonnet** from the University of Leiden (NL) kicked off scientific presentations with a lecture focused on "Ruthenium-based photoactivated chemotherapy for the treatment of cancer: recent developments". This lecture was sponsored by **Anton-Paar**.

Next, **Dr. Darragh McHugh** (University of Galway) presented on "A pH-responsive Zinc Metal-Organic Framework for Triple Negative Breast Cancer Chemotherapy: Insights from a 3D Tumour Model".


**Giulia Ferrari** (Maynooth University) gave a talk on "Deferoxamine-Pt(IV) conjugates for theranostic applications in osteosarcoma".



**Dr. Darren Griffith** (RCSI) was the first invited speaker who show some recent works in his research group with a talk on "Exploiting Click and IEDDA Chemistry in the Development of Pt(II) Anticancer Probes".

Prof. Orla Howe (TUD) chaired the Flash presentation section with three presenters, Tara Mclnerney (UCC), Wanyujin Wang (UCD), Amani Al Riyami (TCD),

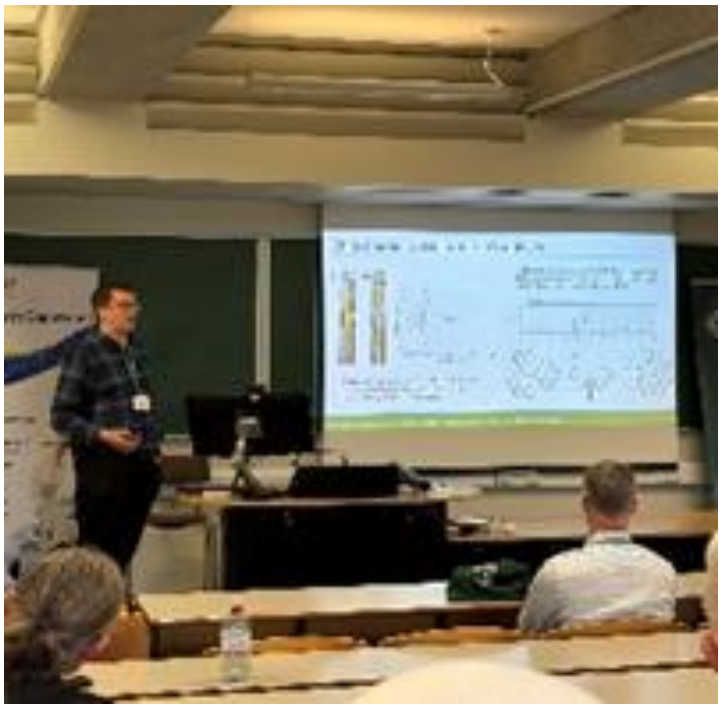


Following lunch and the poster session, the **IBICS AGM** was held with good attendance from members at the symposium. New officers were elected for the coming year, with Prof. Orla Howe taking on the position of President, Prof. Deirdre Fitzgerald-Hughes elected Vice-President, and Dr. Joseph Byrne elected Secretary.

## Session 2 – Chair: Prof. Tia Keys (DCU)

Restarting proceedings after the AGM was our second *invited speaker*, **Dr. Francesca Novara**, Editor in Chief of Wiley-VCH who delivered a presentation on "Opening the Editor's Black Box: Insider Tips for Successful Submissions".

**Daniel Graczyk** (UCD) presented recent work on “Photophysical Study of the DNA Binding of Cr(III) and Os(II) Polypyridyl Complexes with Extended Intercalating Ligands”



**Nidhi Singh** (University of Galway) discussed some recent advances on “Novel Platinum-Based Mitocans for the Treatment of Resistant Cancers: Synthesis, Targeted Delivery and Biological Studies”.

The third invited lecturer (sponsored by **GPE Scientific**) was delivered by **Prof. Angela Scala** (University of Messina, IT) with a lecture whose topic was Metals in hybrid drug delivery nanosystems: role, applications and perspectives

## Session 3 – Chair: Prof. Deirdre Fitzgerald Hughes (RCSI)

Session commenced with a presentation from **Frederica Brescia** (University of Galway) who presented on a new approach to the “Design, Development and Biological Evaluation of Gold(III)-Glycoconjugates as Antiviral Agents against Coronaviruses”.

The next contribution came from Dr. Judith Fodor (TCD) who discussed “Investigation of Transition Metal Complexes with Multimodal Biological Activity for Photodynamic Therapy”.

The **second plenary lecture** (sponsored by **Anton Paar**) was delivered by **Prof. Kevin Kavanagh** (Maynooth University) with a lecture entitled “A tale of two metals: uncovering the mode of action of novel Silver and Gallium complexes”.


## Session 4 – Chair: Dr. Luca Ronconi

The last Session, chaired by outgoing IBICS President Dr. Ronconi, comprised the presentation of **Dr. Darren Beirne** (Maynooth University), who is this years’ winner of the **IBICS Postgraduate Gold Medal Award**, sponsored by **Frontiers in Molecular Biosciences**. Darren’s award lecture centred on his recent PhD work “Pt(IV)–Sunitinib dual action pro-drugs display enhanced activity against” under the supervision of Dr. Diego Montagner.

The symposium was closed out by IBICS president, **Dr. Luca Ronconi**, with the presentation of prizes, his farewell address, and an invitation for all to join the wine reception for further discussion on the excellent presentations delivered throughout the symposium.



*Presentation of gifts to plenary speakers, Prof. Bonnet (left) and Prof. Kavanagh (right).*




*Presentation of gifts to invited speakers, Dr Novara (top), Dr. Griffith (left), and Dr. Scala (right).*

## *Prizes*

The **IBICS Postgraduate Gold Medal,** sponsored by **Frontiers in Molecular Biosciences** was this year awarded to **Dr. Darren Beirne** from Maynooth University (Montagner's group). The Gold Medal is awarded annually to one PhD student who has distinguished themselves across a range of criteria throughout their PhD with a focus on research performance, achievements and impact in the field of medicinal and biological inorganic chemistry across the island of Ireland. The IBICS award selection committee also recognised the high standard of applications with high commendations given to Federica Brescia and Dr. Darragh McHugh from University of Galway.

*Dr. Luca Ronconi (IBICS President), presenting Dr. Darren Beirne with the 2025 IBICS Postgraduate Gold Medal Award, sponsored by Frontiers in Molecular Biosciences.*


Dr. Luca Ronconi (IBICS President), with the highly commended Federica Brescia (left) and Dr. Darragh McHugh (right) with their postgraduate award.

The IBICS president presented three sponsored prizes during the closing remarks of the symposium. Awardees in each category were selected by our independent panel of judges.

Firstly, the **ICI Best Oral Presentation** was awarded to **Daniel Graczyk (UCD)** and the **RSC two poster presentation prizes** were awarded to **Stefania Scurtu (DCU)** and **Esther Akingbagbohun (Maynooth University).**


*ICI Best Oral Presentation Prize was awarded to Daniel Graczyk (UCD).*


*RSC Republic of Ireland Local Section Best Poster Prize was awarded to Stefania Scurtu (left) and Esther Akingbagbohun (right).*

## *The Irish Biological Inorganic Chemistry Society (IBICS)*

The Irish Biological Inorganic Chemistry Society (IBICS) – is a learned Society engaging a multi-disciplinary community of scientists seeking to advance research that crosses the interface between medicinal inorganic chemistry and biology in Ireland. The Society's mission is to develop, foster and promote a strong national network of scientists collaborating in research areas such as biology, chemistry, physics and medicine with an interest in biological inorganic chemistry.

The next symposium of the Irish Biological Inorganic Chemistry Society (IBICS-10) that will also celebrate the 10$^{th}$ anniversary of the IBICS, will take place at TUD during the final quarter of 2026, being led by Prof. Orla Howe and Prof. Bernie Creaven. Please see the IBICS website for event updates (https://ibics.ie). IBICS welcomes any support for its symposia and the future activities of its members.

## *Acknowledgements*

IBICS-9 was made possible by generous financial support from our sponsors: **Anton Paar** (Gold Sponsor), **Frontiers in Molecular Biosciences** (Silver Sponsor), **Clinisciences Group** and **GPE Scientific** (Bronze Sponsors), **Scientific Laboratory Supplies (SLS), Maynooth University** *via* the Impact Dissemination Support Fund**, Royal Society of Chemistry Republic of Ireland Local Section** and **Institute of Chemistry of Ireland.** Many of our sponsors exhibited at the event and contributed to a vibrant meeting.

The local organising committee is grateful to the IBICS Steering Committee for additional support, particularly Luca Ronconi, Deirdre Fitzgerald-Hughes, Orla Howe and Celine Marmion. The local committee also thanks our colleagues at Maynooth University for facilitating our hosting of IBICS-9.

A particular thank you to Giulia Ferrari for the preparation of the programme, to Daryl Reidy for the photographs and to Esther Akingbagbohun for all the logistics.

*IBICS-9 local organising committee, from left: Kevin Kavanagh, Esther Akingbagbohun, Daryl Reidy, Giulia Ferrari and Diego Montagner*

## *Previous Events in this Series*

8th Irish Biological Inorganic Chemistry Society Symposium (IBICS-8), University College Cork: C. S. Burke*, T. McInerney, R. Galway, J. Stack and W. Daly, *Irish Chemical Events*, 2024, **1**, DOI: 10.5281/zenodo.14872697

7th Irish Biological Inorganic Chemistry Society Symposium (IBICS-7), University College Dublin: J. P. Byrne* and S. Kavanagh, *Irish Chemical Events*, 2023, **1**, DOI: 10.5281/zenodo.14052293

Programmes and event reports for all previous IBICS symposia are available at: https://ibics.ie/ibics-symposia

# 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

# Irish Chemical Events

## 4th Medicinal and Biological Chemistry Ireland conference

Report by: Gerd K Wagner*

Event Date: 15/07/2025-16/07/2025

Venue: Queen's University Belfast

Event Type: Conference

Report received: DD/MM/YYYY

DOI: xxx-*EditorWillComplete*-xxx

http://zenodo.org/communities/ice/

ORG LOGO

Organising Committee: Isabel Rozas (Chair),[a] Gerd K Wagner,[b] Marina Rubini,[c] Trinidad Velasco-Torrijos[d]

[a] School of Chemistry, Trinity College Dublin, the University of Dublin, Trinity Biomedical Sciences Institute, 152-160 Pearse St., Dublin 2, Ireland; [b] School of Pharmacy, Queen's University Belfast, Medical Biology Centre, 97 Lisburn Road, Belfast BT9 7BL, United Kingdom; [c] School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland; [d] Department of Chemistry, Maynooth University, Faculty of Science and Engineering, Maynooth, Ireland.

Organisation: held under the auspices of the Medicinal & Biological Chemistry Division of the Institute of Chemistry of Ireland and the European Federation for Medicinal Chemistry & Chemical Biology (EFMC)

***Event Sponsors***

Royal Society of Chemistry, Republic of Ireland Local Section; Institute of Chemistry of Ireland; Almac; Clinigen Ltd; ThermoFisher Scientific; SK Biotek; GPE Scientific Ltd; Trinity College Dublin; The Thomas J Moran Graduate School, Queen's University Belfast

***Summary***

From 15-16 July 2025, the School of Pharmacy at Queen's University Belfast hosted the 4th Medicinal and Biological Chemistry Ireland conference, under the auspices of the Medicinal & Biological Chemistry Division of the Institute of Chemistry of Ireland, and the European Federation for Medicinal Chemistry & Chemical Biology. Following on from successful previous editions at Trinity College Dublin (2016), Dublin City University (2018), and NUI Galway (2022), the meeting exceeded expectations, with 110 participants, 44 submitted abstracts, and strong buy-in from industry.

The scientific programme covered a broad range of topics across chemical biology, medicinal chemistry and drug discovery, from small molecules to protein therapeutics, antibody-drug conjugates, and chemical probes for in vivo real-time optical imaging. The roster of 11 invited speakers included internationally leading scientists as well as rising stars, from these shores and beyond, and from both academia and industry.

As a new element, and in addition to the scientific programme, on its second day the conference also featured a Lunchtime Careers Fair, aimed mainly at Early Career Researchers (ECRs). During the careers fair, participants could attend showcase presentations by ThermoFisher, SK Biotek, GPE Scientific, and EU OpenScreen, as well as a careers "speed dating" event with industry delegates. The speed dating session gave ECRs an opportunity to meet "up close" with industry professionals and ask those questions about a career in industry they had always wanted to ask, but maybe never had the chance. The careers fair was extremely well received by participants and may well become a permanent feature of future editions of this conference.

The conference schedule was rounded off by a social gathering over a pizza and a pint on Tuesday night at the Botanic Inn, including a mini trad session (another conference feature to be retained?)

And, as the final act, the outgoing chair of the Medicinal and Biological Chemistry Division, Isabel Rozas, was recognised with flowers for her immense contribution to the Division, and her tireless efforts to promote the cause of medicinal and biological chemistry in Ireland!

## *Attendees*

With 110 registered delegates, attendance exceeded expectations, with well over half of all participants either PhD students (59) or postdoctoral scientists (11). Efforts had been made specifically to make the conference attractive to ECRs, e.g., through introduction of the careers fair and the opportunity for co-chairing scientific sessions, and these efforts appear to have paid off.

While the majority of participants (78%) hailed, unsurprisingly, from academic institutions or industrial organisations across the island of Ireland, there was also a significant contingent (12%) from Great Britain, as well as individual delegates from as far afield as Hungary and Chile.

Support from industry was strong, not only in the form of sponsorship, but also through the active participation of 12 representatives from a diverse range of industrial organisations large and small. Notably, many of the industrial delegates gave up their time to participate in the careers fair and "careers speed dating" event, for ECRs.

Women were slightly underrepresented, with 46% of all delegates identifying as female.

Target audience: ECRs (postgraduates, postdocs), industrialists, academics

## *Programme*

The scientific programme included a series of 11 invited lectures (Table 1), 4 flash presentations by ECRs selected from the submitted abstracts, and a poster session. The invited lectures were grouped thematically into sessions on Medicinal Chemistry, Chemical Biology & Protein Therapeutics, Chemical Biology & Drug Discovery, and Drug Discovery in Academia, although the boundaries between these themes remained necessarily fluid. ECRs were given the opportunity to co-chair sessions, an opportunity that was enthusiastically taken up by Celia Paramio and Luke Brennan (ICI Young Chemists' Network) and Catherine Webley (QUB).

## *Table 1. Scientific programme*

| | | |
|---|---|---|
| **Session 1: MEDICINAL CHEMISTRY (15 July)** | | |
| **11:10** | Don Weaver | University of Toronto |
| **12:00** | Trinidad Velasco-Torrijos | Maynooth University |
| **12:30** | Joe Byrne | UCD |
| **Session 2: CHEMICAL BIOLOGY & PROTEIN THERAPEUTICS** | | |
| **14:00** | Nicholas Mitchell | University of Nottingham |
| **14:50** | Eddie Myers | University of Galway |
| **15:20** | Graham Cotton | Almac Discovery |
| **Session 3: CHEMICAL BIOLOGY & DRUG DISCOVERY (16 July)** | | |
| **9:00** | Mark Bradley | QMUL |
| **9:50** | Joanna Mcgouran | TCD |
| **10:20** | Daniel O'Donovan | AstraZeneca |
| **Session 4: DRUG DISCOVERY IN ACADEMIA (16 July)** | | |
| **14:15** | Angela Russell | University of Oxford |
| **15:05** | Lorraine Martin | QUB |


*Figure 1. The invited speakers (from left to right): Dr Graham Cotton (Almac), Dr Joanna Mcgouran (TCD), Prof Angela Russell (University of Oxford), Dr Trinidad Velasco-Torrijos (Maynooth University), Prof Mark Bradley (Queen Mary University of London), Prof Lorraine Martin (Queen's University Belfast), Dr Daniel O'Donovan (AstraZeneca), Prof Don Weaver (University of Toronto), Dr Nicholas Mitchell (University of Nottingham), Dr Joe Byrne (UCD) and Dr Eddie Myers (NUI Galway)*


*Figure 2. Left: the flash presenters (from left to right) Guru Vigknesh (University of Galway), Francis M. Barnieh (Bradford University), Periklis Karamanis (University College Dublin), and Timea Baló (Eötvös Loránd University). Right: flowers for Isabel!*

## *Prizes*

The quality of the submitted abstracts was extremely high, and while sponsorship had been secured for no less than four sponsored poster prizes, the judges had a hard time selecting the winners. In the end, they settled on the following contributions by ECRs: Celine Erkey (PhD student, UCD) "Posttranslational Modifications of Human Interferon Gamma for Improved Therapeutics" – Almac Discovery Poster Prize; Nikhil Bajpayee (PhD student, QUB) "A Chemical Toolbox for Targeting b-Strand Mediated Protein-Protein Interactions" – Almac Discovery Poster Prize; Lorcan Rooney (PhD student, QUB) "A Photocleavable Boronic Acid-Based Nanomaterial for the Study of Sialic Acid-Siglec Activation" – ICI Poster Prize; and Ríona Devereux (postdoc, University of Oxford) "Identification of the lipid-protein interactome: A chemo-proteomic approach to understand cardiometabolic dysfunction" – ThermoFisher Poster Prize.


*Figure 3. Left: a snapshot from the poster session in the Thomas J Moran Graduate School. Right: the winners of the poster prizes (from left to right) – Celine Erkey (UCD); Lorcan Rooney (QUB); and Nikhil Bajpayee (QUB). Not in the picture: Ríona Devereux (University of Oxford)*


*Figure 4. Impressions from the social evening and trad session*

## *Feedback*

While many enthusiastic comments about the conference were received informally from delegates, formal feedback was sought specifically about the careers fair, as this was a new addition to the conference schedule. ECRs were sent a questionnaire with 9 questions relating to the careers fair shortly after the end of the conference. 16 responses (23%) were received. All respondents found the careers fair "very useful" (71%) or "somewhat useful" (29%), and just under 40% stated that the careers fair had influenced their decision to attend the conference in the first place. The company showcase presentations were described as "very useful" by 64% of respondents ("somewhat useful": 21%), and the speed dating session by 52% ("somewhat useful": 43%). Aspects that were identified for improvement concerned mainly the time allocated to the careers fair as well as logistics. There were many constructive suggestions that should be taken on board if, as seems desirable, the careers fair becomes a permanent feature of future editions of this meeting.

> "*the careers fair should definitely continue, as many PhD researchers are considering transitioning into industry. Having the opportunity to receive first-hand insights from professionals currently working in industry is very valuable."*
> *"More info about internship […] opportunities"*
> *"more time for the speed dating"*
> *"I really appreciate that it was in small groups. It is easier to speak with the industrials, and others ask questions that I did not think about."*
> *"I particularly liked the speed dating session, because it allowed us to engage directly with the speakers and ask questions in a more relaxed environment."*

## *Acknowledgements*

We wish to reiterate our gratitude to the following organisations for financial support of the conference: The Royal Society of Chemistry, Republic of Ireland Local Section; the Institute of Chemistry of Ireland; Almac; Clinigen Ltd; ThermoFisher Scientific; SK Biotek; GPE Scientific Ltd; and Trinity College Dublin. Without their support, the conference would not have been possible.

We are grateful to the following industry delegates, who gave up their time for the "careers speed dating" event with our early career researchers: Lena Demetre, Daniel O'Donovan, Graham Cotton, Shane Rountree, Victoria Mora, Michael Gurry, Conor Fennell, Tadhg Kelly, and Orla Patton. The careers fair and poster session took place in the Thomas J Moran Graduate School at Queen's, who made their beautiful space available for the conference on a no-cost basis – thank you!

And last not least, I would also like to personally thank my research group, staff in the School of Pharmacy school office, and the events team, catering staff and porters at Queen's University Belfast for their respective contributions to the smooth running of the conference.

## *References*

A blow-by-blow account from both days of the conference, including more pictures, can be found on my personal LinkedIn profile: https://www.linkedin.com/in/gerd-wagner-6807936/

## *Previous Events in this Series*

3rd Medicinal and Biological Chemistry Ireland conference, NUI Galway (2022)
2nd Medicinal and Biological Chemistry Ireland conference, Dublin City University (2018)
1st Medicinal and Biological Chemistry Ireland conference, Trinity College Dublin (2016)

# Inorganic Ireland Symposium 2025

**Friday, 23rd May 2025 | University of Galway**

**Prof. Richard Layfield**
University of Sussex, UK

## Plenary Talks

- **Prof. Richard Layfield,** University of Sussex – 2023 RSC Corday-Morgan Prize
- **Prof. Andrea Erxleben**, University of Galway
- **ICI David Brown Award Lecture** (TBA)

*Register for a one-day event that highlights the breadth, diversity, and excellence of inorganic chemistry research in Ireland.*

*The symposium is dedicated to the memory of **Prof. Pat McArdle**, whose contributions to inorganic chemistry will continue to inspire.*

**Prof. Andrea Erxleben**
University of Galway

***Call for abstracts now open!***

Abstract deadline: **2 May 2025**

Abstract submissions & queries: c.papatriantafyllopo@universityofgalway.ie

**With kind support from:**

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RSC LOCAL SECTION REPUBLIC OF IRELAND

Ollscoil na Gaillimhe University of Galway

# Inorganic Ireland Symposium 2025 Report, University of Galway 23rd May 2025

## Inorganic Ireland 2025

Report by: C. Papatriantafyllopoulou

Event Date: 23/05/2025

Venue: University of Galway, Human Biology Building, Galway

Event Type: Symposium

Report received: 30/05/2025

DOI: 10.5281/zenodo.15556249

http://zenodo.org/communities/ice/

Organising Committee: C. Papatriantafyllopoulou (Chair),[a] C. Marmion,[b] G. Morgan,[c] M. Muldoon,[d] A. McDonald,[e]

[a] University of Galway; [b] Royal College of Surgeons in Ireland; [c] University College Dublin; [d] Queen's University Belfast; [e] Trinity College Dublin

*Event Sponsors*

Royal Society of Chemistry Republic of Ireland Local Section, Institute of Chemistry of Ireland, RSC Dalton Transactions, Complete Laboratory Solutions

**The Inorganic Ireland Symposium 2025** took place on Friday, 23rd May at the University of Galway, bringing together over 55 participants from across Ireland and beyond for a vibrant one-day meeting dedicated to inorganic chemistry. The symposium strengthened national collaborations, provided a platform for early-career researchers to share their work, and celebrated the diversity and excellence of inorganic chemistry research in Ireland.

The programme featured two distinguished plenary lectures by Prof. Richard Layfield (University of Sussex, UK), recipient of the 2023 RSC Corday-Morgan Prize, and Prof. Stuart James (Queen's University Belfast), recipient of the 2025 ICI David Brown Award. A heartfelt tribute lecture by Dr Andrea Erxleben (University of Galway) honoured the memory of Prof. Pat McArdle, to whom the symposium was dedicated. The scientific programme included 3 keynote talks, 14 oral presentations, 5 flash talks, and 18 poster presentations, showcasing excellent research from postgraduate students and postdoctoral researchers across Irish institutions.

Two Early Career Poster Prizes were awarded to Bhawna Kumari (UL) and Judit Fodor (TCD) in recognition of their outstanding contributions.

The symposium was generously supported by the Institute of Chemistry of Ireland (ICI), the Royal Society of Chemistry (RSC) Local Section Republic of Ireland, Dalton Transactions, and Complete Laboratory Solutions (CLS). The event was organised by a national committee chaired by Dr Constantina Papatriantafyllopoulou, with Prof. Celine Marmion, Prof. Mark Muldoon, Dr Grace Morgan, and Dr Aidan McDonald. The organisers extend their gratitude to all attendees, contributors, and sponsors for making this event a memorable success.

# INORGANIC IRELAND 2025

## 23rd May 2025

| | | |
|---|---|---|
| **1st session; chair: Constantina Papatriantafyllopoulou** | | |
| 9:20-9:30 | Welcome | |
| 9:30-10:15 | ***Richard Layfield***, University of Sussex | 2023 RSC Corday-Morgan Prize Lecture: Masked Oxidation States in Lanthanide Organometallic Chemistry |
| 10:15-10:40 | ***Fabio Santani***, Trinity College Dublin | Triggering weak exchange coupling interactions in metalloporphyrins-based quantum logic gates |
| 10:40-11:00 | ***Karlijn Hertsig***, Trinity College Dublin | Greening Quantum Dot Synthesis: A Mild Hydrothermal Route to II-VI Quantum Dots |
| 11:00-11:15 | ***Flash Presentations*** | Sukanya Jana (TCD), Nidhi Singh (UG), Amani Al Riyami (UG) |
| | ***Coffee break*** | |
| **2nd session; chair: John Simmie** | | |
| 11:45-12:30 | ***Andrea Erxleben***, University of Galway | Tribute Lecture to Prof. Pat McArdle |
| 12:20-12:55 | ***Soumya Mukherjee***, University of Limerick | Crystal Engineering of Azolate Coordination Networks for Cleaning Air and Freshwater |
| 12:55-1310 | ***Flash Presentations*** | Judit Fodor (TCD), Victorija Mikaite (UCD), Allan Finlay (UCD) |
| | ***POSTER SESSION*** | |
| **3rd session; chair: Celine Marmion** | | |
| 14:10-14:55 | ***Stuart James***, Queen's University Belfast | ICI David Brown Award 2025 Lecture |
| 14:55-15:15 | ***Darragh McHugh***, University of Galway | OnG7: A Metal–Organic Framework for Potential Chemotherapeutic Delivery in Breast Cancer Treatment |
| 15:15-15:35 | ***Federica Brescia***, University of Galway | Design and development of gold(III)-glycoconjugates as antiviral agents against SARS-CoV-2 |
| 15:35-15:55 | ***Olivia Breed***, University College Dublin | Two centuries of research and all I got was these polymorphs: diverse polymorphism in metal ammonia oxalate hydrate coordination polymers |
| | ***Coffee break*** | |
| **4th session; chair: Diego Montagner** | | |
| 16:30-16:55 | ***Joseph Byrne***, University College Dublin | Presentation title to be confirmed |
| 16:55-17:20 | ***Tandra Ghoshal***, Trinity College Dublin | Fabrication of sub-20 nm $MoS_2$ horizontal nanowire arrays by block copolymer assisted inclusion method |
| 17:20-17:40 | ***Aibhe Boran***, University of Galway | Structural elicidation and morphological exploration of low crystallinity Fe-based MCOFs for $CO_2$ reduction reactions |
| 17:40-18:00 | ***Joshua Thorogood***, Trinity College Dublin | Synthetic magnesium tetrapyrrole radicals for mechanistic studies of Photosystem II |
| **18:00** | **Presentation Awards, closing remarks** | |

## *Attendees*

The symposium welcomed approximately 55 attendees, representing a broad mix of academic levels (undergraduates to senior academics), institutions across Ireland and beyond, and diverse cultural backgrounds. Gender representation was balanced across speakers and audience, with strong participation from early-career researchers and international attendees.

Target audience: academics undergraduates, postgraduates, retired members,

### *List of speakers*

Richard Layfield (University of Sussex)

Stuart James (Queen's University Belfast)

Andrea Erxleben (University of Galway)

Fabio Santani (Trinity College Dublin)

Aibhe Boran (University of Galway)

Soumya Mukherjee (University of Limerick)

Darragh McHugh (University of Galway)

Federica Brescia (University of Galway)

Olivia Breed (University College Dublin)

Joseph Byrne (University College Dublin)

Tandra Ghoshal (Trinity College Dublin)

Joshua Thorogood (Trinity College Dublin)

## *Proceedings*

### Morning Session – *Chair: Constantina Papatriantafyllopoulou*

Richard Layfield (University of Sussex) – **2023 RSC Corday-Morgan Prize Lecture**: Masked Oxidation States in Lanthanide Organometallic Chemistry Fabio

Fabio Santani (Trinity College Dublin) – Triggering Weak Exchange Coupling Interactions in Metalloporphyrin-Based Quantum Logic Gates

Aibhe Boran (University of Galway) – Structural Elucidation and Morphological Exploration of Low Crystallinity Fe-based MCOFs for $CO_2$ Reduction Reactions

### Midday Session – *Chair: John Simmie*

Soumya Mukherjee (University of Limerick) – Crystal Engineering of Azolate Coordination Networks for Cleaning Air and Freshwater

Andrea Erxleben (University of Galway) – Crystallography in Galway – In Memoriam Professor Patrick McArdle.

### Afternoon Session – *Chair: Grace Morgan*

Stuart James (Queen's University Belfast) – **ICI David Brown Award 2025 Lecture**

Darragh McHugh (University of Galway) – OnG7: A Metal–Organic Framework for Potential Chemotherapeutic Delivery in Breast Cancer Treatment
Federica Brescia (University of Galway) – Design and Development of Gold(III)-Glycoconjugates as Antiviral Agents against SARS-CoV-2
Olivia Breed (University College Dublin) – Two Centuries of Research and All I Got Was These Polymorphs: Diverse Polymorphism in Metal Ammonia Oxalate Hydrate Coordination Polymers

## Final Session – *Chair: Diego Montagner*

Joseph Byrne (University College Dublin) – Glycoconjugate Metal Complexes as Anti-Adhesives against Pathogens
Tandra Ghoshal (Trinity College Dublin) – Fabrication of Sub-20 nm $MoS_2$ Horizontal Nanowire Arrays by Block Copolymer Assisted Inclusion Method
Joshua Thorogood (Trinity College Dublin) – Synthetic Magnesium Tetrapyrrole Radicals for Mechanistic Studies of Photosystem II

## *Prizes*

Two poster prizes were awarded at the Inorganic Ireland Symposium 2025, with a focus on recognising excellent research and presentation skills among early career researchers. The recipients of the prizes are Judit Fodor (TCD) and Bhawna Kumari (UL)

*Figure 1. Recipients of the poster prizes: Bhawna Kumari and Judit Fodor.*

*Figure 2. Prof. Stuart James receives the 2025 ICI David Brown Award.*

## About the ICI David Brown Award

This award was established in 2014 to honour Professor David Brown of University College Dublin in recognition of his enormous contribution to inorganic chemistry both nationally and internationally. Professor Brown, together with Professor Bill Davis (TCD) hosted the International Conference on Coordination Chemistry (ICCC) in UCD in 1974. With some funds remaining, Professor Brown set up what became known as the Greystones weekend meetings, which were held in the LaTouche Hotel in Greystones and later in a more formal setting, in Maynooth University, hosted by Dr Malachy McCann every three years until 2005. This was re-launched as a one-day *Inorganic Ireland Symposium* and has been held approximately every two years since then. A highlight of this symposium is the presentation of the ICI David Brown award to a colleague who has made an outstanding contribution to inorganic chemistry.

## Acknowledgements

We gratefully acknowledge the support of all sponsors as listed above, and the host institution, the University of Galway, for providing the venue and facilities. We would like to extend our appreciation to the session chairs, speakers, and all attendees for contributing to the vibrant atmosphere of the event. Special thanks to Manal Alrashidi, Constantinos G. Efthymiou, Darragh McHugh, and Ben Mohan for their pivotal role in organising and running the symposium.

## Previous Events in this Series

The *Inorganic Ireland* symposium series has run approximately every second year in recent times. It is the successor of the Greystones Meetings, set up by Professor David Brown in the 1970s. Reports on some recent symposia are given below:

Inorganic Ireland 2023 (Trinity College Dublin), Programme available on Institute of Chemistry of Ireland website, https://www.chemistry ireland.org/wp-content/uploads/2023/06/Inorganic-Ireland-Symposium-2023-Programme.pdf (Accessed 30/05/2025)

Inorganic Ireland 2021 (Online). *Irish Chemical News*, **2021**, *5*, 34

Inorganic Ireland 2018 (Queen's University Belfast), *Irish Chemical News*, **2019**, *1*, 10.

Inorganic Ireland 2017 (Royal College of Surgeons in Ireland), *Irish Chemical News*, **2017**, *3*, 18.

# 10th Conference for Analytical Sciences in Ireland 2025

3rd and 4th July 2025
Devere Hall, UCC

University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

School of Chemistry
Scoil na Ceimic

10th Conference for Analytical Sciences in Ireland 2025

CASi 2025 – University College Cork July 3rd and 4th 2025

Special Remembrance event for Prof. Jeremy Glennon on July 2nd

A TRADITION OF INDEPENDENT THINKING

University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

School of Chemistry
Scoil na Ceimic

**Welcome to the 10th Conference for Analytical Sciences in Ireland (CASi), University College Cork. On behalf of the RSC Analytical Division, RoI Ireland Sub-Region and the School of Chemistry here in UCC, it is with great pleasure that we can host the event in 2025.**

**There will also be a special remembrance event for Prof. Jeremy Glennon on July 2nd in the Aula Maxima in UCC.**

**CASI brings together a host of world-renowned participants ranging from international plenary, invited speakers to flash presentations and a poster session covering a broad range of analytical topics. Many of the main universities and research institutes on the island of Ireland are well represented, in addition to international guests. We have participation from state bodies and industry across sponsorship support, attendance and research submissions.**

## CASi is being supported by the RSC Republic of Ireland, Analytical Division

# Conference of Analytical Sciences Ireland 2025
# Schedule of Presentations

**3rd July – Day 1**

| Session 1 – Green Analytical Chemistry | | | | Chair: John Clancy (Henkel) |
|---|---|---|---|---|
| 09:30 – 10:00 | Ruth Godfrey | University of Swansey | Keynote | Sustainable Analytical Science: Future-Proofing Methods From Bench to Field |
| 10:00 – 10:15 | Christopher Kent | University College Cork | Speaker | Optimizing parameters for solar electrolysis of water to yield green H2 using Broadband Acoustic Resonance Dissolution Spectroscopy |
| 10:15 -10:30 | Pankaj Kumar | Teerthanker Mahaveer University | Speaker | Graphitic Carbon Nitride-ZnO Nanocomposites as Efficient Cold Field Emission in Green Energy Applications |
| 10:30 – 10:45 | Jessica Smith Osorio | University of Limerick | Speaker | Advancing Quantification Standards: Coulometric Titration Validation for Potassium Hydrogen Phthalate |
| 10:45 – 11:00 | Niamh O'Mahony | University College Cork | Speaker | Rapid determination of the active pharmaceutical Ingredient (API) content of suspension formulations using Broadband acoustic resonance dissolution spectroscopy (BARDS) |

| Session 2 – Biosensing and Sensors | | | | Chair: Micheal Scanlon (University of Limerick) |
|---|---|---|---|---|
| 11:30 – 12:00 | Marion Kennefick | Johnson & Johnson | Keynote | An Overview of Host Cell Proteins in Manufacturing and Analytical Processes |
| 12:00 – 12:15 | Mohamed Sharafeldin | University College Cork | Speaker | Accessible Hepatitis C Virus (HCV) Diagnostics via Unamplified Nucleic Acid Detection |
| 12:15 – 12:30 | Atieh Mousavi | Tyndall National Institute | Speaker | Enabling early detection of ovarian cancer using a novel electrochemical sensing platform |
| 12:30 – 12:45 | Dinakaran Thirumalai | Dublin City University | Speaker | A sensitive non-enzymatic lactate sensor based on pulse electrodeposited nickel oxide on carbon electrode |
| 12:45 – 13:00 | Justina Ugwah | Tyndall National Institute | Speaker | A pilot study evaluating the performance of a prototype impedance sensor integrated on a biopsy needle for breast cancer detection |

Tea/Coffee Networking and Poster Viewing 11:00 – 11:30

Lunch Networking and Poster Viewing 13:00 – 14:00

Conference of Analytical Sciences Ireland 2025
Schedule of Presentations

3rd July – Day 1

| Session 3 – Forensic Analysis | | | | Chair: Elizabeth Gilchrist (University College Cork) |
|---|---|---|---|---|
| 14:00 – 14:30 | Johnathan Spencer | Agilent | Keynote | Next Generation Forensic Screening using Accurate Mass High Resolution Mass Spectrometry |
| 14:30 – 14:50 | Anjan Roy | Coherent Corp (USA) | Invited | Applications of THz-Raman spectroscopy |
| 14:50 -15:05 | Yineng Wang | Tyndall National Institute | Speaker | Development of a mobile CE workstation with a C4D detector for rapid detection of organophosphates under CBRN field conditions |
| 15:05 – 15:20 | John Moran | Forensic Science Ireland | Speaker | Using a portable Near-Infrared Spectroscopy (NIRS) instrument with chemometrics for rapid drugs analysis: A recent evaluation at Forensic Science Ireland |
| 15:20 – 15:35 | John Moriarty | Department of Agriculture | Speaker | Veterinary Toxicology and Geochemical Risk |

Tea/Coffee Networking and Poster Viewing 15:35 – 16:00

| Session 4 – Environmental Analysis | | | | Chair: Eithne Dempsey (Maynooth University) |
|---|---|---|---|---|
| 16:00 – 16:30 | Brett Paul | University of Tasmania | Keynote | Taking Chromatographs out into the Field |
| 16:30 – 16:50 | Isabelle Ourliac-Garnier | Nantes University | Invited | Unravelling Sterol Biosynthesis in Fungi: Where Analytical Chemistry Meets Medical Mycology |
| 16:50 – 17:05 | Micheal Scanlon | University of Limerick | Speaker | Electrosynthesis of Free-Standing Conducting Polymer Thin Films at a Polarized Liquid\|Liquid Interface for Electroanalytical Applications |
| 17:05 – 17:20 | Dean Venables | University College Cork | Speaker | Chemical analysis of the atmosphere — Towards sensitive, fast, and lower cost spectroscopic sensors |

Poster Session and Networking 17:30 – 19:00

Social Event (Mardyke Entertainment Complex) 20:00 – 23:00

UCC School of Chemistry

# Conference of Analytical Sciences Ireland 2025
# Schedule of Presentations

ROYAL SOCIETY OF CHEMISTRY

**4th July – Day 2**

| Session 5 – Separation Science | | | | Chair: Donal Leech (University of Galway) |
|---|---|---|---|---|
| 09:30 – 10:00 | Melissa Hanna-Brown | University College Cork | Keynote | Pills, Pressure, and Parting Ways: Innovative Separation in Modern BioPharma |
| 10:00 – 10:20 | John Lough | University of Sunderland | Invited | Eiroshell™-Enabled Extension to LC Method Development Screening Approaches |
| 10:20 – 10:40 | Ryan Osborne | Pfizer | Invited | An Approach to Method Development in SFC Leveraging Machine Learning for the Development of a Late-Stage Oncology Drug Candidate |
| 10:40 – 10:55 | Ilaria Neri | University of Naples Federico II | Speaker | Biomimetic chromatography-based investigation of environmental contaminants toxicity and biological barrier permeation |

| Session 6 – Bioanalytical Chemistry | | | | Chair: Ciara MacHale (Eli Lilly) |
|---|---|---|---|---|
| 11:30 – 12:00 | Mark Milford | Eli Lilly | Keynote | The Mystery of the Disappearing Excipient: An Analytical Case Study, Investigating a Reduction in Polysorbate Content in a Monoclonal Antibody Drug Substance |
| 12:00 – 12:15 | Ruchi Gupta | University of Birmingham | Invited | Hydrogel Lollipops for Early Detection of Cancer |
| 12:15 – 12:30 | Aine O'Brien | Maynooth University | Speaker | Chemoenzymatic Glycoengineering of Monoclonal Antibodies |
| 12:30 – 12:45 | Alan Ryder | University of Galway | Speaker | Polarized Excitation Emission Matrix (pEEM) spectroscopy for the rapid, non-destructive analysis of proteins |
| 12:45 – 13:00 | Somali Dhal | Tyndall National Institute | Speaker | Optical Evaluation of the Impact of Filtration on Diagnostic Salivary Components |

Tea/Coffee Networking and Poster Viewing 10:55 – 11:30 Lunch, Networking and Poster Viewing 13:00 – 14:00

UCC School of Chemistry

Conference of Analytical Sciences Ireland 2025
Schedule of Presentations

ROYAL SOCIETY OF CHEMISTRY

4th July – Day 2

| Session 7 – Virtual Labs | | | | Chair: Aoife Morin (Dublin City University) |
|---|---|---|---|---|
| 14:00 – 14:30 | Eric Moore | University College Cork | Keynote | Future Proofing Learning and Teaching through Gamification and VR Laboratories |
| 14:30 – 14:50 | Charlotte Hamblet | Labster | Invited | What If Your Toughest STEM Courses Became Your Students' Success Stories? |
| 14:50 – 15:05 | Janine Boetjes | University College Cork | Speaker | Development of a Virtual Reality Capillary Electrophoresis Experiment for Postgraduate Chemistry Education |
| 15:05 – 15:20 | Heather Myler | Beyond Labz | Speaker | How to Teach Scientific Inquiry with Beyond Labz |

## Abstracts Available here:

https://www.ucc.ie/en/media/academic/chemistry/outreach/BookofAbstractsCASi2025.pdf

## CASi 2025 Awards List & Sponsor

- Agilent Presentation Gold Award
- Eli Lilly Presentation Gold Award
- Johnson and Johnson Presentation Gold Award
- RSC Separation Science Group Presentation Award
- Merck, Sharp and Dohme Poster Silver Award
- Particular Sciences Poster Silver Award
- Pfizer Poster Silver Award
- RSC Separation Science Group Poster Award
- Eurachem Ireland Poster Award
- Eurachem Ireland Poster Award
- Analytical Methods Poster Award
- Analyst Poster Award

Agilent · Johnson&Johnson · RSC Interest Group Separation Science · Lilly · MSD · Pfizer · Royal Society of Chemistry · Particular Sciences · Eurachem Ireland · Analytical Methods · Analyst 150

# 10th Conference for Analytical Sciences in Ireland 2025

## Wednesday 2nd July

## Special Remembrance Event for Prof. Jeremy Glennon

**2:30-4:30pm in the Aula Maxima, UCC**

**Prior to event special Tree Planting Ceremony at 1:15pm**

**Lifetime Achievement Award presented to Family of Prof. Glennon at 4:15pm**


Lifetime Achievement Award presented to Jeremy's family, Plaque & Abstracts of his PhD Students Thesis


Prof Eric Moore presents the Lifetime Award to Jeremy's Wife Linda, Daughters Jenny (L), Amy & Partner (R), Son Jack along with Dr Dara Fitzpartick colleague

Ceremony for Jeremy held in the Aula Maxima at UCC on 2nd May

Pictures from the tree planting ceremony on 3rd May down by Cavangh Bridge in the lower grounds with President **John O'Halloran** and members of Jeremy's Family, colleagues from **University College Cork** and beyond.

# School of Chemistry hosts Analytical Chemistry Conference and Remembrance Day for Professor Jeremy Glennon


The School of Chemistry recently played host to the 10th Conference for Analytical Sciences in Ireland (CASI) on July 3rd and 4th which also coincided with a remembrance day for Professor Jeremy Glennon on July 2nd.

Posting on LinkedIn, Professor Eric Moore wrote, "Congratulations to all the participants who attended the 10th Conference for Analytical Sciences in Ireland on the 3rd and 4th July in the Devere Hall, University College Cork! It was a fantastic event with an incredible calibre of presentations (oral and poster). Well done to all our winners! Special thank you to our sponsors for your continued support with this event. It was a welcome return to this conference series for the Republic of Ireland Royal Society of Chemistry Analytical Division. We also remembered the late Professor Jeremy Glennon on a special day in the Aula Maxima on the 2nd of July in UCC and celebrated the occasion with family and friends and the planting of an Oak tree on the lower grounds."

Prof Anita McGuire with Jeremy's family members  Amy, Jenny and Jack

Speaking on the Remembrance event for Professor Jeremy Glennon, Professor Anita Maguire, Head of School said, "This is a very important occasion for Jeremy's friends, colleagues and former members of his research team to come together with Jeremy's family, acknowledge his strengths as a colleague and friend,

his very significant impact on Analytical Chemistry at UCC throughout his career and his support for others especially students and early career researchers. He is greatly missed."

Continuing to speak on the CASI event, Professor Maguire said, "Given UCC's location at the heart of a globally significant pharma and biopharma cluster, Analytical Chemistry is a key discipline within the School of Chemistry providing industry relevant programmes and training at undergraduate and postgraduate levels and through CPD, and with internationally competitive research programmes in in a number of areas including separation science and sensors. In this context hosting the 10th CASI in UCC is very welcome providing an opportunity for researchers, students and PIs in Analytical Chemistry nationally and internationally to share their latest results and develop professional networks across the academic and industry sectors. Well done to Eric, Melissa and all involved in bringing this important conference to UCC."

## Conference Welcome

Welcome to the 10th Conference for Analytical Sciences in Ireland (CASi), at University College Cork (UCC). On behalf of the Royal Society of Chemistry Analytical Division, Republic of Ireland Sub-Region and the School of Chemistry here at University College Cork, it is with great pleasure that we can host the event in 2025. We are also celebrating 25 years since CASi first started back in 2000!


Delegates at CASi

# About CASi

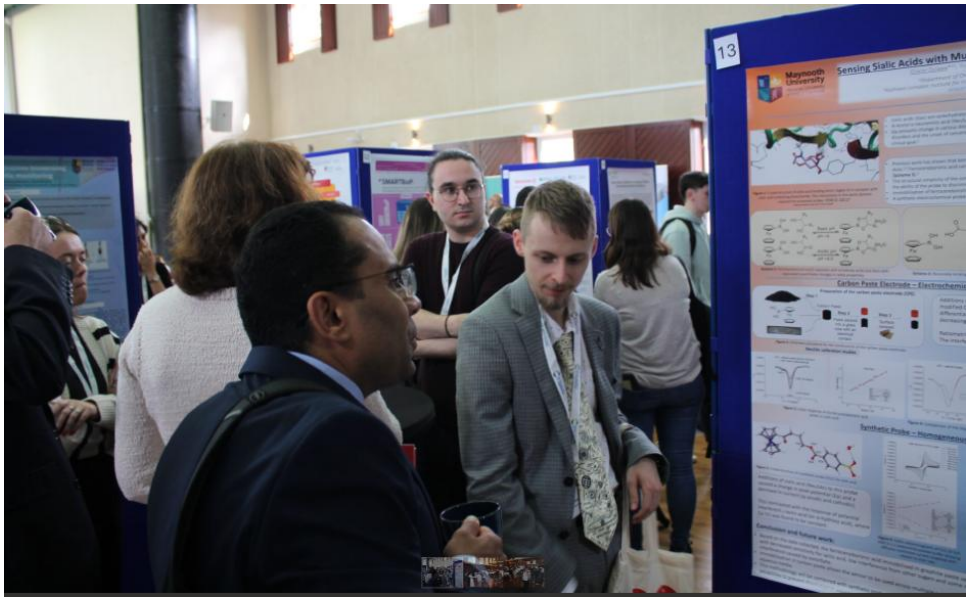
CASi will take place in the Devere Hall, UCC on Thursday and Friday, 3rd and 4th July 2025. This will be the 10th CASi event where around one hundred and fifty researchers from across Ireland and beyond will meet to discuss advances in this interdisciplinary field, bridging the life sciences with Analytical chemistry. The conference will feature several international keynote and invited speakers, as well as contributed talks from Irish researchers and industry. There is also a significant poster session covering a broad range of Analytical topics with 32 posters being presented this year. Many of the main universities and research

institutes on the island of Ireland are well represented, in addition to international guests and participants. We have incredible sponsorship support from industry and a significant presence at the conference with talks and exhibitions. The programme reflects topics of interest to the Irish Analytical Community and speakers will represent experts across a variety of fields with a unique forum to discuss challenges and future opportunities within the academic, industrial and state agency sectors. QR code links to online pdf version.

Finally, none of this is ever possible without the generosity of our sponsors Royal Society of Chemistry, Cork Convention Bureau and our Gold, Silver and Bronze industry level sponsors.

**Social Side of the Conference**

## Poster Session




## Steering Committee: RSC Analytical Division, Republic of Ireland Sub-Region

- Eric Moore, University College Cork (Chair)
- John Clancy, Henkel
- Aoife Morrin, Dublin City University
- Eithne Dempsey, Maynooth University
- Donal Leech, University of Galway
- Blanaid White, Dublin City University
- Aidan Dineen, Metrohm
- Ciara Machale, Eli Lilly
- Kevin Ryan, University of Limerick
- Eoin Gillespie, Atlantic Technological University Silgo
- Siobhan Moane, Technological University of the Shannon


Prof. Eric Moore with Prof. Melissa Hana-Brown (Futures Pharmaceuticals Chair Analytical Chemistry, University College Cork), Keynote Speaker.

# Keynote Speakers

**Green Analytical Chemistry (Session sponsor – RSC Separations Science Group)**

**Dr Ruth Godfrey (Associate Professor in Liquid Chromatography Mass Spectrometry, Medical School, Swansea University**) Ruth is an innovation academic, supporting the R&D of multinational companies, government agencies and SMEs. Her research focuses on analytical technologies and method development for medical/chemical analysis, with her most recent work concerning environmental medicine, mass spectrometry and sample preparation technology development. She has received grant funding (UKRI, EU, industry, charities etc), supervised postgraduate research students (MRes, MPhil and PhD) and performed consultancy work in separation science and mass spectrometry.

**Biosensing and Sensors (Session sponsor – Johnson & Johnson)**

**Dr Marion Kennefick (Associate Director, Johnson & Johnson Innovative Medicine)** Marion currently serves as the Associate Director at Johnson & Johnson Innovative Medicine, where she leads a scientific team focused on Separation Sciences, specializing in method transfer, release, and stability testing for the JNJ clinical portfolio. With extensive experience as a subject matter expert in host cell proteins, Marion has overseen stability initiatives for advanced therapy clinical and commercial programs and has implemented laboratory automation for analytical techniques. With 15 years of experience in the biopharmaceutical industry, Marion holds a PhD in Microbiology, a MSc in Biotechnology, and a BSc in Zoology from University College Cork.

**Forensic Analysis (Session sponsor – Agilent)**

**Mr Johnathan Spencer (LC-MS Applications Scientist, Agilent)** Jonny studied BSc Natural Sciences at the University of Nottingham, where he divided his studies between chemistry and biochemistry. He went on to study MSc Forensic Science at Sheffield Hallam University. Following graduation, he spent 2 years as a Confirmatory Analyst in an anti-doping and forensic toxicology lab, before joining Agilent as an LC-MS Applications Scientist. At Agilent, he focuses on small molecule applications using LC-TQ and LC-QTOF in fields like food, forensic and environmental analysis.

**Environmental Analysis (Session sponsor – Particular Sciences)**

**Prof. Brett Paul (University of Tasmania)** Brett is a BSc, PhD and DSc graduate of the University of Plymouth, U.K. and a Professor of Analytical Chemistry at the University of Tasmania. His research sits at the interface of materials and analytical science, with a focus on analytical platform technologies to explore industrial and environmental systems. Brett is currently Director of the ARC Training Centre for Hyphenated Analytical Separation Technologies (HyTECH), a multi-partner industry supported research centre focussed on analytical technology development to meet complex end-user challenges.

**Separation Science (Session sponsor – Pfizer)**

**Prof. Melissa Hana-Brown (Chair Analytical Chemistry, University College Cork)** Melissa's profile has combined a sandwich of academic and industrial research with a generous dose of professional society/board roles. She started her career in King's College London (Pharmacy) as a separation science lecturer before moving to Pfizer in 2006 where she had various roles (most recently as global Analytical Technology & External Strategic Innovation Lead) and simultaneously taught separation science Masters students as a Visiting Full Professor since 2011. During that same period, she had roles including President of the RSC Analytical Division, Member of RSC Council and she led the Pfizer Analytical Quality by Design work including representing Pfizer in the EFPIA efforts contributing to the recently introduced ICH Q14 guidance. In 2024, Melissa joined UCC as the Futures Pharmaceuticals Chair of Analytical Chemistry and is working hard on re-establishing her academic career, research group (and funding). Melissa's research focus is on separations method development and specifically the journey from 'molecule to green method'.

