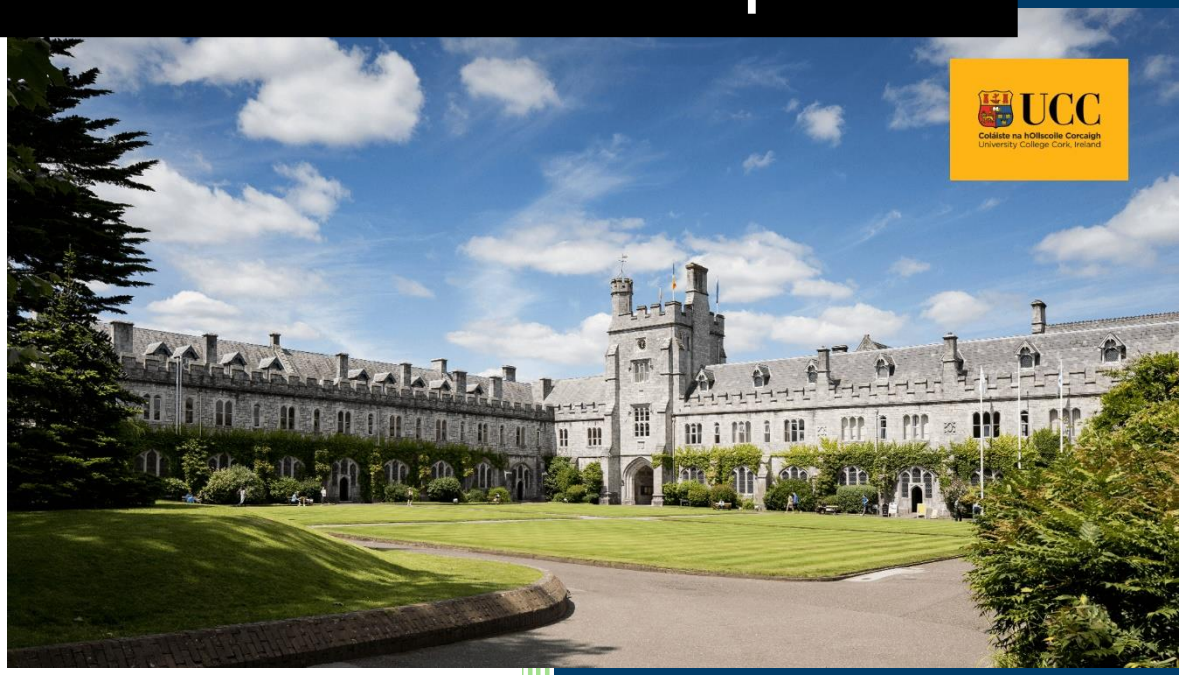
2026

77th Irish Universities Chemistry Research Colloquium



Institute of Chemistry of Ireland

School of Chemistry

University College Cork

23rd – 24th June 2026

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Best Oral Presentation Prizes

Category	Sponsor
Sustainable & Environmental Chemistry	Johnson & Johnson
Synthesis & Catalysis	Eli Lilly
Materials Chemistry	El-Cell
Medicinal Chemistry	APC/VLE Therapeutics
Analytical Chemistry	Pfizer

Best Poster Presentation Prizes

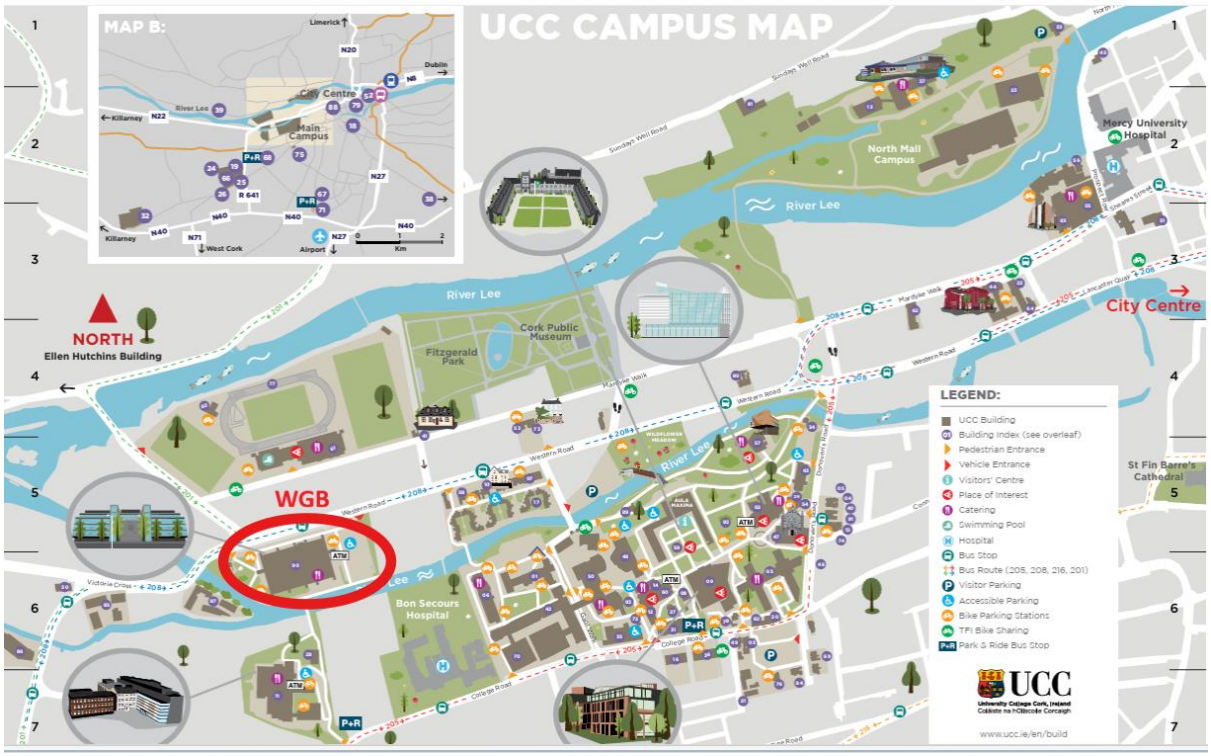
Category	Sponsor
Sustainable & Environmental Chemistry	Johnson & Johnson
Synthesis & Catalysis	Eli Lilly
Materials Chemistry	El-Cell
Medicinal Chemistry	Pfizer
Analytical Chemistry	Eurachem

Special Sponsor Prizes

Category	Sponsor
Overall Best Poster Presentation	Eli Lilly
Best Industry-Relevant Oral Presentation	APC/VLE Therapeutics
Highly Commended Analytical / Measurement Science Poster	Eurachem
Highly Commended Poster Presentation	Scientific Laboratory Supplies

Maps

The Colloquium will be held in the **Western Gateway Building** (marked **WGB**) below.



More detailed maps can be found here [Maps of the UCC Campus | University College Cork]

The social evening on Tuesday 23rd June will be held in **Deep South**, 51 Grand Parade, **T12 H677**.

Please note: If you are **under 23** years of age, please make sure you have **ID** and have given your name to the organisers.