**Bioanalytical Chemistry (Session sponsor – Eli Lilly)**

**Dr Mark Milford (Director Analytical, Eli Lilly)** Mark is an analytical scientist with over 25 years of industrial experience in the protein analytical field. Having gained a PhD from the University of Southampton (UK), Mark's industrial experience has spanned analytical roles in development, commercialization and routine manufacture of biopharmaceuticals, most recently in the analytical testing of monoclonal antibody products. Currently holding a position of Director - Analytical with Eli Lilly, based at the Kinsale manufacturing facility, Mark has technical oversight of analytical aspects of new product introduction and commercialization for biopharmaceutical drug substances, overseeing the analytical method lifecycle and driving analytical control strategy. Mark has a particular interest in analytical procedure development, validation and post-approval lifecycle from a large molecule perspective. As such, Mark holds the position of Industry Expert on the ICH Implementation Working Group for ICHQ2(R2) / ICHQ14, as well as Deputy Topic Lead for the EFPIA ICHQ2(R2) / ICHQ14 Support Group. Mark also holds a position on the EDQM Expert Group 6 – Biological and Biotechnological products, providing regular support for authoring and maintenance of European Pharmacopoeia monographs.

**Virtual Labs (Session sponsor – Labster)**

**Prof. Eric Moore (School of Chemistry, University College Cork)** Eric heads the Separation and Sensing research group in the School of Chemistry at University College Cork focused on chemical and bio-sensing and separation. He leads a multi-disciplinary team of researchers whose principal research activities are focused on developing integrated bio/sensor platforms, separation techniques, surface attached chemistry, electrochemical analysis and micro-fluidics. He is an Academic member within the Life Science Interface group at Tyndall National Institute and a Principal Affiliate at the Environmental Research Institute, University College Cork. He has extensive linkages with the pharmaceutical, biopharmaceutical, biomedical device, environment and food/beverage sectors. He has championed postgraduate education, especially at the MSc level and is dedicated to providing high calibre industry ready graduates. He is currently the Vice Dean for Graduate Affairs in the College of Science, Engineering and Food Science.

# Chemistry Nobel Prizes 2025

**The Nobel Prize in Chemistry 2025 was awarded jointly to Susumu Kitagawa, Richard Robson and Omar M. Yaghi "for the development of metal–organic frameworks"**

Ill. Niklas Elmehed © Nobel Prize Outreach

Susumu Kitagawa

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

Richard Robson

Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach

Omar M. Yaghi

Prize share: 1/3

https://www.nobelprize.org/prizes/chemistry/2025/summary

Press Release: https://www.nobelprize.org/prizes/chemistry/2025/press-release:

**MOF molecular architecture contains rooms for chemistry**
"The Nobel Prize laureates in chemistry 2025 have created molecular constructions with large spaces through which gases and other chemicals can flow. These constructions, *metal–organic frameworks*, can be used to harvest water from desert air, capture carbon dioxide, store toxic gases or catalyse chemical reactions".

**Susumu Kitagawa**, **Richard Robson** and **Omar Yaghi** are awarded the Nobel Prize in Chemistry 2025. They have developed a new form of molecular architecture. In their constructions, metal ions function as cornerstones that are linked by long organic (carbon-based) molecules. Together, the metal ions and molecules are organised to form crystals that contain large cavities. These porous materials are called metal–organic frameworks (MOF). By varying the building blocks used in the MOFs, chemists can design them to capture and store specific substances. MOFs can also drive chemical reactions or conduct electricity.

"Metal–organic frameworks have enormous potential, bringing previously unforeseen opportunities for custom-made materials with new functions," says Heiner Linke, Chair of the Nobel Committee for Chemistry.

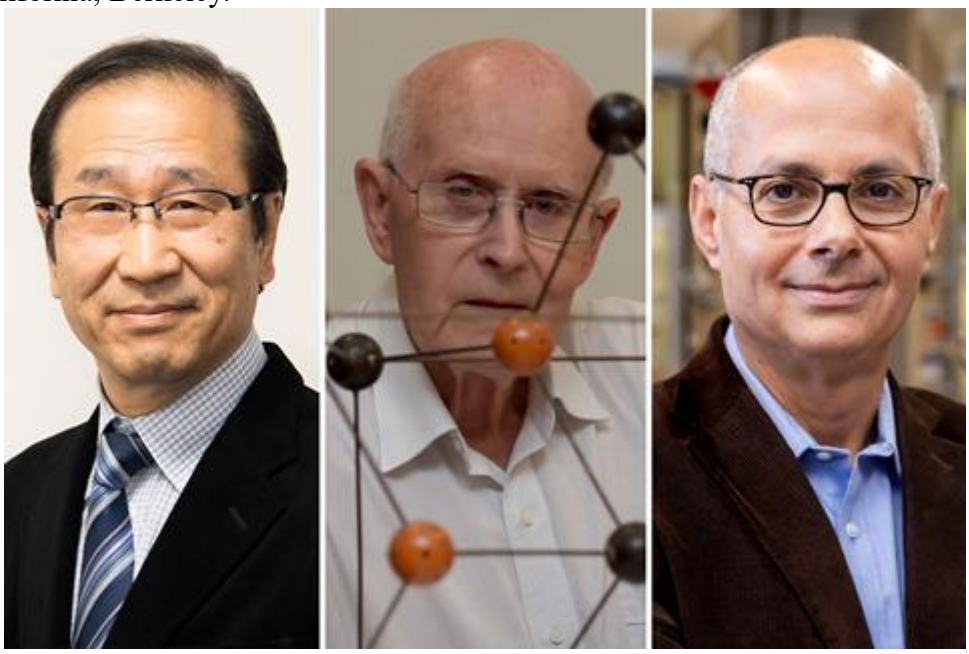
It all started in 1989, when Richard Robson tested utilising the inherent properties of atoms in a new way. He combined positively charged copper ions with a four-armed molecule; this had a chemical group that was attracted to copper ions at the end of each arm.
When they were combined, they bonded to form a well-ordered, spacious crystal. It was like a diamond filled with innumerable cavities.

Robson immediately recognised the potential of his molecular construction, but it was unstable and collapsed easily. However, Susumu Kitagawa and Omar Yaghi provided this building method with a firm foundation; between 1992 and 2003 they made, separately, a series of revolutionary discoveries. Kitagawa

showed that gases can flow in and out of the constructions and predicted that MOFs could be made flexible. Yaghi created a very stable MOF and showed that it can be modified using rational design, giving it new and desirable properties.

Following the laureates' groundbreaking discoveries, chemists have built tens of thousands of different MOFs. Some of these may contribute to solving some of humankind's greatest challenges, with applications that include separating PFAS from water, breaking down traces of pharmaceuticals in the environment, capturing carbon dioxide or harvesting water from desert air.

We at the Institute of Chemistry of Ireland can be very proud that our first Plenary Speaker of the Monday of The EuChemS European Chemistry Congress 9 (ECC9) in Dublin July 2025was **Omar Yaghi** at the University of California, Berkeley.



Source: © Kyoto University, © Paul Burston/University of Melbourne and © Brittany Hosea-Small/UC Berkeley,
Susumu Kitagawa, Richard Robson and Omar Yaghi have won the 2025 Nobel prize in chemistry for discovering and developing MOFs
See link below for graphics and more links:
https://www.chemistryworld.com/news/2025-chemistry-nobel-prize-goes-to-the-scientists-behind-metal-organic-frameworks/4022287.article

This year's Chemistry Nobel prize generated a lot of comment and discussion but due to space limitations only links to some of these can be accommodated in this Issue:

**Chemistry Nobel for scientists who developed massively porous 'super sponge' materials**
8 Oct
Chemistry Nobel for scientists who developed massively porous 'super sponge' materials

**Architects of molecular cages win Chemistry Nobel | Science | AAAS**
8 Oct
Architects of molecular cages win Chemistry Nobel | Science | AAAS

**Nobel Prize in Chemistry for the Development of Metal-Organic Frameworks | The Scientist**
8 Oct
Nobel Prize in Chemistry for the Development of Metal-Organic Frameworks | The Scientist

**Nobel chemistry prize 2025: metal-organic frameworks win for Kitagawa, Robson and Yaghi | Chemistry World**
8 Oct

Nobel chemistry prize 2025: metal-organic frameworks win for Kitagawa, Robson and Yaghi | Chemistry World

**2025 Nobel Prize For Chemistry Awarded For a Whole Lot of Nothing : ScienceAlert**
9 Oct
2025 Nobel Prize For Chemistry Awarded For a Whole Lot of Nothing : ScienceAlert

**An Australian chemist just won the Nobel prize. Here's how his work is changing the world**
9 Oct
An Australian chemist just won the Nobel prize. Here's how his work is changing the world

**Chemistry Nobel winner Kitagawa says downtime helped him think up new material**
9 Oct
Chemistry Nobel winner Kitagawa says downtime helped him think up new material - The Japan Times

**Metal-organic frameworks: Nobel-winning tiny 'sponge crystals' with an astonishing amount of inner space**
9 Oct
Metal-organic frameworks: Nobel-winning tiny 'sponge crystals' with an astonishing amount of inner space

**Nobel Prize in Chemistry 2025 | Metal Organic Frameworks | Latest Update | Drishti IAS English**
8 Oct
(94) Nobel Prize in Chemistry 2025 | Metal Organic Frameworks | Latest Update | Drishti IAS English - YouTube

**Meet the three scientists who have just won the Nobel prize in chemistry | News | Chemistry World**
9 Oct
Meet the three scientists who have just won the Nobel prize in chemistry | News | Chemistry World

**Who won the Nobel Prize in Chemistry (2025)? - Periodic Table of Videos**
10 Oct
(94) Nobel Prize in Chemistry 2025 - Periodic Table of Videos - YouTube

**UC sets record with five Nobel Prizes in one week**
10 Oct
UC sets record with five Nobel Prizes in one week

**How the pioneers of metal-organic frameworks won the Nobel prize**
15 Oct
Chemistry Nobel prize celebrates three scientists who developed versatile metal-organic frameworks | Chemistry World

**The 2025 Nobel Prize in Chemistry Goes to Susumu Kitagawa, Richard Robson, and Omar M. Yaghi**
8 Oct
https://axial.acs.org/cross-disciplinary-concepts/nobel-prize-chemistry-2025

**Former UMich professor Omar Yaghi awarded Nobel Prize in Chemistry**
20 Oct
Former UMich professor Omar Yaghi awarded Nobel Prize in Chemistry

**EuChemS 2025 Nobel Prize in Chemistry awarded for groundbreaking work on metal-organic frameworks**
13 Oct
https://www.magazine.euchems.eu/nobel-prize-chemistry-2025-mofs

**Omar Yaghi: The Live-Wire Nobel Laureate - Rediff.com**
21 Oct
Omar Yaghi: The Live-Wire Nobel Laureate - Rediff.com India News

**Chemistry Nobel Prize winner Susumu Kitagawa reveals Japanese research mindset: 'Don't switch off the light, even…' | - The Times of India**
27 Oct
Chemistry Nobel Prize winner Susumu Kitagawa reveals Japanese research mindset: 'Don't switch off the light, even…' | - The Times of India

**Japanese scientists receive Nobel prizes for medicine, chemistry**
11 Dec
Japanese scientists receive Nobel prizes for medicine, chemistry

**Nobel co-winner Susumu Kitagawa calls for funds for basic research - The Japan Times**
9 Dec
Nobel co-winner Susumu Kitagawa calls for funds for basic research - The Japan Times

**Professor Richard Robson accepts his Nobel Prize in Chemistry**
11 Dec
Professor Richard Robson accepts his Nobel Prize in Chemistry

**Japanese scientists Sakaguchi, Kitagawa receive Nobel prizes in Stockholm - The Mainichi**
11 Dec
Japanese scientists Sakaguchi, Kitagawa receive Nobel prizes in Stockholm - The Mainichi

**Swedish king awards American Saudi scientist, Omar Yaghi, Nobel Prize in Chemistry 2025**
10 Dec
Swedish king awards American Saudi scientist, Omar Yaghi, Nobel Prize in Chemistry 2025

**'I was motivated by solving problems the world didn't care about,' first Saudi Nobel laureate Omar M. Yaghi tells Arab News**
17 Dec
'I was motivated by solving problems the world didn't care about,' first Saudi Nobel laureate Omar M. Yaghi tells Arab News

Chemist Omar M. Yaghi poses with his award during the award ceremony on December 10, 2025, in Stockholm, Sweden. (AFP)

https://cop30.br/en

# 2025 United Nations Climate Change Conference

**The 2025 United Nations Climate Change Conference or Conference of the Parties** to the UNFCCC, more commonly known as COP30, was the 30th session of the United Nations Climate Change Conference. It was held at the Hangar Convention Centre [pt] in Belém, Brazil, from 10 to 21 November 2025.


Agreeing an explicit plan or roadmap for phasing out fossil fuels was the most contentious issue. Oil producing nations blocked any binding language so the COP30 president, André Corrêa do Lago, announced two voluntary roadmaps outside the formal UN process.

The conference text agreed after final negotiations was a compromise. Its main points were:

1. Tripling climate adaptation finance by 2035 but without clarity on who pays.
2. A Just Transition Mechanism (JTM) to support fairness in moving to a green economy.
3. Adoption of 59 global indicators for tracking adaptation progress.

Commentators considered the overall outcome to have been weak.

https://en.wikipedia.org/wiki/2025_United_Nations_Climate_Change_Conference

From 10 to 21 November, the international community gathered for the UN Climate Change Conference (COP30) in Belém, Brazil – a city located in the Amazon region, one of the planet's most vital ecosystems.

The agenda included the consistent implementation of the global energy transition, climate financing, better conservation of endangered rainforests, for example through the COP30 Action Agenda, international forest conservation, sustainable management and supply chains, and improved adaptation to unavoidable climate change.
Ten years after the Paris Agreement, the focus was also on reviewing the new nationally determined contributions (NDCs) of the signatory states for the period up to 2035, which formed an important basis for COP 30.
Here you will find the final press release from the Federal Environment Ministry and the Federal Development Ministry:

**UN Climate Change Conference in Belém: Great progress on implementation, but not enough progress in negotiations**

**https://www.international-climate-initiative.com/en/cop30**

**Given the limitations on space only links can be given in this Issue**

**'A meeting of voices': flotillas head into Belém ahead of Cop30 climate summit**
6 Nov
'A meeting of voices': flotillas head into Belém ahead of Cop30 climate summit | Cop30 | The Guardian

**What to expect at COP30**
What to expect at COP30 | McKinsey & Company

**COP30 will have to be the most important of all climate conferences, says Carlos Nobre**
12 Nov 2025
COP30 will have to be the most important of all climate conferences, says Carlos Nobre

**Five key issues at the UN climate summit in Brazil – and why they matter to you and the planet**
10 Nov
Five key issues at the UN climate summit in Brazil – and why they matter to you and the planet

**Researchers warn of the need for Brazil to turn promises into practical actions at COP30**
19 Nov
Researchers warn of the need for Brazil to turn promises into practical actions at COP30

**The goal of limiting global warming to 1.5 °C cannot be abandoned**
19 Nov
The goal of limiting global warming to 1.5 °C cannot be abandoned

**The fast-fix for global warming that the UN climate summit can't ignore**
18 Nov
The fast-fix for global warming that the UN climate summit can't ignore

**Shared from BBC: UN climate summit drops mention of fossil fuels from draft deal**
21 Nov
COP30: UN climate summit drops mention of fossil fuels from draft deal

**The Earth is getting dimmer**
18 Nov
Earth's albedo effect: How less sunlight reflection accelerates global warming

**Cop30: five reasons the UN climate conference failed to deliver on its 'people's summit' promise**
23 Nov
Cop30: five reasons the UN climate conference failed to deliver on its 'people's summit' promise

**Turkey will host the next UN climate summit – here's how it plans to use its moment in the spotlight**
26 Nov
Turkey will host the next UN climate summit – here's how it plans to use its moment in the spotlight
**What the UN climate summit achieved – and where it failed**
**Cop30: five reasons the UN climate conference failed to deliver on its 'people's summit' promise**
23 Nov
Cop30: five reasons the UN climate conference failed to deliver on its 'people's summit' promise

**COP30: Five key takeaways from a deeply divisive climate summit**
22 Nov
COP30: Five key takeaways from a deeply divisive climate summit

**The World Lost the Climate Gamble. Now What?**
24 Nov
The World Lost the Climate Gamble. Now What? | RealClearScience

**Three reasons why China wants global green leadership after Cop30 – and two reasons it doesn't**
28 Nov
Three reasons why China wants global green leadership after Cop30 – and two reasons it doesn't

**Reflections from COP30: Momentum is stronger than formal commitments suggest**
11 Dec
Driving business value through climate action and adaptation | McKinsey

https://www.mckinsey.com/capabilities/sustainability/our-insights/reflections-from-cop30-momentum-is-stronger-than-formal-commitments-suggest?stcr=590E89ABC61C4996878BEB47A9FED7FF&cid=mgp_opr-eml-alt-mst-mgp-glb--&hlkid=9fe97cb805a9486d8dcaffbf2b67b308&hctky=9170817&hdpid=7388e2aa-e904-46fa-b6bd-c804a0508e38

Family photo of high-level dignitaries attending the Belem Climate Summit (Photo: © UN Climate Change – Kiara Worth)

# COP 30 President André Corrêa do Lago

Ambassador André Corrêa do Lago, president of COP30

**André Aranha Corrêa do Lago** was born in 1959. He has a degree in Economics from the Federal University of Rio de Janeiro (UFRJ) and joined the Brazilian foreign service in 1982. As a career diplomat, he has held functions in different areas at headquarters, in Brasília: international organizations, trade promotion, protocol and energy. As adviser at the Office of the President, between 1991 and 1992, he worked in the organization of the Earth Summit (Rio-92). Abroad, he has been posted to the Brazilian Embassies in Madrid, in Prague, in Washington, in Buenos Aires and to the Brazilian Mission to the EU in Brussels……. https://cop30.br/en/brazilian-presidency


Luiz Inácio Lula da Silva, President of Brazil, welcomes UN Secretary-General António Guterres, to the High-level Segment of Belém Climate Summit (Photo: © UN Climate Change – Kiara Worth)

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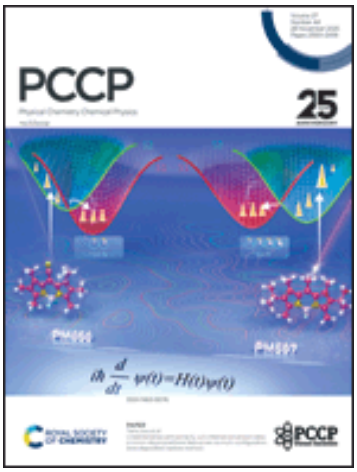


**Physical Chemistry Chemical Physics**
***Phys. Chem. Chem. Phys.***,
30 September 2025, Volume **27**, Issue 44,
Pages 23550-23560
https://doi.org/10.1039/D5CP02771C

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# Universities Research & Publications in Ireland

## University College Cork (UCC) Chemistry Research Publications June-December 2025

(* indicated beside name means contact person)

**The milk metabolome and its potential utilisation for enhanced dairy processing**

Rojas-Gómez, P., Pariyani, R., McCarthy, N. A., Bateman, L. M., O'Mahony, J. A. & O'Callaghan, T. F., International Journal of Dairy Technology. 78, 3, e70058.

Published 28 August2025

DOI: https://doi.org/10.1111/1471-0307.70058

**Abstract**

Background: Milk metabolomics has emerged as a valuable tool in dairy science, offering detailed insight into the molecular composition of milk. Understanding the milk metabolome is increasingly relevant to optimise milk quality, processability and traceability. As the dairy sector intensifies efforts to enhance product functionality and sustainability, metabolic profiling represents a promising approach to link animal physiology, farming practices and changes occurring during processing.

Aims: This review aimed to collate current knowledge regarding the intrinsic and extrinsic factors influencing the milk metabolome and, as a result, how the milk metabolome impacts milk techno-functionality. This review explores primary production variables, such as diet, breed, environment and management practices, and their effects on milk composition and processability.

Methods: A comprehensive literature review of the subject matter was conducted across relevant studies, selected based on their focus on milk metabolomics in the context of dairy production and processing. Emphasis was placed on publications from 2010 to 2025 to capture recent advances and emerging trends.

Major findings: The milk metabolome is affected by multiple intrinsic and extrinsic factors, including species, breed, diet, stage of lactation and health status, each of which influences nutritional value and processability of milk. As such, several milk metabolites, including choline, acetate and myo-inositol, have been correlated with gelation, a key techno-functional indicator. Furthermore, some metabolites have been highlighted as biomarkers of cow feeding systems such as Hippurate, a biomarker of pasture-based feeding.

Scientific and Industrial Implications: Understanding the determinants and consequences of milk metabolome variations offers new opportunities to improve dairy product quality, tailor processing conditions and support the development of farming and traceability strategies.

**The impact of sward type and inorganic nitrogen application rate on the rumen metabolome of dairy cows as determined by nuclear magnetic resonance**

Raghunath Pariyani [a], Gabriele Rocchetti [b], Aidan Lawless [c], Michael Dineen [d], Neil Maher [d], Lorraine M. Bateman [e f], Luigi Lucini [g], Tom F. O'Callaghan [a]

In: **Journal of Dairy Science.** 108, 10, p. 10714-10729 16 p.

Published 22 July 2025

DOI: 10.3168/jds.2025-26678

**Metabolic profiling of bovine colostrum: unravelling the influences of diet and seasonality on functional dairy components**

Raghunath Pariyani [a], Gabriele Rocchetti [b], Aidan Lawless [c], Michael Dineen [d], Neil Maher [d], Lorraine M. Bateman [e f], Luigi Lucini [g], Tom F. O'Callaghan [a]

**Food Chemistry** Volume 493, Part 3, 30 November 2025, 145900

Published 30 November 2023

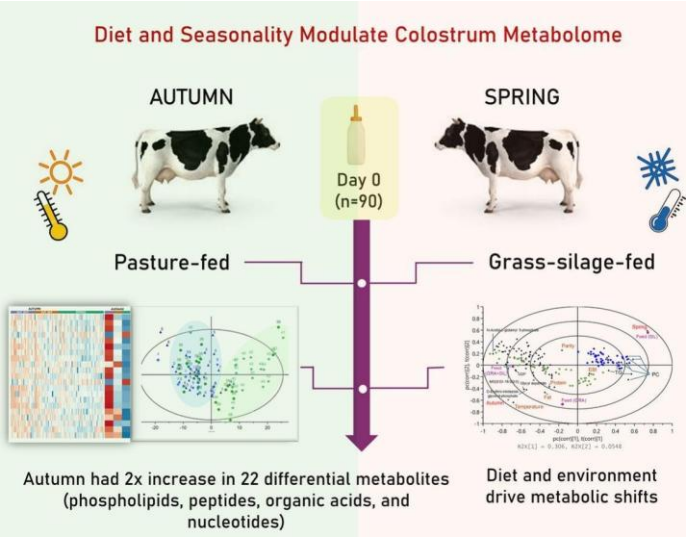
DOI: https://doi.org/10.1016/j.foodchem.2025.145900

**Abstract**

Abstract

Bovine colostrum-based functional foods are gaining recognition for their potential beneficial roles in human health. However, while macronutrient variability has been extensively studied, the impact of seasonality and diet on bioactive metabolome profile of colostrum remains poorly understood. This study employs UHPLC-HRMS to characterize the metabolic profile of colostrum from dairy cows, calving in autumn or spring under distinct environmental and dietary conditions. An untargeted metabolomic analysis demonstrated distinct seasonal variations, with autumn-derived colostrum exhibiting a two-fold increase in 22 metabolites, including phospholipids, bioactive peptides, organic acids, and nucleotides. Glycyl aspartate and D-erythro-imidazole-glycerol-phosphate emerged as key biomarkers distinguishing seasonality of colostrum. Pre-partum diet and environmental temperature were correlated with metabolic differences, whereas parity and genetic merit, represented by the economic breeding index, had minimal influence. These findings highlight the impact of seasonality on the colostrum metabolome, providing novel insights for the future development of colostrum-based functional foods.

**Graphical Abstract**




**Impact of Permeation Enhancers on the Release of Insulin from Tablets in Biorelevant Media**

Andrew Fagan, Lorraine M. Bateman, Abina M. Crean, Joseph P. O'Shea, Lynne S. Taylor*

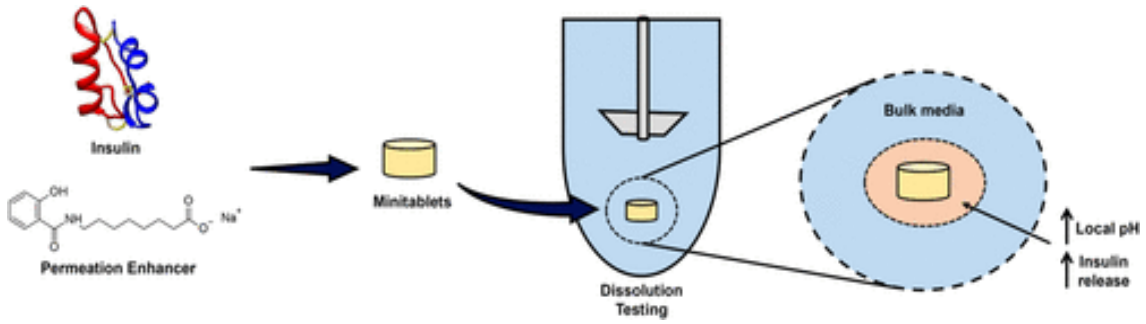
***Mol. Pharmaceutics*** 2025, 22, 7, 3999–4008
Published 17 June 2025
DOI: https://doi.org/10.1021/acs.molpharmaceut.5c00249

**Abstract**

The use of chemical permeation enhancers (PEs) to improve the permeation of peptides across gastric and intestinal epithelia has proven an effective strategy in the development of oral dosage forms of peptides. However, there remains a poor understanding of how the presence of PEs impacts the dissolution characteristics of oral formulations containing peptides, nor is it known how the complex composition of biological media can influence their behaviour *in vivo*. This investigation sought to examine the effect of two widely studied PEs, sodium caprate (C10) and salcaprozate sodium (SNAC), on the release behaviour of a model peptide, insulin, from minitablets in a variety of biorelevant media. First, the equilibrium solubilities of insulin, C10, and SNAC were determined in simulated gastric and intestinal media. Insulin, C10, and SNAC all displayed pH-dependent solubility across a physiologically relevant range of pH conditions. Moreover, at high concentrations, C10 was found to overwhelm the buffer capacity of the simulated media, increasing the pH of fasted state simulated intestinal fluid (FaSSIF) from 6.5 to 9.0, fed state simulated intestinal fluid (FeSSIF) from pH 5.0 to 8.8 and fasted state simulated gastric fluid (FaSSGF) from pH 1.6 to 9.2. Similarly, SNAC caused an increase in the pH of FaSSIF from 6.5 to 7.9, FeSSIF from pH 5.0 to 7.7, and FaSSGF from pH 1.6 to 7.6. Relative to in simulated intestinal media, the solubility of insulin was found to increase significantly in media at pH representative of saturated C10 and SNAC solutions, increasing from 0.1 mg/mL in blank FaSSIF to 14.0 mg/mL in phosphate buffer at pH 7.6 and to 23.7 mg/mL in phosphate buffer at pH 9.2, suggesting that the presence of C10 and SNAC at high concentrations could have a considerable favourable impact on insulin solubility. Furthermore, the release profiles of insulin from

minitablets containing C10 and SNAC were investigated in each of the biorelevant media and compared with the release profiles of insulin from blank minitablets in the absence of PEs. Insulin release from the blank minitablets was found to be media dependent, following an apparent solubility trend. Complete release of insulin was observed in simulated gastric media; however, only between 67 and 82% release was observed in the simulated intestinal media. On the other hand, on the addition of C10 and SNAC to the formulation, greater than 90% release was observed across all media investigated. This difference in release behaviour was determined to be caused by an increase in pH at the surface of the minitablets due to the presence of high local concentrations of C10 and SNAC, respectively, as confirmed by a change in colour of a universal indicator solution. These findings offer a key insight into the influence that C10 and SNAC have on the dissolution characteristics of insulin from an oral dosage form in a variety of simulated gastric and intestinal media.

**Graphical Abstract**




**Direct compression peptide tablets: insights into the importance of permeation enhancer processibility and peptide stability**

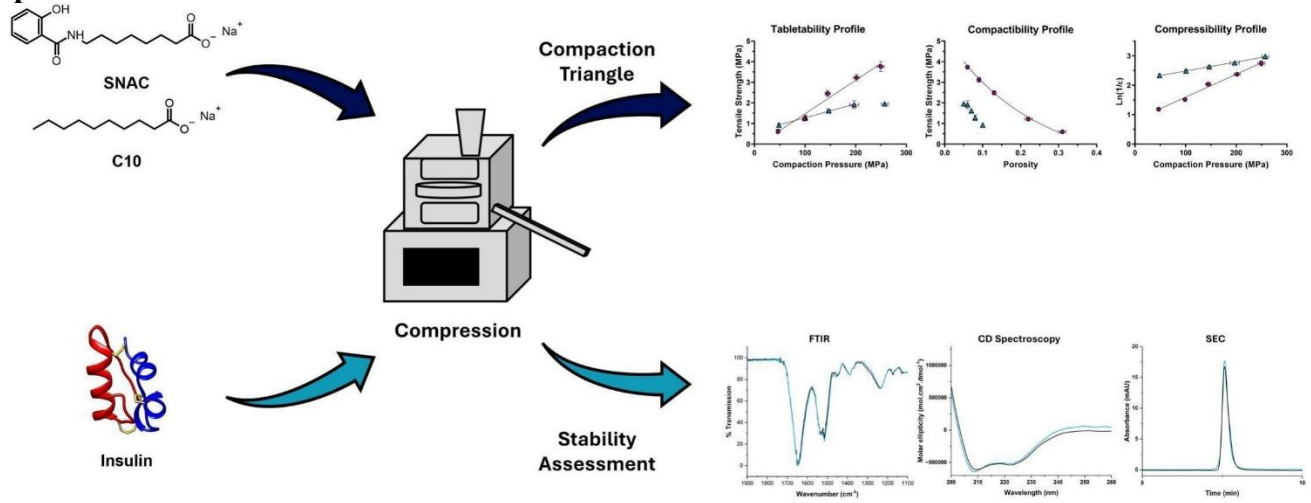
A. Fagan, L. M. Bateman, M. O'Mahony, A. M. Crean, J. P. O'Shea

**International Journal of Pharmaceutics** Volume 685, 30 November 2025, 126257
Published 20 November 2025
DOI: https://doi.org/10.1016/j.ijpharm.2025.126257

**Abstract**

Much of the remarkable advancements in oral peptide delivery have been achieved through the use of chemical permeation enhancers, such as sodium caprate (C10) and salcaprozate sodium (SNAC). However, co-formulation of peptides with permeation enhancers in an oral product introduces several processing and formulation challenges which require further investigation. This investigation sought to rationalise the development of direct compression insulin compacts, using C10 and SNAC as model permeation enhancers, respectively. The physical and mechanical properties of C10 and SNAC were first assessed to evaluate their suitability for processing via direct compression. Overall, C10 displayed passable flow character, however, poor tabletability, compactibility and compressibility profiles were obtained. SNAC, on the other hand, exhibited superior compaction properties, though its flow character was poor. Improvement in the compaction properties of both materials were observed on addition of commonly used direct compression excipients microcrystalline cellulose (MCC) and polyvinylpyrrolidone (PVP) K30, and formulations consisting of 72 % C10/ SNAC, 20 % MCC, 5 % PVP and 3 % insulin were selected for production of direct compression compacts at compaction pressures of 100 and 200 MPa. The compacts produced exhibited complete release within 30 min, and this release behaviour was not significantly affected by the compaction pressure used. Furthermore, the stability of insulin after compaction at 200 MPa, and on storage of the compacts at 40°C/ 75 % RH for 1 month was assessed. Insulin displayed excellent physical stability to mechanical stress, where no evidence of unfolding or aggregation was identified. Moreover, on storage of the formulations at accelerated stability conditions for 1 month, a significant reduction in overall deamidation and aggregation tendency was observed on blending of insulin within the direct compression formulations in comparison to raw insulin material stored under the same conditions, independent of the permeation enhancer used. These results offer a key insight into the influence that formulation components have on the manufacturability of direct compression peptide formulations and the stability of the peptide during compaction and storage.

**Graphical Abstract**

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**Thermodynamic modeling of countercurrent chemical looping reverse water gas shift process for redox material screening**

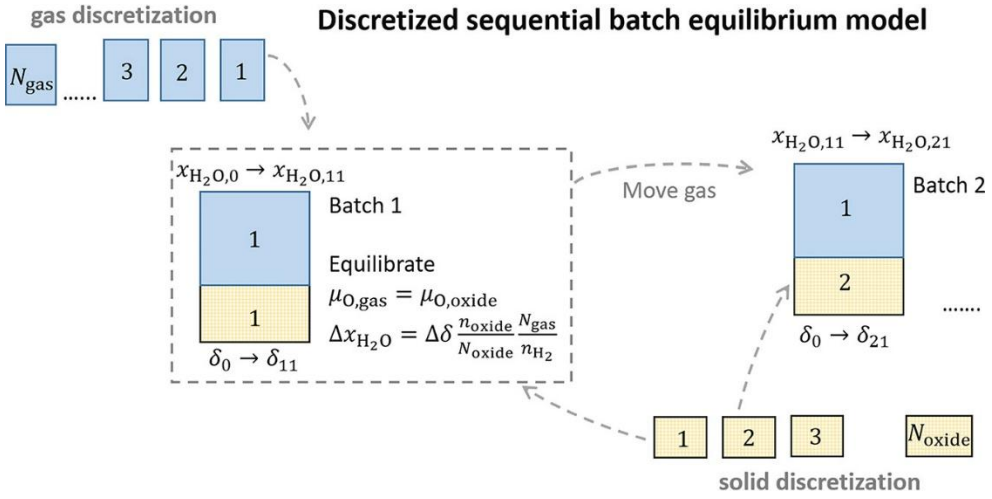
B. Bulfin [a]*, R. Ghotkar [b], A. Lidor [b]*

**Chemical Engineering Journal** Volume 525,
Published 1 December 2025, 170505
DOI: https://doi.org/10.1016/j.cej.2025.170505

**Abstract**

The reverse water gas shift (RWGS) reaction is a key pathway for $CO_2$ utilization, particularly within Power-to-X process chains aimed at sustainable fuel and chemical production. Countercurrent chemical looping (CL-RWGS) using non-stoichiometric oxides can overcome equilibrium limitations of conventional RWGS reactors, enabling significantly higher $CO_2$ conversions. However, modelling the limiting performance of such systems is challenging due to their multiphase nature and coupled spatial and temporal variation in chemical composition. In this work, we present a discretized batch equilibrium model that simulates CL-RWGS reactors as a series of localized equilibrium exchanges between gas and solid elements. The model is numerically stable, computationally efficient, and free of kinetic source terms, making it well-suited for parametric studies and system-level integration. It is validated against established convection–diffusion models and shown to predict reasonable upper bounds on experimental results. Application of the model to a range of oxygen carrier materials identifies cerium–zirconium solid solutions, particularly $Ce_{0.80}Zr_{0.20}O_2$, as a promising class offering superior oxygen storage characteristics compared to state-of-the-art $La_{0.6}Sr_{0.4}FeO_3$. This framework provides a robust platform for materials screening, reactor sizing, and performance optimization in chemical looping systems. The model implementation is available as open-source software to support further research and development.

**Graphical Abstract**



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**A Nickel Telluride Electrochemical Sensor for the Detection of the Antibiotic Ronidazole**

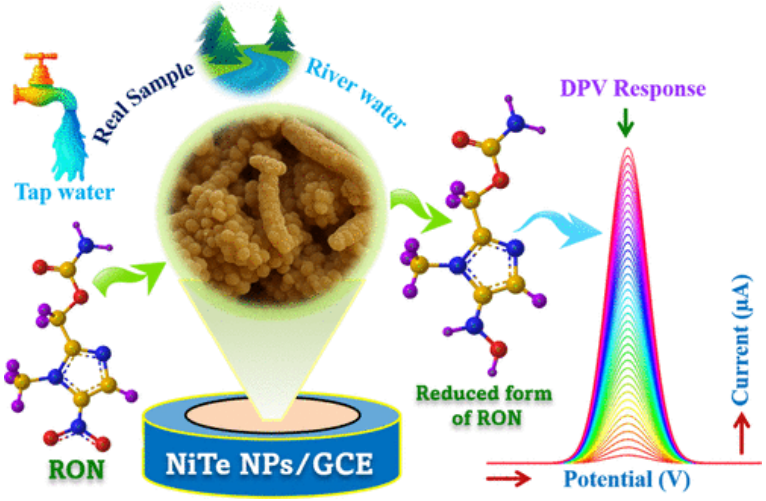
Tara Barwa, Ramaraj Sukanya, Thamaraiselvi Kanagaraj, Gillian Collins, Yiran Luo, Eithne Dempsey, Raj Karthik, Jae-Jin Shim, Carmel B. Breslin*

***ACS Appl. Nano Mater***. 2025, 8, 42, 20523–20533
12 October 2025
DOI: https://doi.org/10.1021/acsanm.5c03794

**Abstract**

The widespread use of nitroimidazole antibiotics such as ronidazole (RON) in human and veterinary medicine raises concerns about environmental persistence and antimicrobial resistance. Sensitive detection of trace RON in water is therefore essential. Here, we report for the first time, nickel telluride nanoparticles (NiTe NPs) as an electrochemical sensor specifically designed for RON detection. NiTe, a transition metal chalcogenide with high conductivity and electrocatalytic activity, was synthesized via a simple hydrothermal method and characterized by X-ray diffraction, field-emission scanning electron microscopy, transmission electron microscopy, and X-ray photoelectron spectroscopy. When drop-cast on a glassy carbon electrode, the NiTe NPs significantly enhanced electron transfer and promoted efficient electrochemical reduction of RON. The sensor achieved a detection limit of 1.5 nM, a wide linear range of 0.01–270 μM, and a sensitivity of 0.489 μA $\mu M^{-1}$ $cm^{-2}$. It also displayed excellent selectivity against common interferents and maintained stability and reproducibility during extended testing. Application to spiked tap and river water confirmed accurate recovery. This work highlights NiTe as an underutilized telluride-based material and establishes its novel application in the environmental monitoring of antibiotic contaminants, addressing a critical gap in electrochemical sensing research.

**Graphical Abstract**

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**Formation of the E-isomer as an impurity in the optimized flow synthesis of a Z-α-thio-β-chloroacrylamide; E/Z photoisomerization in batch and flow, and solid state characterization of both isomers**

Olga C. Dennehy, , Denis Lynch, , U. B.Rao Khandavilli, , Simon E. Lawrence, , Stuart G. Collins, , Anita R. Maguire, , Humphrey A. Moynihan

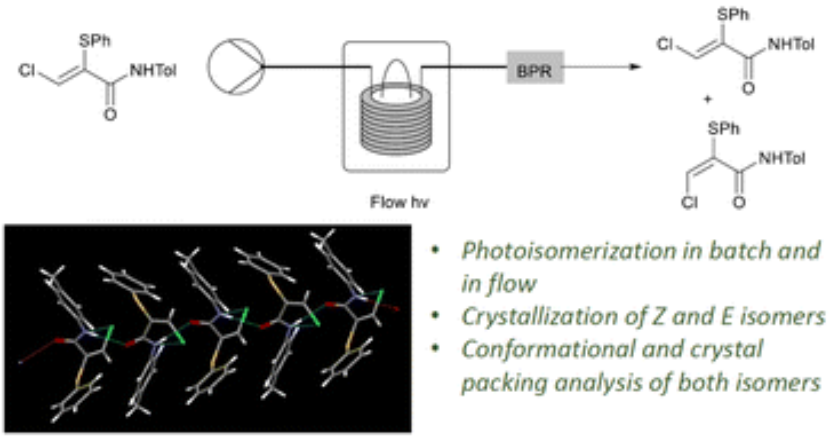
***React. Chem. Eng.***, 2025,**10**, 1878-1886
Published 23 July 2025
DOI: https://doi.org/10.1039/D5RE00137D

**Abstract**

*N*-(4-Methylphenyl)-*Z*-3-chloro-2-(phenylthio)propenamide (***Z*-3**), which is valuable as a reactive substrate for a range of synthetic transformations, can be obtained by a three-step process involving both batch and flow methodologies. Compound ***Z*-3** was isolated as a crystalline material of high purity, however, the *E*-isomer, ***E*-3**, was found to form in solid samples of ***Z*-3** material during storage. Increased ratios of ***E*-3** and pure isolated samples were obtained by photoisomerization in batch and flow modes, with the flow process being optimal in terms of process time. Crystal structure analysis of both the *Z* and *E* isomers highlighted

key differences in molecular conformations and supramolecular interactions with greater deviation from planarity evident in ***E*-3** relative to ***Z*-3**. Analysis of samples of ***Z*-3** by PXRD and DSC after recrystallization from a variety of solvents gave data consistent with the determined crystal structure of ***Z*-3**.

**Graphical Abstract**

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**Isothioureas as Coupling Partners in P–S Bond Formation through Cross-Dehydrogenative Coupling**

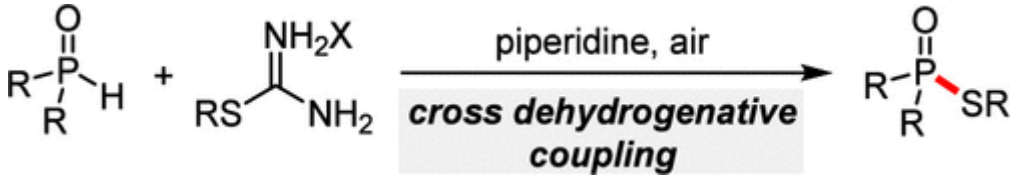
Eimear Courtney, Gian L. Reber, Nikita Liasiuk, David J. Jones*

*Org. Lett.* 2025, XXXX, XXX, XXX-XXX
Published 19 December 2025 (Subscription)
DOI: https://doi.org/10.1021/acs.orglett.5c04813

**Abstract**

Isothioureas have been demonstrated as practical sulfur donors for mild, one-pot P–S bond formation. Treatment with piperidine releases thiolate, which undergoes aerobic oxidation to the corresponding disulfide. Subsequent cross-dehydrogenative coupling with phosphine oxides affords phosphinothioates and related compounds in high yields. The method proceeds under air, tolerates diverse organophosphorus functional groups, and avoids malodorous reagents or external oxidants, providing an efficient and operationally simple route to P–S-containing organophosphorus compounds.

**Graphical Abstract**

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**Operando Acoustic Spectroscopy for Optimizing Gas Evolution In Hydrogen Evolution Reaction and the Oxygen Evolution Reaction Processes**

Christopher Kent, Alex Knowles, Ailbe Ó Manacháin, Colm O'Dwyer, Dara Fitzpatrick*

**ChemElectroChem** Volume12, Issue19 October 3, 2025 e202500215
Published 3 October 2025
DOI: https://doi.org/10.1002/celc.202500215

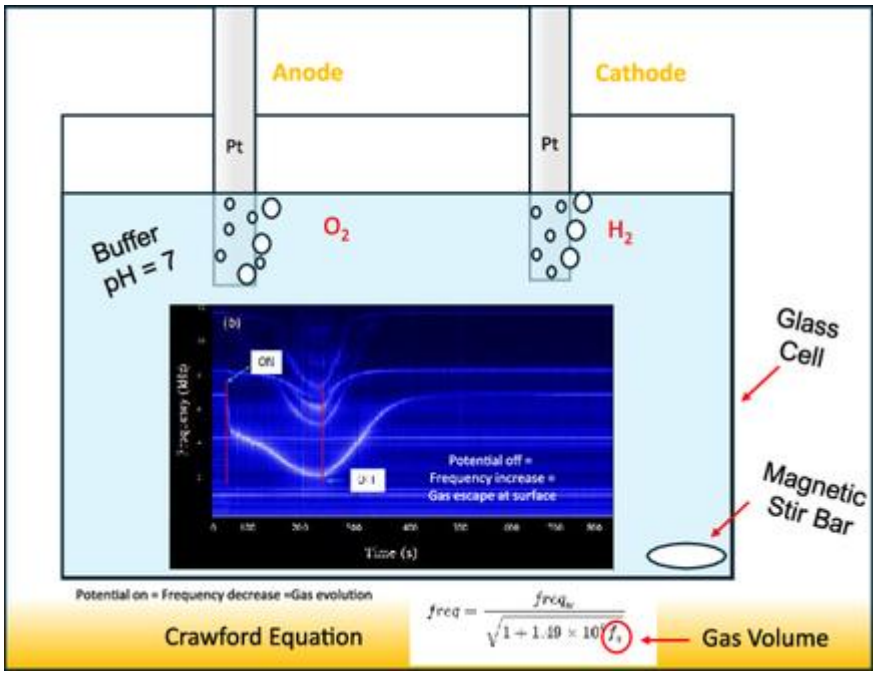
**Abstract**

The use of earth-abundant materials for novel electrodes for solar-driven electrolysis will play a significant role in the future production of hydrogen as a green energy source. The choice of electrolyte will play a major role in how efficient and stable future photoelectrochemical cells (PEC) operate. A new approach to determining PEC efficiency using broadband acoustic resonance dissolution spectroscopy (BARDS) is investigated to analyze the real-time production of hydrogen and oxygen at platinum electrodes in different electrolyte solutions. The parameters investigated include concentration of electrolyte, surface area of the electrode, and the potential applied to the cell. Herein, the suitability of neutral buffer as an electrolyte on a par with either acid or basic electrolytes is shown. This finding allows for the potential design of solar to

hydrogen electrolysers which can operate under mild, neutral, and stable conditions using earth-abundant materials for hydrogen production. It is also shown how BARDS can readily visualize and track gas evolution in real-time and in situ in an open system without the need for gas collection. It is anticipated that the technique can be utilized in the future evaluation of newly developed electrode materials in terms of efficiency, stability, and life span.

**Graphical Abstract**

The graphic enables the visualization of the changes in audible frequency within the cell when the potential is applied at 30 s. The change in frequency is related to the gas volume produced during electrolysis. The gas changes the compressibility of the electrolyte slowing down the speed of sound.

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**Ammonia Sensing via Pseudo Molecular Doping in UV-Activated Ambipolar Silicon Nanowire Transistors**

Vaishali Vardhan, Subhajit Biswas*, Leonidas Tsetseris, Sayantan Ghosh, Ahmad Echresh, S. Hellebust*, Rene Huebner, Yordan M. Georgiev, Justin D. Holmes*

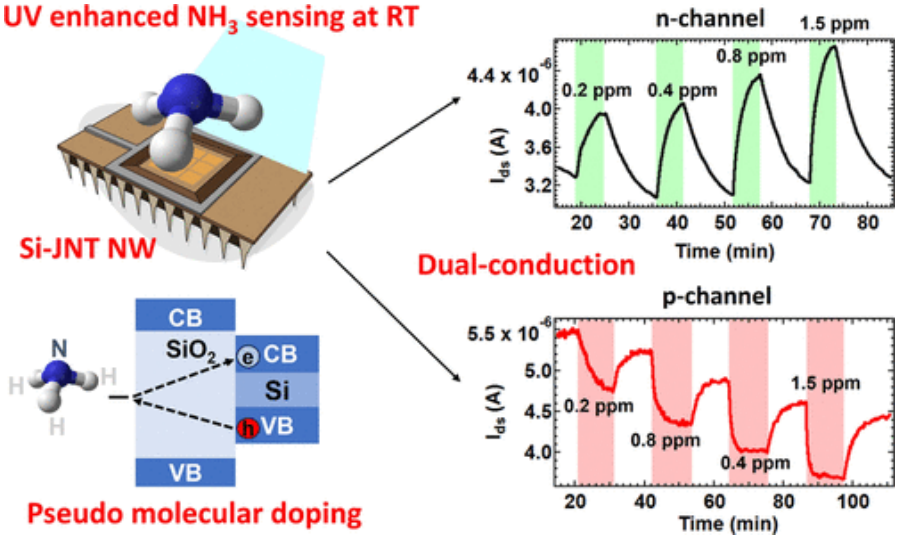
***ACS Appl. Mater. Interfaces*** 2025, 17, 31, 44686–44698
Published 24 July 2025
DOI: https://doi.org/10.1021/acsami.5c08140

**Abstract**

The potential of adsorbed gaseous molecules to create shallow electronic states for thermally excited charge carrier transport and to engineer silicon transistor properties has been largely overlooked compared to traditional substitutional impurities. This paper successfully modifies the electrical properties of ambipolar silicon junctionless nanowire transistors (Si-JNTs) using the reducing properties of ammonia ($NH_3$) for selective detection. Physisorption of $NH_3$ induces a dual response in both *p*- and *n*-type conduction channels of ambipolar Si-JNTs, significantly altering current and key parameters, including the "on" current ($I_{on}$), threshold voltage ($V_{th}$), and mobility (μ). $NH_3$ interaction increases conduction in the *n*-channel and decreases it in the *p*-channel, acting as an electron donor and hole trap, as supported by Density Functional Theory (DFT) calculations. This provides a pathway for charge transfer and ″pseudo″ molecular doping in ambipolar Si-JNTs. This $NH_3$-mediated molecular doping and conduction modulation in Si transistor enabled, for the first time, the electrical detection of gaseous $NH_3$ at room temperature across a wide concentration range (200 ppb to 50 ppm), achieving high sensitivity (200 ppb) and precise selectivity under ultraviolet (UV) light. UV illumination dynamically modulates current and reveals distinct sensing features in the *p*- and *n*-channels of the dual-responsive Si-JNTs. The ambipolar Si-JNT sensor exhibits a fast response time of 1.91 min for 0.8 ppm of $NH_3$ in the hole conduction channel and a high sensitivity of 80% for 0.8 ppm of $NH_3$ in the electron conduction channel. This dual-channel approach optimizes sensor

performance by leveraging the most responsive parameters from each channel. Furthermore, the ambipolarity of Si-JNTs broadens the parameter space for developing a multivariate calibration model, enhancing the selectivity of Si-JNT sensors for $NH_3$ detection.

**Graphical Abstract**

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**Dual-functionality of NiSe2-CoSe2 nanowires for electrochemical charge storage and efficient thermal energy conversion**

Rupa Ranjani Palanisamy, N. Padmanathan, Anjali Ashokan, Amit Tanwar, Subhajit Biswas, Justin D. Holmes, Kafil M. Razeeb*

**Journal of Energy Storage** Volume 121, 15 June 2025, 116568
Published 15 June 2025
DOI: https://doi.org/10.1016/j.est.2025.116568

**Abstract**

Thermo-electrochemical cell coupled with an electrochemical energy storage device creates a comprehensive harvesting system that can convert thermal energy into electrical energy and store it. Thus, the development of electrodes that demonstrate high efficiencies in electrochemical and thermoelectric properties is crucial, as they serve as the fundamental components in energy conversion and storage systems. This study presents the synthesis of NiSe2-CoSe2 (NCS) nanowires on activated carbon cloth (ACC) substrate, for enhanced electrochemical charge storage and ionic-thermoelectric applications. Comparative analysis demonstrates that NCS/ACC electrodes significantly outperform monometallic selenides in both electrochemical performance and thermoelectric applications. The NCS/ACC electrode revealed a maximum charge storage capacity of 112 mA hg−1 at a current density of 1 A g−1. Utilizing 1 M NaOH as an aqueous electrolyte, the NCS/ACC system showcases its pioneering role in thermo-electrochemical cell (TEC), opening avenues for efficient heat-to-electricity conversion. The NCS/ACC-based TEC delivered a Seebeck coefficient of −3.4 mV K−1 and thermal charge storage of −1.02 J. These findings reveal the dual functionality of nickel cobalt selenides, offering promising solutions for thermal energy harvesting and storage in electrochemical systems.

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**Achieving Chemical Recognition, Recycling, and Circularity With Radical Nanostructures**

Arkaprava Das, Ewa Malgorzata Nowik-Boltyk, Tobias Junghöfer, Elke Nadler, Farzan Gity, Paul K. Hurley, Zhimin Yang, Andrzej Rajca, Francesco Tavanti, Arrigo Calzolari, Maria Benedetta Casu

**Advanced Functional Materials**. 35, 37, e04323.
Published 11 Sep 2025
DOI: https://doi.org/10.1002/adfm.202504323

**Abstract**

Although still in its early stages, the production and investigation of 3D magnetic nanostructures signify a major advancement in both fundamental research and practical applications, with immense potential for next-generation technologies. Here, for the fabrication of the 3D nanostructures, an innovative approach

selecting a S = 1/2 4,4′-dicyano-2,2′-biphenylene-fused tetrazolinyl radical is adopted, chemically stable and thermodynamically robust, allowing thin film processing and growth. Interdigitated gold-silicon dioxide hybrid surfaces are used as substrates since gold and silicon dioxide are two technologically relevant materials. The ability to: (1) grow radical nanostructures are demonstrated that retain their magnetic properties, (2) adjust their morphology and size, (3) selectively remove nanostructures from specific substrate regions using distilled water, and (4) return substrates to their pristine condition, making them reusable after washing. This research not only aims to produce innovative 3D nanostructures but also strives to improve efficiency and minimize consumption, aligning with the principles of circular economy. This approach is particularly beneficial for expensive materials, such as gold, or patterned hybrid substrates that require complex fabrication techniques.

**Atomic-Scale Defects and Edge Engineering of ZrSe2Nanosheets: Correlated Microscopy, Spectroscopy and DFT Study with Implications for Quantum Device Applications**

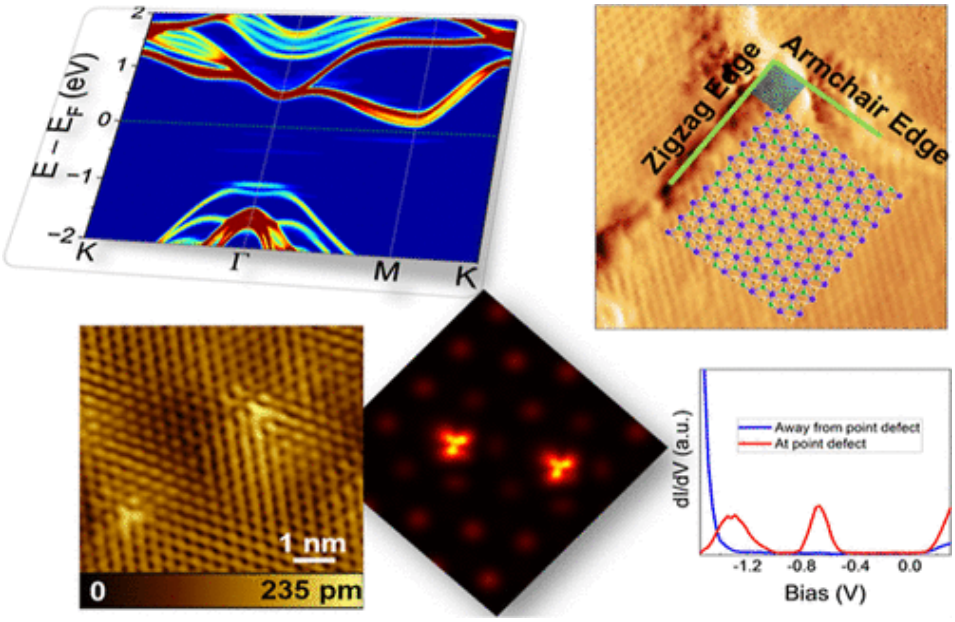
Sharieh Jamalzadeh Kheirabadi*, Luca Persichetti, Lida Ansari, Gabriele Anselmi, Paul K. Hurley, Luca Camilli*, Farzan Gity*

***ACS Appl. Nano Mater.*** 2025, 8, 43, 20848–20857
Published 21 October 2025
DOI: https://doi.org/10.1021/acsanm.5c03451

**Abstract**

We present a comprehensive study of the atomic-scale electronic behavior of $ZrSe_2$, focusing on the effects of intrinsic point defects, grain boundaries, and edge configurations. Using a combination of low-temperature scanning tunnelling microscopy/spectroscopy (STM/STS) and density functional theory (DFT), we identify and characterize the spectroscopic fingerprints of various intrinsic point defects, including vacancies, antisites, and interstitials, and reveal how these features perturb the band edges or introduce in-gap states. These defect-induced features are shown to significantly influence the local electronic properties of $ZrSe_2$. Our analysis of grain boundaries identifies shear-type interfaces that shift the Fermi level without introducing deep in-gap states, thereby preserving the semiconducting character of pristine $ZrSe_2$. In contrast, the edge configuration has a pronounced effect on the electronic structure, with armchair and zigzag edges exhibiting distinctly different behaviors. While the former is characterized by a prominent peak near the valence band edge, indicating the presence of edge-localized states and a clean semiconducting character, the latter instead introduces a significant density of states at midgap and within the upper half of the bandgap. These findings offer atomic-level insights into the interplay between defects, edge chemistry, and electronic behavior in $ZrSe_2$, establishing a framework for defect- and edge-state engineering in two-dimensional semiconductors for nanoelectronics and quantum device applications.

**Graphical Abstract**



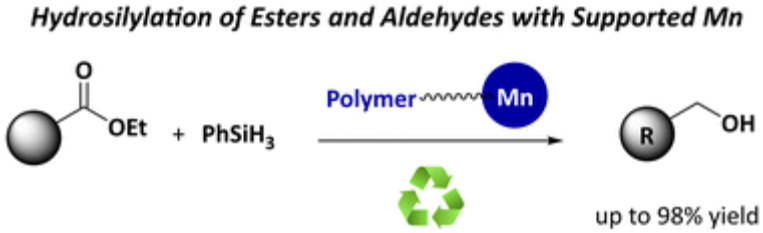
**Polymer-supported manganese-catalysed transformation of esters and aldehydes to alcohols**

V. Kishore Kumar Pampana, [a] Si Lok Ko,[a] Eimear Courtney,[a] Benjamin R. O'Donoghue, [a] David J. Jones, [a] Simon K. Beaumont, [b] Davinder Singh,[c] Charlotte Willans, [d] Ian J. S. Fairlamb, *[d] Jason M. Lynam *[d] and Gerard P. McGlacken *[a]

***Catal. Sci. Technol.***, 2026
Published 5 December 2025
**DOI:** https://doi.org/10.1039/D5CY01174D

**Abstract**
Compared to precious metals, manganese has emerged as a more earth-abundant and potentially safer metal to catalyse important chemical transformations. In contrast to homogeneous Mn catalysts, the use of heterogeneous Mn catalysts, is rare. Herein we describe the preparation of a Mn catalyst supported on a simple phosphine-containing polymer, that efficiently provides alcohols from esters and aldehydes, and facilitates the reduction of amides. Surprisingly, the catalyst gave improved yields upon recycling, which prompted a short study into the structural and oxidative changes of the catalyst using SEM-EDX and XAFS. Breakage of the microspheres and increased Mn oxidation states were observed upon recycling. Ultimately a priming procedure was developed that enabled direct procurement of an active and viable catalyst system.

**Graphical Abstract**



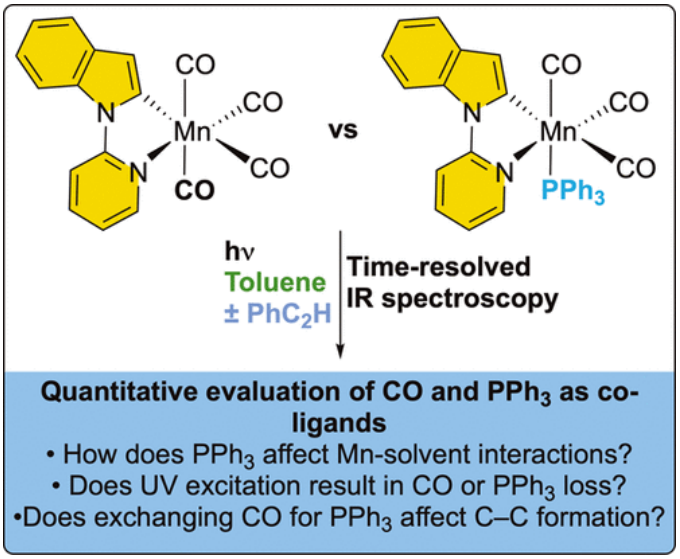

**Probing Mn Precatalyst Activation through Time-Resolved Spectroscopy: A Quantitative Evaluation of the Effects of CO and PPh3 as Coligands on Ultrafast Dynamics and C–C Bond Formation**

Benjamin R. O'Donoghue, Stefan Flesch, Eimear Courtney, Shweta Choudhary, Jonathan B. Eastwood Katrina Mackey, Leticia M. Pardo. Ian P. Clark, Partha Malakar, Gregory M. Greetham, Adrian C. Whitwood, Richard J. Gammons, Gerard P. McGlacken*, Ian J. S. Fairlamb*, Jason M. Lynam*

***Inorg. Chem.*** 2025, 64, 33, 16768–16780
Published 12 August 2025
DOI: https://doi.org/10.1021/acs.inorgchem.5c01443

**Abstract**
An investigation into the effect of a phosphine coligand on the activation of precatalysts for manganese-catalyzed C–H bond functionalization is reported. Although simple precatalysts $[MnBr(CO)_5]$ and $[Mn_2(CO)_{10}]$ are used extensively in these reactions, there is a dearth of alternate precatalyst structures, which has hindered the development of structure–activity relationships. In this work, the effect of substituting a carbonyl ligand for a phosphine ligand is reported. Investigation of the photochemical activation of the precatalyst *fac*-$[Mn(inpy)(CO)_3(PPh_3)]$ (inpy = cyclometalated 1-(pyridin-2-yl)-1*H*-indole) **3** by time-resolved infrared spectroscopy (TRIR) reveals that light-induced dissociation of a CO ligand occurs preferentially over loss of the phosphine. The ultrafast dynamics of the initially formed solvent complex $[Mn(inpy)(CO)_2(toluene)(PPh_3)]$ **9** are described, as is the slower substitution of the coordinated solvent by added pyridine to give $[Mn(inpy)(CO)_2(NC_5H_5)(PPh_3)]$ **10**. Replacing the pyridine with phenylacetylene again results in the substitution of the metal-bound toluene to give the alkyne complex $[Mn(inpy)(\eta^2\text{-}HC_2Ph)(CO)_2(PPh_3)]$ **12**. The alkyne undergoes a migratory insertion reaction into the Mn–C bond on a microsecond time scale with a very similar first-order rate constant to $[Mn(inpy)(CO)_4]$, **2**, demonstrating that this key step in Mn-catalyzed reactions is not affected by the presence of the phosphine ligand.

**Graphical Abstract**

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**Ultrasensitive multiplexed detection of cancer biomarker proteins using SPR imaging**

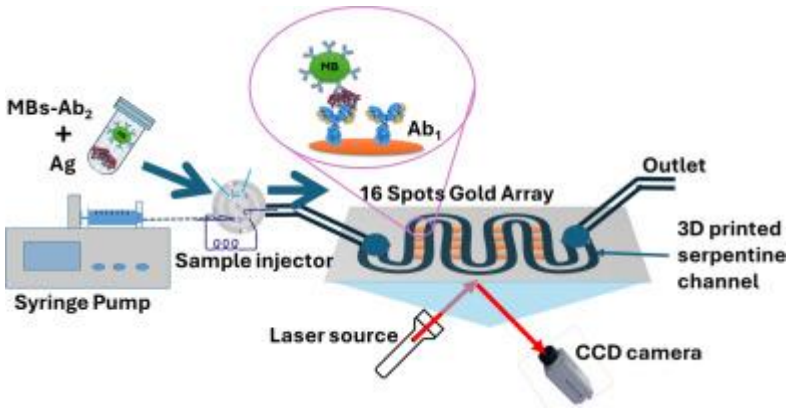
Gulsum Ucak-Ozkaya [a], M. Zeki Durak [b c], Mohamed Sharafeldin [d], James F. Rusling [e f g h]

**Microchemical Journal** Volume 216, September 2025, 114562
Published
DOI: https://doi.org/10.1016/j.microc.2025.114562

**Abstract**

While cancer is one of the leading causes of death worldwide, its diagnosis is still lagging behind lengthy procedures that are both expensive and lack specificity. Herein, we investigate the use of surface plasmon resonance imaging (SPRi) for the multiplexed detection of four cancer biomarkers associated with aggressive prostate cancer. This biomarker panel include prostate-specific antigen (PSA), insulin-like growth factor I (IGF-I), vascular endothelial growth factor (VEGF-D), and monocyte surface antigen (CD14). 16 spots SPR chip array functionalized with primary antibodies ($Ab_1$) against the selected biomarkers, and bovine serum albumin (BSA) as a negative control, was housed in a 3D printed microfluidic channel to control the delivery of sample and reagents. Antigens were first captured, offline, on magnetic beads (MBs) labelled with secondary antibodies ($Ab_2$), and SPRi signals were collected and analyzed while flowing the MBs on the chip. This enabled the collection of real-time data for the association between antigens, captured on MBs, and $Ab_1$ immobilized on the SPR chip, and quantification of the target antigens after reaching equilibrium. This assay was capable of achieving dynamic ranges of 10 fg/mL to 100 pg/mL for PSA, 1 to 100 pg/mL for CD14, 1.1 to 110 pg/mL for IGF-I, and 0.5 to 100 pg/mL for VEGF-D. The multiplexed assay limit of detection (LOD) was found to 7.6 pg/mL for CD14, 5.8 pg/mL for IGF-1, and 5.3 pg/mL for VEGF-D with dynamic ranges of four orders of magnitude up to 125 pg/mL. While we could not apply this system in the analysis of real samples, it demonstrates a high throughput analytical approach with strong potential for identifying prostate cancer at an early stage. The system offers high sensitivity (down to few pg/mL) multiplexed detection of a selected panel of prostate cancer biomarkers.

**Graphical Abstract**

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**A Mobile Analytical Chemistry Workstation with a C4D Sensor for Rapid Detection of Organophosphates Under Field Conditions**

Yineng Wang1,2,3, Xi Cao 1,2,3, Walter Messina1,2,3, Anna Maria Hogan 1,2,3, Justina Ugwah 1,2,3 Eric Moore 1,2,3,*

**Sensors** 2025, 25(11), 3517
Published 3 June 2025
DOI: https://doi.org/10.3390/s25113517

**Abstract**

Timely detection of organophosphates in outdoor environments remains a critical challenge for forensic and environmental monitoring. Traditional methods often require transporting samples to centralised laboratories, delaying essential response actions. In this study, we present a novel mobile analytical chemistry workstation that integrates capillary electrophoresis (CE) with capacitively coupled contactless conductivity detection (C4D) on low-cost polydimethylsiloxane (PDMS) microfluidic chips, enabling rapid and accurate on-site analysis of organophosphates. The system features a streamlined workflow that includes in-field sample collection, microfluidic analysis, and the wireless transmission of data to a central command centre for immediate decision-making. The detection system demonstrates a linear range of 2.5 mM to 20 mM for dimethyl methylphosphonate (DMMP), with an estimated limit of detection (LOD) of 2.5 mM. We evaluate the feasibility of combining CE and C4D under field conditions, highlighting both the strengths and limitations of this integrated platform.

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**Chromatography in the chemical analysis of molecular substances: chemical substance predication and mereology**

Humphrey A. Moynihan

**Foundations of Chemistry** Volume 27, pages 357–372, (2025)
Published 20 September 2025
DOI: https://doi.org/10.1007/s10698-025-09554-0

**Abstract**

High-Performance Liquid Chromatography (HPLC) is widely used in the pharmaceutical and fine chemical industries to establish chemical substance identity. HPLC is an analytical chromatographic technique, i.e., it is used to establish chemical substance identity and purity. Preparative chromatography is used to isolate usable quantities of chemical substances. A sample which gives rise to a chromatographic peak under specified conditions can be said to possess the property of containing the particular chemical substance to which that peak can be assigned. The chemical substance could be said to be part of the analysed sample in the mereological sense. A concern is raised by the possibility noted by Harré and Llored with respect to mereology, that it may be fallacious to infer that the substantive products of an analytical procedure are parts of the substance on which the procedure was performed. Instances arising from preparative chromatography show that that possibility exists, however, the value of analytical chromatography to chemical practice is that the chemical substances which are separated are considered as having being part of the sample analysed. Spatial and temporal aspects of chromatographic assignment of chemical substance properties are considered. A chromatographic peak could also be regarded as an ‘affordance’, i.e., arising from the interaction of the apparatus and the world. Consideration of chromatography in mereological terms is also discussed with relation to issues such as parthood, remainder and relation to concepts of purity, and the applicability of the concepts of fusion and disjointness.

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**Porous carbon nanotube electrodes in 3D printed symmetric supercapacitors with stable electrochemical response**

Siobhán Breen [a], Vijaykumar Jadhav [a], Colm Glynn [a b], Colm O'Dwyer [a c d]

**Electrochemistry Communications** Volume 177, August 2025, 107988
Published August 2025
DOI: https://doi.org/10.1016/j.elecom.2025.107988

**Abstract**

Multi-walled carbon nanotube porous networks offer excellent capacitance and stable electrochemical response in 3D printed symmetric supercapacitors made by fused deposition modelling of conductive thermoset polylactic acid (PLA) current collectors. These electrodes show a stable voltammetric and galvanostatic response with an aqueous KOH electrolyte, without any pretreatment of the graphite-impregnated printed PLA. The printed supercapacitors showed capacitance values of ~80 F $g^{-1}$ with a retention of >96 %.

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**Effect of urea and squaramide IMPDH inhibitors on C. parvum: in vitro trial design impacts the assessment of drug efficacy**

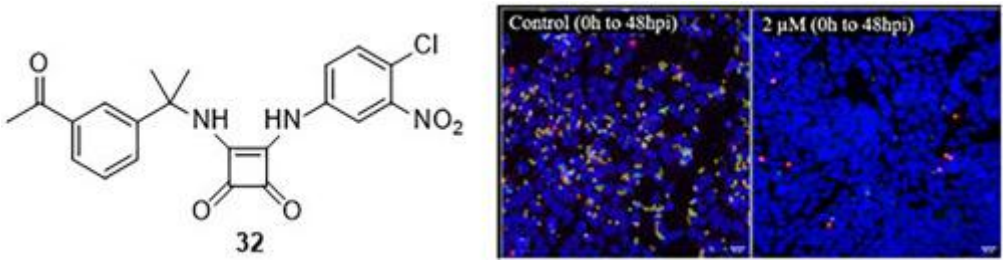
Anne-Charlotte Lenière [a #], Amit Upadhyay [b c d #], Jérôme Follet [a 1]*, Timothy P. O'Sullivan [b c d 1]*

**International Journal for Parasitology: Drugs and Drug Resistance**. Volume 28, August 2025, 100592
Published August 2025
DOI: https://doi.org/10.1016/j.ijpddr.2025.100592

**Abstract**

The protozoan parasite Cryptosporidium is the etiological agent of cryptosporidiosis, a ubiquitous diarrheic disease affecting humans and animals. Treatment options are limited, highlighting an urgent need for novel therapeutics. Despite decades of research and a wide diversity of strategies to tackle parasite metabolic pathways, no completely effective drug has been identified to date. Within targeted parasite enzymatic and metabolic pathways, the synthesis of nucleotide mediated by the inosine 5′-monophosphate dehydrogenase (IMPDH) enzyme is the focus of significant research efforts. Based on our prior studies of bacterial IMPDH inhibitors, we report herein the development and characterisation of novel inhibitors targeting Cryptosporidium parvum IMPDH (CpIMPDH). Specifically, we synthesised heteroaryl-containing urea and squaramide analogues to evaluate their potential in vitro anti-Cryptosporidium activity. Initial screening identified nine active compounds with the most potent candidates achieving IC50 values as low as 2.2 μM. Subsequent time-course experiments revealed that the molecules effectively inhibit parasite invasion and early intracellular development but failed to tackle C. parvum growth when introduced at 30 h post infection. The present work introduces a new family of squaramide-derived IMPDH inhibitors and also interrogates the need to standardise commonly accepted protocols used for assessing anti-cryptosporidial drug activity.

Graphical abstract




**Recent advances in the synthesis of N-acyl sulfonamides**

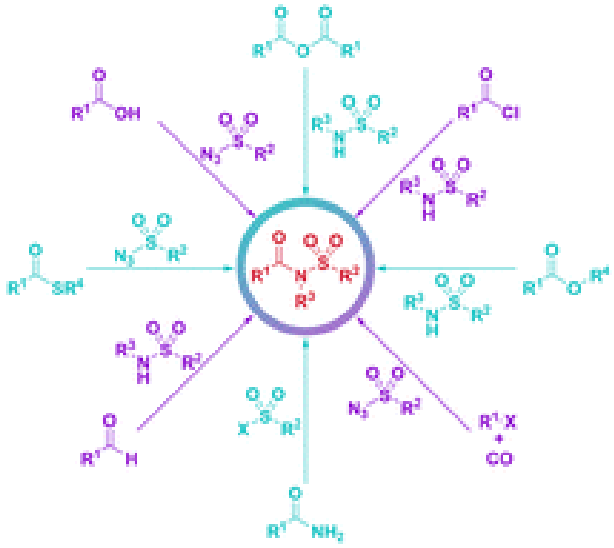
Michelle O'Driscoll, [abc] Gangireddy Sujeevan Reddy [abc] and Timothy P. O'Sullivan [*abc]

***RSC Adv.***, 2025,**15**, 32361-32406
Published 8 September 2025
DOI: https://doi.org/10.1039/D5RA05157F

**Abstract**

The *N*-acyl sulfonamide group is widespread in pharmaceutically active compounds. This is partly due to the ability of *N*-acyl sulfonamides to act as bioisosteric equivalents of carboxylic acids. Accordingly, methods for the efficient preparation of *N*-acyl sulfonamides are of considerable interest to medicinal chemists. In this review, we summarise developments in the synthesis of this pharmaceutically relevant functional group across a broad range of methodologies.

**Graphical Abstract**



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**Effective Oxidation State Analysis for Solids**

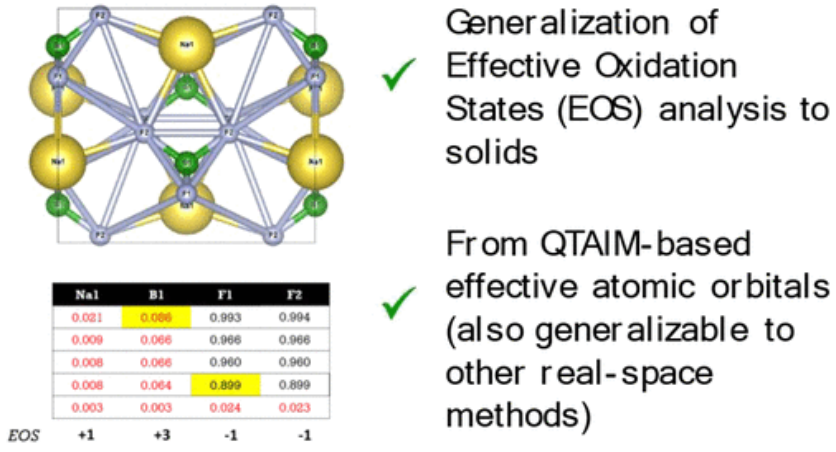
Gerard Comas-Vilà, Leila Pujal, Alberto Otero-de-la-Roza, Davide Tiana, Julia Contreras-Garcia*, Pedro Salvador*

***J. Chem. Theory Comput.*** 2025, 21, 14, 7075–7086
Published 3 July 2025
DOI: https://doi.org/10.1021/acs.jctc.5c00482

**Abstract**

We present the generalization of the effective oxidation state (EOS) method to assign oxidation states from wave function analysis to solid-state calculations. The scheme is realized in the framework of the Quantum Theory of Atoms in Molecules (QTAIM) and makes use of the atomic overlap matrices (AOM) of the atoms of the unit cell, expressed (whenever possible) in terms of maximally localized Wannier functions (MLWFs). The method is generally applicable to ionic solids or molecular crystals. The performance of the new method is assessed using a chemically diverse set of 40 solids, including simple metal oxides, perovskites, hydrides, and high-pressure systems with unusual bonding patterns.

**Graphical Abstract**

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**Promoting urban air quality resilience through communication: A stakeholder needs mapping and prioritisation study informed by design thinking**

Roberto Cibin*, Dean S. Venables*, Marica Cassarino*

**City and Environment Interactions** Volume 27, August 2025, 100209
Published August 2025

DOI: https://doi.org/10.1016/j.cacint.2025.100209

**Abstract**
Air pollution (AP) poses significant global health risks and exacerbates socio-economic inequities, especially in urban contexts. This study mapped stakeholder needs and priorities for developing communication strategies to foster air quality (AQ) resilience, using Cork City, Ireland, as a case study. Employing a Design Thinking approach, the research involved consultations in the form of qualitative interviews and one focus group (n = 62), followed by a quantitative survey (n = 105) to prioritise identified needs. Stakeholders included, among others, residents, policymakers, health professionals, and academics. The needs assessment revealed two key areas related to enhancing communication functions, channels and formats, and addressing policy and systemic issues. Effective AQ communication must address public understanding of AP risks, empower adaptive behaviours, and mobilise civic engagement. Stakeholders emphasised the need for accessible, contextually relevant, and solution-oriented communication.

Systemic needs encompassed enhancing local policies, infrastructure, and governance to support behavioural changes, such as reducing car dependence and promoting sustainable heating practices. Consultations revealed social, cultural, and infrastructural challenges to making AQ communication effective, and underscored the necessity of inclusive, participatory approaches. The need prioritisation results indicate that stakeholders value systemic improvements, such as increased urban green spaces and appropriate public transport infrastructure, alongside tailored communication strategies. This research underscores the importance of integrating communication with systemic interventions to enhance urban AQ resilience. The findings informed co-creation of actionable, equitable AQ communication strategies and contribute to broader debates on environmental sustainability and community resilience. Future work should extend participatory methodologies to diverse contexts and emphasize socio-ecological interactions for effective environmental communication.

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**Promoting air quality-related awareness and behavioural change: A rapid review of communication interventions integrating behavioural, science communication and socio-ecological perspectives**

Roberto Cibin [a], Laura Horgan [a], Luigina Ciolfi [a d], Samantha Dockray [a], Gillian Murphy [a], Dean S. Venables [b c], Marica Cassarino [a c*]

**Environmental Challenges** Volume 20, September 2025, 101237
Published September 2025
DOI: https://doi.org/10.1016/j.envc.2025.101237

**Abstract**
Air pollution (AP) is a global environmental threat to human health and development. Day-to-day behaviours contribute to poor air quality (AQ) but limited public understanding of AQ warrants effective communication strategies to promote awareness and empower positive behavioural change. Through the integration of behavioural, science communication, and socio-ecological frameworks, this rapid review maps existing AQ-related communication interventions and their influence on AQ awareness, protective and/or mitigating behaviours (i.e., avoiding exposure; reducing polluting activities), and civic engagement. We conducted a comprehensive literature search of peer-reviewed and grey literature, including 79 studies for analysis. Findings were synthesised narratively and assessed for quality with the QuADS tool. Despite high heterogeneity in intervention types, most served a persuasion or enablement function, often utilising dissemination modes such as websites or web applications, and most assessed awareness and/or engagement in protective behaviours.

While most interventions focused on individual/household-level actions and interindividual dynamics, only some considered policy-level actions, and very few embedded infrastructural considerations in their communication. Overall, 47 studies reported positive impacts on awareness and/or behaviours, particularly through participatory approaches, although we noted issues associated with promoting meaningful participation and identified influencing psychosocial factors. Evidence of effectiveness for behaviours was often limited by observational designs and the focus on awareness only or self-reported behaviours/intentions. Our findings highlight growing attempts to communicate AQ-related risks and

behavioural solutions through empowering approaches that are sensitive to individual and local circumstances but note the need for further work to foster mitigating behaviours and civic engagement.

**Integrated Absorption Spectroscopic Measurement of 2-Nitrophenol and Naphthalene**

Zhongmei Yang, Meng Wang, Dean S. Venables*, Jun Chen*

***Int. J. Mol. Sci.*** **2025**, *26*(20), 9904
Published 11 October 2025
DOI: https://doi.org/10.3390/ijms26209904

**Abstract**

This study presents a generalized, high-precision measurement system based on Integrated Absorption Spectroscopy (IAS) for determining gas-phase absorption cross sections of low-volatility organic compounds (LVOCs), particularly semi-volatile organic compounds (SVOCs) in the atmosphere. Accurate cross sections and their temperature dependence are essential for modeling atmospheric and high-temperature processes. We coupled a temperature-controlled inlet and cell (473 K) with a nitrogen carrier gas to measure the cross sections of 2-nitrophenol (2-NP) and naphthalene from 250 to 400 nm. At 473 K, peak cross sections for 2-NP were 2.31 × 10−17 cm2/molecule at 260 nm and 1.16 × 10−17 cm2/molecule at 335 nm. For naphthalene, values between 258 and 280 nm decreased from 1.62 × 10−17 to 1.28 × 10−17 cm2/molecule. Thermally induced spectral broadening and reduced peak cross sections align with thermodynamic theory. These high-temperature data resolve discrepancies among low-temperature datasets. For example, our maximum cross section for 2-NP (300–400 nm) is 29% lower than that reported by Chen et al. (293 K), whereas the value from Sangwan and Zhu (295 K) is 86.8% lower than Chen's, supporting the higher reliability of Chen's data. The IAS method thus offers a robust approach for quantifying absorption cross sections under atmospherically relevant conditions.

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**Rethinking environmental boundaries for contaminants of emerging concern**

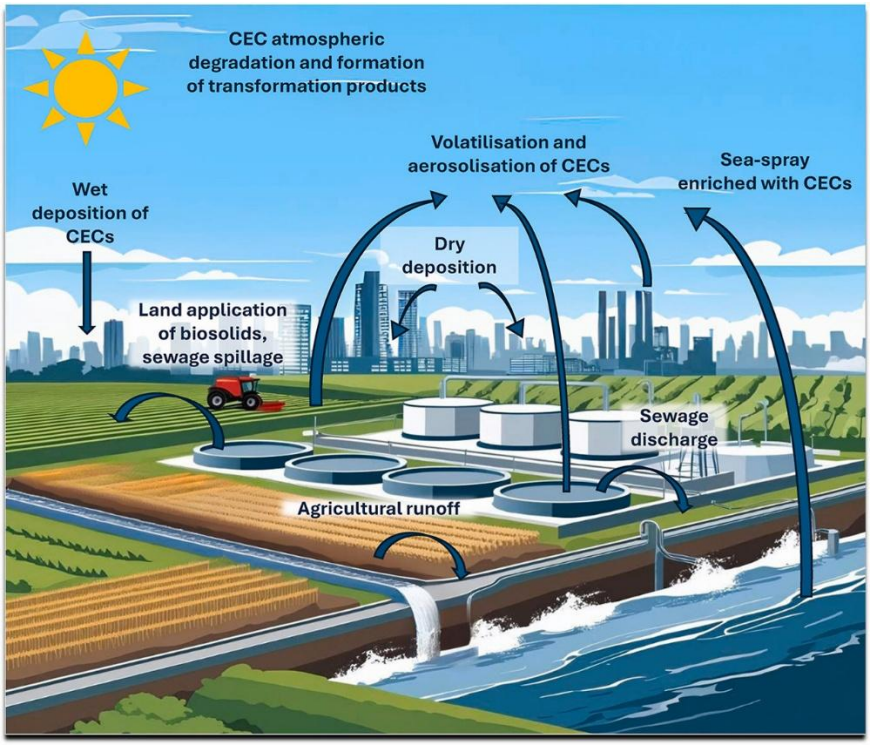
Ivan Kourtchev [a], Max R. McGillen [b], John Wenger [c], Neil M. Donahue [d]

**Atmospheric Environment** Volume 361, 15 November 2025, 121492
Published 15 November 2025
DOI: https://doi.org/10.1016/j.atmosenv.2025.121492

Abstract

The global proliferation of synthetic chemicals has led to the widespread and continuous release of Contaminants of Emerging Concern (CECs) into the environment. CECs include pharmaceuticals, pesticides, personal care products and other industrial chemicals that pose a significant risk to both ecosystems and human health. Regulatory frameworks have predominantly targeted aquatic systems; however, mounting evidence reveals the capacity of many CECs to volatilise, aerosolise and undergo atmospheric transport. This perspective highlights the overlooked atmospheric dimension of CECs and analyses the key physicochemical parameters governing their transfer to the atmospheric domain. The results indicate that many CECs can mobilise from water or soil and undergo atmospheric transport in both the gas- and particle-phase, crossing between several environmental continua as a result. While intrinsic properties such as vapour pressure and partitioning coefficients are central to this analysis, environmental factors such as temperature, humidity, solar radiation, and transformation reactions further modulate the environmental fate and impact of CECs. We emphasise the need for environmental monitoring and regulatory frameworks to incorporate air as a critical vector for CEC dispersion and exposure. Key research priorities identified measurements of CECs in the atmosphere, further development of predictive models, and toxicity evaluation of airborne CECs to better inform policy for protecting public and environmental health.

**Graphic Abstract**


CEC atmospheric degradation and formation of transformation products
Volatilisation and aerosolisation of CECs
Sea-spray enriched with CECs
Wet deposition of CECs
Dry deposition
Land application of biosolids, sewage spillage
Sewage discharge
Agricultural runoff

# Queens University Belfast(QUB) Chemistry Research Publications June-December 2025

## Water-soluble fluorine-free poly(ionic liquid) borate binders for Li-ion battery cathodes Unusual mechanism of aziridine biosynthesis catalysed by the αKG-dependent non-heme enzyme TqaL

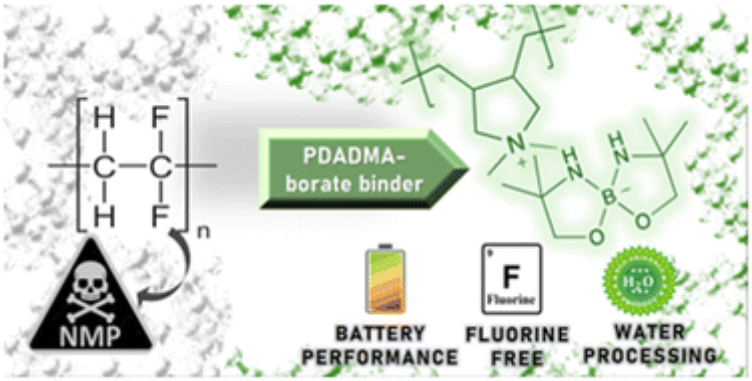
Haris Amir, [a] Ana Clara Rolandi, [b] Gabriele Lingua, [b] Maria Forsyth, [cd] Małgorzata Swadźba-Kwaśny, [a] John D. Holbrey, *[a] David Mecerreyes [bd] and Nerea Casado *[bd]

***RSC Appl. Interfaces***, 2025,**2**, 1702-1714
Published 18 Aug 2025
DOI: https://doi.org/10.1039/D5LF00155B

### Abstract

The development of efficient, eco-friendly lithium-ion battery (LIB) technologies necessitates alternative binder materials to replace conventional polyvinylidene fluoride (PVDF). Five novel water-soluble poly(ionic liquid) (PIL) binders based on poly(diallyldimethylammonium) (PDADMA) with borate counter-anions are presented. The binders—PDADMA–C4B, PDADMA–C3B-A, PDADMA–C3B-B, PDADMA–PyrB, and PDADMA–TriB were synthesised and characterised for thermal stability, electrolyte uptake, adhesion, and electrochemical performance. Among these, PDADMA–C4B demonstrated superior properties, including high thermal stability (>200 °C), significant electrolyte uptake (303%), and low internal resistance, leading to improved cycling performance of LIB. At high C-rates, PDADMA–C4B outperformed PVDF, maintaining structural integrity and higher discharge capacities. Surface analyses confirmed minimal degradation, underscoring the durability of the PDADMA–borate binders. These results highlight PDADMA–C4B as a sustainable, high-performance alternative to fluorinated binders, promoting advancements in LIB technology.

### Graphical Abstract

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## Untying surface chemistry and emulsion stability to construct multifunctional Pickering emulsion SERS sensors for pretreatment-free quantitative analysis in bio-media

Yingrui Zhang, Chunchun Li*, Ruairi Carland, Ziwei Ye, Steven E. J. Bell, Yikai Xu*

**Advanced Science** Volume12, Issue28 2505714
Published 24 July 2025
DOI: https://doi.org/10.1002/advs.202505714

### Abstract

Plasmonic Pickering emulsions have immense potential as enhancing substrates in surface-enhanced Raman spectroscopy (SERS). Traditionally, the functional nanoparticles also act as the emulsion stabilizer, so that their surface chemistry is tied directly to emulsion stability. However, this has meant that adsorption of molecules to the plasmonic nanoparticles destabilizes the emulsion system, which severely limits the use of

Pickering emulsions in SERS. Here, we used a dual-particle approach to create plasmonic Pickering emulsions, in which emulsion stability is maintained solely by one type of nanoparticle so that the other could be used to provide functionality without constraints to its surface properties. This allowed us to construct multiwalled carbon nanotubes-Au@Prussian blue Pickering emulsion SERS sensors with integrated internal standards and filtration functionalities, which enabled quantitative, biphasic and multiplex analysis of discrete molecules in serum. The synthetic approach used in this work can be readily extended to form Pickering emulsions carrying functional components with arbitrary surface functionalities, which paves the way for advanced applications in sustainability and healthcare.

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## Unusual mechanism of aziridine biosynthesis catalysed by the αKG-dependent non-heme enzyme TqaL

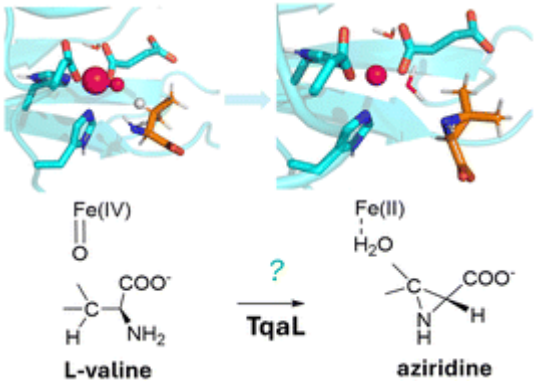
Warispreet Singh* Meilan Huang*

***Phys. Chem. Chem. Phys.***, 2025,**27**, 9620-9630
Publication 14 May 2025 In:
DOI: https://doi.org/10.1039/D4CP03708A

### Abstract

Aziridines are present in many synthetic pharmaceuticals. The synthesis of the aziridine ring remains challenging due to its highly strained three-membered ring structure. Recently, a non-heme αKG-dependent enzyme, TqaL, has been demonstrated to catalyze the synthesis of aziridines from L-Val. However, the detailed reaction mechanism of the enzyme remains elusive. Herein, we reported, for the first time, the mechanism of oxidative cyclisation for aziridine synthesis catalyzed by TqaL. Following the HAA step, the reaction proceeded *via* a unique concerted process with a single electron transfer from the isopropyl radical to the Fe(III)–OH motif, which was coupled with the electrophilic attack of the primary amine substrate on the tertiary isopropyl radical and simultaneous proton transfer from the substrate amine to the hydroxyl group of the Fe(III)–OH to give the aziridine. This research would provide a valuable structural basis for tailoring the non-heme αKG-dependent enzyme for the biosynthesis of highly active aziridine derivatives as pharmaceuticals.

### Graphical Abstract

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## Untying Surface Chemistry and Emulsion Stability to Construct Multifunctional Pickering Emulsion SERS Sensors for Pretreatment-Free Quantitative Analysis in Bio-Media

Yingrui Zhang, Chunchun Li*, Ruairi Carland, Ziwei Ye, Steven E. J. Bell, Yikai Xu*

***Advanced*** *Science* Volume12, Issue28 2505714
Published July 24, 2025
DOI: https://doi.org/10.1002/advs.202505714

### Abstract

Plasmonic Pickering emulsions have immense potential as enhancing substrates in surface-enhanced Raman spectroscopy (SERS). Traditionally, the functional nanoparticles also act as the emulsion stabilizer, so that their surface chemistry is tied directly to emulsion stability. However, this has meant that adsorption of molecules to the plasmonic nanoparticles destabilizes the emulsion system, which severely limits the use of Pickering emulsions in SERS. Here, we used a dual-particle approach to create plasmonic Pickering emulsions, in which emulsion stability is maintained solely by one type of nanoparticle so that the other could be used to provide functionality without constraints to its surface properties. This allowed us to construct multiwalled carbon nanotubes-Au@Prussian blue Pickering emulsion SERS sensors with integrated internal standards and filtration functionalities, which enabled quantitative, biphasic and multiplex analysis of discrete molecules in serum. The synthetic approach used in this work can be readily extended to form Pickering emulsions carrying functional components with arbitrary surface functionalities, which paves the way for advanced applications in sustainability and healthcare.

---

## The Electrochemical Characterization of Functionalized Isoindolinones

Daniel. E. Smith, Ashley J. Basson, Niamh J. Owen, Mark Potter, Mark G. McLaughlin, Kathryn E. Toghill*

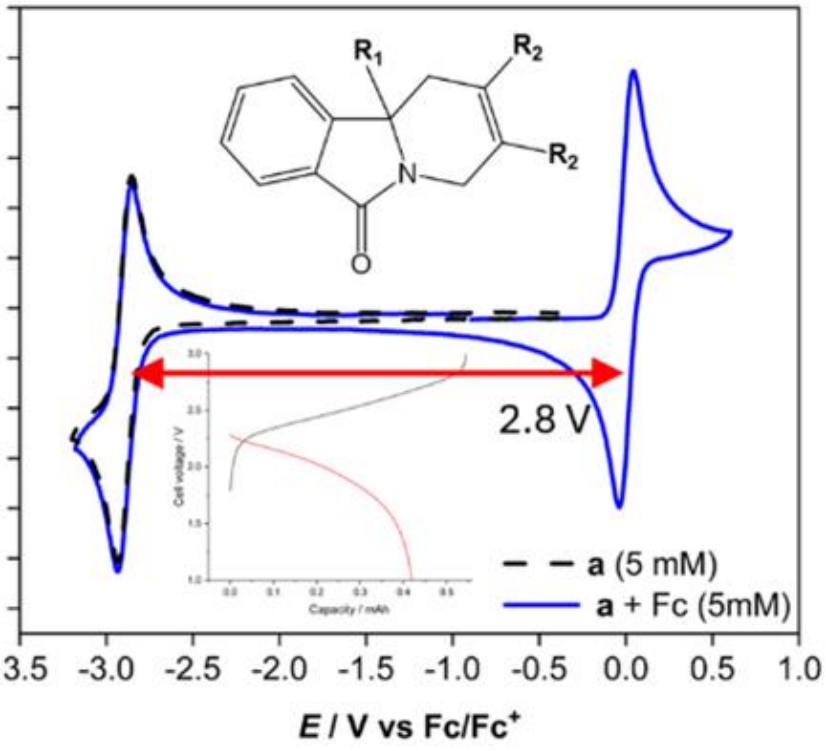
**ChemElectroChem** Volume12, Issue12 e202500044
Published June 10, 2025
DOI: https://doi.org/10.1002/celc.202500044

### Abstract

This study considers the electrochemical and physical properties of six functionalized isoindolinones, synthesized using a facile, green route. The compounds show redox activity at a highly negative potential with quasireversible redox potentials of ≈−2.8 V versus $Fc/Fc^+$, a potential in the region of alkali metal deposition and intercalation. For those molecules with a specific structural motif, the electrochemical behavior is electrochemically quasireversible, attributed to the formation of a carbanion radical stabilized on the carbonyl group. The electrochemical properties of the reversible compounds are assessed, with the lead-performing compound extensively characterized galvanostatically to assess its candidacy for nonaqueous, high-voltage energy storage.

### Graphical Abstract

A new class of redox organic molecules called isoindolinones are evaluated electrochemically for their use in high-voltage nonaqueous organic flow batteries. The molecules are characterized by a reversible and highly negative formal potential in the region of −2.8 V versus ferrocene/ferrocenium.



## Systematic refinement of experimental practices to improve repeatability in flow battery cycling

Hugh O'Connor, Alexander H. Quinn, Fikile R. Brushett, Oana Istrate, Stephen Glover, Josh J. Bailey & Peter Nockemann

***Discov. Electrochem.* 2, 23 (2025).**
Published 11 June 2025
DOI: https://doi.org/10.1007/s44373-025-00036-8

### Abstract

Flow batteries represent one of the leading options for large-scale, long-duration energy storage. In recent years, research into this technology has accelerated, with numerous innovative studies focusing on electrolytes, membranes, and electrode materials. Despite this, there is presently no clear set of testing protocols followed during full-cell testing of flow batteries and the experimental techniques detailed in published literature are often insufficient to reproduce results. Furthermore, testing to quantify the repeatability of experiments is not often reported. In this work, various aspects of an experimental procedure developed from the peer-reviewed literature are refined, with voltage efficiency, coulombic efficiency, energy efficiency, and electrolyte utilization used as indicators of repeatability. A set of improved testing protocols are presented for researchers to consider when conducting charge–discharge testing, and additional factors to be reported and studied in the context of repeatability are suggested.

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## Symmetric and asymmetric ligands for FeIII spin crossover – the influence of the C2 axis

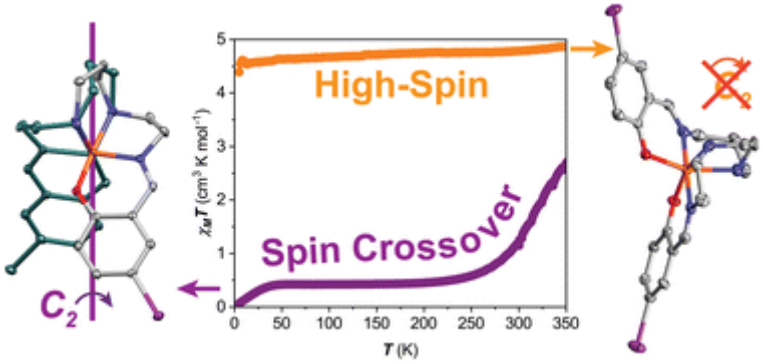
Conor T. Kelly, *[a] Emmelyne Cuza, [a] Eoin Pasquetti,[a] Niall Quinn,[a] Michael Griffin,[a] Peter Nockemann, [b] Helge Müller-Bunz,[a] Julia Bruno-Colmenarez, [a] Solveig Felton, [c] Zoi G. Lada [d] and Grace G. Morgan *[a]

***Dalton Trans.***, 2025,**54**, 14522-14532
Published 10 Sep 2025
DOI: https://doi.org/10.1039/D5DT01833A

### Abstract

Modulation of the local strain and geometry in $Fe^{III}$ Schiff base complexes has been shown to allow the stabilisation of both the high spin (HS) and low spin (LS) states, along with thermal spin crossover (SCO). Complexes with hexadentate Schiff base ligands can be readily modified by changing the length of the tetraamine backbone linker. We report here 34 complexes of the symmetric $[Fe^{III}(R\text{-sal}_2232)]^+$ and asymmetric $[Fe^{III}(R\text{-sal}_2223)]^+$ families, where the former typically support the HS state, along with a handful of SCO examples, and the latter only supports the HS state. Magnetic measurements reveal that one symmetric example, $[Fe^{III}(5\text{-I-sal}_2232)]ClO_4$**1.5**, undergoes thermal SCO close to room temperature. We compare the structural distortion and spectroscopic properties in these examples, to identify the factors that influence spin state choice. This reveals the importance of molecular symmetry, by way of a $C_2$ axis bisecting the complex which is present in the samples which stabilise the LS state so far. The aforementioned example and three others, one reported previously, have short metal–ligand bond lengths suggesting adoption of the LS state coupled with the presence of a $C_2$ axis. The additional strain in the $[Fe^{III}(R\text{-sal}_2223)]^+$ complexes due to the asymmetric nature of the backbone results in significantly greater distortion around the $Fe^{III}$ centre which inhibits the stabilisation of the less distorted LS state. Computational analysis of the $[Fe^{III}(5\text{-I-sal}_2232)]^+$ and $[Fe^{III}(5\text{-I-sal}_2223)]^+$ isomers reveals that the HS state is more stable in the asymmetric $[Fe^{III}(5\text{-I-sal}_2223)]^+$ species, whereas the energy difference between the HS and LS state for the $[Fe^{III}(5\text{-I-sal}_2232)]^+$ cation is sufficiently small to allow for SCO to occur.

### Graphical Abstract

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## Sustainable valorisation of waste-derived plastic rich materials into porous carbon materials for adsorption cooling applications

Małgorzata Sieradzka [b], Wojciech Kalawa [a], Chunfei Wu [c], Marcin Sowa [a], Tomasz Bujok [a], Aneta Magdziarz [b], Agata Mlonka-Mędrala [a]*

**Journal of Environmental Chemical Engineering** Volume 13, Issue 6, 119279
Published Dec 2025
DOI: https://doi.org/10.1016/j.jece.2025.119279

### Abstract

The thermochemical valorisation of waste materials rich in plastics offers a sustainable approach for waste reduction and the generation of high-value products, aligning with the European Green Deal and circular economy principles. This study investigates the conversion of three solid waste streams: refuse-derived fuel (RDF) from municipal (RDF_MW) and industrial (RDF_IW) sources and tyre-derived fuel (TDF) into activated carbons for application in adsorption cooling systems. A two-step activation process, combining pyrolysis at 600 °C with subsequent steam (850 °C) or chemical (KOH at 800 °C) activation, was employed to enhance porosity and surface area. RDF_IW-derived carbon activated with KOH achieved a maximum BET surface area of 955 m²/g, while methanol adsorption tests showed an uptake exceeding 40 %. Heavy metal analysis revealed significant Zn contamination in TDF (up to 37,415 mg/kg), while Cr, Pb, and Sn were prominent in RDF samples; chemical activation reduced Zn content by up to 70 %. Performance testing in methanol-based adsorption chillers showed that RDF_IW_H2O and RDF_IW_KOH samples achieved specific cooling powers (SCP) of 53.5 W/kg and 88.9 W/kg, and coefficients of performance (COP) of 0.631 and 0.673, respectively, comparable to commercial activated carbons (CWH-22: SCP = 95.5 W/kg, COP = 0.615). These findings demonstrate the dual benefit of valorising heterogeneous waste into functional sorbents while enabling energy-efficient, low-grade thermal cooling systems.

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## Surface Interactive Assembly of Ruthenium Based Janus Bimetallic Nanoparticles With Active Dual-Function Sites for Efficient Use in CO2 Utilization

Heesu Kim, Seongjun Lee, Boseok Seo, Min Xu, Mane Rasika, Chanmin Lee, John T.S. Irvine*, Minkyu Kim*, Yukwon Jeon*

**Advanced Functional Materials** Volume35, Issue 27 2418874
Published 3 Jul 2025
DOI: https://doi.org/10.1002/adfm.202418874

### Abstract

Noble bimetallic nanoparticles (NPs) are nowadays essential in various applications, like $CO_2$ utilization by dry reforming of methane (DRM), due to their unique and potential properties. A synthesis method for Ru based Janus-structured NPs is presented via surface interactive assembly of deposited Ru and emerged Ni species from carefully tailored perovskite oxide support. As noble-metals typically result in the alloy, an exclusive formation mechanism is introduced by utilizing Ru energetically favorable for the Janus phase by lower ground state energy from interactions between the strongly embedded cluster and perovskite surface. Consequently, noticeable Janus NPs, controllable in size and composition with active configuration by dual-

function sites and interface strains, are well-produced with high distribution. DRM performance highly exceeds conventional Ru over 5 times in TOFs for both $CO_2$ and $CH_4$ with improved stability maintaining $H_2$/CO for 100 h without sintering at harsh reaction conditions, which comprehensively exhibits distinct advantages over recent works. Fundamental studies indicate combined electronic d-band structures proving distinctive $CO_2$ dissociation and $CH_4$ activation, involving efficient dehydrogenation and CO production via surface oxygenation, considerably suppresses coking. This approach presents a potential avenue to surmount constraints on designing bimetallic NPs in any structured oxide systems for effective materials in various low carbon relevant industries.