77th Irish Universities Chemistry Research Colloquium

23rd - 24th June 2026, University College Cork

Western Gateway Building

Tuesday 23rd June		
09:30 – 10:15	**Registration** - main foyer Western Gateway Building	
Western Gateway Building (WGB) G05		
10:15 – 10:30	**Welcome** *Prof Anita Maguire, Head of School*	
10:30 – 11:15	**Plenary Speaker** ***Dr. Shelly Conroy,*** Associate Professor in Functional Thin Films & Microscopy, Imperial College London *"Chemistry at Charged Interfaces: Dynamics Driving Energy and Quantum Technologies"*	
11:15 – 11:45	**Coffee Break & Poster Set-up**	
	WGB G01	**WGB G03**
11:45 – 13:30	**Sustainable and Environ. Chemistry** *Chair: Prof James O'Sullivan, UCD* Christopher Kent (UCC) Rocco Villano (UCD) Praveen Kumar Selvam (UGAL) Amir Ben Brik (UCC) Daniel Molloy (UCD) Conor Dorney (UCC)	**Synthesis and Catalysis** *Chair: Dr Mary Deasy, TUD* Amy Twomey (UCC) Brian Durkan (RCSI) Ashwini Mishra (UCD) Fiona Kinsella (UCC) Aoibhínn Downes (UCD) Rebecca O'Keeffe (UCC)
13:30 – 14:15	**Lunch**	
	WGB G05	
14:15 – 15:00	**Plenary Speaker** ***Dr. Jessica Doherty,*** *Associate R&D Manager, Product Engineering, Stryker* "Stepping Stones; From Academia to Industry"	
	WGB G01	**WGB G03**
15:00 – 17:00	**Materials Chemistry** *Chair: Dr Nikolay Petkov, MTU* Yekaterina Tskhe (TCD) Amrutha Varshini Hariharan (UGAL) Kaynat Alvi (UCC) Aodhán Dugan (QUB) Marilia Dalla Benetta (MU) Christian Corcoran (MTU) Joseph Monahan (MU)	**Medicinal Chemistry** *Chair: Dr David Jones, UCC* Emily Hill (UL) Sebastian Pim (RCSI) Pei-Hsuan Wu (TUD) Aoife Cotter (UL) Andreea Cislaru (MU) Surangana Kashyap (QUB) Rebecca Lynn (DCU)
17:00 – 18:30	**Poster Session & Drinks Reception** - main foyer WGB	
19:30	**Social Evening - Deep South**	

77th Irish Universities Chemistry Research Colloquium

23rd - 24th June 2026, University College Cork

Western Gateway Building

Wednesday 24th June		
Western Gateway Building (WGB) G05		
09:00 – 09:45	**Science Communication Talk** ***Dr. Matthew Partridge**, Senior Enterprise Fellow and Director of Outreach in the School of Chemistry and Chemical Engineering at the University of Southampton* "The Why, the How, and the Cartoons of Science Communication"	
	WGB G01	**WGB G03**
09:45 – 10:40	**Medicinal Chemistry** *Chair: Dr Lorraine Bateman, UCC* Niamh Hickey (UL) Ciara McEvoy (MU) Karina Chan (RCSI)	**Synthesis and Catalysis** *Chair: Prof Declan Gilheany, UCD* Oana Popa (UCD) Éabha McMahon (UCC) Sarah Smoni Varghese (UCD)
10:40 – 11:00	**Coffee Break**	
	WGB G01	**WGB G03**
11:00 – 12:15	**Materials Chemistry** *Chair: Dr Brendan Bulfin, UCC* Martina Piletti (UCC) Niamh O'Shea (TCD) Muhammad Adnan (UL) Neil Curtis (UCC)	**Analytical Chemistry** *Chair: Dr Eoin McGillicuddy, TUD* Edel Whelton (UCC) Emily Harlin (MU) Devansh Shah (UCC) Md Rasel (UCC)
	WGB G05	
12:15 – 12:45	**ICI PG Awardees Lecture**	
12:45 – 13:15	**Prizegiving & Colloquium Closing Ceremony**	
14:00 – 14:30	**ICI Young Chemist Network AGM**	
14:30 – 15:00	**Keynote – Prof Denise Rooney** (Maynooth University)	
15:00 – 15:30	**Eli Lilly info session -** 24 month PhD Program	
15:30 – 16:00	**EDI Knowledge Quiz and Accessibility Audit Quiz**	
16:00 – 16:15	**Quiz Prizes**	

Oral Abstracts

Tuesday 23rd June

11:45 – 13:30 WGB G01

Sustainable and Environ. Chemistry

Chair: *Prof James O'Sullivan, UCD*

Christopher Kent (UCC)

ASSESSING NOVEL ELECTRODES FOR GREEN H2 PRODUCTION USING BROADBAND ACOUSTIC RESONANCE DISSOLUTION SPECTROSCOPY (BARDS) AND HIGH SPEED PHOTOGRAPHY

Rocco Villano (UCD)

ENHANCED MULTI-CARBON PRODUCTION VIA PULSED SYNGAS ELECTROREDUCTION ON AG DECORATED ZNO NANOPARTICLES

Praveen Kumar Selvam (UGAL)