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## Solar-Driven Atmospheric Water Production Through Hierarchically Ordered Porous Carbon for Self-Sustaining Green Hydrogen Production

Bo Fu, Jifang Zhang, Neil Robinson, Zhen Zhang, Zhengju Zhu, Mengyang Dong, Xinyuan Zhang, Jian Kang, Paul Michalski, Zeyang Zhao, Jiapeng Ji, Yiming Xu, Kaidi Zhang, Xinyu Wang, Shan Chen, Haolan Xu*, Porun Liu*, Huajie Yin*, Huijun Zhao*

**Advanced Materials** **Volume37, Issue 44** e11336
Published 6 Nov 2025
DOI: https://doi.org/10.1002/adma.202511336

### Abstract

Green hydrogen production by proton exchange membrane water electrolysis (PEMWE) powered by clean energy is a promising and environmentally friendly technology. However, it relies on a high-purity water source, which is limited in regions facing water scarcity. Here, a coupled self-sustaining solar-enabled system is reported that couples atmospheric water harvesting with PEM water electrolysis (AWH-PEMWE), offering a novel pathway for clean water generation and green hydrogen production. The atmospheric water harvester (AWH) component utilizes N and O co-doped hydrophilic ordered porous carbon, engineered with an interconnected hierarchical porous structure with prosperous channels for efficient mass transport. It enables effective interfacial solar evaporation for water release, achieving a record-high water harvesting capacity of 0.49 L $kg^{-1}$ $h^{-1}$ at 40% relative humidity (RH). During outdoor tests, the AWH-PEMWE system reaches a peak green hydrogen production rate of 204 mL $h^{-1}$ at midday using only atmospheric water as feedstock. Remarkably, the system remains operational under ultra-low humidity conditions down to 20% RH, addressing the challenge of water availability in arid environments. Importantly, the system operates without the need for carrier gases or external energy input accessories, enabling a fully solar-driven process with zero carbon emission throughout the hydrogen production cycle.

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## Self-Assembled Multifunctional Supraparticle Films for Label-Free Direct SERS Quantitation of Weakly Adsorbing Molecules in Serum

Yingrui Zhang, Yingrui Zhang, Chunchun Li, Weilong Liu, Yunpeng Huang, Ziwei Ye*, Steven E. J. Bell, Yikai Xu*, Xiang Ma

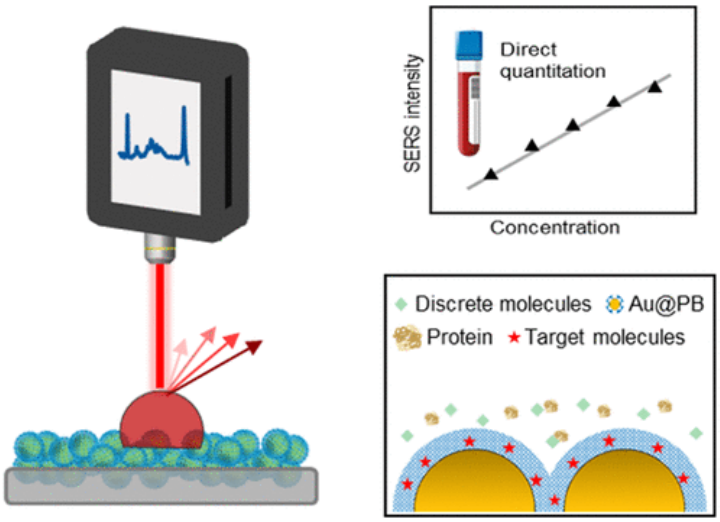
***ACS Appl. Mater. Interfaces*** 2025, 17, 44, 61550–61558
Published 23 Oct 2025
DOI: https://doi.org/10.1021/acsami.5c17582

### Abstract

Detecting and quantifying molecular species at trace levels is crucial for understanding fundamental processes in chemistry and biology; however, the complexity of real-life samples renders their direct analysis extremely challenging. Here, we demonstrate a surface-enhanced Raman spectroscopic approach for the direct on-site detection and quantification of trace analytes in real-life samples. The key to our approach is the creation of multifunctional plasmonic films via interfacial self-assembly using colloidal Au@Prussian blue (PB) supraparticles as the functional building block. The supraparticles contain 3-dimensional hot-spots that give rise to strong plasmonic near-field enhancement, while the PB shell acts simultaneously as a molecular sieve and internal standard to induce selective analyte adsorption and to calibrate signal fluctuations. This enables direct identification and quantitation of a range of weakly adsorbing targets in

biological and environmental samples using a portable Raman spectrometer, which paves the way for rapid on-site chemical analysis in important applications, including therapeutic drug monitoring and environmental analysis.

## Graphical Abstract

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## Ritter reactions in continuous flow catalysed by a solid-supported sulfonic acid catalyst

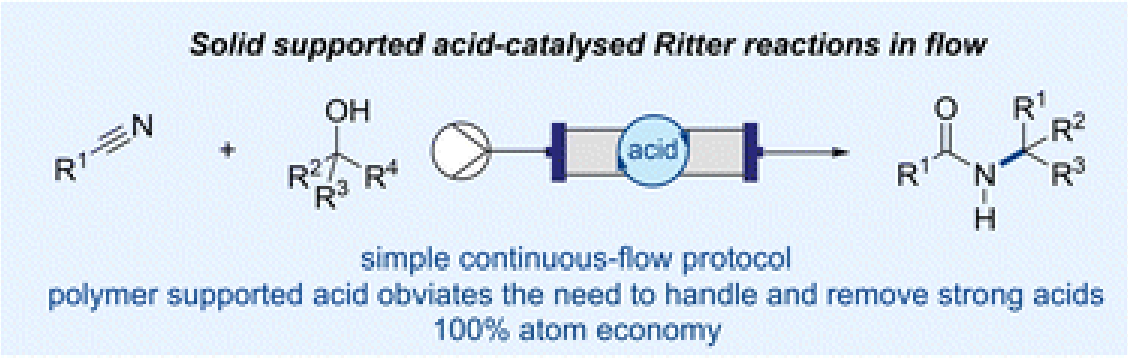
Lara J. Nolan,[abc] Ailbhe A. Ryan,[abc] Seán Dempsey,[abc] Megan Smyth,[c] Thomas S. Moody,[bc] Scott Wharry,[c] Karen Fahey,[b] Paul Dingwall,[a] David W. Rooney,[a] Jillian M. Thompson,*[a] Mark J. Muldoon*[a] and Peter C. Knipe*[a]

***Catal. Sci. Technol.***, 2026, Advance Article
Published 29 Dec 2025
DOI: https://doi.org/10.1039/D5CY01306B

## Abstract

The Ritter reaction allows the 100% atom economical synthesis of amides *via* acid-catalysed coupling between nitriles and alcohol substrates. However, this reaction has traditionally required harsh acid catalysts which must be separated from the product stream. Here, we demonstrate that commercial polymer-supported Brønsted acids catalyse the Ritter reaction under continuous flow conditions. The products are generated in high yield and free from acidic catalyst impurities. Continuous flow conditions deliver high yields in significantly shorter reaction times compared with batch reactions (1 hour *vs.* 24 hours) and the catalyst remains effective after 43 hours of continuous operation.

## Graphical Abstract

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## Rice grain quality alteration through manipulation of parboiling procedures to affect the concentration of macro- and micro- nutrient elements, B-vitamins, inorganic toxicants, and bacterial contamination

Andrew Meharg [a 1]*, Mukhlesur Rahman [b c], Manus Carey [a 2], Kathryn Ralphs [a 3], Jonathan McComb [a], Coal ain McCreanor [a], Mahmud Sumon [b], Rafiqul Islam [b], Mohammed Uddin [d], Muhammad Siddique [e], Saiful Isl am [f], Caroline Meharg [a 4*]

**Food Chemistry** Volume 479, 1 July 2025, 143782
Published 1 July 2025
DOI: https://doi.org/10.1016/j.foodchem.2025.143782

### Abstract

A Bangladesh village rice parboiling plant was used to investigate how to improve essential elements and B-vitamin content of rice, while reducing the toxicants arsenic and cadmium, and potential bacterial pathogens. A $2^5$ -factorial experiment was conducted where husked and de-husked rice was parboiled at different pre-parboiling soaking times, pre-parboiling soaking temperatures, parboiled through either boiling or steaming, and parboiled for 2 different times. Three rice cultivars were used. Using wholegrain, rather than rough rice, with 15 mins of parboiling, gave the optimal reduction in inorganic arsenic (25 %), as compared to widely used rough rice parboiling procedures. This combination of treatments also enhanced calcium (circa. 200 %) and iron (circa. 50 %), but lost circa. 50 % of potassium. The wholegrain parboiling procedures reduced vitamin B1 and B6 compared to rough rice parboiling, but made no difference for B2 and B3. *Bacillus* and *Enterobacter* related sequences showed highest levels of abundance, and were identified in 100 % and 77 % of non-parboiled rice samples, respectively. The overall implications of this study was that wholegrain, as compared to rough rice, parboiling should be adopted, but the B-vitamin and potassium intakes of the receiving populace need to be considered.

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## Quantification of Antibiotic Diffusion in Biofilms Using Gold Nanostar Surface-enhanced Raman Spectroscopy

Wafaa Aljuhani, Yingrui Zhang, Matthew P. Wylie, Colin P. McCoy, Steven E. J. Bell*

***Advanced science*** **Volume13, Issue 2** e10346
Published 9 January 2026 (first Published 21 OCT 2025
DOI: https://doi.org/10.1002/advs.202510346

### Abstract

The increased resistance to antibiotics shown by bacteria in biofilms is believed to be partly the result of the limited penetration of antibiotics. However, there are no well-established techniques which allow quantitative, label-free monitoring of antibiotic transport in biofilms. Here, it is shown that surface-enhanced Raman spectroscopy (SERS) with gold nanostars (NS) can be used for the detection of levofloxacin (Levo) in *Staphylococcus aureus* biofilms at clinically relevant concentrations. Ex situ studies showed that although matrix interference reduced the sensitivity compared to aqueous solutions, quantitative detection remained possible. With intact biofilms, monitoring the SERS signals from layers of NS embedded at specific depths allowed the time-dependence of the penetration of Levo from the surface to the embedded layer to be measured and the diffusion coefficient of Levo to be calculated. The measured value of $D = 2.79 \pm 0.79 \times 10^{-9}$ cm$^2$ s$^{-1}$ is over three orders of magnitude lower than in aqueous solutions. This work is the first demonstration that SERS can be a powerful method for investigating antibiotic transport in biofilms, offering new insights into resistance mechanisms and supporting the development of more effective antimicrobial strategies.

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## Novltex: A New Class of Antibiotics with Potent Activity against Multidrug-Resistant Bacterial Pathogens─Design, Synthesis, and Biological Evaluation

Esra Malkawi, Anish Parmar, Sanjit Das, Enas Newire, Charlotte M. Jones, Kate A. Morrison, Milandip Karak, Frédéric Blanc, Nicholas Harper, Rajamani Lakshminarayanan, Zhi Sheng Poh, Navin K. Verma, Jennifer Unsworth, Dallas E. Hughes, Losee Lucy Ling, Stephen A. Cochrane, William Hope, Ishwar Singh*

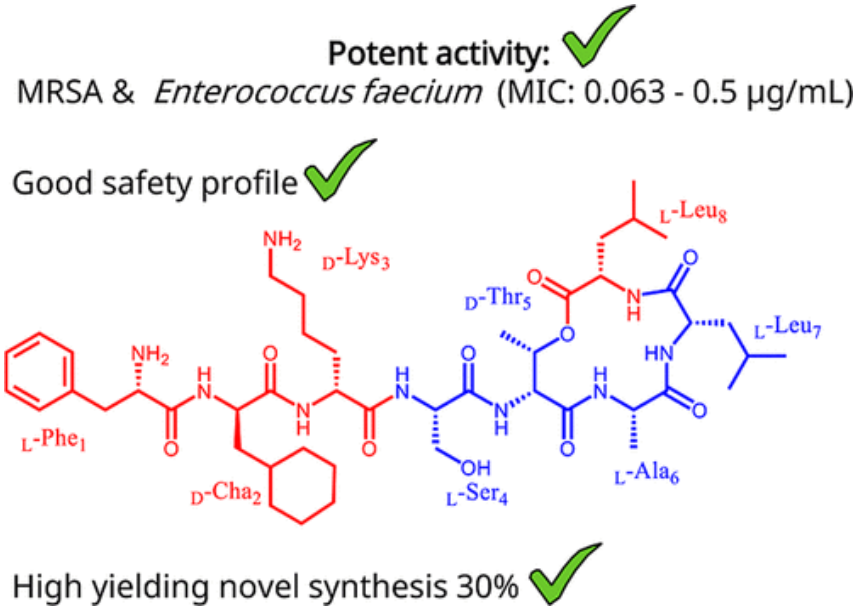
***J. Med. Chem.*** 2025, 68, 18, 19143–19152

Published 16 Sep 2025
DOI: https://doi.org/10.1021/acs.jmedchem.5c01193

## Abstract

Increasing spread of multidrug-resistant (MDR) bacteria demands antibiotics that combine potent activity with scalable synthesis. Novo29 (clovibactin) is promising but suffers from low yield (1%), dependence on costly and noncommercial d-hydroxy-asparagine (d-Hyn$_5$), and lengthy syntheses. We report "Novltex", a novel class of antibiotic that fuses the Leu$_{10}$-teixobactin macrocycle to the Novo29 N-terminus tail, replacing d-Hyn$_5$ with inexpensive threonine. Our efficient synthesis delivers 30% yield with faster coupling cycles (~10 min), enabling rapid and low-cost scale-up. A 16-member analogue library systematically probing amino-acid configuration identified analogue **4** (d-Leu$_2$) as the initial lead, informing the rational design of analogue **12** (d-cyclohexylalanine$_2$). Analogue 12 displays potent antibacterial activity (minimum inhibitory concentration (MIC) 0.12–0.5 μg/mL) against World Health Organization (WHO)-priority pathogens, including methicillin-resistant *Staphylococcus aureus (*MRSA) and *Enterococcus faecium*, surpassing several licensed antibiotics while maintaining an excellent safety profile. Lipid II-binding assays confirm the conservation of the parent mechanism. Novltex, therefore, offers a practical, high-yielding, and cost-efficient platform for the development of next-generation antibiotics targeting MDR infections.

## Graphical Abstract

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## Novel Synthetic Strategies Towards Analogues of Cadaside and Malacidin Antibiotic Peptides

Katharina Webhofer[1], Darsha Naidu[1,2], Milandip Karak[3], Stephen A. Cochrane[3], Christopher J. Morris[1] and Rachael Dickman[1,*]

***Biomolecule s*** **2025,** *15*(11), 1497
Published 22 Oct 2025
DOI: https://doi.org/10.3390/biom15111497

## Abstract

With antibiotic resistance becoming an increasingly pressing issue, the search for novel antimicrobial drugs is more important than ever before. The recently discovered calcium-dependent lipopeptides cadaside A/B and malacidin A/B have promising activity against resistant Gram-positive bacteria. With limited reports of synthetic routes towards these peptides available in the literature, especially for cadasides, we herein report a novel on-resin synthesis strategy. We used this strategy to produce fifteen simplified malacidin and cadaside analogues. In addition, both minimum inhibitory concentration and thin layer chromatography assays were conducted to determine antimicrobial activity and advance our understanding of these peptides' structure–activity relationships.

## Multicharged zwitterions form superior antifouling interfaces

Declan Meehan, Jessica McMaster, Ayantika Kundu, Matthew P. Wylie, Joseph S. Vyle, Karl J. Hale, Marijana Blesic*

***Advanced science*** Early View Online Version of Record before inclusion in an issue
e14739
Published 24 Oct 2025
DOI: https://doi.org/10.1002/advs.202514739

### Abstract

The long-term prevention of unwanted protein and microbial accumulation on surfaces, including medical devices, remains a significant and largely unresolved challenge. Decades of research into antifouling surfaces have suggested that addressing this issue will require a sustained approach focused on incremental advances in chemical design. The creation of highly hydrophilic surfaces has long been recognized as a key strategy, initially pursued through polyethylene glycol-functionalized coatings. More recently, zwitterionic groups have emerged as effective antifouling moieties. However, the limited chemical diversity of zwitterion-forming chemical entities has constrained further progress. In this study, an alternative approach to enhancing surface hydrophilicity is presented by employing multicharged zwitterionic molecules (**MZWs**), which increase the density of charged hydrophilic groups per monomer unit. Surfaces functionalized with **MZWs** exhibited 40–45% lower protein adsorption compared to benchmark single zwitterionic molecules. Remarkably, the synthesized **MZWs** spontaneously assemble into vesicular aggregates (130–170 nm) without the need for additives or any form of external force. These findings strongly support further exploration of **MZW**-functionalization as a novel strategy to enhance antifouling performance, while remaining readily adaptable via minor modifications to existing synthetic routes used for the incorporation of conventional zwitterions into polymers, self-assembled monolayers, hydrogels, and nanocarriers.

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## Methanolysis of polyethylene terephthalate (PET) using non-stoichiometric protic ionic liquids

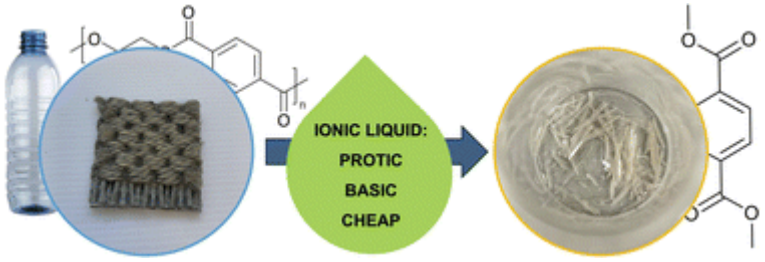
Emma McCrea, [a] Peter Goodrich,[a] John D. Holbrey [a] and Małgorzata Swadźba-Kwaśny *[a]

***RSC Sustainability***, 2025,**3**, 3987-3996
Published 31 Jul 2025
DOI: https://doi.org/10.1039/D5SU00316D

### Abstract

Methanolysis of polyethylene terephthalate (PET) to dimethyl terephthalate (DMT), carried out in a microwave reactor, was catalysed by an inexpensive and recyclable non-stoichiometric protic ionic liquid, formulated from sulfuric acid and triethylamine. The influence of the catalyst composition (excess of acid or base), reaction temperature and time, as well as methanol excess, on the conversion of PET and the yield of DMT, was investigated. Under optimised conditions (3 h, 180 °C), waste PET from milled plastic bottles was depolymerised, reaching 100% PET conversion and 98% isolated yield of DMT. Pure DMT was separated through recrystallisation directly from the reaction mixture. Preliminary experiments with carpet waste (dyed mixed polymer waste, without milling) gave results on par with those achieved for PET bottles, with 100% PET conversion and 97% of DMT (isolated yield).

### Graphical Abstract



## Mechanochemically engineered CaO-CeO2 dual-function catalysts for sustainable glycerol carbonate production without solvents

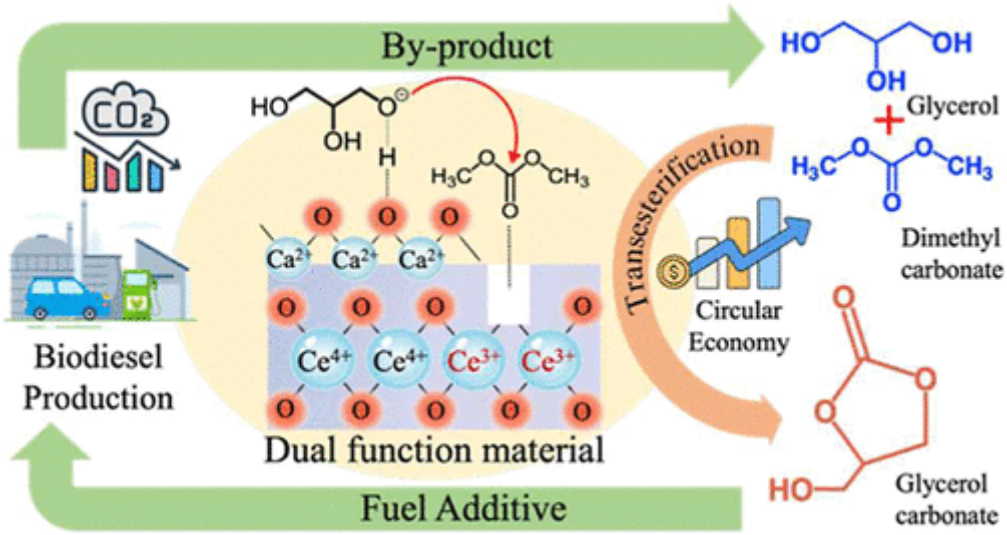
Patcharaporn Inrirai, Runzhe Yu, Daniel Goma Jiménez, Nancy Artioli, Haresh Manyar*

***Energy Fuels*** 2025, 39, 26, 12676–12688
Published 19 Jun 2025
DOI: https://doi.org/10.1021/acs.energyfuels.5c01580

### Abstract

Upgrading biorefinery-derived waste such as glycerol to fuel-additives and high-value products is essential to further enhance the productivity, profitability, and circularity of the biorefinery concept to achieve a green and sustainable net-zero world. This study explores the catalytic conversion of glycerol into glycerol carbonate using calcium oxide–cerium oxide ($CaO–CeO_2$) dual-function catalytic materials. Herein, a clean and efficient approach was developed to synthesize $CaO–CeO_2$ materials using a green mechanochemical method and then utilize these as catalyst in sustainable and solvent-free synthesis of glycerol carbonate to enhance the circular economy of biorefineries while reducing their carbon footprint. The catalysts were comprehensively characterized using XRD, FTIR, ICP, $N_2$ sorption, $CO_2$-TPD, and SEM/EDS analyses and evaluated for their catalytic activity. Among the catalysts studied, 40 wt % $CaO–CeO_2$ exhibited the highest catalytic activity, achieving 95% glycerol conversion and 99% selectivity to glycerol carbonate under optimized conditions (10 wt % catalyst loading relative to glycerol, 90 °C, 60 min, and a glycerol/ DMC molar ratio of 1:3). This catalyst showed excellent reusability, maintaining high conversion over four cycles. The transesterification reaction followed irreversible second-order reaction kinetics with an activation energy of 46.9 kJ $mol^{-1}$. The synergistic interplay between the basic sites of the $Ca^{2+}–O^{2-}$ pair and the oxygen vacancies in the $CeO_2$ matrix at the $CaO–CeO_2$ interface work in tandem to enhance the catalytic activity for glycerol carbonate production. We have developed a highly efficient, cost-effective, and environment-friendly approach for the sustainable production of glycerol carbonate from glycerol.

### Graphical Abstract

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## Mechanisms of using NaCl-CaCl2 molten solar salts in enhancing the integrated CO2 capture and utilization via reverse water gas shift (ICCU-RWGS) process with CaO alone

Xiaotong Zhao, Bo Zong, Jia Hu, Yulan Han, Yingrui Zhang, Chunfei Wu*

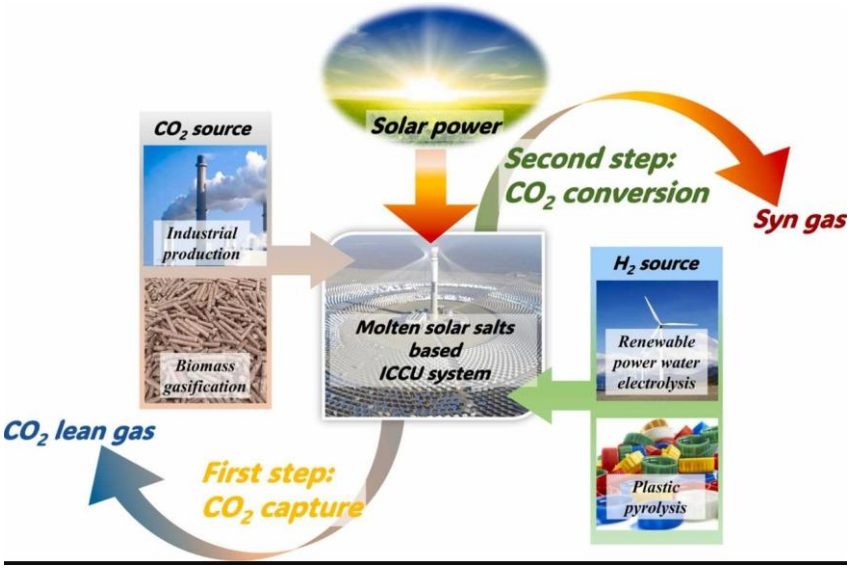
**Applied Catalysis B: Environment and Energy** Volume 367, 15 June 2025, 125100
Published 15 June 2025
DOI: https://doi.org/10.1016/j.apcatb.2025.125100

### Abstract

This study explored the integration of $NaCl-CaCl_2$ molten solar salts with CaO in the integrated $CO_2$ capture

and utilization via reverse water gas shift reaction (RWGS). It was demonstrated that the molten salt system significantly improves $CO_2$ capture capacity and CO generation rate compared to CaO alone. The system achieved a $CO_2$ conversion of 56.99 % at 650 ℃, with a notable average $CO_2$ capture rate of 0.64 mmol $g^{-1}$ $min^{-1}$ and CO generation rate of 0.23 mmol $g^{-1}$ $min^{-1}$. The co-melting behavior of NaCl-$CaCl_2$-CaO was found to be the main reason for enhancing $CO_2$ capture through the TG-DSC test. XPS analyses confirmed that the eutectic melting of the salts disrupts the crystalline structure of CaO, leading to $CO_2$ and metals bonding through adsorbed oxygen rather than lattice oxygen. Combined with the mechanistic insights provided by in-situ DRIFTS and in-situ Raman, it was confirmed that the easier desorption of adsorbed oxygen is the key factor behind the enhanced CO generation during the RWGS stage in the molten salt environment. These findings provide foundational insights for the future design of solar-driven $CO_2$ capture and conversion molten salt systems.

## Graphical Abstract

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## Lipid II unlocked: strategies for obtaining a major antibiotic target

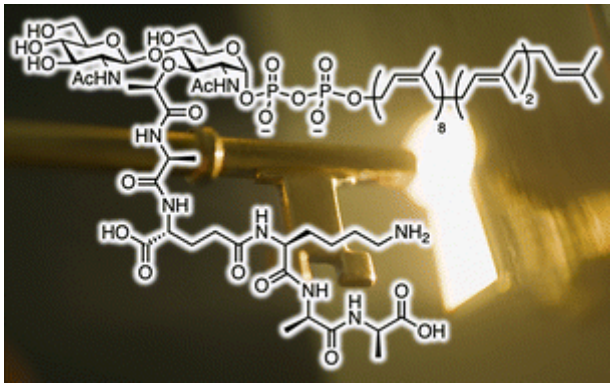
Luke J. Tyrie,[a] Milandip Karak *[a] and Stephen A. Cochrane *[a]

***Chem. Commun.***, 2025,**61**, 17787-17809
Published 17 Oct 2025
DOI: https://doi.org/10.1039/D5CC04843E

## Abstract

Antimicrobial resistance (AMR) is a major global concern. It caused nearly five million deaths in 2019 and is projected to be responsible for up to ten million annually by 2050. A deeper understanding of how antibiotics interact with their molecular targets is essential to addressing this threat, as it can facilitate rational drug design. One major antibiotic target is lipid II, a highly conserved and essential precursor in bacterial cell wall biosynthesis. As the final monomeric intermediate in peptidoglycan biosynthesis, lipid II has become an important target for antibiotic discovery. However, accessing lipid II remains technically challenging. In this review, we examine the three main strategies used to obtain lipid II: direct extraction from bacteria, enzymatic or chemoenzymatic assembly using purified or partially purified biosynthetic machinery, and total chemical synthesis. We discuss the strengths and limitations of each method, scalability, and structural control, and highlight notable approaches that are expanding the accessibility of lipid II and its analogues. These advances are critical not only for antibiotic research but also for understanding bacterial physiology at the molecular level.

## Graphical Abstract



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## Iron catalysts enhanced by ultrasound for methane decomposition and hydrogen generation

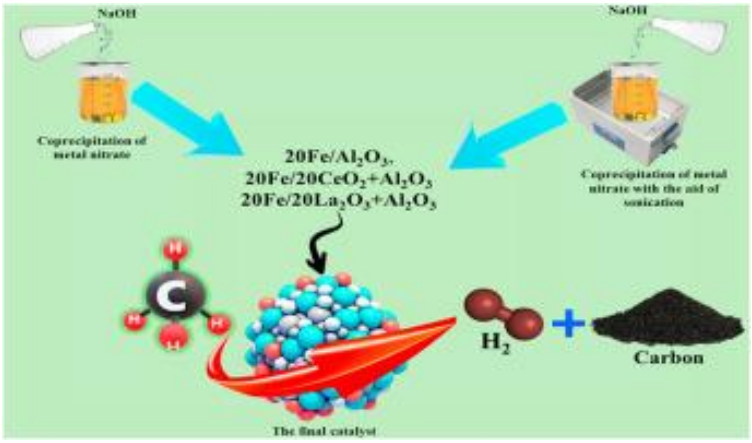
Ahmed A. Ibrahim [a], Hamid Ahmed [a], Anis H. Fakeeha [a], Ahmed E. Abasaeed [a], Ahmed S. Al-Fatesh [a]*, Ahmed I. Osman [b]*

**International Journal of Hydrogen Energy** Volume 137, Pages 851-860
Published 12 June 2025
DOI: https://doi.org/10.1016/j.ijhydene.2024.05.079

### Abstract

Clean hydrogen production offers a viable alternative in the transition to a greener and more sustainable energy future. This study introduces a novel method for enhancing $Fe/Al_2O_3$ catalysts using $La_2O_3$ and $CeO_2$ doping, aimed at improving hydrogen production via methane decomposition. It addresses the critical challenge of modulating metal-support interaction. Employing ultrasonication in the catalyst preparation, we observed through XRD, $H_2$-TPR, $H_2$ chemisorption, Raman spectroscopy, TGA, and TPO analyses that $La_2O_3$ addition prevents $FeAl_2O_4$ formation and increases Fe reduction and active sites. Catalysts assisted by ultrasound outperform traditional methods, exhibiting a consistent and significant increase in conversion and yield efficiencies. The $La_2O_3$-modified catalysts outperformed the standard $Fe/Al_2O_3$ catalyst in methane decomposition. At 800 °C, they demonstrated enhanced activity and stability under demanding conditions, achieving a methane conversion of 93% and hydrogen yield of 84%. This approach boosts hydrogen production and contributes to the development of sustainable and efficient energy solutions.

### Graphical Abstract

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## Ionic liquid gels: catalysts for sustainability in synthesis, energy, electronics and medicine

Patricia C. Marr, Andrew C. Marr

**Philosophical Transactions of the Royal Society of London Series A**
Publication status Accepted - 05 Aug 2025

## Abstract
This opinion paper reflects upon highlights in ionic liquid gel research for green and sustainable chemistry. Discussed are some key observations from research into ionic liquid gels in catalysis, and insights into potential future uses and areas for development. It is noted that some IL gels have a remarkable ability to hold onto precious metals when used to entrap catalysts (nanoparticulate metals and complexes with minimal leaching) allowing heterogenized homogeneous catalysts to be reused, recycled and easily separated. Herein we present observations that ionic liquid gels can actively absorb and retain metals from solution. Evolving trends in research into liquids comprised of ions will be reviewed and a future in which the ionic liquid gels themselves are green and sustainable materials is hypothesized, which will accelerate their adoption as NaturIL gels in synthesis, materials, electronics and medicine.

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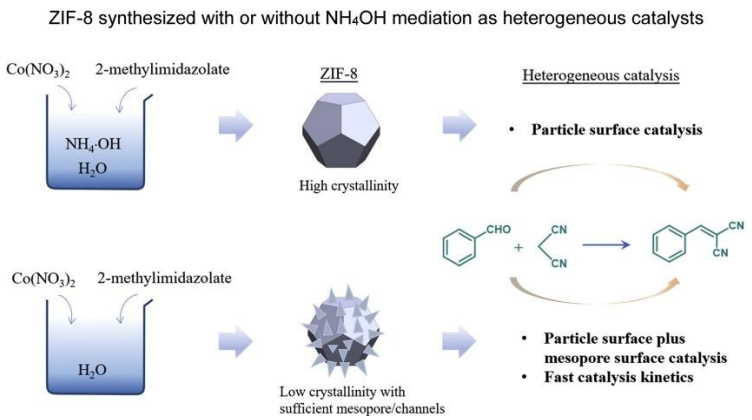
# Influence of crystal textures in metal-organic frameworks (MOFs) on catalysing heterogeneous Knoevenagel condensation reaction

Qingwei Meng [a], Petra J. van Koningsbruggen [b], Daniel Jozef Nowakowski [a], Jinesh C. Manayil [a], Tony Bridgwater [a], Bo Xiao [c], Qingchun Yuan [a b]*

**Chemical Engineering Journal Advances** Volume 23, 100788
Published August 2025
DOI: https://doi.org/10.1016/j.ceja.2025.100788

## Abstract
Metal-organic frameworks (MOFs) have received long-term research attention due to their exceptionally high specific surface areas and customizable active sites. These properties are typically critical indices for evaluating porous materials in applications such as adsorptive separation or heterogeneous catalysis. High crystallinity and specific surface area have been the focus of MOF synthesis. MOF crystals rich in small micropores may not be sufficient for effective heterogeneous catalysis, especially when the reactants are too large to access the micropores. This study examined ZIF-8 MOF (Zeolite Imidazole Frameworks, a representative and extensively studied MOF) crystal textures for their heterogeneous catalytic performance in the Knoevenagel condensation of benzaldehyde and malononitrile to form benzylidene malononitrile. The ZIF-8 samples were synthesized in aqueous media at a room temperature with or without the mediation of a small amount of ammonia. The obtained ZIF-8 samples were characterized by XRD, ATR, $N_2$-adsorption, TGA and STEM. Although the ammonia-mediated ZIF-8-$NH_4OH$ samples exhibited superior crystallinity and high specific surface areas compared to the non-mediated ones, these are not beneficial for their catalytic kinetics in the Knoevenagel condensation of benzaldehyde and malononitrile. In contrast, the ZIF-8 crystals synthesized without ammonia meditation exhibited open mesoporous characteristics, which provided greater accessibility of the reactants to the catalytic active sites on the internal surface. This resulted in significantly faster catalytic conversion, comparable to that achieved in homogeneous catalysis. For the first time, this work systematically demonstrates the critical role of open mesopore formation within MOF crystal particles in promoting heterogeneous catalytic kinetics. The research findings open a new guideline for heterogeneous catalyst development from MOFs.

## Graphical Abstract
ZIF-8 synthesized with or without $NH_4OH$ mediation as heterogeneous catalysts.



## Hydroxylation mechanism of lignin-derived aromatic substrates catalyzed by plant P450 cinnamate 4-hydroxylase

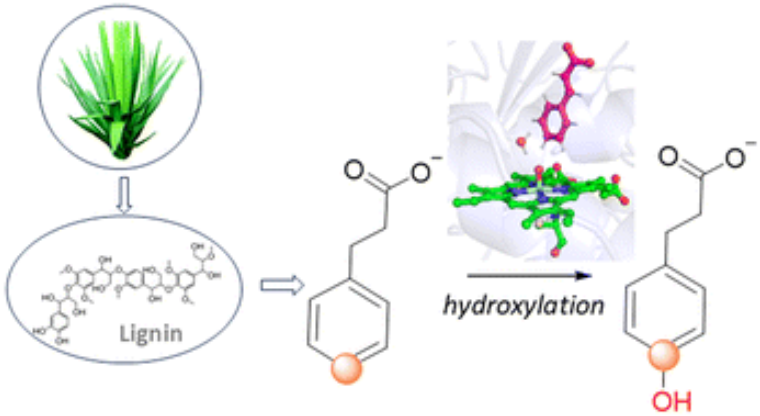
Sónia F. G. Santos,[ab] Paul James,[b] Rajesh Reddy Bommareddy,[b] Yunhong Jiang,[b] Jun Li,[c] Chun Li,[d] Warispreet Singh*[b] and Meilan Huang *[a]

***Catal. Sci. Technol.***, 2025,**15**, 7067-7078
Published 2 Oct 2025
DOI: ***Catal. Sci. Technol.***, 2025,**15**, 7067-7078

### Abstract

Cytochrome P450 cinnamate 4-hydroxylase (C4H) is a pivotal enzyme in the phenylpropanoid pathway, playing a critical role in regulating lignin biosynthesis in plants. In contrast to the hydroxylation reactions catalyzed by human P450 enzymes, which have been extensively studied, the mechanistic understanding of plant P450-mediated hydroxylation of aromatic substrates remains limited. In this study, using comprehensive atomistic molecular dynamics (MD) simulations, we elucidated the binding pose of the native substrate *trans*-cinnamic acid and identified key residues contributing to the substrate specificity of the enzyme, which include Arg213 and a conserved hydrophobic pocket comprising Val118, Phe119, Val301, Ala302, Ile367 and Phe484. Additionally, we investigated the catalytic mechanism using hybrid quantum mechanics/molecular mechanics (QM/MM) calculations, evaluating all plausible C4H-catalysed pathways for aromatic hydroxylation. Our results reveal that among all investigated mechanisms, the most favourable pathway involves direct hydroxylation *via* electrophilic attack coupled with a proton shuttle. These findings provide valuable insights into the catalytic mechanism of C4H, which would pave the way for modifying lignin biosynthesis to regulate various lignin contents in plants, unlocking its potential applications in sustainable bioremediation and biomanufacturing.

### Graphical Abstract

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## Highly regioselective, ligand-differentiated platinum-catalysed hydrosilylation of propynamides

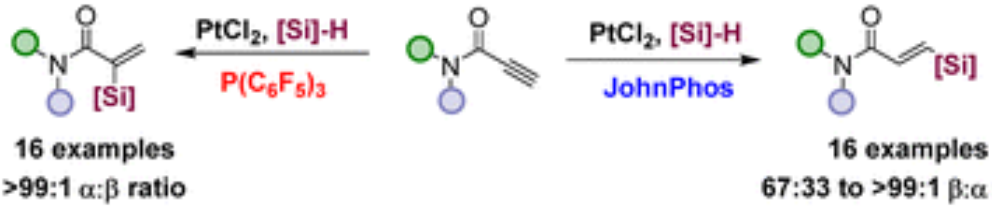
Elizabeth L. R. Leonard,[ab] Megan E. Boyd,[b] Geoffrey R. Akien [a] and Mark G. McLaughlin *[b]

***Chem. Commun***., 2025,61, 14121-14124
Published 13 August 2025
DOI: https://doi.org/10.1039/D5CC03832D

### Abstract

We present, for the first time, a highly regio- and stereoselective ligand-divergent hydrosilylation reaction. The methodology produces diverse amido-vinyl silanes from readily available propynamides. Employing platinum catalysis utilizing commercially available ligands, silyl-α,β-unsaturated amides are produced in synthetically useful yields (up to 91%). This methodology allows, for the first time, an unprecedented ligand differentiated hydrosilylation methodology to form β-(*E*)-silyl-α,β-unsaturated amides in high regioselectivity and α-silyl-α,β-unsaturated amides with complete regioselective control (>99 : 1).

## Graphical Abstract

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## High-active CoPi-Ov nanolayer promotes photoelectrochemical glycerol oxidation for efficient dihydroxyacetone production

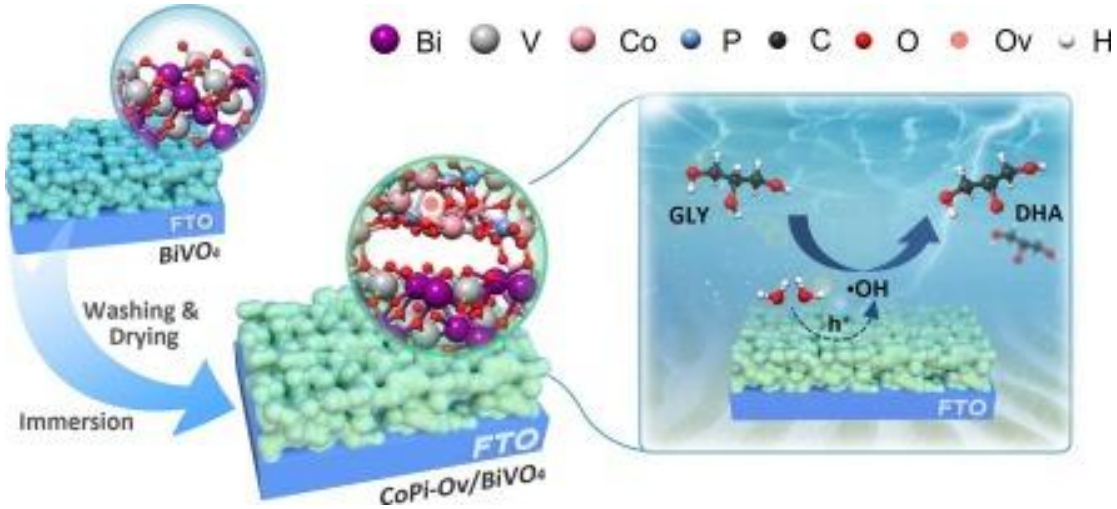
Zihu Kang [a], Yujie Shen [b], Yue Zheng [a], Kairui Ma [a], Zhi Zhang [a], Meilan Huang [b]*, Xia Tao [a]*

**Chemical Engineering Journal** Volume 515, 163904
Published 1 July 2025
DOI: https://doi.org/10.1016/j.cej.2025.163904

## Abstract

The increasing global consumption of biofuels calls for efficient transformation of the main by-product glycerol (GLY) in the biodiesel and bioethanol industry process. Photoelectrochemical (PEC) oxidation of GLY to high value-added C3 products like preferred dihydroxyacetone (DHA) over a $BiVO_4$ photoanode remains challenging, due to the low photocurrent density and/or selectivity and thus insufficient DHA productivity (<400 mmol $m^{-2}$ $h^{-1}$). Herein, we report the PEC GLY oxidation to DHA over a heterogeneous photoanode of the cobalt phosphate nanolayer with rich oxygen vacancies (Ov) anchored on $BiVO_4$ (CoPi-Ov/$BiVO_4$). The conversion achieves the highest DHA production rate of 454.9 mmol $m^{-2}$ $h^{-1}$ among reported $BiVO_4$-based photoanode to date. We demonstrate that the CoPi-Ov nanolayer is featured with amorphous morphology and enriched Ov facilitating photo-induced charge separation and hole transport, thereby providing more active sites for GLY oxidation reaction (GOR). TR-FTIR, radical recognition assays and DFT calculations verify that the Co atoms in CoPi-Ov preferentially interact with the middle hydroxyl of GLY to form carbon-centered radicals, promoting the oriented production and desorption of DHA. This study highlights a GOR system, starting from facile photoanode synthesis to the design of high-active photoelectrocatalyst enlightened by structure-activity relationship, which potentiates biomass valorization to generate valuable products.

## Graphical Abstract



## Gas exclusion zones in Type II porous liquids

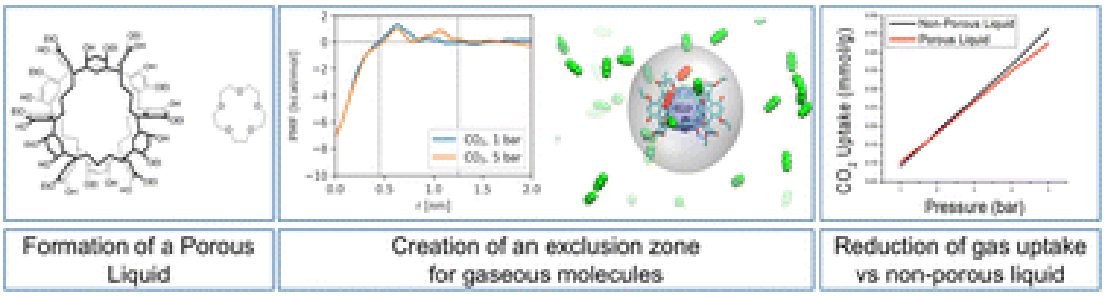
Cathal F. Kelly,[a] Sergio F. Fonrouge,[b] José L. Borioni,[c] Mario G. Del Pópolo,[b] Émer M. F. Rooney,[a] Deborah E. Crawford,[d] K. Travis Holman[e] and Stuart L. James *[a]

***Chem. Sci.***, 2026,**17**, 1341-1348
Published 19 Nov 2025
DOI: https://doi.org/10.1039/D5SC06588G

### Abstract

Porous liquids combine permanent porosity with fluidity and may ultimately find uses which are not possible for conventional liquids or porous solids. An important general characteristic of porous liquids studied to date is that they exhibit very high gas solubilities. Here, we examine this aspect in more detail than has been done previously, in particular with regard to $CO_2$ and $CH_4$ solubility in the Type II porous liquid $Noria_{OEt}$@15C5 (15C5 = 15-crown-5). Whilst this porous liquid exhibits increased $CH_4$ solubility compared to neat 15-crown-5, counterintuitively it actually exhibits equal or lower $CO_2$ solubility than the neat solvent 15C5 at pressures above 1 bar. Molecular dynamics modelling reveals that although the pore space does provide a good binding site for gas molecules, there is an 'exclusion zone' around the pore space within which binding of $CO_2$ molecules is disfavoured compared to binding within the bulk solvent. The unfavourable binding in this region arises from a number of effects, including (i) steric exclusion from the bulky covalent framework of the $Noria_{OEt}$ host, and (ii) ordering of 15C5 solvent molecules in the solvation shell around the $Noria_{OEt}$. The first porous liquid to be based on the host Cryptophane-A, Cryptophane-A@Cyrene, was prepared in the expectation that the smaller framework bulk of Cryptophane-A compared to that of $Noria_{OEt}$ should result in a smaller exclusion zone. Correspondingly, this porous liquid did indeed exhibit improved $CO_2$ uptake compared to its neat solvent, supporting the assertion that the exclusion zone is at least in part due to exclusion of gas from the framework of the host. Overall, the work provides a more sophisticated understanding of gas solubility in Type II PLs and suggests some additional design considerations for achieving high solubility for a given gas. It also shows that, as well as being able to increase the solubility of certain gases PLs can also conceivably be designed to suppress the solubility of gases under some conditions, which could be useful in tuning selective dissolution.

### Graphical Abstract

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## First-principles insights into the direct synthesis of acetic acid from CH4 and CO2 over TM-Si@2D catalysts

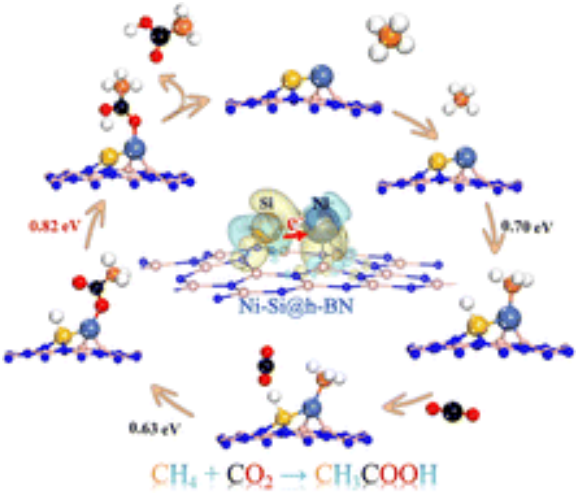
Mingyuan Zhang,[a] Linxia Cui,[a] Yang Jiang,[a] Rui Gao,[a] Haigang Hao*[a] and Meilan Huang *[b]

***Chem. Commun.***, 2025,**61**, 19836-19839
Published 28 Oct 2025
DOI: https://doi.org/10.1039/D5CC04864H

### Abstract

The direct synthesis of acetic acid from natural gases has attracted great attention. However, achieving selective C–C coupling remains a major challenge. We designed doped single-atom transition metal catalysts on 2D materials, guided by DFT calculations on the reaction pathways for acetic acid synthesis *via* $CH_4/CO_2$ coupling. Among the catalysts examined, Ni–Si@h-BN shows strong electron synergy in $CH_4$ activation and C–C coupling under the E–R mechanism, confirmed by kinetics.

## Graphical Abstract

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## Fast-Tracking Transition-State Localization via Reaction Directional Analysis

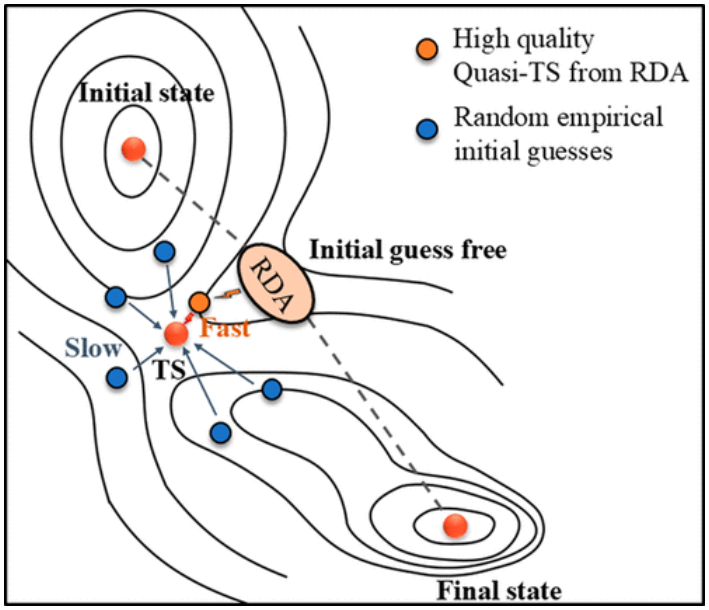
Peipei Zhang, Chenxi Guo*, P. Hu*

***J. Chem. Theory Comput.*** 2025, 21, 24, 12686–12695
12 Dec 2025
DOI: https://doi.org/10.1021/acs.jctc.5c01784

## Abstract

Transition-state localization is critical for elucidating chemical reaction mechanisms but remains one of the most computationally demanding challenges in theoretical chemistry. Here, we introduce a novel method, reaction directional analysis-dimer (RDA-D), which integrates reaction directional analysis (RDA) with the dimer method to achieve efficient and reliable transition state searching. Reaction directional analysis generates high-quality quasi-transition-state structures directly from only the initial and final state geometries, combining dynamic interpolation, structural optimization, and directional analysis. These quasi-transition-state structures then serve as starting points for refinement via the dimer method. Benchmark tests on a diverse set of gas-phase and catalytic reactions on surfaces demonstrate that RDA-D is, on average, 5.83 times faster than the Nudged Elastic Band (NEB) method in CPU time and reduces the number of gradient evaluations by a factor of 4.74. Moreover, reaction directional analysis eliminates the need for predefined reaction coordinates or chemically intuitive initial guesses, providing a robust, scalable, and automation-friendly framework for transition-state localization.

## Graphical Abstract



## Exploring the potential of chemically matched fragments as internal standards for quantitative SERS with Panobinostat

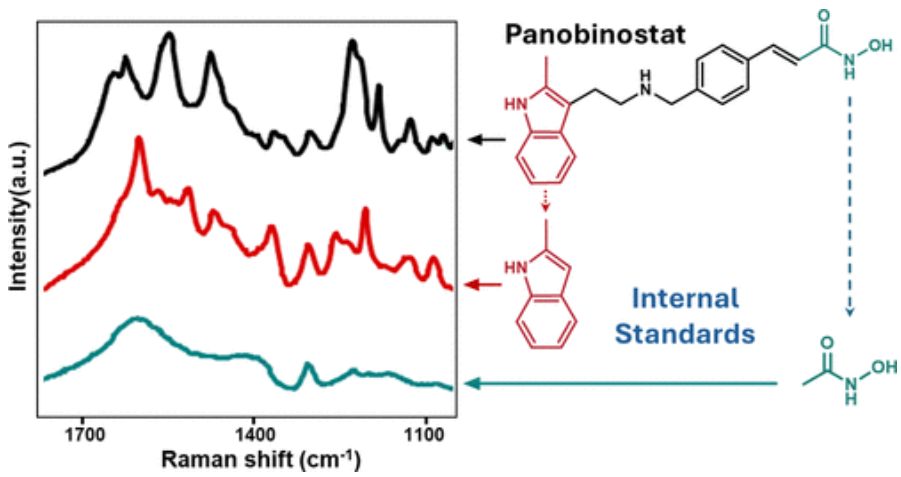
Yiming Huang, Yikai Xu, Chunchun Li, Steven E. J. Bell*

***Anal. Chem***. 2025, 97, 34, 18490–18498
Published 21 August 2025
DOI: https://doi.org/10.1021/acs.analchem.5c02017

### Abstract

Surface-enhanced Raman spectroscopy (SERS) has great potential for therapeutic drug monitoring (TDM) due to its high sensitivity; however, achieving accurate and robust quantitative data remains challenging. The most effective approach for quantitative SERS is to use internal standards (IS). Isotopologues are particularly effective; however, these or closely related analogues of the target compound are often unavailable. We have addressed this problem by using fragments of the target compound as the IS. Here, 2-methylindole (2-MI) was identified as the most suitable fragment for Panobinostat (Pano). Tests with an enhancing colloid that degraded significantly over a 4-week period showed that the 2-MI IS allowed changes in the absolute intensity of the Pano signal over time to be corrected and that the standard error achieved with the degrading enhancing medium matched that of results obtained with the fresh colloid. The calibration range could be extended by using either low ($4 \times 10^{-7}$ M) or high ($10^{-5}$ M) concentrations of 2-MI, both of which gave linear log/log Pano calibration curves ($R^2 = 0.993$ and 0.998, respectively) although these curves had different slopes. In contrast, thiophenol (TP), a nonchemically matched IS, gave reasonable results at a low ($10^{-6}$ M) concentration ($R^2 = 0.942$) but completely failed at a high ($10^{-5}$ M) concentration due to surface saturation. These findings can be rationalized using a model where, at submonolayer concentrations, both the target and IS adsorb to the nanoparticle surface in proportion to their concentrations; however, at higher concentrations, competition for active sites on surface alters the relative intensities observed. This fragment-based approach significantly increases the availability of chemically matched IS for large target molecules and therefore significantly broadens the range of compounds where robust quantitative SERS analysis is possible.

### Graphical Abstract

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## Evaluation of rice husk biochar influence as a partial cement replacement material on the physical, mechanical, microstructural, and radiation shielding properties of ordinary concrete

Alaa A. Mahmoud, Alaa A. El-Sayed, Islam N. Fathy, Samer Fawzy, Mansour Alturki, Maged E. Elfakharany, Mohamed A. Abouelnour, K. A. Mahmoud, Hany A. Dahish, Soliman M. ElTalawy & Islam M. Nabil

***Scientific Reports*** volume 15, Article number: 27229 (2025)
Published 26 Jul 2025
DOI: https://doi.org/10.1038/s41598-025-11987-8

## Abstract

The construction industry's urgent need for sustainable alternatives to ordinary Portland cement (OPC) has spurred significant interest in supplementary cementitious materials (SCMs). Therefore, this study investigates the synergistic effects of rice husk ash (RHA) and extracted microsilica (EMS) as partial replacements for cement in high-strength concrete (HSC). RHA was produced by controlled combustion of rice husk (RH) at 600–700 °C, while EMS was obtained through an optimized extraction process. Along with control mix (CM), three ternary mixes incorporating 15–35% RHA and 5–15% EMS were investigated to evaluate their effects on the mechanical and durability properties, as well as microstructural characteristics. Experimental results demonstrated that samples containing 20% (5% EMS + 15% RHA) and 35% (10% EMS + 25% RHA) as cement replacement exhibited enhanced performance, increasing the 28-day compressive strength by 11.56% and 5.98%, respectively, as compared to conventional concrete. Durability assessments of the optimal mixes revealed a significant reduction in water absorption (WA) and permeability. Physiochemical characterization confirmed the increased formation of dense calcium silicate hydrate (CSH) gels and a reduction in portlandite content, indicating high pozzolanic reactivity. However, the 50% replacement mix (15% EMS + 35% RHA) showed inferior performance due to the particle agglomeration and higher porosity. This study shows that the strategically formulated combinations of EMS and RHA blends (up to 35%) can produce sustainable HSC with improved mechanical properties and durability while mitigating environmental impacts. These findings provide valuable insights for advancing eco-friendly construction materials, supporting global sustainability initiatives in infrastructure development.

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## Engineering sustainable adsorption processes: batch vs. fixed-bed systems for pollutant removal

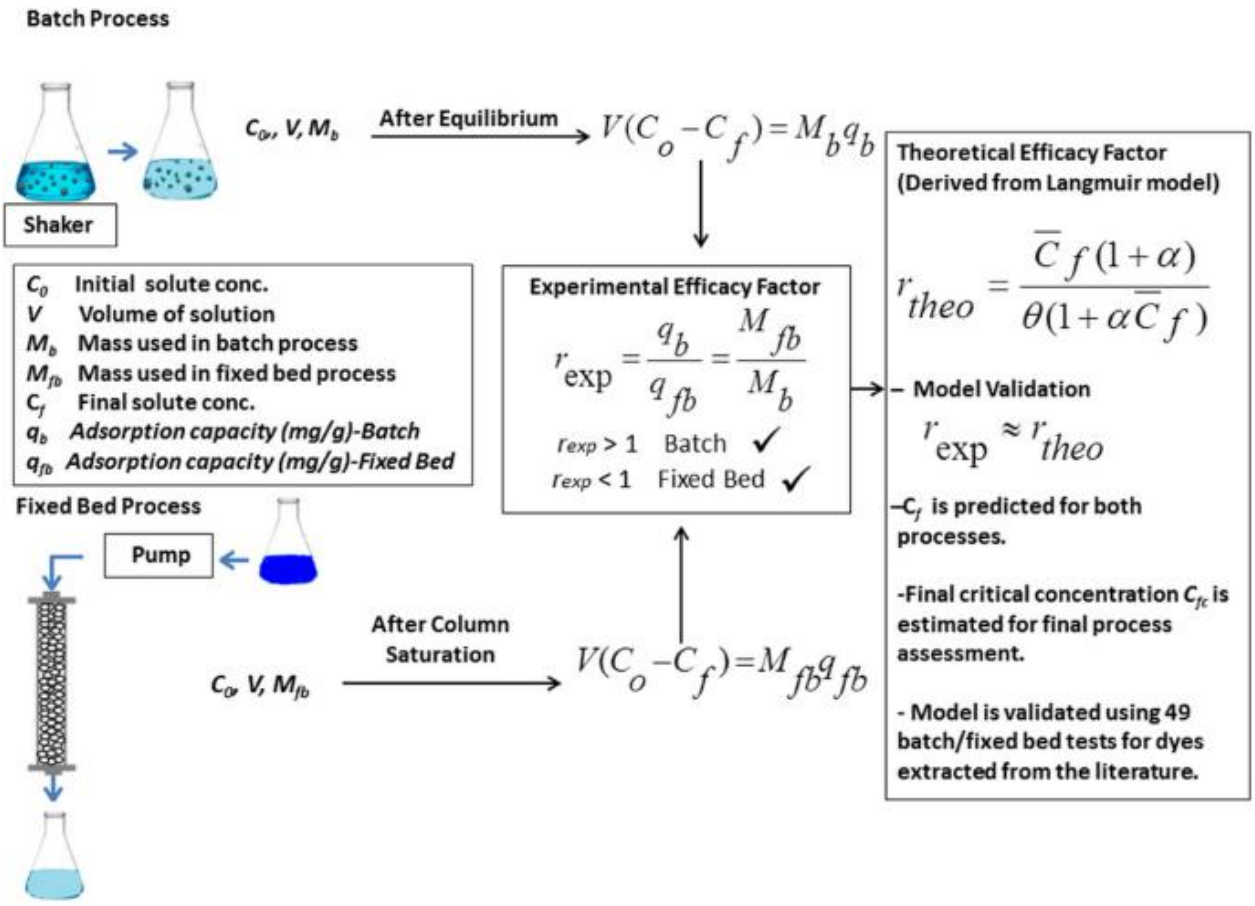
Khaled Al-Zawahreh, Ahmad B. Albadarin, Chirangano Mangwandi & Esam Ayed Wshah

***Environ Sci Pollut Res*** **32**, 18944–18960 (2025)
Published 5 Aug 2025
DOI: https://doi.org/10.1007/s11356-025-36800-x

## Abstract

In this work, we present a practical framework for selecting between batch and fixed-bed adsorption processes to achieve efficient pollutant removal while minimizing adsorbent consumption. To evaluate performance, we introduce an experimental efficacy factor ($r_{exp}$), defined as the ratio of adsorption capacity under batch conditions ($q_b$) to that under fixed-bed conditions ($q_{fb}$), under identical operating conditions. A theoretical efficacy factor ($r_{theo}$) was also derived using the Langmuir model, and its close agreement with $r_{exp}$ confirms the reliability of the approach for assessing and comparing adsorption process efficiency. Performance assessment was based on the final pollutant concentration, $C_{fc}$, defined as the critical concentration at which equal masses of adsorbent are used in both systems. The two processes were evaluated by comparing $C_{fc}$ values against a defined threshold limit of 5.0 mg/L. The model's validity was tested using data from 31 different adsorbents assessed under both batch and fixed-bed conditions. The screened adsorbents—including activated carbon, chitosan, resin, collagen, and a wide range of bioadsorbents—demonstrated high dye uptake capacities, ranging from 30.0–1070.0 mg/g in batch mode and 5.0–920.0 mg/g in fixed-bed mode. Among them, polymeric resin showed the highest retention, with capacities of 1076.0 mg/g (batch) and 917.0 mg/g (fixed-bed). Although $r_{exp}$ values suggested that the fixed-bed process was effective in many cases, the batch process showed a clear advantage where the $C_{fc}$ values in batch systems were consistently below the threshold, indicating more effective pollutant removal. The proposed model provides a valuable framework for selecting appropriate adsorption methods, particularly when synthetic adsorbents are costly. Overall, it supports informed decision-making and process optimization in adsorption-based pollutant removal.

## Graphical Abstract

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## Emerging metal–organic framework-based materials for photocatalytic and electrocatalytic NH3 synthesis: Design principles, structure-activity correlation, and mechanistic insights

Ximing Li [a b], Lin Tian [a], Qibing Dong [a], Zhe Wang [b], Kathryn Ralphs [b], Catharine Esterhuysen [c], Peter K.J. Robertson [b], Detlef W. Bahnemann [a d e], Guanjie He [f], Chuanyi Wang [a]*

**Coordination Chemistry Reviews** Volume 534, 216543
Published 1 July 2025,
DOI: https://doi.org/10.1016/j.ccr.2025.216543

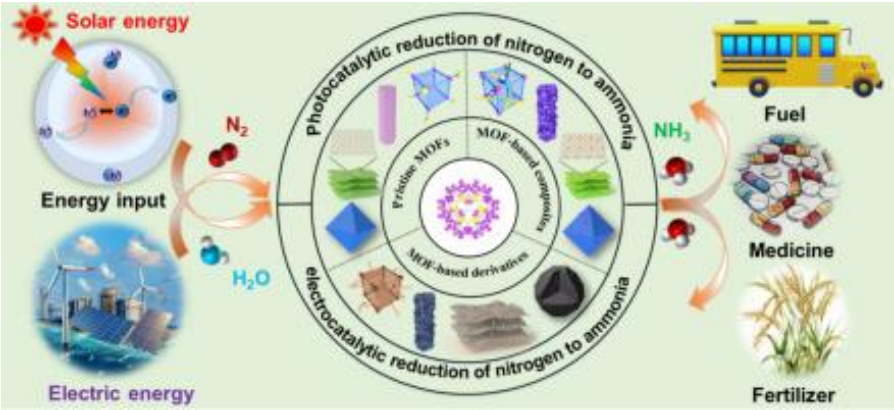
## Abstract

Sustainable ammonia ($NH_3$) synthesis through artificial nitrogen fixation has gained significant attention as a promising alternative to the energy-intensive Haber-Bosch process, offering a greener pathway for $NH_3$ production. In particular, to optimize the economic sustainability pathway of $NH_3$ synthesis technology, it is paramount to engineer novel catalysts. Emerging MOFs are a type of lightweight porous network materials with tunable channels, high surface areas, and designable components, which offer intriguing functionalities in photo- and electro-driven $N_2$ reduction reaction (NRR) by lowering reaction potentials and accelerating reaction rates. Although some progress has been achieved in this area, fundamental issues remain to be addressed to better understand the relationship between the structures, properties, catalytic activity, and potential applications of MOF-based catalysts. Herein, based on the comprehensive design concept, the latest advancements in MOF-based material design principle, structural modulation mechanism, and reaction engineering are systematically summarized to elucidate the structure-activity correlations in NRR. It begins with the MOF-based material design principles, which encompass synthesis strategies, material properties, and the transition from laboratory to large-scale continuous production progress. Following that, in terms of structural modulation mechanism, particular emphasis is placed on the analysis of crystal structure, atomic configuration, and electronic properties, aiming to gain a deeper understanding of the transport and reaction processes of charge carriers. Furthermore, the structure-activity correlations and reaction engineering are

elaborated for NRR. Finally, a comprehensive analysis of the prospects and challenges associated with MOF-based catalysts in NRR is presented, along with detailed solutions.

## Graphical Abstract

Sustainable $NH_3$ synthesis through photo/electro-driven $N_2$ reduction using MOF-based catalysts offers a green route for ammonia production. This review outlines the design principles, structural modulation mechanisms, and reaction engineering of MOF-based catalysts for NRR, aiming to advance innovative and efficient solutions toward ammonia synthesis.

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# Efficacy of mechanochemically prepared ceria-zirconia catalysts in ketonisation of acetic acid

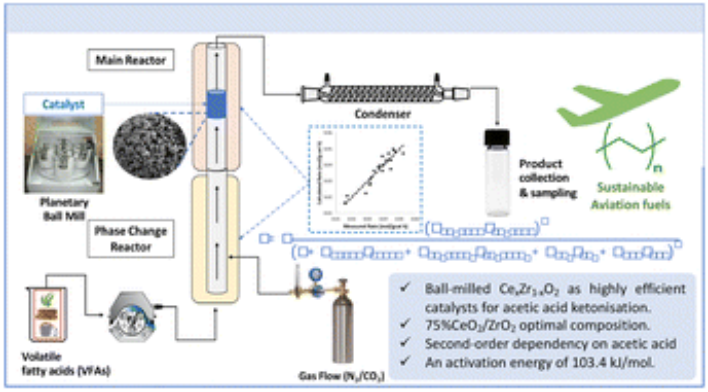
Krutarth Pandit,[ab] Gunjan Deshmukh,[a] Dipti Wagh,[a] Vikram Chatake,[c] Aniruddha Pandit,[c] Supriyo Kumar Mondal,[b] Atul Bari,*[b] Nancy Artioli[ad] and Haresh Manyar *[a]

***React. Chem. Eng.***, 2025,**10**, 1994-2003
Published 10 Jun 2025
DOI: https://doi.org/10.1039/D4RE00181H

## Abstract

This work presents a comprehensive study on the catalytic and kinetic aspects of the ketonisation of acetic acid, a model volatile fatty acid, using $Ce_{1-x}Zr_xO_2$ as catalysts. Volatile fatty acids are promising biomass derived feedstock for production of drop-in sustainable aviation fuels through a series of cascade reactions, with ketonisation as the first step followed by aldol condensation and subsequent hydrogenation. A series of $Ce_{1-x}Zr_xO_2$ catalysts for ketonisation were prepared using a mechanochemical technique of ball milling, and their performance was evaluated for varying Ce/Zr mole ratios. Among the catalysts tested, $Ce_{0.75}Zr_{0.25}O_2$ exhibited the highest conversion and selectivity towards the desired product, acetone. The catalyst characterisation showed the formation of nano-aggregates with an average particle size of 340.8 nm and a specific surface area of 66.2 $m^2\ g^{-1}$. The kinetics of the reaction indicated a second-order dependence on acetic acid, while the products (acetone, water, and $CO_2$) exhibited negative orders, suggesting competitive adsorption on the active sites of the catalyst. The activation energy for the reaction was determined to be 103.4 kJ $mol^{-1}$ suggesting the surface reaction as the rate controlling step. These findings provide valuable insights into the catalytic behaviour and kinetics of the ketonisation reaction.

## Graphical Abstract



## Dual-functional La2NiO4 impregnation for enhancement of catalytic activity and microstructure in SOEC fuel electrodes

Lu Zhou [a 1], Cheng Li [a 1], Liyuan Fan [b], Dilshod Nematov [c], Lichao Jia [a]*

**Sustainable Materials and Technologies** Volume 46, December 2025, e01759
Published December 2025
DOI: https://doi.org/10.1016/j.susmat.2025.e01759

### Abstract

Achieving high efficiency and long-term durability in solid oxide electrolysis cells (SOECs) requires innovative electrode engineering. In this study, we report a simple and scalable impregnation strategy to enhance the performance and stability of SOECs by modifying the conventional Ni-YSZ fuel electrode with $La_2NiO_4$. Under operating conditions, $La_2NiO_4$ undergoes in-situ decomposition, forming a nanocomposite of Ni nanoparticles embedded within $La(OH)_3$ substrate. This unique structure provides abundant catalytic sites for $H_2O$ dissociation and suppresses Ni coarsening, thereby ensuring stable electrochemical performance. The impregnated electrode delivered a high current density of $-1.36$ A $cm^{-2}$ at 1.3 V and 750 °C, while exhibiting significantly enhanced stability with a low degradation rate of only 0.25 mV $h^{-1}$ over 200 h, significantly outperforming the unmodified electrode counterpart. Electrochemical and microstructural analyses further confirmed reduced polarization resistance and excellent microstructural robustness. These findings highlight the promise of this impregnation approach for developing high-performance, durable SOEC electrodes, advancing sustainable hydrogen production technologies.

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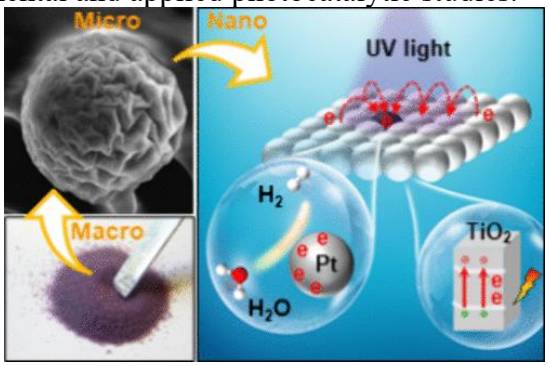
## Disentangling the effect of key parameters in hydrogen evolution for rational design of metal-semiconductor photocatalysts via self-assembly

Chunchun Li, Ziwei Ye*, Shan Xu, Nathan Skillen, Yingrui Zhang, Zehong Xu, Colby Chang, Jinlong Zhang Peter K. J. Robertson, Steven. E. J. Bell*, Yikai Xu*

***ACS Appl. Mater. Interfaces*** 2025, 17, 34, 49069–49078
Published 13 Aug 2025
DOI: https://doi.org/10.1021/acsami.5c14789

### Abstract

Fabrication of high-performance metal–semiconductor photocatalysts is a challenging problem in nanoengineering since it requires development of methods, which create strong metal–semiconductor contacts and accessible catalytic surfaces while simultaneously allowing control of the physical properties of the metal nanoparticle cocatalysts. Here, we introduce a convenient self-assembly approach for preparing highly active metal-$TiO_2$ photocatalysts, which meets all these requirements. More specifically, preformed Au/Pt and $TiO_2$ nanoparticles were used to generate Pickering emulsions, which were converted in situ into polymer microbeads covered in a mixed surface layer of tightly packed metal and $TiO_2$ nanoparticles with photocatalytic properties. A key benefit of our synthetic approach is that it allowed the physical parameters of the photocatalyst to be controlled independently. This made the materials an ideal model system to investigate structure–property relationships in photocatalysis, which allowed us to rationalize the effect of metal size, loading, surface chemistry, and composition on hydrogen evolution efficiency. Understanding the interplay of these factors allowed the creation of photocatalysts to move away from trial-and-error and enabled us to rationally design and prepare composite photocatalysts with exceptional activity. More broadly, our self-assembly approach can be readily extended to the creation of other metal–semiconductor systems, which will pave the way for both fundamental and applied photocatalytic studies.




### Graphical Abstract

## Direct transformation of biomass into levulinic acid using acidic ionic liquids: an example of sustainable and efficient waste valorization

Marta Przypis, Agata Wawoczny, Karolina Matuszek, Anna Chrobok, Małgorzata Swadźba-Kwaśny, Danuta Gillner*

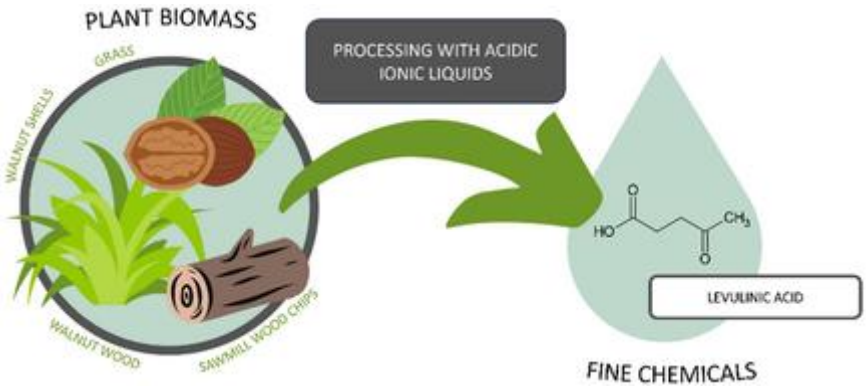
**ChemSusChem** Volume18, Issue17 2025 e202500951
Published 1 Sep 2025
DOI: https://doi.org/10.1002/cssc.202500951

### Abstract

The intensification of the use and conversion of renewable raw materials, including plant biomass, into valuable products is one of the major goals of the Sustainable Development Strategy. Levulinic acid (LA), classified as one of the top twelve biobased platform chemicals of the future, can be produced from lignocellulose; however, this process is often complex. Herein, a novel and effective pathway for the direct transformation of lignocellulosic biomass into LA under mild conditions, without pretreatment, is presented. Selected waste lignocellulosic biomass, including sawmill chips, grass, and walnut waste, as well as model cellulose, is converted to LA using acidic ionic liquids (ILs). Among the evaluated ILs, [Hmim($HSO_4$)($H_2SO_4$)$_2$] provided the highest product yields even at 50–70 °C. The ILs used herein are significantly more efficient in converting cellulose and biomass compared to conventional sulfuric acid. The highest yield of LA is obtained from sawmill chips, reaching 64.04 mol% of LA.

### Graphical Abstract

The study highlights the potential of acidic ionic liquids for sustainable and efficient biomass conversion to levulinic acid (LA). The process in the presence of [Hmim] [($HSO_4$)($H_2SO_4$)$_x$], especially with $x$=1 or 2, can be carried out efficiently under mild conditions. The highest yield of LA is obtained in the conversion of sawmill chips using [Hmim($HSO_4$)($H_2SO_4$)$_2$] at 70 °C (64.04 mol% of LA).

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## Development of molecularly imprinted polymers via dual polymerisation strategies for targeted isolation of Ethyl p-Methoxycinnamate from Kaempferia galanga L. extract

Marisa Dwi Ariani [a], Ade Zuhrotun [b], Panagiotis Manesiotis [c], Aliya Nur Hasanah [a d]*

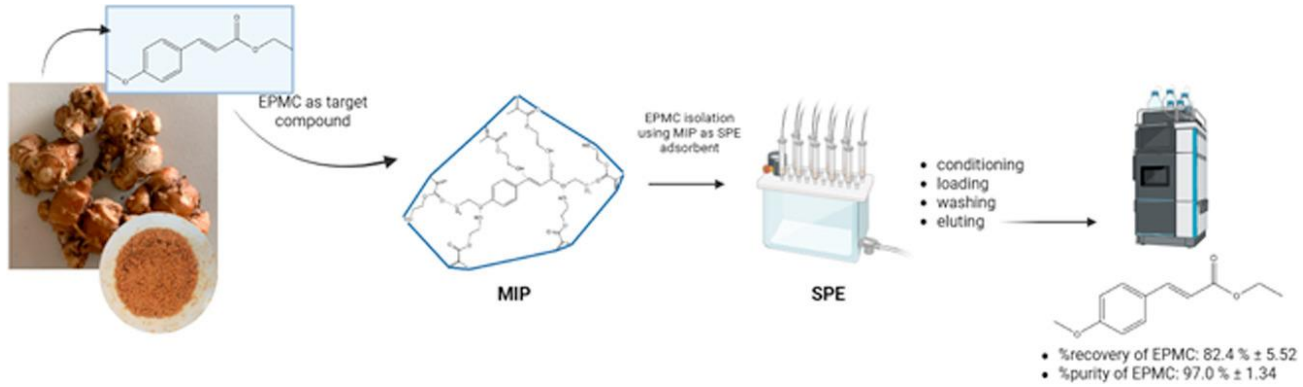
**Talanta Open** Volume 12, 100580
Published December 2025
DOI: https://doi.org/10.1016/j.talo.2025.100580

### Abstract

he rhizome of *Kaempferia galanga* L. contained ethyl p-methoxycinnamate (EPMC) as a major component of its essential oil. Despite the abundance of EPMC in the plant, conventional isolation methods yielded only 0.5 – 2.5 %. This study developed molecularly imprinted polymers (MIPs) via bulk and suspension polymerisation to enhance the selective isolation of EPMC from *K. galanga* extracts. Six functional monomers were screened for their binding affinity with EPMC. 2-hydroxyethyl methacrylate (HEMA) in chloroform and methacrylic acid (MAA) in *n*-hexane were selected for further investigation. Stoichiometric analysis established optimal template-to-monomer ratios of 1:6 for HEMA and 1:7 for MAA. Eight MIP formulations and their corresponding non-imprinted polymers (NIPs), were synthesised using these monomers via both

polymerisation methods. Characterisation using Fourie Transform Infra-Red (FTIR), Scanning Electron Microscope (SEM), Brunauer-Emmett-Teller (BET), and Particle Size Analysis (PSA) revealed that bulk polymers exhibited larger, irregular, and non-uniform particles compared to those produced by suspension polymerisation. Adsorption studies confirmed that the MIPs follow Freundlich isotherms, with MIP B2 (bulk, MAA, 1:7 ratio) exhibiting the highest binding affinity (KF = 0.081 mg/g). MIP B2 also demonstrated superior performance in the solid-phase extraction of EPMC from extracts, achieving recoveries of up to 82.4 % ± 5.52 and imprinting factors above 1.3. Selectivity tests confirmed strong discrimination of EPMC over structural analogues. In conclusion, MIP B2 offers a selective, efficient, and scalable method for EPMC isolation. These findings supported the continued development of tailored MIPs for natural product purification and provided a foundation for future optimisation of monomer-initiator systems and polymerisation parameters.

## Graphical Abstract

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## Cyanopyridinium-based ionic liquids and their mixtures for ethylene and ethane separation

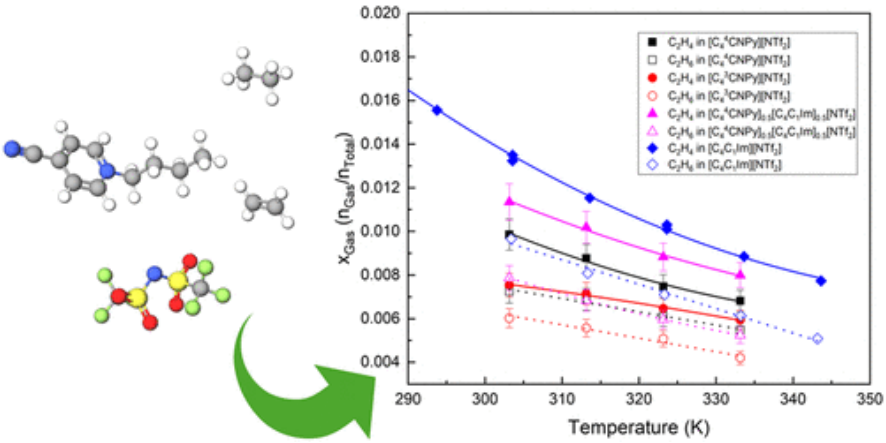
Sam H. McCalmont, Guillaume Simon, H. Q. Nimal Gunaratne, Margarida Costa Gomes, David M. Wilkins, John D. Holbrey, Leila Moura*

***ACS Sustainable Chem. Eng***. 2025, 13, 30, 11770–11783
Published 24 Jul 2025
DOI: https://doi.org/10.1021/acssuschemeng.5c01481

## Abstract

The solubility of ethane and ethylene was determined in a series of cyanopyridinium ionic liquids known to form charge-transfer complexes with polyaromatic hydrocarbons to determine their potential to form specific interactions with the unsaturated gas. The solubilities of ethylene and ethane in 1-butyl-4-cyanopyridinium bis(trifluoromethane)sulfonimide ($[C_4{}^4CNPy][NTf_2]$) and 1-butyl-3-cyanopyridinium bis(trifluoromethane)sulfonimide ($[C_4{}^3CNPy][NTf_2]$) were measured using an isochoric saturation method. The mole fraction solubility of ethane in the ionic liquids ranged from $6.0 \times 10^{-3}$ to $7.2 \times 10^{-3}$ and from $7.5 \times 10^{-3}$ to $9.9 \times 10^{-3}$ for ethylene in $[C_4{}^3CNPy][NTf_2]$ and $[C_4{}^4CNPy][NTf_2]$ at 0.1 MPa and 313 K, respectively. The small preferential solubility of ethylene over ethane in the ionic liquids results in ideal ethylene separation selectivities between 1.2 and 1.4, which is in the same range as typical physisorbent ionic liquids of the same type and molecular weight, indicating that there is no significant preferential interaction between the ionic liquids and ethylene. The calculated thermodynamic properties of solvation reveal that the solvation of both gases is entropically driven. To promote cyanopyridinium–ethylene interactions and decrease the possibility of steric constrictions to the interactions, 1-butyl-4-methylimidazolium bis(trifluoromethane)sulfonimide ($[C_4C_1Im][NTf_2]$) was added as diluent to $[C_4{}^4CNPy][NTf_2]$. This IL mixture was found to behave almost ideally based on isothermal titration nanocalorimetry results. The solubility of ethylene or ethane in the mixture was found to be the weighted average of the corresponding solubilities in the two pure ionic liquids, still indicating that no specific ethylene–ionic liquid interactions were formed. Molecular dynamics (MD) simulations of the systems were performed and revealed that the slightly higher ethylene solubility in $[C_4{}^4CNPy][NTf_2]$ is due to a slightly stronger association with this cation compared to the 3-isomer.

## Graphical Abstract

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## Composition-structure relationships for calcium aluminosilicate glasses

Subhashree Panda, Meili Liu, Rudra N. Purusottam, Jamie D. Walls, Luis Ruiz Pestana & Prannoy Suraneni
***Mater Struct* 58**, 187 (2025)
Published 25 Jun 2025
DOI: https://doi.org/10.1617/s11527-025-02693-y

### Abstract

Calcium aluminosilicate (CAS) glasses serve as ideal model systems for understanding the composition-structure relationships underpinning the performance of supplementary cementitious materials (SCMs) due to their simpler chemistry and reduced phase heterogeneity. Here, we investigate the structure of a broad compositional range of CAS glasses, including unprecedented high-CaO compositions, using X-ray diffraction (XRD), solid-state nuclear magnetic resonance (NMR), and Fourier transform infrared (FTIR) spectroscopy. With increasing CaO content, the XRD hump maxima shifts towards higher diffraction angles and causes downfield shifts in the $^{29}$Si and $^{27}$Al NMR isotropic shift maxima, indicating reduced interatomic distances and decreased electron density around Si and Al nuclei, respectively. These trends, consistent with a depolymerized structure that is more compact and contains a higher number of non-bridging oxygens, also correlate strongly with changes in Si–O-Si and Al–O–Al bond angles predicted by atomistic simulations. FTIR spectra reveals shifts in T-O-T' bond vibrations to lower wavenumbers with increasing CaO, signifying a transition to less polymerized $Q^n$ (Si, Al) species. Collectively, our results demonstrate the role of CaO in promoting network depolymerization, a crucial factor for SCM reactivity, and provide valuable insights into the structural evolution of CAS glasses as a function of composition.

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## CO2-sensitive inks for the rapid measurement of total viable count (TVC) using micro-respirometry

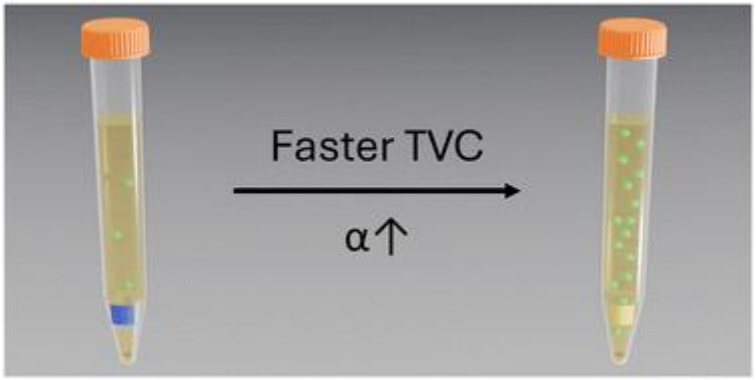
Sean Cross, [a] Christopher O'Rourke [a] and Andrew Mills *[a]
***Sens. Diagn.***, 2025,**4**, 767-778
Published 3 Jul 2025
DOI: https://doi.org/10.1039/D5SD00078E

### Abstract

At present, micro-respirometry for measuring total viable count, $O_2$ μR-TVC, is based on the time taken, TT, for an inoculum to significantly reduce the dissolved $O_2$ level (typically from 21% to ≤ 10.5%). Here, a simple kinetic model relevant to μR-TVC is presented which describes the growth of the bacteria from an initial inoculum, $N_o$, to a maximum level, $N_{max}$, and concomitant consumption of $O_2$ and generation of $CO_2$, in which the half-way time point, $t^*_{1/2}$, corresponds to $N_{max}/N_o = 0.5$, at which point $\%O_2 = \%CO_2 = 10.5\%$. The model shows that it is not possible to reduce the TT in $O_2$ μR-TVC below $t^*_{1/2}$, as TT increases above $t^*_{1/2}$ with

increasing sensitivity of the $O_2$ sensor. In contrast, the same model shows that if a $CO_2$ sensor is used instead, TT can be reduced significantly below $t_{1/2}^*$ and consequently $CO_2$ μR-TVC could be made much faster than conventional $O_2$ μR-TVC. To test this model prediction, a range of colourimetric $CO_2$ sensors of varying sensitivity, $\alpha$, were prepared and used to make $CO_2$ μR-TVC measurements. The results confirm that the greater the sensitivity of the sensor, the shorter the TT, as predicted by the kinetic model. Two $CO_2$ indicators, one of moderate sensitivity and one of high sensitivity were used to generate straight-line log(CFU $mL^{-1}$) *vs.* TT calibration plots, which can then be used to determine the unknown TVCs of subsequent samples. The future of $CO_2$ μR-TVC as a possible new, faster alternative to conventional $O_2$ μR-TVC is discussed briefly.

## Graphical Abstract

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## CO2 capture mechanism of [DBUH][Im] under humid conditions

Dominic Burns [a #], Hye-Kyung Timken [b], Huping Luo [b], Evan Hatakeyama [b], Bong-Kyu Chang [b], Małgorzata Swadźba-Kwaśny [a], John D. Holbrey [a]*

**Journal of Ionic Liquids** Volume 5, Issue 2
Published 2025
DOI: https://doi.org/10.1016/j.jil.2025.100179

### Abstract

Abstract
This work reports on the $CO_2$ absorption properties of the superbase derived protic ionic liquid (PIL) made from 1,8-diazabicyclo(5.4.0)undec-7-ene (DBU) and imidazole (Im). The results show distinct absorption mechanisms under dry and humid conditions. Under dry conditions, $CO_2$ capture results in formation of a carbamate with the imidazolate anion and the base IL can be regenerated at relatively low temperatures, below 100 °C. In contrast, under humid conditions, $CO_2$ is initially absorbed forming bicarbonate, $[HCO_3]^-$, which induces solidification and inhibits $CO_2$ desorption below *ca*. 95 C, however successive absorption/desorption cycles can be achieved using a temperature swing between 95 and 160 °C where the bound $CO_2$ cycles between bicarbonate and carbonate.

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## CO2 capture by carboxylate ionic liquids: fine-tuning the performance by altering hydrogen bonding motifs

Mohammad Yousefe, [a] Katarzyna Glińska,[a] Michael Sweeney,[b] Leila Moura, [b] Małgorzata Swadźba-Kwaśny [b] and Alberto Puga *[a]

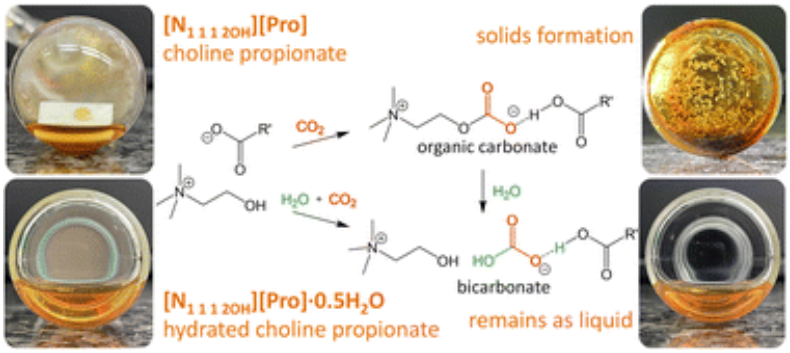
***RSC Sustainability***, 2025,**3**, 2952-2961
Published 17 Jun 2025
DOI: https://doi.org/10.1039/D5SU00108K

### Abstract

The use of ionic liquids (ILs) for $CO_2$ capture has drawn significant attention due to their tuneable structural design and non-volatility. Among these, carboxylate ionic liquids, particularly in the presence of water as a

hydrogen bond donor, show great promise due to their effective chemical sorption mechanism, leading to bicarbonate, and low regeneration energy requirements. The additional presence of hydroxyl groups in their structures is expected to affect both hydrogen bonding network and $CO_2$ capture capacity. This study systematically investigates the role of hydroxyl moieties in tetraalkylammonium cations of carboxylate ionic liquid hydrates on their physicochemical properties and $CO_2$ solubility. The ILs studied are based on the trimethylpropylammonium cation or choline as a hydroxyl-containing analogue, paired with either acetate or propionate. The solubilities of $CO_2$ in each IL at different $H_2O$/IL hydration ratios were determined by a headspace gas chromatography method. The effects of water, in addition to those of cationic hydroxyl, on $CO_2$ capture performance were evaluated. To this end, nuclear magnetic resonance and infrared spectroscopy results are presented and analyzed to propose distinct chemical sorption mechanisms in either scenario.

## Graphical Abstract

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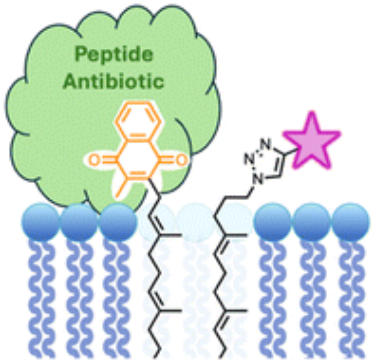
## Chemical diversification of polyprenyl quinones for mechanistic studies on menaquinone-binding peptide antibiotics

Eilidh J. Matheson, [a] Roy A. M. van Beekveld,[b] Paolo Innocenti,[c] Nathaniel I. Martin, [c] Markus Weingarth [b] and Stephen A. Cochrane [*a]

***Chem. Sci.***, 2025,**16**, 13629-13635
Published 3 July 2025
DOI: https://doi.org/10.1039/D5SC03363B

## Abstract

Polyprenyl quinones, such as ubiquinone and menaquinone, are essential membrane-embedded redox cofactors that are involved in electron transport and found across all domains of life. However, their highly hydrophobic structure, which includes a quinone head-group and long polyprenyl tail, has limited their chemical derivatization for biological studies. Here, we report a versatile synthetic approach for the chemical diversification of natural polyprenyl quinones, enabling the introduction of various reporter groups including fluorophores, quenchers, NMR-active nuclei, and photoaffinity and bioaffinity tags. These functionalized analogues retain their membrane-associating properties and enable new applications in antibiotic discovery. We show that fluorescently labelled menaquinone analogues retain their strong binding affinity to the menaquinone-binding peptide antibiotics lysocin E and lysomeb (MBA2). Incorporation of BODIPY–quinones into vesicles allowed visualization of the peptide–quinone interaction, revealing their effects on membrane integrity and quinone aggregation. This study expands the chemical toolbox for polyprenyl quinones, enabling targeted functionalization of these essential biomolecules and facilitating further exploration of their roles in biological systems.




## Graphical Abstract

## Binding dynamics of biomimetic zinc–cyclen ionic liquid catalyst to enhance CO2 hydrolysis kinetics

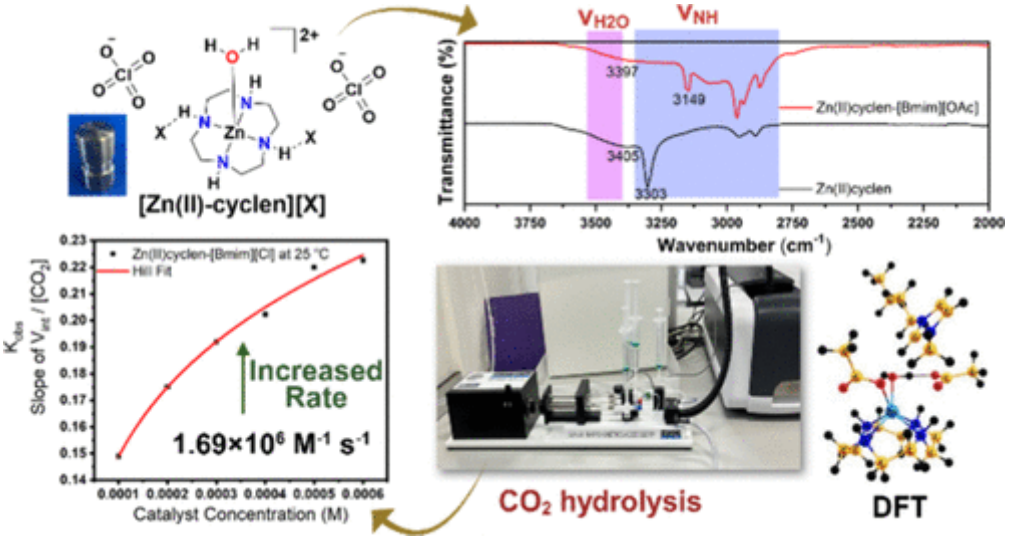
Novina Malviya*, Ravi Kumar, Matthias Stein, Małgorzata Swadźba-Kwaśny

*ACS Sustainable Chem. Eng.* 2025, 13, 40, 17014–17025
Published 30 Sep 2025
DOI: https://doi.org/10.1021/acssuschemeng.5c07574

## Abstract

An alternative approach to catalytic hydrolysis of $CO_2$ is presented, using a biomimetic Zn(II)cyclen system formulated with an ionic liquid (IL). A matrix of Zn(II)cyclen catalysts, formulated with ILs and Group 1 metal salts, was prepared by mechanochemistry. Their catalytic activity in the hydrolysis of $CO_2$ was assessed through stopped-flow kinetic measurements to provide real-time insights into the reaction dynamics. Zn(II)cyclen-[Bmim][OAc] catalyst, where [Bmim][OAc] is 1-butyl-3-methylimidazolium acetate, exhibited turnover rates of $2.02 \times 10^5$ $M^{-1}$ $s^{-1}$ at 25 °C and $1.69 \times 10^6$ $M^{-1}$ $s^{-1}$ at 75 °C, exhibiting both excellent performance and thermal stability. This performance exceeds that of previously reported Zn(II)cyclen catalysts and the Carbonic anhydrase (CA) enzyme. A combination of spectroscopic techniques and computational modeling was used to comprehensively understand how binding dynamics influence catalytic behavior. It has been shown that both ions cooperate in activating the zinc-bound water molecule, and the anion exhibits strong hydrogen bonding to the NH group of the cyclen ring. Finally, the presence of IL prevented $Zn^{2+}$ leaching at elevated bicarbonate concentrations (up to 1 M).

## Graphical Abstract

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## A sustainable-by-design process for the selective photooxidation of ethylbenzene in a scalable agitated baffle reactor

Gary Morrison, Nayan Jyoti Mazumdar, Nancy Artioli, Megan Smyth, Scott Wharry, Thomas S. Moody, Jonty Thornton, Edward Bainbridge, Nikolay Cherkasov, Haresh Manyar*

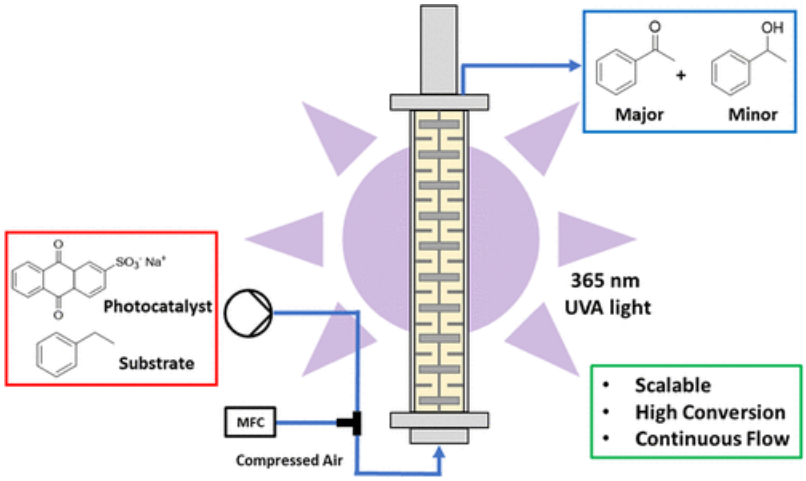
***ACS Omega* 2025**, 10, 36, 42083–42091
Published 6 Sep 2025

DOI: https://doi.org/10.1021/acsomega.5c07359

## Abstract

This study presents a sustainable-by-design approach for the selective photooxidation of ethylbenzene under continuous flow conditions using sodium anthraquinone-2-sulfonate (SAS) as a water-soluble photocatalyst. The reaction was conducted in a scalable agitated baffle reactor (SABRe) under ultraviolet (UV)-A irradiation (365 nm), enabling enhanced mixing, illumination, and gas–liquid contact. To systematically optimize the process, a four-factor central composite design based on response surface methodology (RSM) was employed, evaluating the influence of catalyst loading, liquid and gas flow rates, and light intensity. The study revealed that oxygen mass transfer from air is a key limiting factor, which was successfully addressed by implementing counter-current gas–liquid flow and increased agitation speeds. These modifications led to a significant improvement in ethylbenzene conversion and selectivity toward acetophenone. The SABRe reactor achieved a space–time yield (STY) of 14.8 g $L^{-1}$ $h^{-1}$, representing a threefold improvement over the conventional microchannel reactor configuration. Under optimized conditions, an extended 8 h continuous operation processed 1.44 L of feed solution, delivering an 87% isolated yield with ≥98% product purity. The modular and scalable nature of the SABRe platform, combined with efficient process intensification strategies, underscores its potential for sustainable chemical manufacturing and future scale-up via a numbering-up approach for photocatalytic C–H functionalization using our intensified continuous flow technology.

## Graphical Abstract

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## Advances in SOEC electrodes, electrolytes, and stacks: a review of materials innovation and intellectual patent trends

Cheng Li [a b], Jiabin Wang [b], Liyuan Fan [c], Lichao Jia [b], Ye Yang [a*]

## Abstract

Solid oxide electrolysis cell (SOEC), as electro-thermal-chemical energy conversion devices, offer high energy conversion efficiency, flexible deployment, and environmental friendliness, making them a key focus of international energy research. This paper reviews the progress made in the past five years in key cell materials and stack components across major SOEC research nations, including China, the United States, Denmark, Germany, Japan, and South Korea. The current research landscape in these countries is examined through an analysis of patent data. Finally, the paper presents an outlook on future directions for SOEC development.

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## Adsorption thermodynamics of methane reforming over solid oxide fuel cell anodes

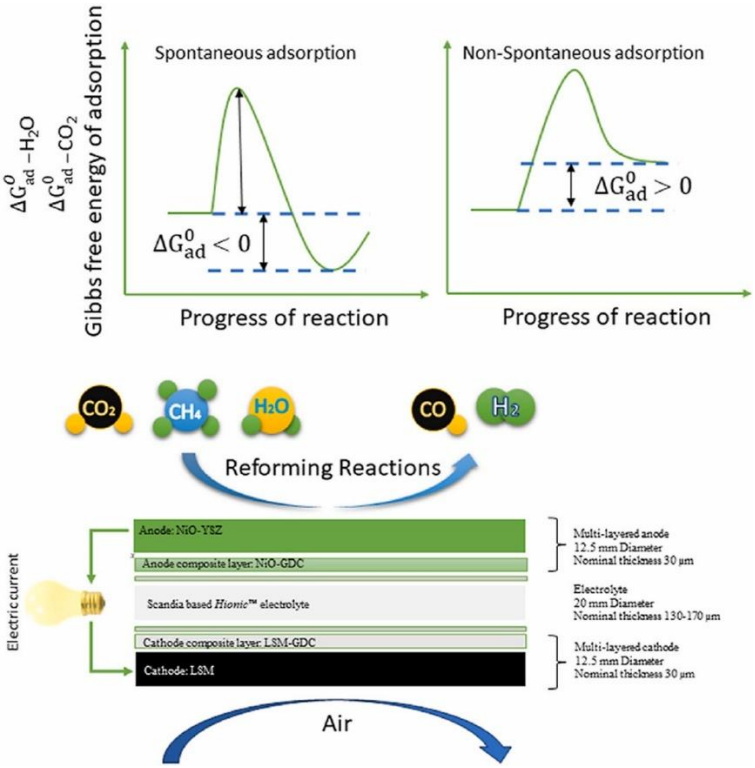
Saeed Moarrefi [a], Mohammad Rajabi Naraki [b], Mohan Jacob [a], Nilay Shah [c], Stephen Skinner [d], Lichao Jia [e], Shou-Han Zhou [f], Weiwei Cai [g], Liyuan Fan [h]

**Journal of Power Sources** Volume 655, 1 November 2025, 237905
Published 1 November
DOI: https://doi.org/10.1016/j.jpowsour.2025.237905

## Abstract

Adsorption kinetics and thermodynamics on nickel base anode materials remain underexplored under reforming conditions when fuelled directly with methane. The kinetics determine how quickly and effectively reactant gases interact on the anode surfaces, affecting the behavior of subsequent electrochemical reactions. However, the complexity of these interactions under operating conditions have led to a limited number of detailed studies in this area. Thus, further investigation into adsorption kinetics could unlock new possibilities for optimizing fuel cell performance. This study examines the adsorption Gibbs free energy of reactants on the anode in solid oxide fuel cell to assess the electrocatalyst activity. Our findings reveal that $H_2O$ exhibits more favorable adsorption conditions than $CO_2$ on the catalyst surface, and increased temperature and current density lead to different surface adsorption behaviours. The results show that steam reforming prevents coke formation on the fuel cell anode more effectively than dry reforming. This proposed method can also be used to examine the coke resistance and the performance of anode structures during the investigation and development stages for fuel cell research. The study provides valuable insights into anode performance and offers a foundation for future advancements in SOFC technology.


## Graphical Abstract

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## Achieving nearly 100 % CO2 conversion via CaCO3-carbon reverse Boudouard reaction in an integrated CO2 capture and utilization process using carbon as the reducing agent (C-ICCU)


Xiaotong Zhao [a], Jia Hu [a], Bo Zong [a], Yuanyuan Wang [a], Junhan Lu [a], Chunfei Wu [a]*



**Chemical Engineering Journal** Volume 522, 168153
Published 15 October 2025
DOI: https://doi.org/10.1016/j.cej.2025.168153

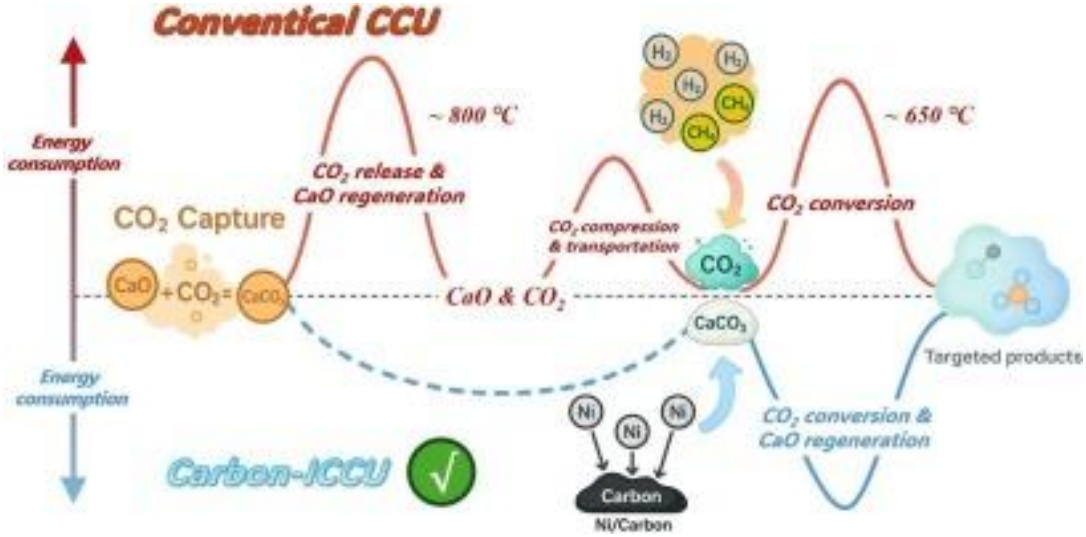


## Abstract

Hydrogen-driven $CO_2$ utilization technologies have attracted significant attention in recent years. However, large-scale implementation is constrained by the high energy demands and limited availability of sustainable $H_2$ sources, which are often derived from fossil fuels or rely on energy-intensive water electrolysis. To address this challenge, we propose an alternative approach by introducing solid carbon as a reductant in the integrated $CO_2$ capture and utilization (ICCU) process via the reverse Boudouard reaction. In this study, we investigate the feasibility and mechanism of this carbon-mediated ICCU (C-ICCU) pathway by examining the reaction

between $CaCO_3$ and nickel-supported carbon materials (Ni/activated charcoal and Ni/graphite). Our experimental results reveal that the $CaCO_3$&Ni/carbon system achieves nearly 100 % $CO_2$ conversion at 600 °C, with sustained high performance at elevated temperatures (90 % at 650 °C and 88 % at 800 °C for Ni/graphite). Notably, the presence of nickel significantly enhances the direct reactions between $CaCO_3$ and carbon, circumventing the need for thermal decomposition of $CaCO_3$, which otherwise introduces unconverted $CO_2$. In contrast, non-catalytic systems exhibit minimal $CO_2$ conversion, underscoring the critical role of metal catalysts in this process. In-situ DRIFTS, Raman, and XPS analyses demonstrate that Ni facilitates a direct interfacial reaction between $CaCO_3$ and carbon, circumventing the need for $CaCO_3$ to thermally decompose into $CO_2$. This catalytic mediation avoids the high-temperature decomposition typically required (>800 °C) and enables an alternative, lower-temperature reaction pathway. This study not only demonstrates the high efficiency of the C-ICCU route but also establishes a novel catalytic mechanism for $CO_2$ reduction using solid carbon, paving the way for more sustainable and $H_2$-independent carbon capture and utilization strategies.

## Graphical Abstract

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# Royal College of Surgeons in Ireland (RCSI) Chemistry Research Publications June-December 2025

## Desulfurative Acetoxylation of Alkyl Benzyl Phenyl Sulfides

Daniele Canestrari, Umamaheswara Rao Boddu, Gangaram Pallikonda, Mauro F. A. Adamo*
***Chemistry*** **2025**, *7*(4), 131
Published 18 Aug 2025
DOI: https://doi.org/10.3390/chemistry7040131

### Abstract

The reaction of thiophenylsulfides with diacetoxyiodobenzene, iodine and light produced corresponding acetoxylated products, allowing the formation of new C-O bonds from starting materials other than carbonyls in high yields. Hence, under these conditions, thiophenylsulfide underwent displacement/substitution by an acetate. $^{1}$H-NMR studies of the reaction carried out with exclusion of each single reactant pointed at two operative pathways and to the involvement of an intermediate that was assigned as an acetoxy sulfonium (IV) species.

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## Fulfilling Multiple Roles in PROTAC Design: The Emerging Potential of Oligonucleotides (Preprint)

Daniel Alencar Rodrigues, Gustavo Salgado Pires, Urbi Roy, Eric Conway, Pedro de Sena Murteira Pinheiro
ChemRxiv Nov 2025 Version 1
Published 20 Nov
DOI:
10.26434/chemrxiv-2025-g3qfc

### Abstract

The field of targeted protein degradation (TPD) has emerged as a novel therapeutic approach based on event-driven pharmacology, rather than on continuous occupancy or inhibition of a target. Proteolysis-targeting chimeras (PROTACs) are one of the main TPD modalities, enabling a protein of interest (POI) to be brought into proximity with an ubiquitin ligase, which facilitates ubiquitination of the target protein, leading to its degradation. The design of PROTACs involves the development of heterobifunctional compounds composed of three parts: a POI ligand, a linker, and an E3 ligase ligand. To date, PROTAC technology has been applied to degrade a wide range of targets, with particular interest in previously “undruggable” targets, such as transcription factors. In this context, oligonucleotides have emerged as potential POI binders for transcription factors, since these targets naturally bind to DNA to modulate gene expression. This has led to the development of oligonucleotide-based degraders. Moreover, the role of oligonucleotides has expanded beyond their use as POI ligands. Several strategies have been explored to overcome inherent challenges such as poor stability and limited drug delivery. Currently, novel approaches also demonstrate the potential of nucleotides to function as linkers, where they can exert control over the spatial orientation between the POI ligand and the E3 ligase ligand, thereby optimizing ternary complex formation. In addition, nucleotides can also serve as E3 ligase ligands. Oligonucleotides represent a promising approach in PROTAC design, capable of fulfilling multiple functional roles.

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## Inhibition of HDAC6 alters fumarate hydratase activity and mitochondrial structure

Andrew Roe, Catríona M. Dowling, Cian D’Arcy, Daniel Alencar Rodrigues, Yu Wang, Matthew Hiller, Carl Keogh, Kate E. R. Hollinshead, Massimiliano Garre, Brenton Cavanagh, Kieran Wynne, Tianyan Liu, Zhixing Chen, Emma Kerr, Marie McIlroy, Jochen H. M. Prehn, Ingmar Schoen, Tríona Ní Chonghaile
***Nat Commun*** **16**, 6923 (2025)
Published 28 July 2025

DOI: https://doi.org/10.1038/s41467-025-61897-6

## Abstract
Fumarate hydratase (FH), a key node of mitochondrial metabolism, is also a tumour suppressor. Despite its prominent roles in tumourigenesis and inflammation, its regulation remains poorly understood. Herein, we show that histone deacetylase 6 (HDAC6) regulates FH activity. In triple-negative breast cancer cells, HDAC6 inhibition or knockdown results in alterations to mitochondrial cristae structure, as detected by live-cell super-resolution STED nanoscopy and electron microscopy, along with the release of mitochondrial DNA. Mass-spectrometry immunoprecipitation reveals multiple mitochondrial HDAC6-interactors, with FH emerging as a top hit. Super-resolution 3D-STORM shows HDAC6 interactions with FH in mitochondrial networks, which increases after perturbation of HDAC6 activity with BAS-2. Treatment with BAS-2 leads to fumarate accumulation by $^{13}C$ glucose labelling, along with downstream succination of proteins and cell death. Together, these results identify HDAC6 inhibition as a regulator of endogenous FH activity in tumour cells and highlight it as a promising candidate for indirectly targeting tumour metabolism.

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## Recent Advances in the Synthesis and Biological Applications of Prenylated Chalcones

Mouna Hind Laiche*, James W. Barlow*

***Int. J. Mol. Sci.*** **2025**, *26*(20), 9845
Published 10 Oct 2025
DOI: https://doi.org/10.3390/ijms26209845

## Abstract
Prenylated chalcones, a subclass of chalcones distinguished by the addition of one or more prenyl (3-methylbut-2-enyl) groups, have attracted significant attention due to their promising biological activities. The origins, chemical diversity, and synthetic routes used to prepare naturally occurring and synthetic prenylated chalcones are discussed in this review paper, alongside their diverse pharmacological properties, as reported over the past 10 years (2015–2025), mainly emphasising their strong anti-cancer, anti-inflammatory, anti-bacterial, anti-fungal, anti-parasitic, and anti-malarial effects. We address their structure–activity relationships (SARs) to interrogate how prenylation affects the pharmacological activity of these chalcones.

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## Poly(ethylene Glycol)-Based Peptidomimetics (Pegtides) of Antimicrobial Peptides

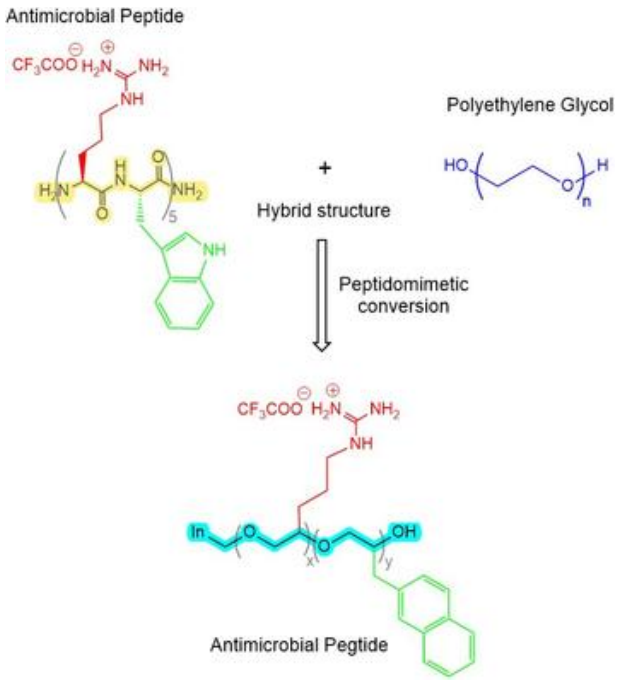
Conor Shine, John R. F. B. Connolly, Robert D. Murphy, Hazel Lafferty, Abdalmalek Alfnikh, Ned P. Buijs, Hawraa Shahrour, Nathaniel I. Martin, Eoghan O'Neill, George Amarandei, Jimmy Muldoon, Marc Maresca, Deirdre Fitzgerald-Hughes, Marc Devocelle*

**ChemBioChem** **Volume 26, Issue 21** e202500258
Published 8 November 2025
DOI: https://doi.org/10.1002/cbic.202500258

## Abstract
Cationic amphipathic poly(ethylene glycol)-based polymers are generated with synthetic efficiencies allowing their evaluation as antimicrobial peptide (AMP) mimetics. Accordingly, statistical copolymers with cationic units consistently functionalized with guanyl groups, but different side-chain lengths, and hydrophobic units displaying long aliphatic, branched, and/or aromatic side chains are produced and tested for their antimicrobial and hemolytic properties. The results obtained indicate that candidates with activities and selectivity commensurate to some AMPs can be obtained and that further development of this novel type of antimicrobial peptidomimetics, pegtides, is warranted for clinical and/or biotechnological applications.

## Graphical Abstract
Polyethylene glycol (PEG) is commonly used to improve the pharmacokinetics and pharmacodynamics of therapeutic candidates by conjugation. Here PEG is exploited for peptidomimetic conversion of antimicrobial peptides (AMPs), as candidate antibacterial agents, by replacing their polyamide backbone.

The pegtides obtained thereby can be readily synthesized from inexpensive starting materials and demonstrate properties commensurate of AMP mimetics.

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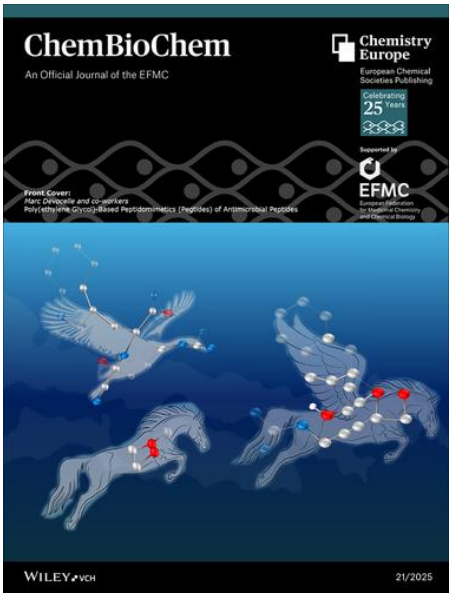
## Front Cover: Poly(ethylene Glycol)-Based Peptidomimetics (Pegtides) of Antimicrobial Peptides (ChemBioChem 21/2025)

Conor Shine, John R. F. B. Connolly, Robert D. Murphy, Hazel Lafferty, Abdalmalek Alfnikh, Ned P. Buijs, Hawraa Shahrour, Nathaniel I. Martin, Eoghan O'Neill, George Amarandei, Jimmy Muldoon, Marc Maresca, Deirdre Fitzgerald-Hughes, Marc Devocelle*

**ChemBioChem** Volume 26, Issue 21 November 8, 2025 e70108
Published 8 Nov, 2025
DOI: https://doi.org/10.1002/cbic.70108

### Graphical Abstract

Hybridising an Antimicrobial Peptide (AMP) with polyethylene glycol (PEG), to replace the peptide's polyamide backbone by PEG, produces a Pegtide as an AMP mimetic. By analogy, the molecules are represented as combining the features of a bird (AMP) and a horse (PEG) in a winged horse (Pegasus) and folded to match the shapes of the Swan, Equuleus and Pegasus constellations, respectively. More details can be found in the Research Article by Marc Devocelle and co-workers



## Novel Platinum(II) Tetrazine Complex Capable of Live-Cell IEDDA Reaction

Paul D. O'Dowd, Dan Wu, Alby Benny, Ellen King, Alice Harford, Brendan Twamley, Olga Piskareva, Donal F. O'Shea, Darren M. Griffith*

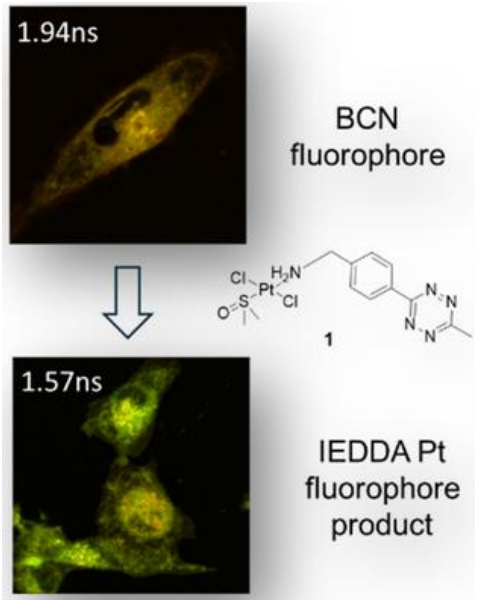
**ChemBioChem** Volume 26, Issue 18, 2025 e202500376
Published 18 Sep
DOI: https://doi.org/10.1002/cbic.202500376

### Abstract

The development of the first Pt(II) tetrazine complex, *trans*-[Pt(II)$Cl_2$(dmso)($CH_3$-Tz-Bz-$NH_2$)] (**1**), is reported, which exhibits good in vitro cytotoxicity against MDA-MB-231 cells and successfully undergoes inverse electron demand Diels–Alder (IEDDA) reactions with *trans*-cyclooctene (TCO) and bicyclononyne (BCN) derivates in solution. We demonstrate a live-cell IEDDA reaction of **1** with a $BF_2$-azadipyrromethene fluorophore (NIR-AZA) possessing a BCN handle. A live-cell bioorthogonal reaction is established using fluorescence lifetime imaging microscopy (FLIM), through a fluorescence lifetime change of 0.3 ns from $BF_2$-azadipyrromethene fluorophore starting material to IEDDA Pt fluorophore reaction product. As there is a distinct difference in fluorescence lifetimes between starting material and product, this approach removes the necessity for designing challenging off to on fluorogenic Pt probes and washing steps when developing bioorthogonal cell-imaging strategies for Pt complexes.

### Graphical Abstract

The first Pt(II) tetrazine complex, *trans*-[$PtCl_2$(dmso)($CH_3$-Tz-Bz-$NH_2$)] (1), is reported, showing good cytotoxicity against MDA-MB-231 cells and undergoing IEDDA reactions with TCO and BCN derivatives. A live-cell IEDDA reaction in MDA-MB-231 cells with a BCN-bearing $BF_2$-azadipyrromethene fluorophore is tracked via FLIM, owing to a 0.3 ns lifetime shift.

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## Inhalable Nanotechnology-Based Drug Delivery Systems for the Treatment of Inflammatory Lung Diseases

Doaa Elsayed Mahmoud[1], Seyedeh Hanieh Hosseini[2], Hassaan Anwer Rathore[1], Alaaldin M. Alkilany[1], Andreas Heise[3], Abdelbary Elhissi[1,*]*

***Pharmaceutics*** **2025**, *17*(7), 893
Published 9 Jul 2025
DOI: https://doi.org/10.3390/pharmaceutics17070893

### Abstract

This review explores recent advancements in inhaled nanoparticle formulations and inhalation devices, with

a focus on various types of nanoparticles used for inhalation to treat inflammatory lung diseases and the types of devices used in their delivery. Medical nebulizers have been found to be the most appropriate type of inhalation devices for the pulmonary delivery of nanoparticles, since formulations can be prepared using straightforward techniques, with no need for liquefied propellants as in the case of pressurized metered dose inhalers (pMDIs), or complicated preparation procedures as in the case of dry powder inhalers (DPIs). We demonstrated examples of how formulations should be designed considering the operation mechanism of nebulizers, and how an interplay of factors can affect the aerosol characteristics of nanoparticle formulations. Overall, nanoparticle-based formulations offer promising potential for the treatment of inflammatory lung diseases due to their unique physicochemical properties and ability to provide localized drug delivery in the lung following inhalation.

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## Polycaprolactone–Itaconic Acid Resins for Additive Manufacturing of Environmentally Degradable 3D and 4D Materials by Thiol-ene Photopolymerization

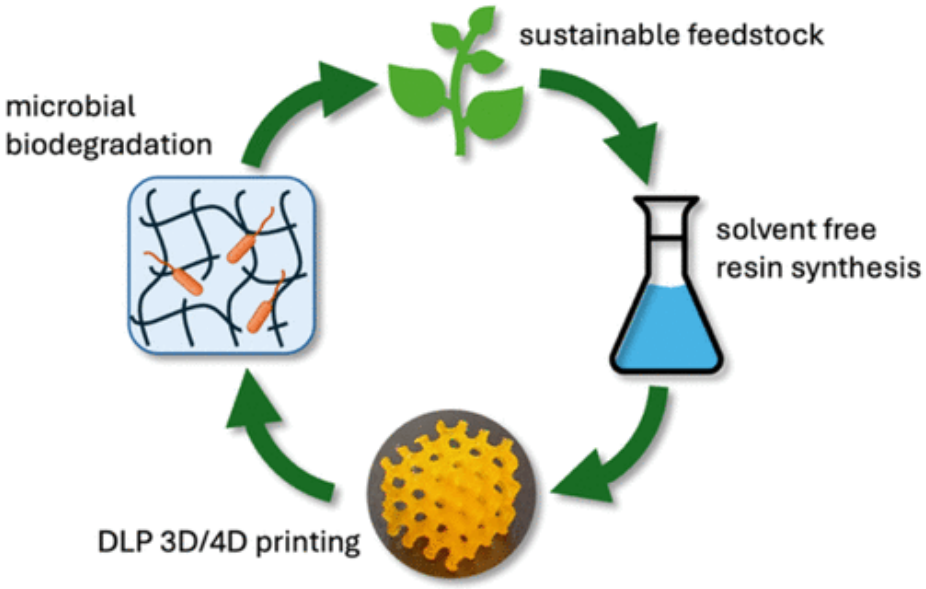
Bo Li, Gianluca Bartolini Torres, Baptiste Martin, Nicholas Taylor, Eugen Barbu, Annette Christie Andreas Heise*

***Macromolecules*** 2025, 58, 16, 8887–8897
Published 5 August 2025
DOI: https://doi.org/10.1021/acs.macromol.5c01310

### Abstract

Digital light processing (DLP) has emerged as a powerful tool for advanced manufacturing, enabling the fabrication of intricate 3D polymer structures and, more recently, responsive 4D architectures that adapt to environmental stimuli. However, current DLP technologies rely heavily on acrylate-based photocurable resins, which pose significant sustainability challenges from resin synthesis to end-of-life disposal. To address these issues, we present a novel solvent-free approach to functionalizing polycaprolactone (PCL) using biomass-derived itaconic acid (IA). The unsaturated moiety of IA enables efficient photopolymerization via thiol-ene chemistry in both dioxane and the sustainable solvent γ-valerolactone, affording excellent printability. In the resulting cross-linked networks, IA end-groups serve not only as photocurable sites but also as functional handles that confer environmental responsiveness, as demonstrated by pH-triggered 4D transformations and dye uptake. To simulate end-of-life conditions, we demonstrated hydrolysis and microbial degradation of the cross-linked materials in a sewage-derived inoculum, supporting the potential for biomass regeneration in a circular materials framework. This strategy provides a sustainable route to producing functional, mechanically robust resins for 3D and 4D printing, offering a reduced environmental impact without compromising performance.

### Graphical Abstract

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## Light-Based 3D Printing of Polyesters: From Synthesis to Fabrication

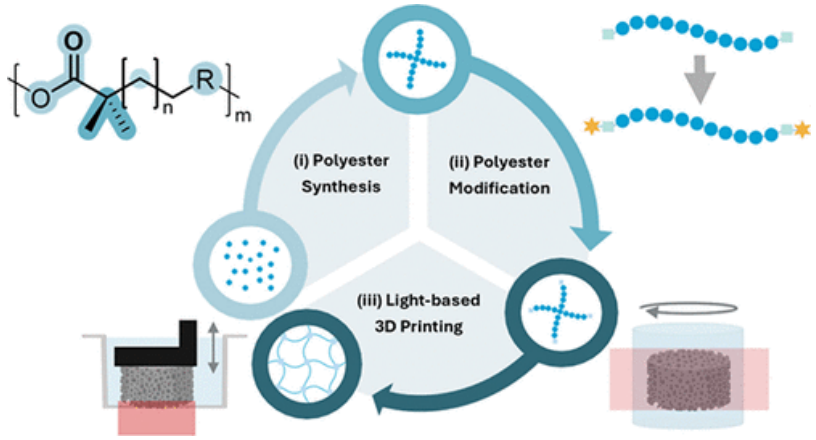
Quinten Thijssen*, Astrid Quaak, Bart Bijleveld, Bo Li, Lenny Van Daele, Andreas Heise, Sandra Van Vlierberghe*

***Chem. Rev.*** 2025, XXXX, XXX, XXX-XXX
Published 23 Dec 2025
DOI: https://doi.org/10.1021/acs.chemrev.5c00611

### Abstract

Polyesters represent a versatile class of materials whose biodegradability, biocompatibility, mechanical tunability, and broad chemical design space have made them valuable across a wide range of application areas, including tissue engineering, biomedical engineering, sustainable manufacturing, and soft robotics. Light-based 3D printing has further expanded their potential by enabling precise spatial control across nano- to macroscales, supporting the fabrication of resorbable implants, drug-delivery systems, microneedle arrays, and stimuli-responsive materials. This review discusses the essential steps toward light-based 3D printing of polyesters from synthetic strategies for producing these materials to functionalization methods that render them suitable for light-based 3D printing. Particular attention is given to the synthetic origin of the polyester, the way photoreactive groups are introduced and organized within the network, and how the formulation of the resulting photoresin together govern the ultimate photoreactivity, degradation behavior, print resolution, and mechanical performance. Advantages and limitations of current photochemical approaches are discussed across different light-based 3D printing technologies. With continuing advancements in manufacturing, the field of light-based 3D printing of polyesters shows substantial promise, poised to redefine material design, and influence a broad range of future technologies.

### Graphical Abstract

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## RAFT-Mediated 3D Printing of Polylactones/Itaconate Elastomers with Polypeptide Surface Functionalization

Gianluca Bartolini Torres, Tianlai Xia, Dengwei Yu, Quinten Thijssen, Sandra Van Vlierberghe, Bo Li*
Andreas Heise*

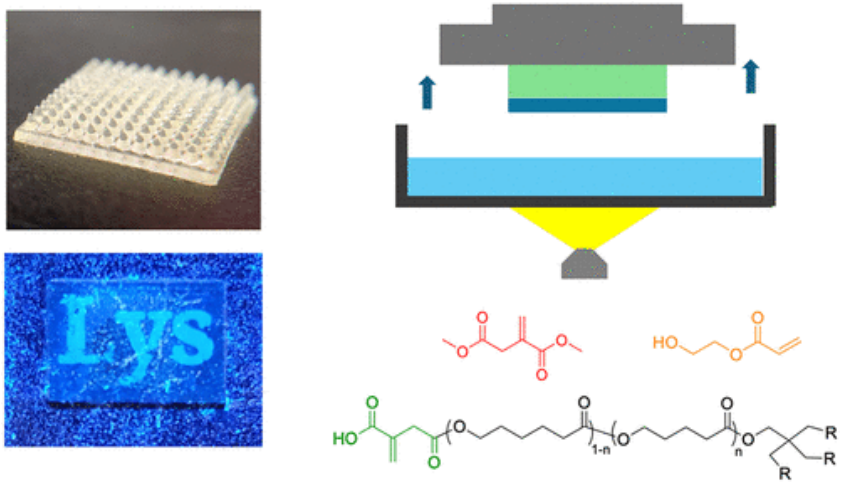
***ACS Polym. Au*** 2025, 5, 6, 956–966
29 Oct 2025
DOI: https://doi.org/10.1021/acspolymersau.5c00117

### Abstract

Reversible addition–fragmentation chain transfer (RAFT) polymerization has gained interest in vat photopolymerization, particularly for enabling postprinting surface functionalization via reactivation of the RAFT agent. In this work, we report the development of RAFT photopolymerizable resins containing up to 50% renewable content using sustainable dimethyl or dibutyl itaconate as primary monomers combined with hydroxyethyl acrylate as a reactive comonomer. A 4-arm polyester cross-linker end-functionalized with itaconic acid (IA), poly(caprolactone-*co*-valerolactone)-IA, was synthesized and incorporated into the resin formulation. Photorheology confirmed efficient polymerization, and mechanical characterization revealed

elastomeric properties for networks derived from dimethyl itaconate. Digital light processing (DLP) of this formulation enabled the 3D printing of flexible structures, including microneedles. The presence of pendant carboxylic acid groups in the cross-linker imparted pH-responsiveness to the printed objects, allowing for reversible swelling and size changes in response to environmental pH, demonstrating 4D behavior. Leveraging the controlled nature of RAFT polymerization, a two-stage printing approach was employed. After printing with the itaconate-based ink, a switch to a methacrylated polylysine ink enabled surface biofunctionalization. Successful grafting of polylysine was confirmed by atomic force microscopy (AFM) and FTIR spectroscopy. Preliminary results demonstrate antimicrobial activity of the cationic surfaces, as well as the ability to spatially control surface functionalization, exemplified by patterned attachment of fluorescent polylysine.

## Graphical Abstract

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## Alendronate-Based Polypeptide Hydrogels with Osteogenic Potential for Digital Light Processing

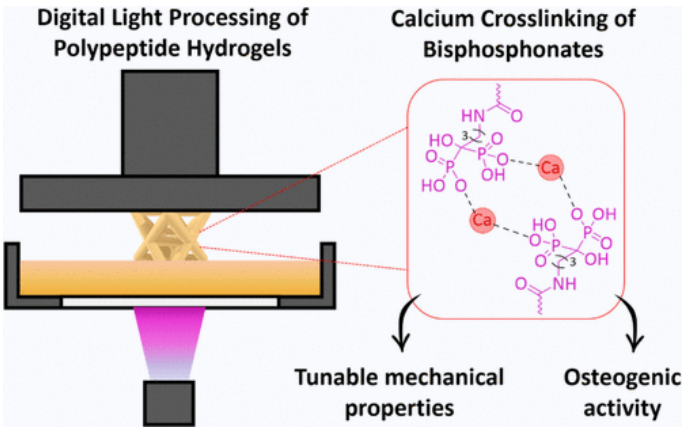
Muireann Cosgrave, Avelino Ferreira, Ciara M. Murphy, Andreas Heise*, Robert D. Murphy*

*ACS Appl. Mater. Interfaces* 2025, 17, 49, 67123–67131
Published 24 November 2025
DOI: https://doi.org/10.1021/acsami.5c16898

## Abstract

In this work, we present an alendronate star polypeptide formulation capable of digital light processing high-resolution 3D hydrogel structures. Through the use of embedded bisphosphonate moieties from the alendronate, which has a high affinity for divalent calcium ($Ca^{2+}$) ions, a second ionic network is introduced within the hydrogel. A significant enhancement of hydrogel mechanical properties is observed, reaching Young's modulus values toward those observed for native bone. Furthermore, the presence of $Ca^{2+}$ supports mineralization, fostering osteogenesis in seeded rat mesenchymal stem cells (rMSCs), indicating the potential to promote effective bone tissue regeneration.

## Graphical Abstract



## The Design and Development of an Injectable Thermoresponsive Hydrogel for Controlled Simvastatin Release in Bone Repair Applications

Christopher R. Simpson [1], Helena M. Kelly [1,2], Ciara M. Murphy [1,3,4,*]

***Gels*** **2025**, *11*(12), 995
Published 10 Dec 2025
DOI: https://doi.org/10.3390/gels11120995

### Abstract

Osteoporotic vertebrae are a uniquely challenging tissue for local delivery due to the complex geometry of cancellous bone, the proximity of the spinal cord, and the need for reliable site retention. These challenges can be met with the use of stimuli responsive, state transiting formulations by leveraging their unique capacity for minimally invasive implantation as a liquid, sol–gel transition in response to stimuli, and finally, release of a loaded therapeutic. Here, we present the formulation development of a thermosensitive methylcellulose–collagen hydrogel, functionalised with controlled release simvastatin, recently shown to enhance osteogenesis while also impeding osteoclast activity. We first optimised a formulation with collagen content of 0.4% *w*/*v* to achieve a thermosensitive system with sol–gel transition at 29 °C, shear-thinning/injectable properties, low cytotoxicity, and high biocompatibility. Incorporation of nano-hydroxyapatite for enhanced bone tissue mimicry revealed optimal performance at 100% *w*/collagen content, showing long-term hydrolytic stability, maintaining more than 100% of its mass after 28 days. A loading concentration of 1 mg of simvastatin to 1 g of hydrogel displayed sustained release of simvastatin over 35 days. Finally, the release of simvastatin from the hydrogel into in vitro conditions prevented the formation of osteoclasts but failed to boost osteogenesis. Together these findings reveal a series of desirable stimuli-responsive hydrogel properties, achieving minimally invasive application coupled with sustained release of a hydrophobic compound, which is potentially useful for spatially complex bone regeneration. Further this work demonstrates the challenge of dosing sustained release systems to achieve simultaneous osteogenesis and anti-osteoclastogenic effects.

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## Platinum(II ) complexes of aryl guanidine-like derivatives as potential anticancer agents: between coordination and cyclometallation

Patrick O'Sullivan[a] Viola Previtali[a] Brendan Twamley[a] Celine J. Marmion[b], Aidan R. McDonald[a] and Isabel Rozas*[a]

**RSC Adv**., 2025, 15, 3427
DOI: DOI: 10.1039/d5ra00310e

### Abstract

The preparation of a wide variety of Pt( II) complexes with aryl guanidines and their potential application as anticancer agents have been explored. A relatively facile synthesis of cyclometallated Pt(II ) complexes of arylguanidines, preparation of Pt(II) guanidine coordination complexes and an in situ activation of platinum arylguanidine complexes with acetonitrile to create a bidentate aryl iminoguanidine Pt( II) complex were achieved. Cyclometallation methodology was extended to create a water-stable conjugate incorporating two Pt( II) ions and a diaryl bis-guanidine DNA minor groove binder. Several crystal structures were obtained confirming these complexation modes. The cyclometallated Pt(II) complexes were particularly stable to aqueous environments and were tested for Reactive Oxygen Species generation and anticancer activity in a leukaemia cancer cell line.

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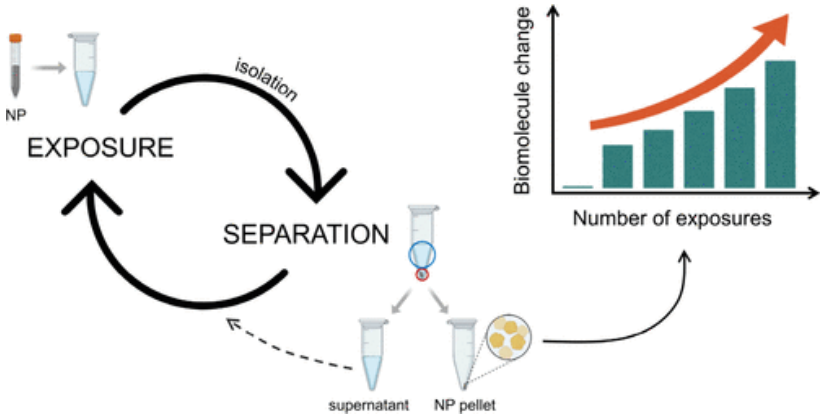
## Multiple Exposures of Plasma to Nanoparticles: A Novel Tool to Personalize Biomolecular Coronas and Fractionate Fluids

Alberto Martinez-Serra, Jack Cheeseman, Asia Saorin, Mahmoud G. Soliman, Marko Dobricic, Daniel I. R. Spencer, Marco P. Monopoli*

***Anal. Chem***. 2025, 97, 27, 14132–14141
Published 30 June 2025
DOI: https://doi.org/10.1021/acs.analchem.4c05573

## Abstract
Nanoparticles (NPs) have emerged as a valuable tool for biomarker discovery due to their ability to interact with biological fluids and form biomolecular coronas. In this study, we introduce a multiple exposure method that uses NPs to fractionate biological fluids and obtain personalized coronas. By repeatedly exposing plasma to silica NPs, we observed a progressive change of the biomolecule profile in both the pellet and supernatant. The varying protein and glycan composition of the corona was characterized using techniques such as SDS–PAGE, mass spectrometry, and UHPLC. Notably, the corona's composition evolved with each exposure cycle, reflecting the selective binding of proteins and glycosylated molecules from a corona of high-affinity biomolecules to a more diverse corona with very distinct structures. By tracing the sequential modification of protein and glycan composition, we believe that the method can be useful to trace specific biomarker profiles, offering a noninvasive alternative to conventional diagnostic processes with the potential to become a useful tool for disease monitoring and advanced biomedical applications.

## Graphical Abstract

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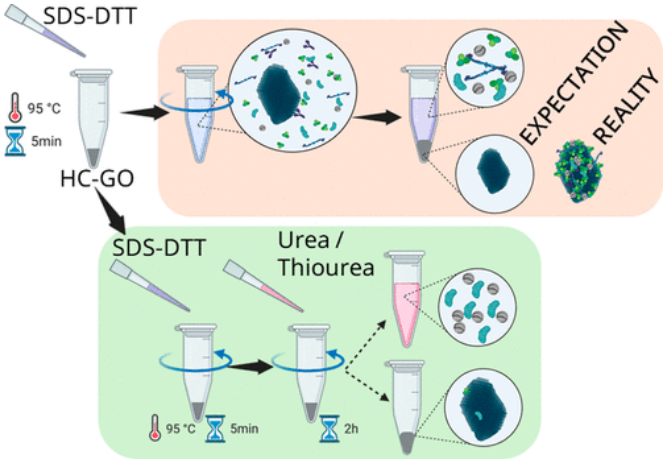
## A Redefined Protocol for Protein Corona Analysis on Graphene Oxide

Asia Saorin, Ahmed Subrati, Alberto Martinez-Serra, Beatriz Alonso, Michael Henry, Paula Meleady, Sergio E. Moya, Marco P. Monopoli*

***ACS Nanosci****. Au* 2025, 5, 5, 388–397
Published 24 Jul 2025
DOI: https://doi.org/10.1021/acsnanoscienceau.5c00052

## Abstract
It is well established that the biomolecular corona affects the biological behavior of nanomaterials, including cellular uptake, toxicity, and biodistribution. However, the unique physicochemical properties of advanced materials, such as graphene oxide, challenge the effectiveness of standard protocols for biomolecular corona characterization, which may lead to incomplete biomolecule recovery and biased experimental results. Protein analysis is one of the broadest techniques in the characterization of the biomolecular corona, providing important information about the composition and behavior of proteins adsorbed onto nanomaterial surfaces. Two widely accepted protein analysis methods include SDS-PAGE and mass spectrometry, and both require the complete elution of the proteins from the nanoparticle surface during denaturation steps. In this work, limitations of widely used SDS-based elution methods with GO were identified, and an improved protocol using chaotropic agents (urea and thiourea) was developed. The stepwise extraction allowed for near-complete protein desorption. Under the modified protocol, strongly bound proteins that are more hydrophobic have been proved to be underestimated using the standard method. This further reiterates the necessity for the development of methodologies tailored to the specific materials under study which accurately characterize the protein corona. Our results highlight the need for standardization and optimization of protocols to ensure reproducibility and reliability in nanosafety studies, hence promoting the safe and sustainable use of advanced materials in biological and environmental systems.

## Graphical Abstract

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## The cellular response of the bronchial epithelium shapes the protein corona of inhaled nanoparticles

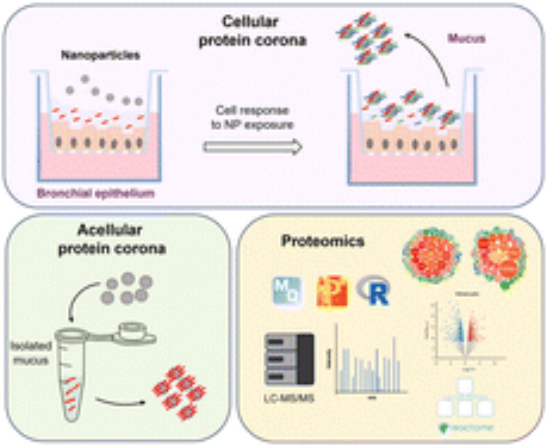
Daniel Sanchez-Guzman, †[a] Chloé Chivé,[a] Olivier Taché,[b] Marco P. Monopoli,[c] Armelle Baeza-Squiban[a] and Stéphanie Devineau *[ab]

***Nanoscale***, 2025,**17**, 24682-24698
Published 7 Oct 2025
DOI: https://doi.org/10.1039/D5NR02590G

## Abstract

Protein adsorption to nanoparticles is a key molecular event that influences their fate, biodistribution and toxicity. In the lung, a mucus layer protects the bronchial epithelium from inhaled pollutants. However, the effect of cell exposure to nanoparticles on the formation of the protein corona in the bronchial mucus is not well understood. This study aimed to uncover how the bronchial epithelial cell response shapes the biomolecular corona on inhaled nanoparticles and whether cell adaptation remodels the nano/bio interface. We reproduced a realistic scenario of lung exposure to silver nanoparticles (AgNPs) *in vitro* using a 3D human bronchial epithelium model. AgNPs were incubated in the isolated bronchial mucus or directly exposed to Calu-3 cells at the air–liquid interface. The stability of AgNPs in the mucus was characterized by small-angle X-ray scattering, dynamic light scattering, and transmission electron microscopy. The protein corona formed during the exposure of the bronchial epithelium to nanoparticles was analyzed using quantitative mass spectrometry and Reactome pathway analysis as a function of NP concentration and exposure time. Proteomic analysis revealed major differences in the biomolecular corona formed *in situ* compared to the corona formed in isolated bronchial mucus. Unique proteins expressed in the apical secretome of Calu-3 cells exposed to AgNPs were identified in the protein corona formed *in situ*. The stress response of the epithelial cells led to a complete reshuffling of the protein corona after initial deposition of AgNPs on mucus. Our results demonstrate that the cellular response of the bronchial epithelium plays a critical role in shaping the protein corona of inhaled particles. The remodeling of the nano/bio interface by cellular secretory mechanisms during exposure calls for a renewed focus on the role of cells and NP-cell interactions in biomolecular corona studies using advances 3D models.

## Graphical Abstract



## A machine learning tool to analyze spectroscopic changes in high-dimensional data

Alberto Martinez-Serra[a 1]*,
Gionni Marchetti[b c 1]*, Francesco D'Amico[d]*, Ivana Fenoglio[e]*, Barbara Rossi[d]*, Marco P. Monopoli[a]*, Giancarlo Franzese[b c]*

**International Journal of Biological Macromolecules** Volume 330, Part 3, 148095
Published November 2025
DOI: https://doi.org/10.1016/j.ijbiomac.2025.148095

### Abstract

When nanoparticles (NPs) are introduced into a biological solution, layers of biomolecules form on their surface, creating a corona. Understanding how the protein's structure evolves into the corona is essential for evaluating the safety and toxicity of nanotechnology. However, the influence of NP properties on protein conformation is not well understood. In this study, we propose a new method that addresses this issue by analyzing multi-component spectral data (UV Resonance Raman, Circular Dichroism, and UV absorbance) using machine learning (ML). We apply the method to fibrinogen, a crucial protein in human blood plasma, at physiological concentrations while interacting with hydrophobic carbon or hydrophilic silicon dioxide NPs, revealing striking differences in the temperature dependence of the protein structure between the two cases. Our unsupervised ML method (a) does not suffer from the challenges associated with the *curse of dimensionality*, and (b) simultaneously handles spectral data from various sources. The method offers a quantitative analysis of protein structural changes upon adsorption. It enhances the understanding of the correlation between protein structure and NP interactions, which could support the development of nanomedical tools to treat various conditions.

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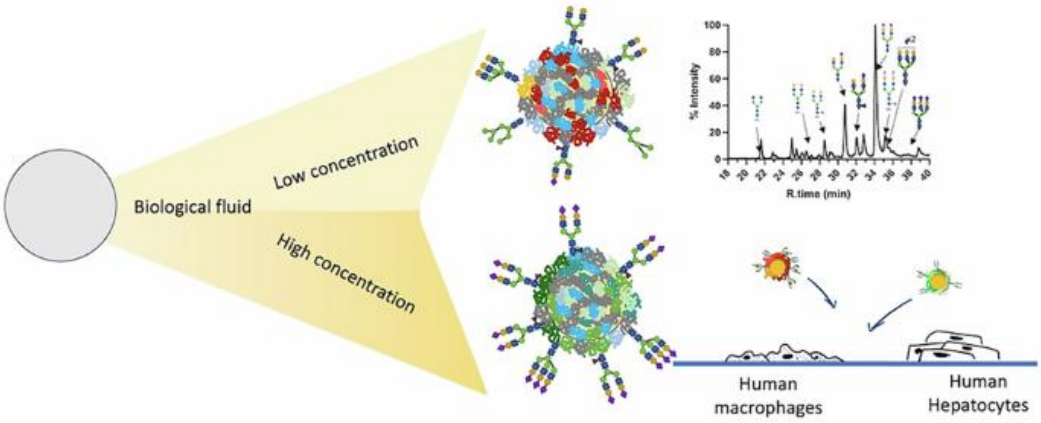
## Terminal sialic acids in the nanoparticle corona modulate cellular uptake

Marko Dobricic, Alberto Martinez-Serra, Claudia Durall, Anna Nakonechna, Jack Cheeseman, Roger Preston, James S. O'Donnell, Daniel I. R. Spencer, Teodor Aastrup, Marco P. Monopoli*

***Communications Chemistry*** **volume 8**, Article number: 308 (2025)
Published 14 Oct 2025
DOI: https://doi.org/10.1038/s42004-025-01677-x

### Abstract

Advances in engineering functional structures at the nanoscale have led to the generation of a wide range of nanoparticles (NPs) with promising therapeutic applications. However, when NPs come into contact with a biological environment, they strongly interact with the available biomolecules, such as glycoproteins. Their adsorption on the NP's surface forms the " biomolecular corona". Recent findings have shown that the glycosylation of the corona affects NPs' stability, and it is unclear whether it can engage with receptors present in the body. By dissecting the corona's glycan composition with enzymatic approaches, we demonstrate, through differential centrifugal sedimentation and quartz crystal microbalance, that differences in the monosaccharide sialic acid content change the NP-corona interactions with isolated glycan receptors. Furthermore, flow cytometry data confirmed this behaviour in relevant cell lines. Overall, these findings highlight the role of the biomolecular corona glycosylation in NP's interaction, suggesting advanced parameters to predict their biological fate.




### Graphical Abstract

# Magnesium Ion-Mediated Regulation of Osteogenesis and Osteoclastogenesis in 2D Culture and 3D Collagen/Nano-Hydroxyapatite Scaffolds for Enhanced Bone Repair

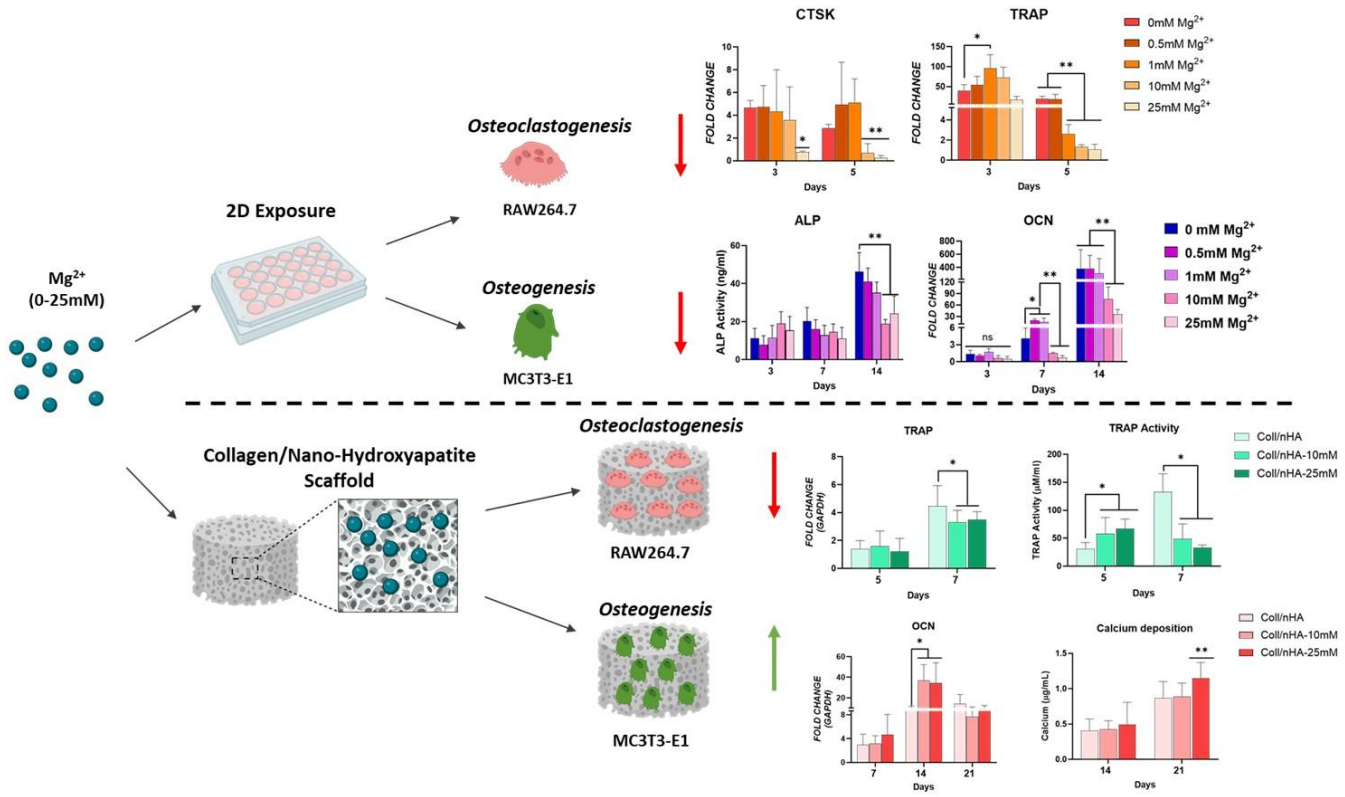
Sílvia Sá Paiva[1,2,†], Avelino Ferreira[1,†], Eavan Pakenham[1], Kulwinder Kaur[1,3], Brenton Cavanagh[4], Fergal J. O'Brien[1,2,5] , Ciara M. Murphy[1,2,5,*]

***J. Funct. Biomater.*** **2025**, *16*(10), 363
29 Sep 2025
DOI: https://doi.org/10.3390/jfb16100363

## Abstract

Bone regeneration depends on a delicate balance between osteoblast-driven bone formation and osteoclast-mediated resorption, coordinated by complex biochemical cues. Magnesium ($Mg^{2+}$) is known to modulate these processes. However, despite extensive research, its ability to simultaneously enhance osteogenesis and inhibit osteoclast activity remains unclear. In this study, we first investigated the effect of extracellular $Mg^{2+}$ (0, 5, 10, 25, 50 mM) on osteoblast and osteoclast differentiation in 2D culture to determine whether a single $Mg^{2+}$ dosing regimen can simultaneously promote osteogenesis while inhibiting osteoclast differentiation and maturation. A concentration dependent effect of $Mg^{2+}$ was observed on both cell types, with increasing $Mg^{2+}$ concentrations up to 25 mM significantly reducing osteoclast formation yet concurrently inhibiting osteogenic differentiation. At 50 mM, $Mg^{2+}$ exhibited cytotoxic effects on both cell types. We then leveraged the osteogenic properties of biomimetic collagen/nano-hydroxyapatite (Coll/nHA) scaffolds by incorporating $Mg^{2+}$ into the nHA phase to enable localised, controlled delivery. At a scaffold-loaded equivalent of 25 mM $Mg^{2+}$, we observed enhanced bone matrix deposition alongside reduced osteoclast maturation, indicating a synergistic effect between $Mg^{2+}$ and nHA in promoting osteogenesis. While no optimal synergistic dose was identified in 2D culture, these findings demonstrate that Coll-nHA scaffolds offer a promising strategy for localised $Mg^{2+}$ delivery to enhance osteogenesis and suppress osteoclastogenesis. Importantly, the ease of scaffold modification opens the door to incorporating additional bioactive molecules, further advancing their potential in bone tissue engineering applications and the development of next-generation biomaterials for bone regeneration.

## Graphical Abstract



# Lanthanum vs samarium doping into hydroxyapatite nanoparticles for bone tissue engineering: Experimental and theoretical investigations

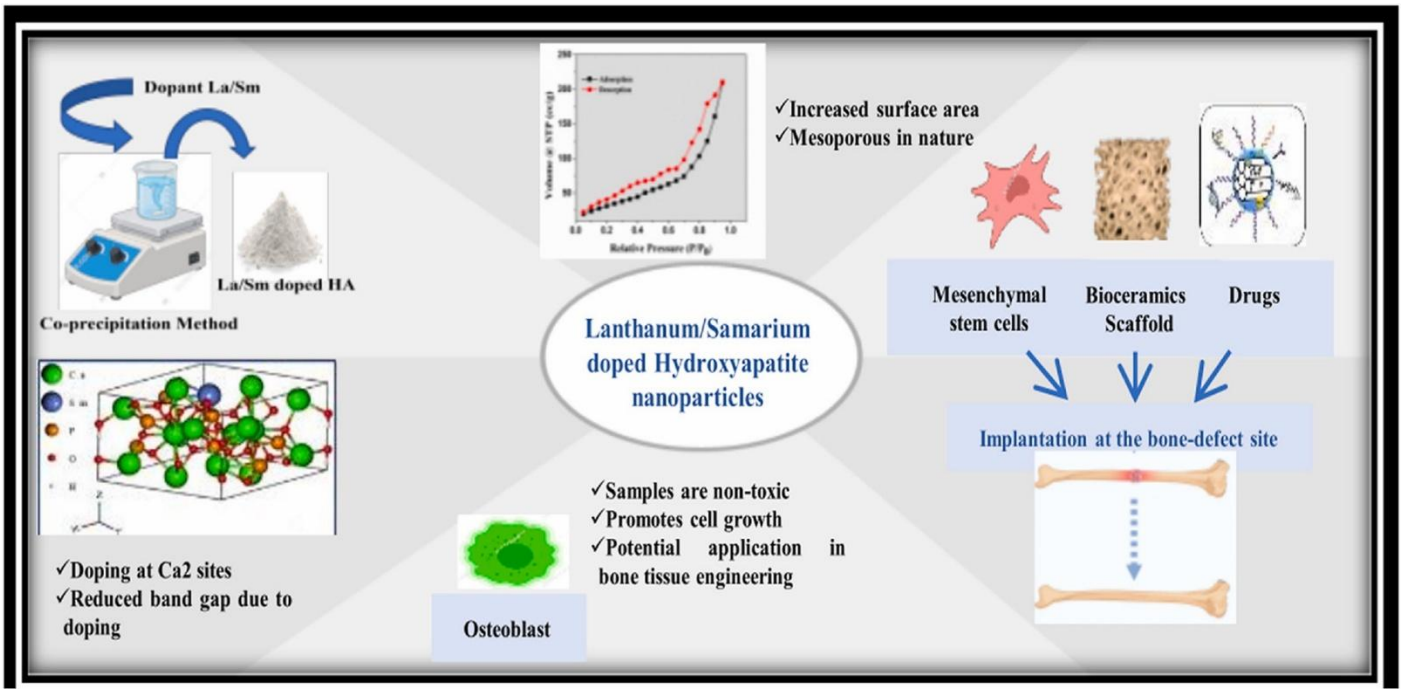
Kanika Chandel [a], Jasvir Singh [a], Kulwinder Kaur [b c], Ciara M. Murphy [c d e], Gurdev Preet Singh [a], K.J. Singh [a]

**Ceramics International** Volume 51, Issue 25, Part A, Pages 44189-44204
Published October 2025
DOI: https://doi.org/10.1016/j.ceramint.2025.07.150

## Abstract

Lanthanide ions doped hydroxyapatite nanoparticles are well-established in biomedical applications. While lanthanide elements are closely grouped in the periodic table and share many similar characteristics, small differences in their effective ionic radii can lead to changes in the physiochemical and biological properties of hydroxyapatite (HA) substitutes. Lanthanum doped hydroxyapatite (HA-La) and samarium doped hydroxyapatite (HA-Sm) nanoparticles of moderate crystallinity (~60–64 %) have been successfully synthesized using the co-precipitation technique. The effects of doping the above-mentioned lanthanide ions on the structural, morphological, drug release and *in vitro* biocompatibility properties of hydroxyapatite samples were investigated experimentally using powder XRD, FTIR, TEM, BET surface area analyser, XPS, UV–Visible spectroscopy, Alamar blue and Pico green assays. Besides, the prepared samples were also modelled for making the theoretical investigations on the density of states and band structures. XPS analysis confirmed the successful incorporation of $La^{3+}$ and $Sm^{3+}$ into the HA lattice without the formation of secondary oxide phases. BET analysis showed almost 35 % increase in surface area for HA-La (from 89.3 $m^2/g$ to 120.4 $m^2/g$) as compared to hydroxyapatite. Drug release studies using ciprofloxacin demonstrated prolonged release behaviour, with HA-La releasing 90 % of the drug over 72 h. Furthermore, theoretical investigations reveal that the doping of hydroxyapatite with lanthanum and samarium leads to the narrowing of the band gap from 5.2 to 4.61 eV. *In vitro* studies with rat mesenchymal stem cells showed enhanced biocompatibility, with HA-La exhibiting of 21 % increase in cell viability and almost 11 % higher DNA content after 7 days compared to control hydroxyapatite. While some previous studies have reported reduced cell viability for lanthanide-doped hydroxyapatite, our findings demonstrate enhanced biocompatibility, with increased cell viability and DNA content. The superior cell viability and proliferation on HA-La suggests its enhanced biocompatibility, making it more suitable for promoting cell growth and tissue regeneration.

## Graphical Abstract



## The Design and Development of an Injectable Thermoresponsive Hydrogel for Controlled Simvastatin Release in Bone Repair Applications

Christopher R. Simpson [1], Helena M. Kelly [1,2,] Ciara M. Murphy[1,3,4,]*

***Gels*** **2025**, *11*(12), 995
Published 10 Dec 2025
DOI: https://doi.org/10.3390/gels11120995

### Abstract

Osteoporotic vertebrae are a uniquely challenging tissue for local delivery due to the complex geometry of cancellous bone, the proximity of the spinal cord, and the need for reliable site retention. These challenges can be met with the use of stimuli responsive, state transiting formulations by leveraging their unique capacity for minimally invasive implantation as a liquid, sol–gel transition in response to stimuli, and finally, release of a loaded therapeutic. Here, we present the formulation development of a thermosensitive methylcellulose–collagen hydrogel, functionalised with controlled release simvastatin, recently shown to enhance osteogenesis while also impeding osteoclast activity. We first optimised a formulation with collagen content of 0.4% *w*/*v* to achieve a thermosensitive system with sol–gel transition at 29 °C, shear-thinning/injectable properties, low cytotoxicity, and high biocompatibility. Incorporation of nano-hydroxyapatite for enhanced bone tissue mimicry revealed optimal performance at 100% *w*/collagen content, showing long-term hydrolytic stability, maintaining more than 100% of its mass after 28 days. A loading concentration of 1 mg of simvastatin to 1 g of hydrogel displayed sustained release of simvastatin over 35 days. Finally, the release of simvastatin from the hydrogel into in vitro conditions prevented the formation of osteoclasts but failed to boost osteogenesis. Together these findings reveal a series of desirable stimuli-responsive hydrogel properties, achieving minimally invasive application coupled with sustained release of a hydrophobic compound, which is potentially useful for spatially complex bone regeneration. Further this work demonstrates the challenge of dosing sustained release systems to achieve simultaneous osteogenesis and anti-osteoclastogenic effects.

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## 3D-Printing of Electroconductive MXene-Based Micro-Meshes in a Biomimetic Hyaluronic Acid-Based Scaffold Directs and Enhances Electrical Stimulation for Neural Repair Applications

Ian Woods, Dahnan Spurling, Sandra Sunil, Anne Marie O'Callaghan, Jack Maughan, Javier Gutierrez-Gonzalez, Tara K. McGuire, Liam Leahy, Adrian Dervan, Valeria Nicolosi, and Fergal J. O'Brien*

**Adv. Sci.** 2025, e03454
Published Jul 2025
DOI: https://dx.doi.org/10.1002/advs.202503454

### Abstract

No effective treatments are currently available for central nervous system neurotrauma although recent advances in electrical stimulation suggest some promise in neural tissue repair. It is hypothesized that structured integration of an electroconductive biomaterial into a tissue engineering scaffold can enhance electroactive signaling for neural regeneration. Electroconductive 2D $Ti_3C_2T_x$ MXene nanosheets are synthesized from MAX-phase powder, demonstrating excellent biocompatibility with neurons, astrocytes and microglia. To achieve spatially-controlled distribution of these MXenes, melt-electrowriting is used to 3D-print highly-organized PCL micro-meshes with varying fiber spacings (low-, medium-, and high-density), which are functionalized with MXenes to provide highly-tunable electroconductive properties ($0.081 \pm 0.053$-$18.87 \pm 2.94$ S/m). Embedding these electroconductive micro-meshes within a neurotrophic, immunomodulatory hyaluronic acid-based extracellular matrix (ECM) produced a soft, growth-supportive MXene-ECM composite scaffold. Electrical stimulation of neurons seeded on these scaffolds promoted neurite outgrowth, influenced by fiber spacing in the micro-mesh. In a multicellular model of cell behavior, neurospheres stimulated for 7 days on high-density MXene-ECM scaffolds exhibited significantly increased axonal extension and neuronal differentiation, compared to low-density scaffolds and MXene-free controls. The results demonstrate that spatial-organization of electroconductive materials in a neurotrophic scaffold

can enhance repair-critical responses to electrical stimulation and that these biomimetic MXene-ECM scaffolds offer a promising new approach to neurotrauma repair.

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## Method for Targeted Cellular Seeding of Tubular Tissue-Engineered Scaffolds for Tracheal Regeneration Approaches

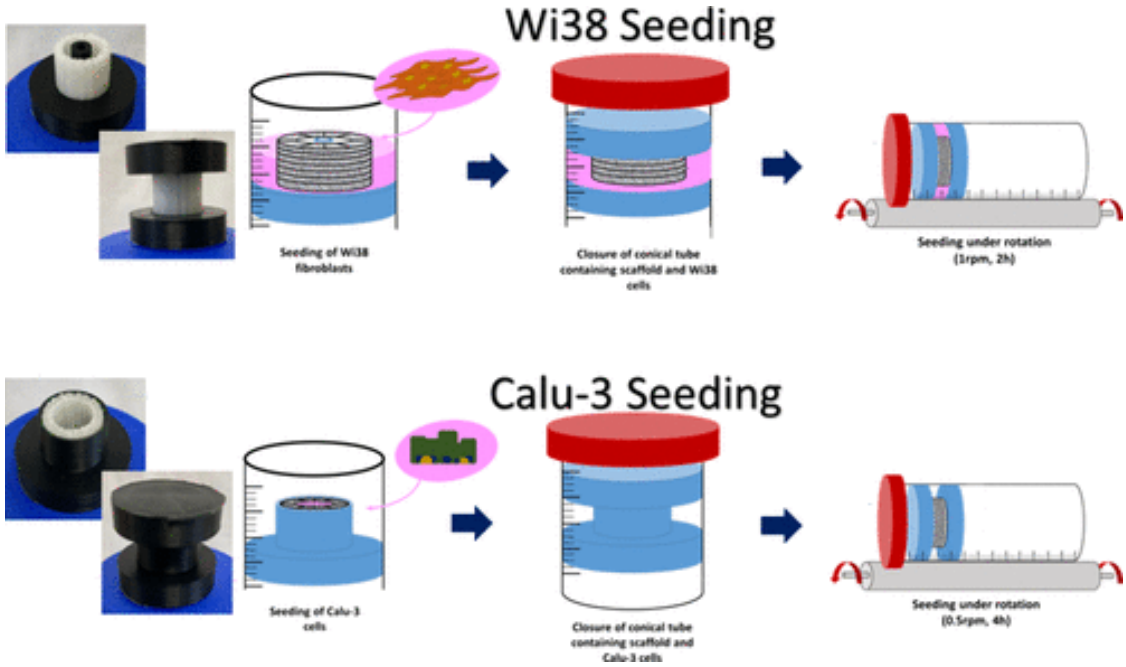
Luis Soriano, Mark Lemoine, Brenton Cavanagh, Anna Johnston, Tehreem Khalid, Fergal J. O'Brien, Cian O'Leary, Sally-Ann Cryan*

***ACS Biomater. Sci. Eng***. 2025, 11, 9, 5293–5305
Published 7 August 2025
DOI: https://doi.org/10.1021/acsbiomaterials.5c00365

## Abstract

Effective tracheal tissue engineering benefits from scaffolds that mimic the native structure of the tissue, provide mechanical stability, and support spatially controlled cell seeding to encourage tissue regeneration. This study presents a novel approach for fabricating tubular scaffolds for tracheal regeneration that integrates a 3D-printed polycaprolactone (PCL) backbone with a freeze-dried collagen-hyaluronic acid (CHyA) layer. Two scaffold geometries (tubular and c-shaped) were produced and mechanically characterized, and it was demonstrated that PCL reinforcement significantly enhanced scaffold structural robustness and durability. To achieve spatially selective cell seeding, custom-designed PLA accessories facilitated the precise deposition of respiratory epithelial cells (Calu-3) onto the inner layer and lung-derived fibroblasts (Wi38) onto the outer layer of the scaffolds. Monoculture experiments showed successful cell localization, while sequential seeding established an effective coculture system with enhanced epithelial coverage and sustained fibroblast viability. This study validates a scalable and customizable method for manufacturing mechanically robust tubular scaffolds with precise spatial cell organization, providing a promising platform for tracheal tissue engineering and potentially other tubular applications such as vascular or gastrointestinal regeneration. Future work will focus on validating this method with primary human cells, incorporating air–liquid interface cultures to enhance epithelial differentiation, and scaling up the constructs to anatomically relevant sizes to advance clinical translation.

## Graphical Abstract



## 2D Boron Nanoplatelets as a Multifunctional Additive for Osteogenic, Gram-Negative Antimicrobial and Mechanically Reinforcing Bone Repair Scaffolds

Jack Maughan, Harneet Kaur, Lucy Prendeville, Tian Carey, Cian O'Connor, Kevin Synnatschke, Juan Carlos Palomeque, Ian Woods, Fergal J. O'Brien, Jonathan N. Coleman*

**Small science** Volume 5, Issue 12 e202500409
Published 4 November
DOI: https://doi.org/10.1002/smsc.202500409

### Abstract

Two-dimensional boron offers unique advantages in bone tissue engineering, unlocking capabilities that conventional additives struggle to achieve. Herein, the 2D morphology and intrinsic bioactivity of boron nanoplatelets are leveraged, to be incorporated into collagen-based scaffolds and simultaneously achieve osteogenic, mechanically reinforcing, and antimicrobial effects, with a shift toward neurogenic, angiogenic, and anti-inflammatory signaling. Boron nanoplatelets, synthesized from nonlayered precursors using liquid-phase exfoliation, are combined with collagen to form boron-collagen scaffolds (BColl). Boron significantly reinforces the collagen matrix, beneficial for mechanoresponsive bone cells. Osteoblasts and mesenchymal stem cells exhibit healthy morphology and proliferation on BColl films and scaffolds, with extended culture leading to increased alkaline phosphatase release and significantly increased calcium deposition, indicating enhanced osteogenesis. *E. coli* viability decreases significantly on BColl films, demonstrating their potential to limit postimplantation infections. Finally, angiogenic, neurogenic, and anti-inflammatory signaling, with dose-dependent upregulation of vascular endothelial growth factor-A, nerve growth factor-beta, and interleukin-10, and downregulation of interleukin-6 are observed, highlighting boron's potential to drive pro-reparative processes. Taken together, these data showcase boron's potential for next-generation bone biomaterials, by offering multifunctional benefits to clinically relevant aspects of bone regeneration such as mineralization, angiogenesis, and innervation, while improving the mechanical and antimicrobial properties of natural polymer scaffolds.

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## A Tailored-made BODIPY Scaffold for STED Super-resolution Microscopy

Martina Fresia, Eden Booth, Massimiliano Garre, Andrea Fin, Marco Blangetti, Donal O'Shea

**ChemRixiv** 07 November 2025, Version 1
Published 7 Nov 2025
DOI: 10.26434/chemrxiv-2025-gcs34

### Abstract

The development of bright and photostable fluorophores tailored for stimulated emission depletion (STED) microscopy remains a major challenge in bioimaging. Here, we report a rationally designed BODIPY scaffold optimized for STED applications through a three-step telescoped synthesis. The introduction of α-thiophene substituents at the BODIPY core was found to be crucial for achieving the spectral and photophysical properties required for efficient depletion using a 775 nm laser. Compared to the parent core-unsubstituted compound, the α-thiophene-modified dye exhibits a pronounced, red-shifted emission and suppressed non-radiative decay, leading to high quantum yield, remarkable photostability, and minimal sensitivity to polarity or viscosity. Following incubation with HeLa Kyoto cells, efficient staining of multiple lipophilic intracellular membranes and organelles was observed. 2D and 3D STED imaging of various subcellular regions in live cells such as the nuclear membrane, endoplasmic reticulum, lipid droplets and mitochondria demonstrated that resolution below the diffraction limit of a confocal microscope was readily achievable. Notably, in the case of mitochondria both the outer and inner cristae membranes could be resolved and 3D reconstruction illustrated the tunnel like characteristics of nuclear membrane invagination. Overall, this work establishes α-thiophene substitution as a powerful molecular engineering strategy to convert environment-sensitive BODIPY fluorophores into a robust, STED-compatible platform. The modular synthetic approach further provides a versatile red-fluorescent scaffold for developing next-generation fluorophores tailored to specific biological targets and super-resolution techniques.

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## Double Click for Chirality: Chiral Dibenzo-cycloocta-bis-triazoles via Strain-Promoted Alkyne-Azide Cycloaddition

Sebastian Pim+,[a] Aaron D. G. Campbell+,[b] Dmitry Levshov,[c] Wouter Herrebout,[c]
Gonzalo Durán-Sampedro,[a] Michael J. Hall,*[b] Roly J. Armstrong,*[b] and Donal F. O'Shea*[a]
**ChemPhotoChem**
Posted 1 May 2025
DOI: doi.org/10.1002/cptc.202500042

### Abstract

The synthetically convenient strain promoted double azide cycloaddition of the Sondheimer-Wong diyne produces resolvable chiral dibenzo-cycloocta-bis-triazoles whose stereogenicity, to date, has gone unrecognised. Enantiomers were separable by chiral HPLC and showed no racemization at 100 °C. This unique method to produce chiral substrates was exploited for the synthesis and resolution of a chiral fluorescent BF2-azadipyrromethene, with absorption and emission spanning the important spectral range of 600 to 700 nm. The fluorophore properties were studied utilising X-ray structural analysis, electronic circular dichroism spectra and DFT calculations.

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## Lipid Mapping of Cell Mitosis by Non-covalent Migratory Fluorescence Labelling

Anais Bourgès, Massimiliano Garre, Donal O'Shea
**ChemRxiv** Version 1
Posted 9 July 2025
DOI:
10.26434/chemrxiv-2025-9khqw

### Abstract

The concept of non-covalent migratory fluorescence labelling is introduced to spatially and temporally map intracellular lipids throughout a cell division cycle. This hands-off approach utilizes a small molecule BF2-azadipyrromethene fluorophore, NM-ER, to first label the nuclear membrane and endoplasmic reticulum of cells at interphase but which can migrate with the lipid components of these structures throughout mitosis as they disassemble, redistribute and reassemble prior to daughter cell separation. Through this unique approach to image capture, key prometaphase events such as lipid intrusion into the nucleus and nuclear membrane disassembly are observable, as are the stages of nuclear membrane reassembly in telophase and lipid distribution during cytokinesis. When used alone NM-ER can distinguish each phase of cell mitosis from lipid staining patterns, is compatible with STED super resolution imaging, and with an emission max of 648 nm makes it useable with other common GFP and nuclear DNA stains. The non-covalent NM-ER label remains associated with the originating lipid components as they undergo architectural reorganizations and changes in subcellular localization associated with mitosis. As lipid-based cell structures are influenced by numerous biological processes and mechanical forces, our approach to fluorescence imaging could offer novel perspectives into their different roles.

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## Endogenous Labelling of Extracellular Vesicles and Image Capture of their Interactions with Acceptor Cells

Donal O'Shea, Eden Booth, Massimiliano Garre, Dan Wu
**ChemRxiv** Version 1
Posted 18 Sep 2025
DOI:
10.26434/chemrxiv-2025-4t29r

### Abstract

Despite their significance in both physiological and pathological contexts, the mechanisms governing extracellular vesicle (EV) uptake and cytosolic cargo delivery remain incompletely understood. Here, we report the development of a $BF_2$-azadipyrromethene-based near-infrared fluorophore for the endogenous

labelling of EVs, enabling their interaction with acceptor cells to be observed using both intensity and fluorescence lifetime imaging microscopies. Through endogenous labelling dye aggregate free EVs can be readily isolated and confirmed through their emission wavelengths (λmax 720 nm) and lifetime (2.7 ns). These photophysical properties permitted clear discrimination between aggregated and disaggregated forms of the fluorophore in complex biological environments. Endogenously labelled EVs containing the disaggregated fluorophore were incubated with unlabelled acceptor cells and imaged by both intensity and lifetime microscopy, confirming identical intensity and lifetime values to the free disaggregated dye. Incubation at 4 °C, which slows cellular processes, enabled visualization of initial EV-plasma membrane interactions, while at 37 °C efficient transfer of the fluorophore into acceptor cells was observed, evidenced by increased emission intensity and matching characterised spectral–lifetime signatures. Our results establish endogenous labelling as an efficient method to introduce a fluorophore into the lumen of EVs thereby providing a robust platform for real-time visualization of EV communication with acceptor cells.

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# Dublin City University ((DCU) Chemistry Research Publications June-December 2025

## A trackable trinuclear platinum complex for breast cancer treatment

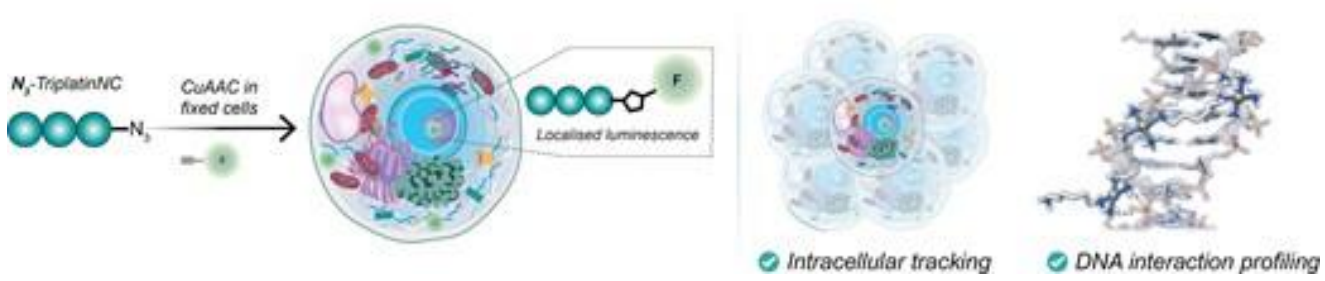
Sinéad O'Carroll, Creina Slator, Raphael E F de Paiva, Conor Newsome, Bethany Searle, Sriram KK, Sylvia Whittle, Thomas E Catley, Stefano Scoditti, Katarzyna Mnich, Erica J Peterson, Bin Hu, Jennifer E Koblinski, Afshin Samali, Vickie McKee, Alice L B Pyne, Fredrik Westerlund, Nicholas P Farrell*, Andrew Kellett*

***Nucleic Acids Research***, Volume 53, Issue 13, 22 July 2025, gkaf628
Published 16 Jul 2025
DOI: https://doi.org/10.1093/nar/gkaf628

### Abstract

Cancer remains a leading cause of death, with triple-negative breast cancer (TNBC) being particularly significant due to limited treatment options. As such, there is interest in anticancer polynuclear platinum(II) complexes, attributed to their unique DNA-binding modes and potential against therapy-resistant cancer phenotypes. However, a persistent challenge with polynuclear compounds is their lack of cellular trackability, hindering their effectiveness and monitoring in clinical settings. Here, we report the preparation of a new azide-appended trinuclear platinum complex, $N_3$-TriplatinNC, and characterize its DNA-targeting, cytotoxicity, and topoisomerase relaxation properties from the nanoscale to the macroscale. Using single-molecule biophysics and in-liquid atomic force microscopy, $N_3$-TriplatinNC was identified as a powerful DNA recognition agent with remarkable potential towards the TNBC cell line, MDA-MB-231. Installation of the azide handle on the polynuclear complex was achieved using a first-in-class approach to produce a complex that retained analogous biological activity to the parent TriplatinNC. Importantly, the azide handle facilitates *in situ* click chemistry for tracking cellular localization, with subsequent xenograft studies demonstrating *in vivo* antitumoural potential.

### Graphical Abstract




## Visualizing stress granule dynamics with an RNA guanine quadruplex targeted ruthenium(II) peptide conjugate†

Rhianne C. Curley‡ , Lorcan Holden‡ and Tia E. Keyes *

***RSC Chem. Biol.***, 2025, **6**, 1403-1413
Published 19 June 2025
DOI: 10.1039/D5CB00008D

### Abstract

Stress granules (SGs) are membraneless ribonucleoprotein assemblies that form in response to cellular stress. They have been linked to cell survival and cancer progression, though many questions remain regarding their structure, function and therapeutic potential. Live-cell fluorescence imaging is key to advancing understanding of SGs, but there are very few small-molecule probes reported that selectively image these organelles. RNA G-quadruplex (rG4) folding is believed to play a role in initiation of SG formation. Thus, to create a probe for SGs, we conjugated a G4 binding domain peptide from RNA helicase associated with AU-rich element (RHAU) to a luminescent $[Ru(bpy)_2(PIC\text{-}COOH)]^{2+}$, Ru-RHAU. Ru-

RHAU is designed to target rG4s and thus SGs in live cells. Studies *in cellulo* demonstrate that Ru-RHAU can induce SG formation in a concentration and time dependent manner, and immunolabelling confirmed the complex remains associated with rG4s in the SGs. The SG stimulation is attributed to stabilization of rG4 by Ru-RHAU consistent with rG4's role in SG formation. Ru-RHAU shows low cytotoxicity under imaging conditions, facilitating prolonged observation in live cells. Interestingly, under more intense photoirradiation, Ru-RHAU induces phototoxicity through an apoptotic pathway. Ru-RHAU is a versatile tool for probing SG dynamics and function in cellular stress responses and has heretofore unconsidered potential in phototherapeutic applications targeting SGs.

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## Ink synthesis and inkjet printing of manganese electrodes on laser textured aluminium foil: The effect of laser texturing parameters on surface roughness and printability

Anesu Nyabadza [a b c]*, Suman Chatterjee [a c], Suganya Pitchai Muthusamy [c], Sean Ryan [d e], Jesus Inocente Medina Santos [d e], Valeria Nicolosi [d e], Dermot Brabazon [a b c], Mercedes Vazquez [a b c]

**Journal of Materials Research and Technology** Volume 37, July–August 2025, Pages 4514-4531
Published July–August 2025
DOI: https://doi.org/10.1016/j.jmrt.2025.07.120

### Abstract

Inkjet printing of manganese on aluminium provides a cost-effective method for electrode fabrication in sensing and capacitor applications, leveraging aluminium's conductivity and manganese's electrochemical activity. However, existing studies often isolate ink formulation, substrate preprocessing, and inkjet printing, overlooking their interdependence. This study integrates all three aspects, using femtosecond laser texturing to enhance surface roughness and improve printability. A full-factorial design optimized laser parameters, achieving a roughness of 8.487 μm–16 times that of pristine aluminium—using a 70 μm hatch spacing, laser energies of 27–36 mJ, and scan speeds of 15–25 mm/s. Manganese ink was synthesised via laser ablation in IPA, producing spherical nanoparticles (64 nm) with a viscosity of 2.86 mPa s. A design of experiments approach determined optimal inkjet printing conditions: 15 kHz jetting frequency, 50 °C print bed, 60 s interlayer delay, and 1270 DPI. This is the first study to integrate laser texturing for printability enhancement with control of ink formulation via laser processing. The process ensured target properties were met during ink formulation, including a specific surface area of ≥30 $m^2/cm^3$, at least 90 % of nanoparticle size <100 nm, and viscosity <5 mPa s, all achieved within 65 min of laser ablation.

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## CACHE Challenge #2: Targeting the RNA Site of the SARS-CoV-2 Helicase Nsp13

Multiple Authors: see the paper via the DOI.

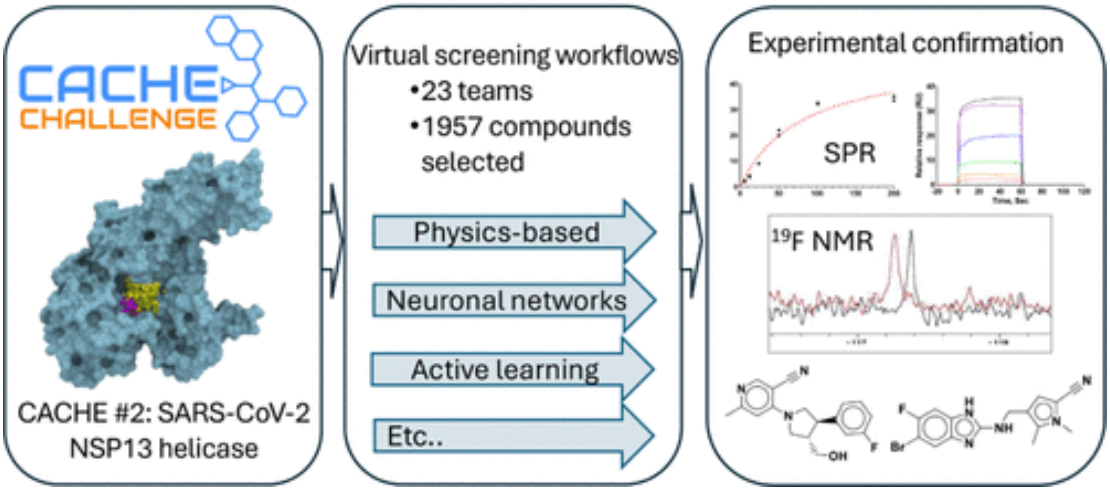
***J. Chem. Inf. Model***. 2025, 65, 13, 6884–6898
Published 20 June 2025
DOI: https://doi.org/10.1021/acs.jcim.5c00535

### Abstract

A critical assessment of computational hit-finding experiments (CACHE) challenge was conducted to predict ligands for the SARS-CoV-2 Nsp13 helicase RNA binding site, a highly conserved COVID-19 target. Twenty-three participating teams comprised of computational chemists and data scientists used protein structure and data from fragment-screening paired with advanced computational and machine learning methods to each predict up to 100 inhibitory ligands. Across all teams, 1957 compounds were predicted and were subsequently procured from commercial catalogs for biophysical assays. Of these compounds, 0.7% were confirmed to bind to Nsp13 in a surface plasmon resonance assay. The six best-performing computational workflows used fragment growing, active learning, or conventional virtual screening with and without complementary deep-learning scoring functions. Follow-up functional assays resulted in identification of two compound scaffolds that bound Nsp13 with a $K_d$ below 10 μM and inhibited *in vitro* helicase activity. Overall, CACHE #2 participants were successful in identifying hit compound scaffolds targeting Nsp13, a central component of the coronavirus replication-transcription complex. Computational design strategies recurrently successful across the first two CACHE challenges include linking or growing docked or crystallized fragments and docking small and diverse libraries to train ultrafast

machine-learning models. The CACHE #2 competition reveals how crowd-sourcing ligand prediction efforts using a distinct array of approaches followed with critical biophysical assays can result in novel lead compounds to advance drug discovery efforts.

## Graphical Abstract

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## Photophysical Properties and Protein Binding Studies of Piperazine-Substituted Anthracene-BODIPY Dyads for Antimicrobial Photodynamic Therapy

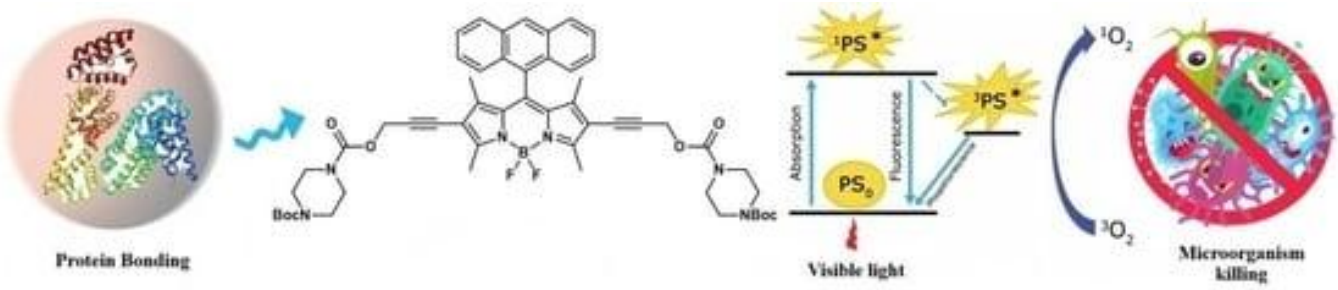
Stephen O'Sullivan[1]*,Leila Tabrizi[1]*, Kaja Turzańska[2]*, Ian P. Clark[3]*, Deirdre Fitzgerald-Hughes[2,*]* Mary T. Pryce[1,*]*

***Molecules*** **2025**, *30*(13), 2727
Published 25 June 2025
DOI: https://doi.org/10.3390/molecules30132727

### Abstract

This work presents the synthesis, characterisation, photophysical properties, time-resolved spectroscopic behaviour, and biological evaluation of two structurally distinct heavy-atom-free BODIPY-anthracene dyads (**BDP-1**) and the newly designed 2,6-bis[1-(tert-butyl) 4-(prop-2-yn-1-yl) piperazine-1,4-dicarboxylate] BODIPY-anthracene (**BDP-2**), incorporating 2,6-alkynyl-piperazine substituents for potential application in antimicrobial photodynamic therapy. **BDP-1** exhibits absorption and emission maxima at 507 nm and 516 nm, respectively, with a Stokes shift of 344 $cm^{-1}$ in dichloromethane (DCM), characteristic of unsubstituted BODIPYs. In contrast, **BDP-2** undergoes a red-shift in the absorption maximum to 552 nm (Stokes shift of 633 $cm^{-1}$), which is attributed to the extended conjugation from the introduction of the alkyne groups. Time-resolved infrared spectroscopy confirmed efficient spin-orbit charge transfer intersystem crossing, and nanosecond transient absorption studies confirmed the formation of a long-lived triplet state for **BDP-2** (up to 138 µs in MeCN). A binding constant ($K_b$) of $9.6 \times 10^4$ $M^{-1}$ was obtained for **BDP-2** when titrated with bovine serum albumin (BSA), which is higher than comparable BODIPY derivatives. **BDP-2** displayed improved hemocompatibility compared to **BDP-1** (<5% haemolysis of human erythrocytes up to 200 $\mu g \cdot mL^{-1}$). Antimicrobial activity of **BDP-1** and **BDP-2** was most potent when irradiated at 370 nm compared to the other wavelengths employed. However, **BDP-2** did not retain the potent (6 log) and rapid (within 15 min) eradication of *Staphylococcus aureus* achieved by **BDP-1** under irradiation at 370 nm. These findings demonstrate the rational design of **BDP-2** as a biocompatible, and heavy-atom-free BODIPY offering promise for targeted antimicrobial photodynamic therapeutic applications.

## Graphical Abstract

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## Assessment of IoT low-cost sensor networks for long-term outdoor and indoor air quality monitoring: a case study in Dublin

Jiayao Chen [a]*, Óscar González [b], David O'Connor [c], Lindsay Tallon [d], Francesco Pilla [a]

**Atmospheric Pollution Research** Volume 16, Issue 11, November 2025, 102651
Published 22 Jul 2025
DOI: https://doi.org/10.1016/j.apr.2025.102651

### Abstract

This study provides a framework for Internet of Things based low-cost sensors (LCS) network implementation, using office environments in Dublin, Ireland, as a case study for long-term indoor air quality (IAQ) monitoring. It covers options and key decisions related to sensor technology, reporting systems and data management. Environmental and indoor data were collected from 1 June 2023 to 20 June 2024, using Smart Citizen Kit 2.1 and PurpleAir devices, and data retrieved from cloud-based data platforms for analysis. The standard deviation and coefficient of variation were calculated to evaluate intra-sensor precision. To improve data quality of LCS various correction models were tested, considering the impact of temperature and relative humidity. A multilinear model with additive relative humidity, using the piecewise regression, provided better performance ($R^2 > 0.7$, RMSE <5 μg/m$^3$) and accuracy (>0.88) for 24-h fine particulate matter ($PM_{2.5}$) and inhalable particulate matter ($PM_{10}$). This study bridges the data gap by incorporating multi-brand LCS network for further application in outdoor supplementary and IAQ reporting. The results showed corrected indoor $PM_{2.5}$ data in offices complies with WHO air quality guidelines, and carbon dioxide ($CO_2$) levels in naturally ventilated conditions remained below 800 ppm. Additionally, diurnal patterns reveal elevated levels of $CO_2$ and total volatile organic compounds during core office hours, while the contrasting patterns for $PM_{2.5}$ suggest outdoor infiltration as the dominant source. This study demonstrates the potential of data-driven techniques for real-time IAQ monitoring and reporting, providing valuable insights to promote healthier IAQ for occupants.

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## Spatial N-glycan rearrangement on α5β1 integrin nucleates galectin-3 oligomers to determine endocytic fate

Massiullah Shafaq-Zadah*, Estelle Dransart, Ilyes Hamitouche, Christian Wunder, Valérie Chambon, Cesar A. Valades-Cruz, Ludovic Leconte, Nirod Kumar Sarangi, Jack Robinson, Siau-Kun Bai, Raju Regmi, Aurélie Di Cicco, Agnès Hovasse, Richard Bartels, Ulf J. Nilsson, Sarah Cianférani-Sanglier, Hakon Leffler, Tia E. Keyes, Daniel Lévy, Stefan Raunser, Daniel Roderer*, Ludger Johannes*

***Nature Communications*** volume 16, Article number: 9461 (2025)
Published 27 Oct 2025
DOI: https://doi.org/10.1038/s41467-025-64523-7

### Abstract

Membrane glycoproteins frequently adopt different conformations when altering between active and inactive states. Here, we discover a molecular switch that exploits dynamic spatial rearrangements of N-glycans during such conformational transitions to control protein function. For the conformationally switchable cell adhesion glycoprotein $\alpha_5\beta_1$ integrin, we find that only the bent-closed state arranges N-glycans to nucleate the formation of up to tetrameric oligomers of the glycan-binding protein galectin-3. We propose a structural

model of how these galectin-3 oligomers are built and how they clamp the bent-closed state to select it for endocytic uptake and subsequent retrograde trafficking to the Golgi for polarized distribution in cells. Our findings reveal the dynamic regulation of the glycan landscape at the cell surface to achieve oligomerization of galectin-3. Galectin-3 oligomers are thereby identified as functional decoders of defined spatial patterns of N-glycans on specifically the bent-closed conformational state of $\alpha_5\beta_1$ integrin and possibly other integrin family members.

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## Visualizing stress granule dynamics with an RNA guanine quadruplex targeted ruthenium(ii) peptide conjugate†

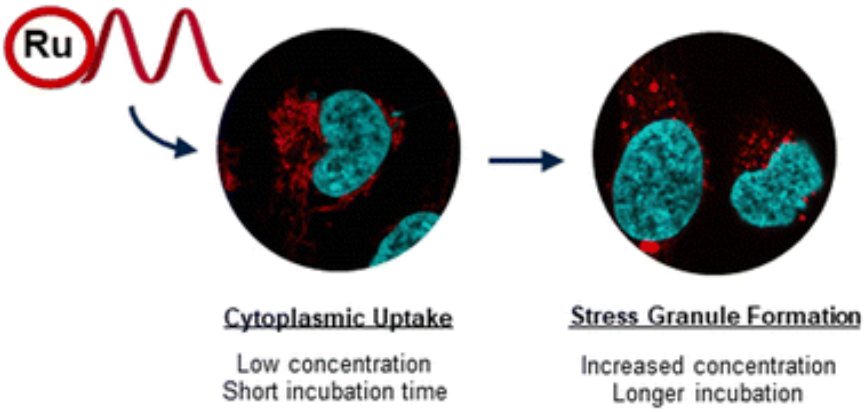
Rhianne C. Curley,‡[a] Lorcan Holden‡[a] and Tia E. Keyes *[a]

***RSC Chem. Biol.***, 2025,**6**, 1403-1413
Published 19 Jun 2025
DOI: https://doi.org/10.1039/D5CB00008D

### Abstract

Stress granules (SGs) are membraneless ribonucleoprotein assemblies that form in response to cellular stress. They have been linked to cell survival and cancer progression, though many questions remain regarding their structure, function and therapeutic potential. Live-cell fluorescence imaging is key to advancing understanding of SGs, but there are very few small-molecule probes reported that selectively image these organelles. RNA G-quadruplex (rG4) folding is believed to play a role in initiation of SG formation. Thus, to create a probe for SGs, we conjugated a G4 binding domain peptide from RNA helicase associated with AU-rich element (RHAU) to a luminescent $[Ru(bpy)_2(PIC\text{-}COOH)]^{2+}$, Ru-RHAU. Ru-RHAU is designed to target rG4s and thus SGs in live cells. Studies *in cellulo* demonstrate that Ru-RHAU can induce SG formation in a concentration and time dependent manner and immunolabelling confirmed the complex remains associated with rG4s in the SGs. The SG stimulation is attributed to stabilization of rG4 by Ru-RHAU consistent with rG4's role in SG formation. Ru-RHAU shows low cytotoxicity under imaging conditions, facilitating prolonged observation in live cells. Interestingly, under more intense photoirradiation, Ru-RHAU induces phototoxicity through an apoptotic pathway. Ru-RHAU is a versatile tool for probing SG dynamics and function in cellular stress responses and has heretofore unconsidered potential in phototherapeutic applications targeting SGs.

### Graphical Abstract




## Ultrafast light-switch properties of a G-quadruplex binder: [Ru(phen)2(tpphz-DC3)]4+

Philip A. Morgenfurt,†[a] Avinash Chettri,††[bc] Lorcan Holden,[a] Benjamin Dietzek-Ivanšić §*[bc] and Tia E. Keyes *[a]

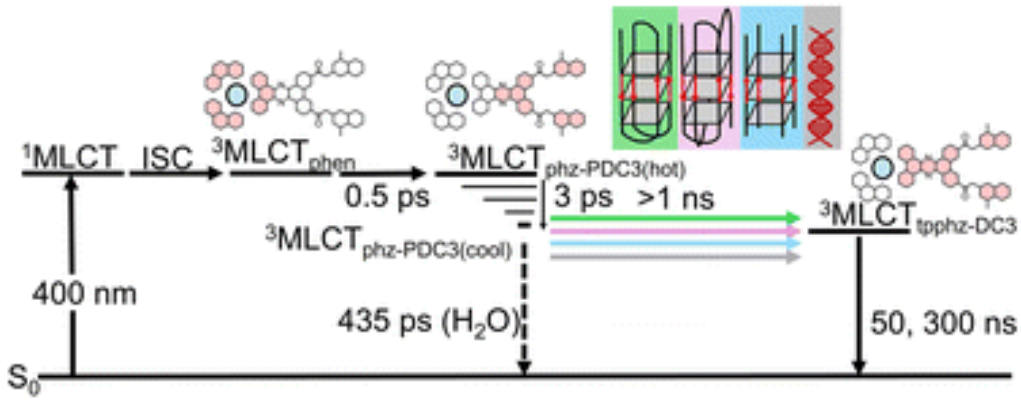
***Inorg. Chem. Front.***, 2025,**12**, 8375-8387
Published 22 August 2025
DOI: https://doi.org/10.1039/D5QI01553G

### Abstract

Light-switch probes, where the probe only emits light on binding to its target, are highly attractive in bioimaging as they provide for outstanding contrast, especially in the interrogation of a discrete and dynamic

distributed structure like G-quadruplex DNA. Here, we examine the photophysical properties of a G-quadruplex (G4) selective probe comprising a light-switch Ru(II) dipyridylphenazine complex co-assembled with the well-known G4 selective ligand PDC3; $[Ru(phen)_2PDC3]^{4+}$ (**RuPDC3**), using femtosecond and nanosecond transient absorption spectroscopy, complemented by steady-state spectroscopy and spectro-electrochemistry. We compared the photophysics of RuPDC3 with that of a well-known photo-switch $[Ru(bpy)_2(dppz)]^{2+}$, **Rudppz**, and observed marked differences in their behaviours. Whereas in **Rudppz**, the $^3$MLCT state is either localized on the phenanthroline or the phenazine unit, we show that in **RuPDC3**, this state has charge delocalised over the entire PDC3 unit. We then compared the ultrafast dynamics of this complex with **Rudppz** when associated with duplex and G4 DNA of different topologies and observed notable differences in trends in the exited-state dynamics in both **RuPDC3** and **Rudppz** with G4 for the first time. **RuPDC3** shows greater variation in excited-state dynamics with G4 topology and offers the prospect of elucidation of topology by ultrafast imaging.

## Graphical Abstract

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## Triplet–Triplet Annihilation Upconversion Is Impeded in Liposomes that Prevent Sensitizer and Annihilator Co-Confinement

Amrutha Prabhakaran, Keshav Kumar Jha, Rengel Cane E. Sia, Mateusz Kogut, Jacek Czub, Julien Guthmuller, Colm Smith, Christopher S. Burke, Benjamin Dietzek-Ivanšić, Tia E. Keyes*

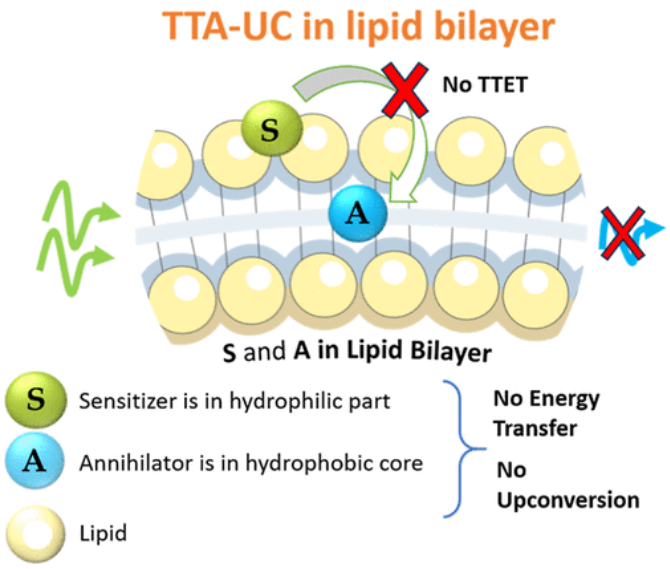
***J. Phys. Chem. B*** 2025, 129, 25, 6220–6232
Published 12 June 2025
DOI: https://doi.org/10.1021/acs.jpcb.5c01826

## Abstract

Triplet–triplet annihilation upconversion (TTA-UC) implemented in liposomes may be a promising tool in drug delivery and sensing. Indeed, we recently demonstrated that colocalization of lipophilic reagents to the membrane hydrophobic core improves the TTA-UC efficiency in liposomes compared to solution. Here, we examined if the counter is true, i.e., we evaluate if TTA-UC is inhibited when the sensitizer and annihilator occupy different regions within a single leaflet of a liposome membrane. To test this hypothesis, we used a Ru(II) complex, with tridentate ligand 2,6-di(quinolin-8-yl)pyridyl) (bqp) $[Ru(bqp)(bpq\text{-}oct)]^{2+}$(Ru-bqp-oct) where oct is a C8 alkyl chain appended to facilitate integration into the liposome, as a sensitizer and diphenylanthracene (DPA) as an annihilator. TTA-UC from this pair was evaluated and compared in solution and liposomal nanovesicles. This Ru(II)-bqp complex was selected for its exceptionally long-lived emission and high triplet quantum yield, due to its expanded N-Ru-N bite angles. In solution, TTA-UC was efficient with a quantum yield of 3.11%, but in liposomes, no anti-Stokes shifted emission was observed even with an increased concentration of sensitizer and annihilator in the membrane. Molecular dynamics simulations were used to understand this effect and confirmed poor co-orientation of sensitizer and annihilator in the membrane was responsible for lack of TTA-UC in the membrane. DPA was determined to orient at the hydrophobic core, while the cationic Ru complex is embedded shallowly at the membrane interface, the closest approach of donor and acceptor in the membrane was determined as 0.7 nm. This work highlights the critical importance of colocalization of sensitizers and annihilators, even within a single membrane leaflet to

facilitate Dexter energy transfer through collision in membrane-constrained TTA-UC systems and the value of MD simulations in system design.

## Graphical Abstract

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## Receptor modulated assembly and drug induced disassembly of amyloid beta aggregates at asymmetric neuronal model biomembranes

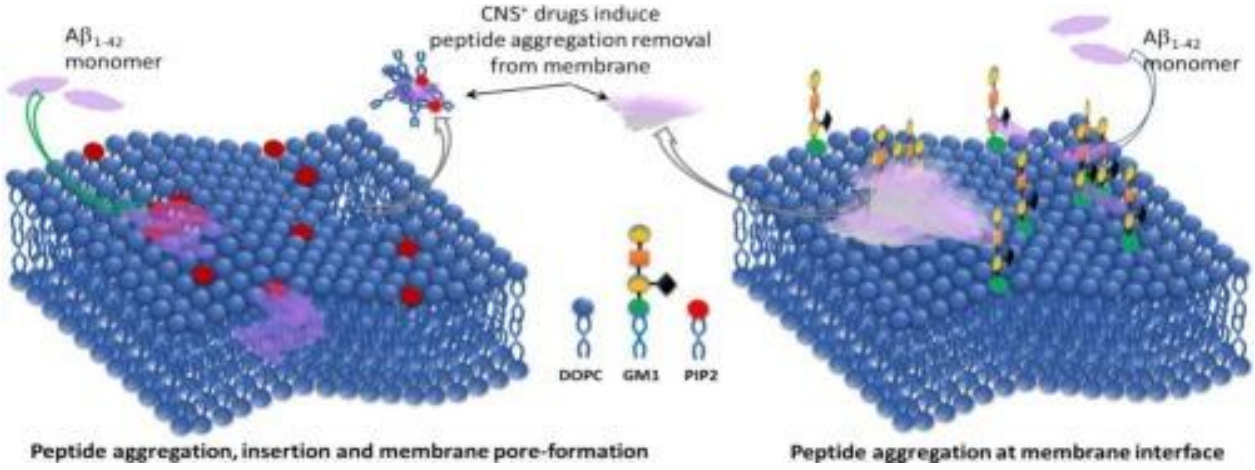
Nirod Kumar Sarangi [a b], Subrata Mondal [a b], Tia E. Keyes [a]*

**Biophysical Chemistry** Volume 322, July 2025, 107441
Published July 2025
DOI: https://doi.org/10.1016/j.bpc.2025.107441

## Abstract

Amyloid peptide non-fibrillar oligomers cause neurotoxicity and may contribute to Alzheimer's disease (AD) pathogenesis. Mounting evidence indicates that $A\beta_{1-42}$ oligomers disrupt and remodel neuronal membrane, causing neuronal cell death. The involvement of individual neuronal membrane constituents in real-time $A\beta_{1-42}$ aggregate assembly is unclear due to complexity of neuronal cell membrane. We used non-Faradaic electrochemical impedance spectroscopy (EIS) to track monomeric $A\beta_{1-42}$ peptide binding and aggregation pathways in real-time in asymmetric micropore suspended lipid bilayer membranes with anionic phospholipids and glycosphingolipids. Anionic DOPC:PIP2 pore suspended membrane showed pore-formation within 2 h of incubation, but peptide insertion occurred over 6 h, with an onset time of ~6–8 h for peptide aggregation at the membrane surface. Among different gangliosides, peptide binding to GM1- and GM3-containing membranes did not result pore development, but receptor mediated peptide aggregation formation caused membrane admittance to decrease within 2 h. In contrast, partial peptide insertion in the membrane surface increases membrane admittance at GD1a and mixed GSL membranes, arresting aggregation. Time-lapsed AFM imaging at asymmetric solid supported lipid bilayers (aSLBs) corroborated EIS findings, capturing pore-formation and receptor mediated peptide assembly routes. Fluorescence lifetime imaging (FLIM) imaging and spatial resolved single-point fluorescence correlation spectroscopy (FCS) at aSLBs revealed membrane-peptide interaction, assembly, and peptide induced membrane reorganization. Treatment with antidepressants fluoxetine and imipramine therapeutics, in synergy, which are cost-effective and capable of crossing the central nervous system (CNS+), resulted in the disassembly of membrane mediated $A\beta_{1-42}$ aggregates, but not fibrils. Overall, the data suggests that membrane-mediated aggregate disassembly at the correct timing of AD progression may halt or reverse amyloid assembly through the use of repurposed drugs.

## Graphical Abstract

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## Spatial N-glycan rearrangement on α5β1 integrin nucleates galectin-3 oligomers to determine endocytic fate

Massiullah Shafaq-Zadah, Estelle Dransart, Ilyes Hamitouche, Christian Wunder, Valérie Chambon, Cesar A. Valades-Cruz, Ludovic Leconte, Nirod Kumar Sarangi, Jack Robinson, Siau-Kun Bai, Raju Regmi, Aurélie Di Cicco, Agnès Hovasse, Richard Bartels, Ulf J. Nilsson, Sarah Cianférani-Sanglier, Hakon Leffler, Tia E. Keyes, Daniel Lévy, Stefan Raunser, Daniel Roderer, Ludger Johannes

***Nat Commun*** **16**, 9461 (2025)
Published 27 OCT 2025
DOI: https://doi.org/10.1038/s41467-025-64523-7

### Abstract

Membrane glycoproteins frequently adopt different conformations when altering between active and inactive states. Here, we discover a molecular switch that exploits dynamic spatial rearrangements of N-glycans during such conformational transitions to control protein function. For the conformationally switchable cell adhesion glycoprotein $\alpha_5\beta_1$ integrin, we find that only the bent-closed state arranges N-glycans to nucleate the formation of up to tetrameric oligomers of the glycan-binding protein galectin-3. We propose a structural model of how these galectin-3 oligomers are built and how they clamp the bent-closed state to select it for endocytic uptake and subsequent retrograde trafficking to the Golgi for polarized distribution in cells. Our findings reveal the dynamic regulation of the glycan landscape at the cell surface to achieve oligomerization of galectin-3. Galectin-3 oligomers are thereby identified as functional decoders of defined spatial patterns of N-glycans on specifically the bent-closed conformational state of $\alpha_5\beta_1$ integrin and possibly other integrin family members.

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## Machine learning-based process quality control of screen-printed titanium dioxide electrodes

Anesu Nyabadza [a] [b], Lola Azoulay-Younes [b] [c], Mercedes Vazquez [a] [b], Dermot Brabazon [a] [b]

**Results in Materials** Volume 26, June 2025, 100692
Published June 2025
DOI: https://doi.org/10.1016/j.rinma.2025.100692

### Abstract

AI-based quality control has gained attention in the manufacturing industry due to its ability to improve speed and accuracy. AI can analyze a printed electrode and classify it as either good or bad quality within milliseconds, much faster than humans and conventional methods (random sampling and control charts). Herein, machine learning methods including Random Forest (RF), Support Vector Machine (SVM), and Feedforward Neural Network (FNN) are used to address a quality control problem involving the classification of screen-printed $TiO_2$ electrodes based on image data. Multivariate data analysis techniques such as factor analysis were employed to evaluate the effectiveness of the features extracted from these images. Characterization techniques like FTIR, 4-point probe, and microscopy were used to study the printed

electrodes and provide accurate labeling. A dataset comprising ~300 electrodes was created to train the AI models. The SVM model demonstrated the best performance, achieving 100 % accuracy and recall, followed by the FNN model with 99 % accuracy. Models were optimized and accelerated through feature engineering and extraction techniques, allowing them to be trained in under 1 min. This rapid training capability makes these models highly suitable for real-world quality control applications where hundreds of electrodes are produced per minute.

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## Machine learning for quality control of Tin-Copper electrodes

Anesu Nyabadza [a b], Lola Azoulay-Younes [b c], Mercedes Vazquez [b c], Dermot Brabazon [a b]

**Measurement** Volume 250, 117191
Published 15 June 2025
DOI: https://doi.org/10.1016/j.measurement.2025.117191

### Abstract

Screen printing is the most common technique for manufacturing printed electrodes, yet machine learning applications in its quality control are underexplored. Herein, $SnO_2$-CuO microparticle-nanoparticle-based electrodes were printed on paper substrates and categorised as bad, medium, or good. The optimal chemical composition of the formulated inks and the maximum operating temperatures of the electrodes (up to 150 °C) were investigated. The inks were formulated using various ratios of $SnO_2$ powder (particle size 325 µm), glycerine and Polyvinyl alcohol (PVA) glue. The highest conductivity recorded was 80 $S.m^{-1}$ achieved for an ink composed of 1 g $SnO_2$ powder, 3 g glycerine, 0.03 PVA glue, and heat treated at 150 ºC for 30 min. Random forest (RF), support vector machine (SVM) and Feedforward neural networks (FNN) models achieved approximately 80 % accuracy and recall. Synthetic Minority Over-sampling Technique with Edited Nearest Neighbors and hyperparameter tunning methods were used to eliminate model overfitting by balancing the dataset. An ensemble model that can classify about 100 electrodes in under 100 ms and can correctly classify bad electrodes with an average accuracy of 92 % was developed. This ensemble model was demonstrated as a feasible solution for real world fast-paced manufacturing environments.

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## Zinc electrode manufacturing quality control with machine learning: Using SMOTE & image augmentation to prevent overfitting

Lola Azoulay-Younes [a b c], Anesu Nyabadza [a b], Mercedes Vazquez [a b], Dermot Brabazon [b c]

Journal of Engineering Research Volume 13, Issue 4, Pages 3822-3832
Published December 2025
DOI: https://doi.org/10.1016/j.jer.2025.01.002

### Abstract

This study investigates machine learning-based quality control for ZnO electrode manufacturing via screen printing. Traditional machine learning models such as Random Forest (RF), XGBoost, Support Vector Machine (SVM), and Logistic Regression (LR), known for their speed, are rarely used for image-based machine learning since they are designed for numerical and categorical data. Here, images of ZnO electrodes were converted to numerical form via feature extraction using filters, allowing these models to achieve competitive accuracy and recall values of up to 96 % and 95 %, respectively. Images were labeled according to conductivity tests and print quality analysis via optical microscopy and visual inspection. The initial dataset, which contained 356 “bad” and 100 “good” electrode images, was balanced using Synthetic Minority Over-sampling Technique and image augmentation to reduce overfitting. The best performing model was the RF due to its highest testing accuracy (0.96), F1 score (0.96), and low overfitting. The worst model was LR due to its lowest testing accuracy (0.85) and F1 score (0.81), despite being the fastest model. The RF model balanced performance (accuracy of 96 %) and speed, classifying 100 images in under 2 ms.

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# University of Galway Chemistry Research Publications June-December 2025

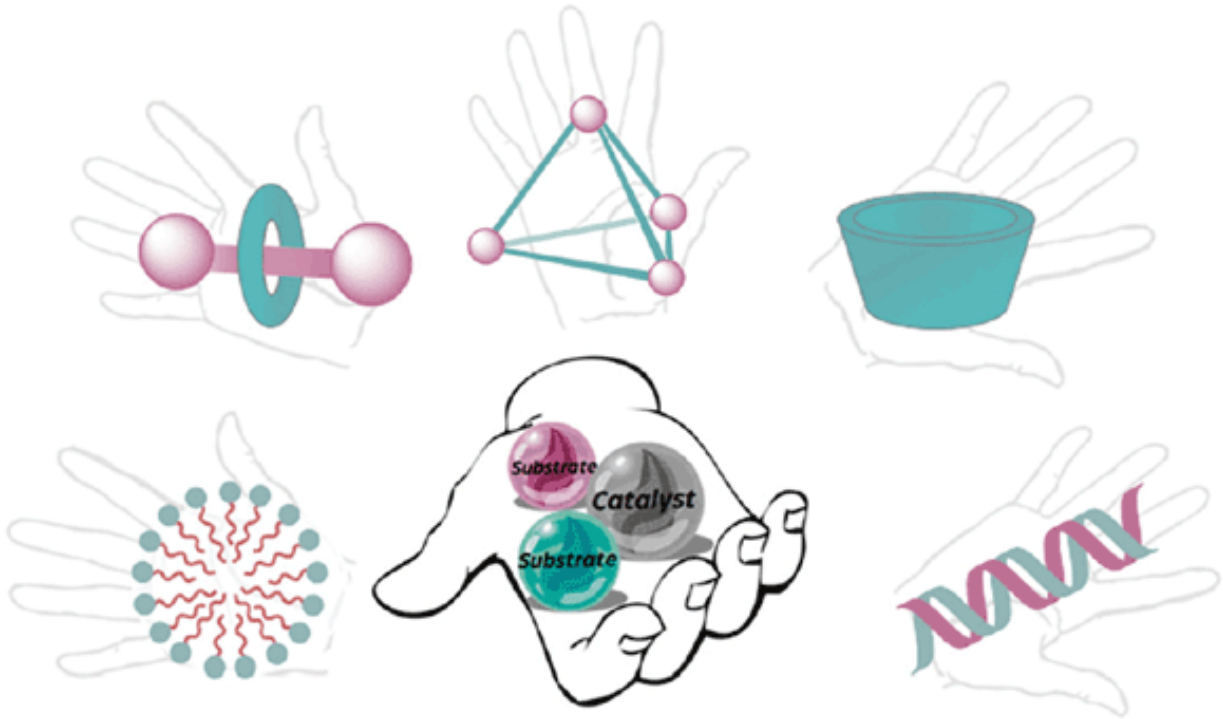
## Supramolecular Chemistry: An Enabling Tool for Asymmetric Catalysis

Laura Cunningham*
**Synlett** 2025; 36(09): 1189-1200
Published 2025 (19 Feb)
DOI: DOI: 10.1055/a-2513-2141 (Subscription)

### Abstract

Asymmetric synthesis and supramolecular chemistry are cornerstones of modern organic chemistry. The combination of both fields to develop new approaches to enantioselective catalysis has gained considerable momentum in recent years. Herein, we highlight some of the advantages offered by various supramolecular architectures over conventional chiral catalysts and reflect on obstacles that currently limit widespread use of supramolecular tools in asymmetric synthesis.

### Graphical Abstract




Dedicated to the memory and achievements of the late Prof. Dervilla M. X. Donnelly, a trailblazer of Irish chemistry

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## Structural determination of MCOFs: status, challenges and perspectives

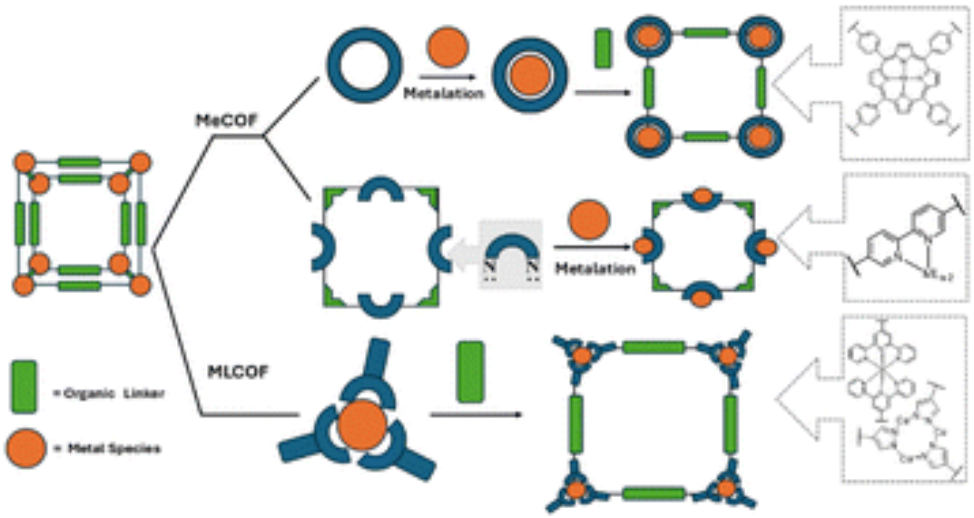
A. Boran, R. González-Gómez, S. Hennessey, P. Farràs
***Chem. Sci.***, 2025,**16**, 12227-12241
Published 24 June 2025
DOI: https://doi.org/10.1039/D5SC03670D

### Abstract

Porous materials have many promising characteristics, including tuneable chemical and optical properties, modifiable porosities and large surface areas. Long-range order frameworks have effective evaluation methods as a result of their crystallinities and in this context, nanoscale analysis, namely single-crystal X-ray

diffraction, is a particularly useful approach for optimising the structure–property relationships. Metal–covalent organic frameworks (MCOFs), synthesised by incorporating a metal complex into a stable covalent organic framework (COF) backbone, have shown considerable promise for a variety of applications. Nonetheless, their wide-scale implementation remains hindered due to difficulties in structurally mapping them; their typically reduced crystallinities result in major challenges for their structural determination. By classifying MCOFs as metalated COFs (MeCOFs) and metalloligand COFs (MLCOFs), the characterisation of these lower crystallinity frameworks can be carried out according to their distinctive architecture using a combination of complementary structural analysis techniques. This perspective highlights examples of a synergistic approach to the structural elucidation of MLCOFs to overcome obstacles related to their crystalline nature, generating an atomic map through a combination of nano and macroscale characterisation procedures supported by theoretical modelling tools. The effective use of structural characterisation methods is considered in this perspective, which can reveal key information regarding the structure–activity relationships as they relate to MLCOFs.

## Graphical Abstract

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## Functionalizing Injectable Hydrogels with Cobalt-Based Metallacarboranes for Targeted Delivery in Triple-Negative Breast Cancer

Neville Murphy, Roberto González-Gómez, Nivethitha Ashok, Enda O'Connell, Howard Fearnhead, William J. Tipping, Karen Faulds, Wenming Tong, Abhay Pandit, Róisín M. Dwyer, Duncan Graham, Pau Farràs*

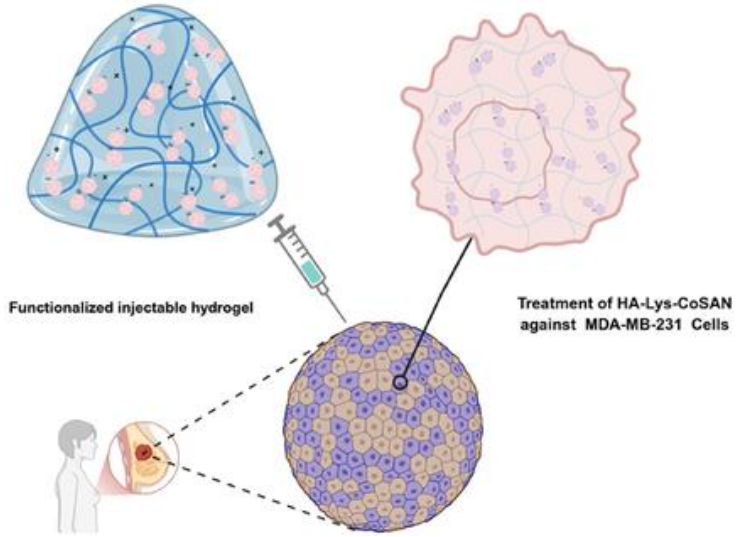
**ChemBioChem** Volume 26, Issue 21 e202500589
Published 8 November, 2025

### Abstract

Cobalt-based metallacarboranes have emerged as potential candidates for cancer treatment owing to their unique structural properties. In this study, a biocompatible delivery platform is developed by noncovalently incorporating cobalt metallacarborane (CoSAN) into hyaluronic acid (HA) functionalized with lysine (Lys). HA-Lys **2** enables the electrostatic interaction of CoSAN while retaining its cytotoxic activity, as confirmed by cellular assays using MDA-MB-231 triple-negative breast cancer cells. Elemental mapping via energy-dispersive X-ray spectroscopy (EDX) confirms the successful and homogeneous incorporation of CoSAN to lead HA-Lys-CoSAN **3**, and the composite is further characterized using diffusion-ordered nuclear magnetic resonance (NMR) spectroscopy (DOSY). Stimulated Raman scattering (SRS) microscopy data demonstrate comparable cellular uptake in MDA-MB-231 cells of free and HA-loaded CoSAN. Additionally, release studies under physiologically relevant conditions show a sustained release profile over 24 h with pH dependency to mimic normal and tumor microenvironments. The present study describes a viable method for integrating metallacarboranes into a polymeric drug delivery system without compromising their anticancer properties, thereby advancing their potential for future therapeutic use.

## Graphical Abstract

This study reports a biocompatible HA–lysine hydrogel loaded with cobalt metallacarborane (CoSAN) for targeted release into triple-negative breast cancer cells. The system maintains CoSAN cytotoxicity, as confirmed by cell assays and imaging, representing an attractive approach toward a localised TNBC treatment.

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## Circumventing Radical Generation on Fe–V Atomic Pair Catalyst for Robust Oxygen Reduction and Zinc–Air Batteries

Lan Ran, Yichen Zhang, Dr. Wenming Tong, Long Chen, Dr. Maoyu Wang, Prof. Hua Zhou, Dr. Pau Farràs*, Dr. Shanyong Chen*, Prof. Xiaoqing Qiu*

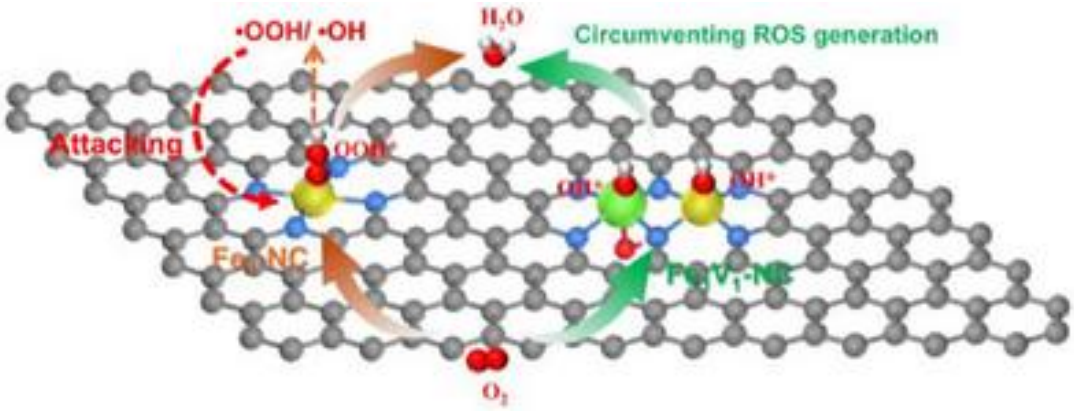
**Angewandte Chemie** Volume64, Issue45 November 3, 2025 e202514542
First Published 4 Sep 2025
DOI: https://doi.org/10.1002/anie.202514542

### Abstract

Iron–nitrogen–carbon (Fe–N–C) catalysts are considered the most active platinum-free alternative for oxygen reduction reaction (ORR), yet the generated reactive oxygen species (ROS) from general mechanistic pathway rapidly impair the ORR activity and stability of Fe–N–C. Herein, we establish and report an ORR pathway-switching strategy to circumvent ROS generation and fundamentally improve the activity and stability of Fe–N–C via DFT guided catalyst design. The constructed Fe–V atomic pair catalyst ($Fe_1V_1$-NC) with $N_2Fe$-$N_2$-$VN_2$ configuration enables side-on adsorption of $O_2$ and subsequent direct-breaking of the O═O bond to form O*, thereby avoiding the formation of ROS radicals. Importantly, there is intersite electron interaction between $FeN_4$ and $VN_4$, which further boosts the ORR activity. Consequently, $Fe_1V_1$-NC exhibits outstanding ORR activity with onset and half-wave ($E_{1/2}$) potentials at 1.02 and 0.89 V versus RHE, respectively, in 0.1 M KOH. Record-high stability is achieved on $Fe_1V_1$-NC with a minimal decay in $E_{1/2}$ by 16 mV over 50000 cycles, surpassing Fe–N–C counterpart and most of the catalysts reported to date. The $Fe_1V_1$-NC-based zinc-air battery reported here demonstrates exceptional durability up to 400 h at 10 $mA \cdot cm^{-2}$. This work identifies the intrinsic correlation between ORR pathway, activity, and stability, advancing development of stable catalytic systems.

## Graphical Abstract

The designed Fe–V atomic pair catalyst ($Fe_1V_1$-NC) proceeds via direct O═O breaking pathway and thus circumvents the ROS radical generations, fundamentally enhancing ORR stability for perdurable zinc–air batteries.

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## An experimental and kinetic modeling study of ethyl tert-butyl ether. Part I: High temperature pyrolysis and oxidation chemistry

Jiaxin Liu [a 1], Jin-Tao Chen [a 1], Maryam Khan-Ghauri [b], Joseph E. Jacobs [b], Claire M. Grégoire [b], Olivier Mathieu [b], Eric L. Petersen [b], Peter K. Senecal [c], Chong-Wen Zhou [a], Henry J. Curran [a]*

**Combustion and Flame** Volume 281, November 2025, 114394
Published Nov 2025
DOI: https://doi.org/10.1016/j.combustflame.2025.114394

### Abstract

A comprehensive experimental and kinetic modeling study of the combustion of ethyl *tert*-butyl ether (ETBE) is conducted over a wide range of engine-relevant conditions. Part I focuses exclusively on the high-temperature chemistry including relevant experimental pyrolysis and high-temperature oxidative validation targets. Part II focuses on the low- to intermediate temperature chemistry of ETBE and uses ignition delay times to validate the mechanism. CO time-history profiles from highly-diluted ETBE pyrolysis are measured behind reflected shock waves with a spectroscopic laser diagnostic in the 1235–1528 K temperature range near atmospheric pressure. Laminar flame speed (LFS) measurements of ETBE oxidation in air are conducted at 1 and 3 atm in the equivalence ratio range of 0.7–1.6. Reaction classes involving unimolecular decomposition, hydrogen atom abstraction, fuel radical $\beta$-scission and isomerization reactions are included to describe the high-temperature chemistry using the GalwayMech1.0 core $C_0$–$C_4$ chemistry. Sensitivity analyses reveal that the rate constant of the elimination reaction ETBE ⇌ $IC_4H_8$ + $C_2H_5OH$ is very important to species profile predictions, followed by the two C–O bond breaking channels. Hence, pressure- and temperature-dependent rate constants for the two alcohol elimination channels: (a) ETBE ⇌ $IC_4H_8$ + $C_2H_5OH$ and (b) ETBE ⇌ $TC_4H_9OH$ + $C_2H_4$ were calculated using quantum chemistry. Similarly, the C–O bond $\beta$-scission reaction of ETBE radical, ETBE-S ⇌ $T\dot{C}_4H_9$ + $CH_3CHO$ was also calculated in this study. The LFS predictions are dominated by the $C_0$–$C_2$ core chemistry with the fuel chemistry not appearing to be sensitive.

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## A focus on the first-stage ignition of n-pentane

Pengzhi Wang [a], Jesus Caravaca-Vilchez [b], Tibor Nagy [c], Shijun Dong [d]*, Xiaobei Cheng [d], Karl Alexander Heufer [b], Henry J. Curran [a]

**Combustion and Flame** Volume 277, July 2025, 114207
Published July 2025
DOI: https://doi.org/10.1016/j.combustflame.2025.114207

### Abstract

It is important to investigate the first-stage ignition of alkane fuels as it is responsible for the cool flame heat release in combustors, particularly engines. In the present study, a new set of ignition delay time (IDT) data of *n*-pentane is measured in a rapid compression machine (RCM) at $\varphi$ = 1.0, $p$ = 30 atm, and $T$ = 685–994 K. Moreover, the species concentration profiles of major intermediate species, including alkenes, cyclic ethers,

and aldehydes are measured in an RCM at a two-stage ignition condition ($T$ = 730 K) using an updated 2 × fast-acting-valves sampling system. A new kinetic model has been developed to simulate this data. Both the core chemistry and thermochemistry of the low-temperature species associated with *n*-pentane have been systematically updated. It is found that updating the $H\dot{O}_2 + H\dot{O}_2$ reaction, which leadstwo ȮH radicals and $O_2$, has no obvious influence on the 1st-stage ignition but significantly affects the prediction of the total IDT. This is because ȮH radicals are mainly produced from the formation and consumption of carbonyl-hydroperoxide species before the 1st-stage ignition; $H\dot{O}_2$ radical recombination and the reaction $H_2O_2$ (+M) ↔ ȮH + ȮH (+M) become the main source of ȮH radical production only at/after the 1st-stage ignition. The updated thermochemistry data inhibit both the 1st-stage and total IDTs due to the shift towards reactant in the equilibrium of the $R\dot{O}_2 \rightleftharpoons$ OOH reaction. The key reactions involved in the low-temperature chemistry are optimized using the Optima++ code within the uncertainty limits of reviewed rate constants in the literature. The present model can predict the experimentally measured data well and shows an improvement compared to previous models.

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## Development of flexible nanoporous gold electrodes for the detection of glucose

Denise Demurtas [a], Julia Alvarez-Malmagro [a], Arvind Rathore [b], Tanushree Mandal [c], Andrés Felipe Quintero- Jaime [a],
Serguei Belochapkine [a], Anna Lielpetere [d], Kavita Jayakumar [c], Dónal Leech [c], Wolfgang Schuhmann [d], Nicolas Mano [e], Claudine Boiziau [b], Edmond Magner [a]

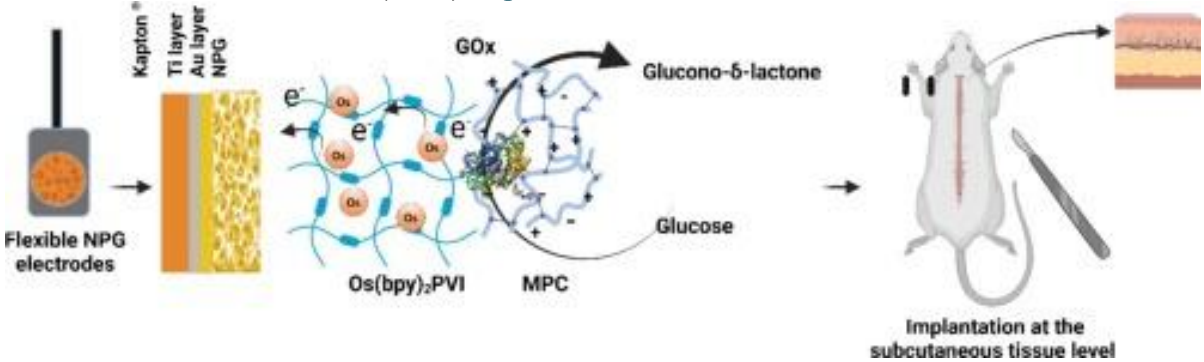
**Bioelectrochemistry** Volume 165, October 2025, 108949
Published Oct 2025
DOI: https://doi.org/10.1016/j.bioelechem.2025.108949

### Abstract

The development of implantable glucose sensors is of significant interest in the management of diabetes. This work focuses on developing an implantable, biocompatible nanoporous gold electrode prototype based on Kapton® for the subcutaneous detection of glucose. The electrodes were first modified with a layer containing glucose oxidase and Os(2,2′-bipyridine)$_2$Cl·PVI (Os(bpy)$_2$Cl PVI). An additional polymeric layer *co*ntaining poly(2-methacryloyloxyethyl phosphorylcholine-co-glycidyl methacrylate) was then added to reduce biofouling and foreign body reaction effects. The modified electrode had a $V_{MAX}$ of 211 ± 13 μA cm$^{-2}$ and a $K_{Mapp}$ of 6.1 ± 0.8 mM in pseudo physiological conditions, with a linear detection range from 1 to 4 mM and a sensitivity of 28.6 ± 2.1 μA cm$^{-2}$ mM$^{-1}$. In artificial plasma, the response of the sensor was saturated at 3 mM, with a $V_{MAX}$ of 113 ± 10 μA cm$^{-2}$ and a $K_{Mapp}$ of 2.1 ± 0.4 mM with a linear detection range from 1 to 2.5 mM and a sensitivity of 14.6 ± 3.3 μA cm$^{-2}$ mM$^{-1}$. Mechanical stress testing demonstrated that there was a 40 % reduction of the redox polymer coverage after 320 deformation events, however the catalytic activity was still detectable after 160 events. Minimal cytotoxicity effects of the electrodes were observed. When subcutaneously implanted the electrodes showed fairly good mechanical stability after one week and detachment of the metallic layer on some electrodes after 21 days, probably due to electrode bending. A limited foreign body reaction was observed. These results indicated that the electrodes could be implanted for a period of up to 1 week.

### Graphical Abstract

Created in BioRender. Demurtas, D. (2024) https://BioRender.com/h71x011



## Synthesis of an N-Galactosyl Norbornane Aziridine and its Potent Mixed Inhibition of Aspergillus oryzae β-Galactosidase

Aaron McCormack, Ronan Gavin, Mikael Bols*, Paul V. Murphy*

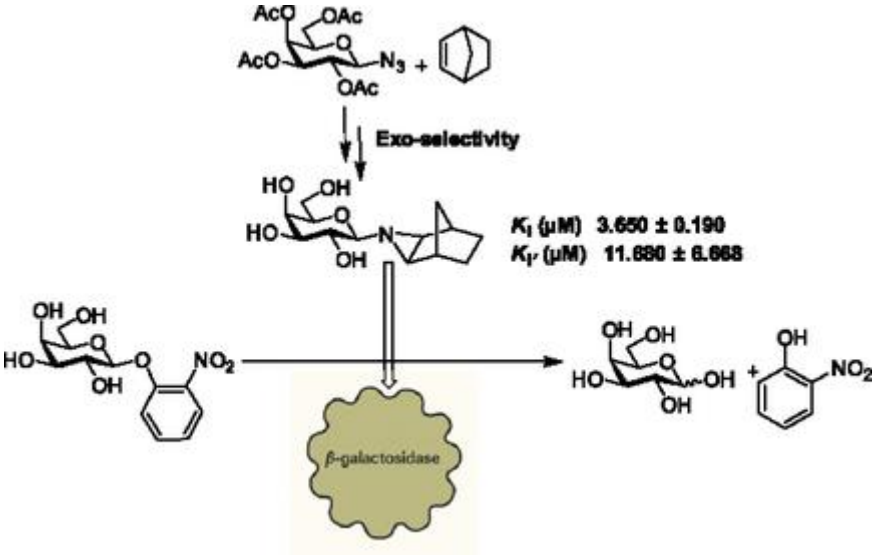
**ChemBioChem** Volume 26, Issue 23 November 27, 2025 e202500623
Published 27 Nov 2025
DOI: https://doi.org/10.1002/cbic.202500623

### Abstract

Aziridine-bearing cyclic polyols are established as irreversible covalent inhibitors of glycosyl hydrolases and have been employed as activity-based probes. In the present study, the stereoselective synthesis of a novel *N*-galactosyl aziridine derivative on a norbornane scaffold and its subsequent evaluation as an inhibitor of glycosyl hydrolase activity are described. The diastereoselective Huisgen cycloaddition between 2,3,4,6-tetra-*O*-acetyl-β-d-galactopyranosyl azide and norbornene yields *exo*-triazoline intermediates of norbornane. Following the removal of the acetyl protecting groups and a silica gel-mediated decomposition of the triazoline intermediates, *exo N*-galactopyranosyl norbornane aziridine (*N*-(β-d-galactopyranosyl)-*exo*-3-azatricyclo[3.2.1.$0^{2,4}$]octane, NGNA) is obtained. Enzymatic assays demonstrate that NGNA exerts potent mixed-mode inhibition of *Aspergillus oryzae* β-galactosidase, while exhibiting significant selectivity over green coffee bean α-galactosidase.

### Graphical Abstract

An *N*-galactosyl aziridine is found to have μM range mixed inhibition constants ($K_i$ and $K_i$') for a fungal β-galactosidase.

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## Disrupting membranes, controlling cell fate: the role of pore-forming proteins in cell death and therapy

Sonia Iranpour, Maryam Arif, Eva Szegezdi*

**Apoptosis** Volume 30, pages 1961–1988, (2025)
Published 21 July 2025
DOI: https://doi.org/10.1007/s10495-025-02133-w

### Abstract

Pore-forming proteins (PFPs), characterized by their ability to form pores or disrupt membranes are now recognized as key executioners of cell death, either as effectors of the immune system (non-cell-autonomous function), or of regulated cell death programs (cell autonomous function). To perforate membranes, most PFPs transition from water-soluble monomers or oligomers into multimeric and often supramolecular complexes, a process achieved via substantial structural transition of the PFP. Although they share the general ability to perforate cellular or intracellular membranes, PFPs differ in their membrane-binding preferences, the structural and functional characteristics of the pores they form (such as pore size, pore structure and ability to trigger membrane rupture) and the cell death mechanism they induce or execute.

Herein, we review the specific traits of all key human PFPs, including their membrane specificity, regulation of their activity and the structure of the membrane pores they form, followed by insights into the therapeutic potential of PFPs and harnessing their abilities for cancer therapy.

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## Specific and non-specific interactions of fibronectin with zwitterionic peptoid brushes studied by molecular dynamics simulation

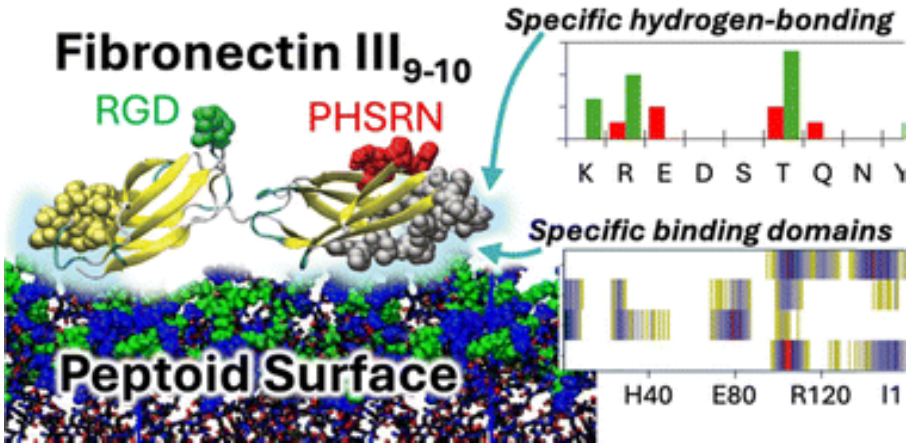
David L. Cheung, *[a] Phillip B. Messersmith [bcd] and King Hang Aaron Lau *[e]

***Phys. Chem. Chem. Phys.***, 2025,**27**, 25116-25126
Published 5 Nov 2025
DOI: https://doi.org/10.1039/D5CP02324F

### Abstract

Zwitterionic polymer brushes represent a prominent class of surfaces to prevent non-specific protein interactions. However, residual protein binding and cell attachment can still be observed. Peptide-mimetic "peptoids" constitute a versatile sequence-specific platform for developing specific protein binding motifs as well as antifouling brushes. Nonetheless, molecular level insight into their protein interactions is generally lacking. Using atomistic molecular dynamics (MD) simulation, we analyse the interactions of fibronectin type-III (FnIII) 9- and 10-domains with a zwitterionic peptoid brush and compare it with polysarcosine, the well-known and uncharged elementary peptoid and potential PEG replacement. Experimental protein adsorption trends are used to determine the peptoid chain densities simulated. For each combination of peptoid and chain density, 9 independent simulations with different starting protein orientations are performed. The simulation results are consistent with experimental measurements over different chain densities, and they identified $FnIII_{9\text{-}10}$ regions and specific amino acids with typical involvement in interactions with polysarcosine and the zwitterionic variant. Moreover, stronger interactions are seen for the zwitterionic peptoid design, and the protein's integrin binding motifs face away from the surface, nearly opposite in direction to the sequence segments interacting with the peptoids. These observations give new insight into protein–peptoid interactions and suggest the possibility of designing peptoid sequences for presenting cell-binding protein motifs and mediating cell attachment.

### Graphical Abstract




## Protein Recognition and Assembly by a Phosphocavitand

Colin P. Wren, Ronan J. Flood, Niamh M. Mockler, Martin Savko, Maura Malinska, Qiang Shi, Peter B. Crowley*

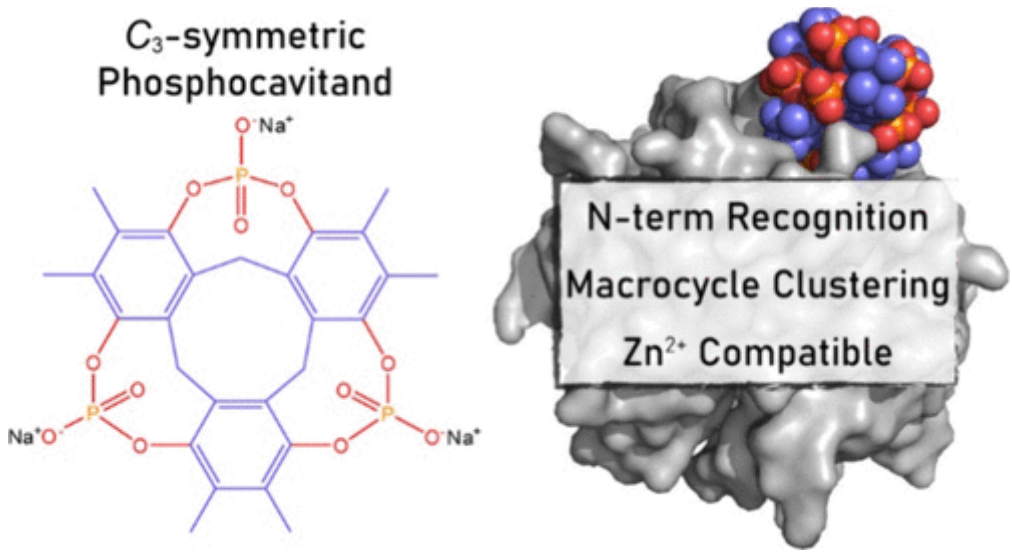
***J. Am. Chem. Soc***. 2025, 147, 31, 28107–28116
Published 22 July 2025
DOI: https://doi.org/10.1021/jacs.5c08121

### Abstract

Controlled protein assembly is an enabling technology, in particular, for biomaterials fabrication. Here, we report protein recognition and assembly by a phosphate-containing macrocycle (**pctx**). We show that the $C_3$-symmetric phosphocavitand is a versatile receptor for N-terminal residues or arginine but not lysine. Using atomic resolution X-ray diffraction data, we reveal the precise details of N-terminal complexation in the β-

propeller protein *Ralstonia solanacearum* lectin (RSL). In some cocrystal structures, a tetrahedral cluster of the phosphocavitand occupies one end of the β-propeller fold, providing a node for protein assembly. The macrocycle cluster is compatible with different types of precipitants, a broad pH range, and zinc complexation. We demonstrate system control with an arginine-enriched RSL that alters the overall assembly due to selective arginine complexation by **pctx**. A lysozyme–**pctx** cocrystal structure also demonstrates arginine complexation by the macrocycle. An alternative macrocycle cluster occurs with an engineered RSL bearing an extended N-terminus. In this structure, involving zinc ligation at the N-terminus, the macrocycle forms trimeric clusters and four such clusters form cage-like substructures within the tetrahedral protein framework. Thus, N-terminal complexation in combination with phosphocavitand self-assembly provides new routes to protein crystal engineering.

## Graphical Abstract

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## Probing the Adsorption of Fibronectin onto Model Biomaterial Surfaces using Molecular Dynamics Simulations

Viswanath Vittaladevaram, David Cheung

**ChemRxiv** Jul 28, 2025 Version 1
Published 28 Jul 2025
DOI: https://doi.org/10.26434/chemrxiv-2025-w3x3w

## Abstract

Fibronectin is a versatile extracellular matrix glycoprotein, which fulfils many roles in cell adhesion and growth. Adsorption of fibronectin on biomaterial surfaces can influence the eventual biological fate of implanted medical devices or be used in to modify the biological activity of surfaces. Understanding the behaviour of fibronectin on surfaces relies on knowledge of its conformation and orientation of fibronectin and how this is affected by surface chemistry. Using atomistic molecular dynamics simulations, the behaviour of type-III fibronectin fragments, containing heparin binding sites, is investigated on models of biomaterial surfaces. Stronger adsorption is seen on the more hydrophobic ethyl acrylate terminated surface compared to a surface terminated with methyl acrylate groups. This shows that minor changes to the surface chemistry can lead to significant changes to protein behaviour, with the removal of a methyl group from the surface significantly reducing the tendency for protein adsorption. Even for the more hydrophobic surface, polar and charged residues were involved in surface adsorption, potentially due to favourable interactions with acrylate groups in the surface. This new information may be used to improve the design of biomaterials with tailored interactions with proteins.

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## An Oxygen-Insensitive Electrochemical Biosensor for l-Lactate Using a Novel Flavin Mononucleotide-Dependent Lactate Dehydrogenase

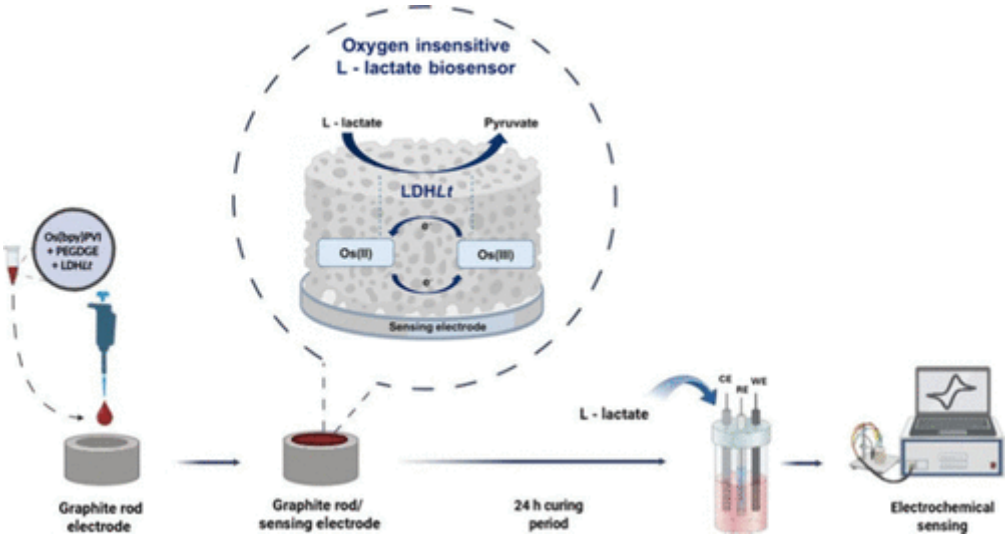
Reshma Kidayaveettil, Christopher Schulz, Alfons K. G. Felice, Leander Suetzl, Dónal Leech*

***ACS Electrochem.*** 2025, 1, 10, 2209–2216
Published 22 Aug 2025
DOI: https://doi.org/10.1021/acselectrochem.5c00247

### Abstract

Accurate and rapid quantification of l-lactate is essential in clinical diagnostics, bioprocess monitoring, and food quality control. Electrochemical biosensors are well suited for sensing due to their scalability, rapid response, and high sensitivity. Among these, mediated electron transfer-based enzymatic sensors offer distinct advantages by employing redox mediators to facilitate efficient electron exchange between enzymes and electrode surfaces, thereby overcoming the limitations of direct electron transfer. Despite these advantages, deployment of traditional lactate detecting enzyme systems, such as oxygen-dependent lactate oxidase (LOx) and $NAD^+$-dependent lactate dehydrogenases (LDHs) is hindered by oxygen interference, cofactor instability, and complex assay conditions. To address these challenges, we report the development of an oxygen-insensitive l-lactate biosensor incorporating a novel flavin mononucleotide (FMN)-dependent LDH (LactaZyme Type LDH*Lt*) immobilized within an osmium redox polymer matrix as mediator. This biosensor is unaffected by the presence of oxygen, with a signal loss of 2.1 ± 2.9 % for 5 mM l-lactate when changing from nitrogen sparging to oxygen sparging, whereas LOx-modified electrodes show a loss of 25 ± 13 % under the same conditions. The LDH*Lt* biosensor also exhibits an enhanced electrocatalytic performance over the LOx biosensor, with a sensitivity of 0.16 ± 0.01 mA $cm^{-2}$ $mM^{-1}$ and a maximum current density of 2.15 ± 0.07 mA $cm^{-2}$. Notably, it also maintains reliable operation across a broad pH and temperature range. These results establish the LDH*Lt*-based biosensor as a robust and practical platform for l-lactate detection in complex sample matrices.

### Graphical Abstract




## First Crystal Structure of an Aspartame Cocrystal

Nazanin Fereidouni, Marwah Aljohani, Andrea Erxleben*

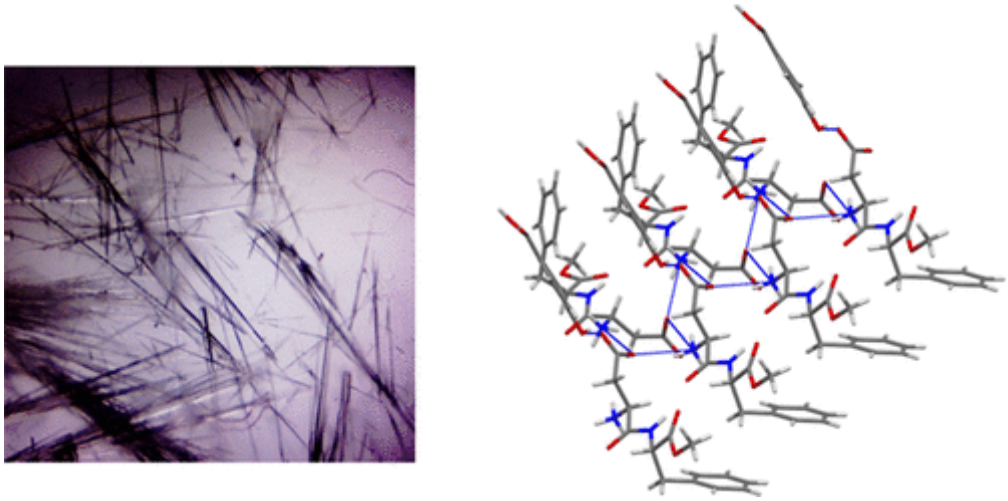
***Cryst. Growth Des.*** 2025, 25, 15, 5954–5959
Published 29 July
DOI: https://doi.org/10.1021/acs.cgd.5c00373

### Abstract

Aspartame crystallizes as very long, thin needles. The crystallization behavior of extreme needle formers not only causes problems in industrial processing and handling but is also of interest in fundamental research. Cocrystallization is a popular approach to expand the solid-state landscape of a compound and often leads to improved physicochemical properties such as stability, dissolution behavior, particle size, and morphology.

No crystal structure of an aspartame cocrystal has been reported in the literature up to now. In this work, a comprehensive screening study for aspartame cocrystals was performed. Cocrystals with fumaric acid and 4-hydroxybenzoic acid were detected by powder X-ray diffraction analysis. Growing X-ray suitable cocrystals, however, proved extremely difficult, as both cocrystals, like aspartame, crystallized as very fine needles. Nevertheless, in the case of 4-hydroxybenzoic acid, crystals of sufficient quality for single-crystal X-ray analysis could be grown, and the first crystal structure of an aspartame cocrystal is reported. In the cocrystal aspartame·4-hydroxybenzoic acid dihydrate (**1**), the coformer forms the OH···$^{-}$OOC synthon with aspartame. The aspartame zwitterions in **1** are connected through charge-assisted $NH_3^{+}$···$^{-}$OOC hydrogen bonds into a spiral along a $2_1$ screw axis, the same structural feature that drives the needle growth of aspartame and that seems to be the reason why the isolation of X-ray-quality cocrystals of aspartame is so challenging.

## Graphical Abstract



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## Screening the Irish Marine Biorepository Identifies a New Bryostatin Analog as Potent Inhibitor of Activated B-Cells Diffuse Large B-Cell Lymphom

Laurence K. Jennings, Filippo Spriano, Maggie M. Reddy, Luciano Cascione, Elisa Civanelli, Andrea Rinaldi, Francesco Bertoni,* and Olivier P. Thomas*

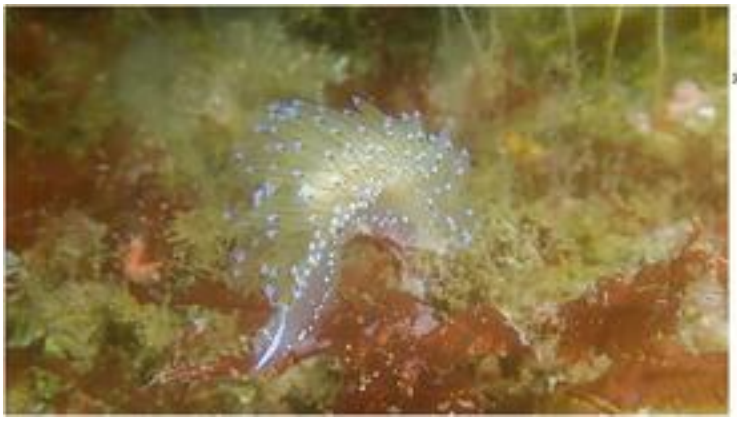
**ChemBioChem** Volume 26, Issue 19 October 3, 2025 e202500500
First Published 11 Sep 2025
DOI: https://doi.org/10.1002/cbic.202500500

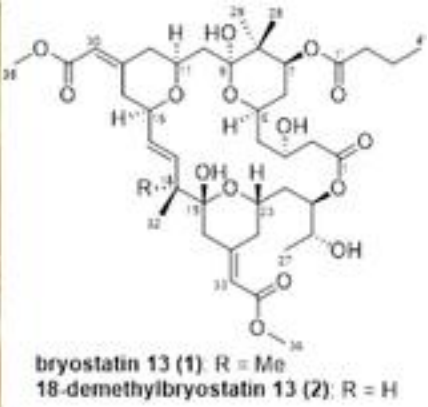
## Abstract

Activated B-cell diffuse large B-cell lymphoma (ABC-DLBCL) is an aggressive cancer with poor response to standard chemotherapy. In search of new therapeutic leads, a library of 435 fractions prepared from the Irish marine biorepository was screened against 2 ABC-DLBCL cell lines (TMD8 and OCI-Ly10) and a non-cancerous control cell line (CB33). Active fractions are prioritized based on potency and selectivity. Among them, fractions from the nudibranch *Antiopella cristata* and the ascidian *Diplosoma listerianum* exhibit the most potent and selective cytotoxicity. Bioassay-guided fractionation of *D. listerianum* led to the identification of the known loliolide and epiloliolide. On the other hand, *A. cristata* yielded several bryostatin analogs, including bryostatin 13 and a new natural product, its 18-demethylated analog. Both compounds demonstrated nanomolar cytotoxicity against ABC-DLBCL cell lines with minimal activity in CB33. Transcriptomic profiling showed significant gene expression changes, particularly for the 18-demethylated analog, implicating modulation of key signaling pathways. This study identifies *A. cristata* as a novel and highly enriched source of bioactive bryostatins and supports the dietary sequestration hypothesis in nudibranchs, highlighting the value of marine invertebrates as reservoirs of selective anticancer agents for drug discovery.

## Graphical Abstract

Bryostatin analogs are found to be accumulated in the nudibranch *Antiopella cristata* collected in Irish waters. These are found to be potent inhibitors of activated B-cells diffuse large B-cell lymphoma.





**bryostatin 13 (1)**: R = Me
**18-demethylbryostatin 13 (2)**: R = H

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