HIGH ENTROPY METAL OXIDES AS ELECTROCATALYSTS FOR ALKALINE WATER SPLITTING

Amir Ben Brik (UCC)

PHOTOOXIDATION OF NAPHTHALENE–BENZENE MIXTURES: PRODUCT DISTRIBUTIONS AND SOA FORMATION ACROSS DIVERSE ATMOSPHERIC CONDITIONS

Daniel Molloy (UCD)

What To Do with Lightning in a Bottle: Non-Thermal Plasma for Treatment of Aqueous PFAS

Conor Dorney (UCC)

A LOW-COST CEAS SPECTROMETER FOR IN-SITU ROADSIDE NITROGEN DIOXIDE

ASSESSING NOVEL ELECTRODES FOR GREEN H_2 PRODUCTION USING BROADBAND ACOUSTIC RESONANCE DISSOLUTION SPECTROSCOPY (BARDS) AND HIGH SPEED PHOTOGRAPHY

Mr. Christopher Kent[1,2], Dr. Ailbe Ó Manacháin.[1,2,3], Prof. Colm O'Dwyer.[1,3], Dr Dara Fitzpatrick.[1,2]
Presenter email address: 116222725@umail.ucc.ie

[1]*School of Chemistry, The Kane building, University College Cork, Cork City, Ireland,*
[2]*Analytical and Biological Chemistry Research Facility, University College Cork, Cork City, Ireland,*
[3]*Enviromental Research Institute, Ellen Hutchins Building, Lee Road, University College Cork, Cork City, Ireland.*

Improving hydrogen production efficiency through electrochemical and photoelectrochemical (PEC) systems encompasses numerous parameters including electrolyte composition, electrode materials, surface coatings, and architectural design. The geometric shape of novel electrodes is a key parameter when optimizing hydrogen production from solar powered electrolysis for green hydrogen. The ability to minimize bubble retention on an electrode surface is a crucial factor in maximizing the available surface area for electrolysis to take place. Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS) coupled with high speed photography (HSP) can be used to assess critical bubble diameter at the point of detachment, for an array of different custom 3D printed architectures and materials. HSP is used with the aid of J image® and SPSS® software to measure bubble diameter on novel electrodes to identify the optimum configuration. Herein, we show that the optimum geometry to reduce bubble retention and maximize bubble production is "Octet big" architecture.[1] This finding allows for the design of more efficient hydrogen producing electrodes which enhance the output of photo electrochemical cells (PEC).

References

(1) Ferguson, M.; Lonergan, A.; Kent, C.; Fitzpatrick, D.; O'Dwyer, C. Hydrogen Evolution Reaction Bubble Traffic in Coated 3D-Printed Microlattice Electrodes. *ACS Electrochem.* **2026**, acselectrochem.6c00029. https://doi.org/10.1021/acselectrochem.6c00029.

ENHANCED MULTI-CARBON PRODUCTION VIA PULSED SYNGAS ELECTROREDUCTION ON AG DECORATED ZNO NANOPARTICLES

Rocco Villano[1], Saman Mutahir[1], Yuval Fishler[1], Jeannie Z. Y. Tan[2], Juan José Villora-Picó[3], Xuyun Guo[4], James A. Sullivan[1], Haresh Manyar[3], Valeria Nicolosi[4], Leila Negahdar[1]* email: rocco.villano@ucdconnect.ie

[1] School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland

[2] Research Centre for Carbon Solutions (RCCS), Heriot–Watt University, Edinburgh, UK

[3] School of Chemistry and Chemical Engineering, Queen's University Belfast

[4] Nanomaterials & Advanced Microscopy, School of Chemistry, CRANN, AMBER & I-Form, Trinity College Dublin 2, Dublin, Ireland

Sustainable multi-carbon production through syngas electroreduction is particularly attractive, as they offer significantly higher economic value and broader functional applications than single-carbon products.[1] In this study, Ag/ZnO nanoparticles were synthesized and characterized with high resolution Transmission Electron Microscopy (TEM) coupled with Electron Energy-Loss Spectroscopy (EELS) detector to confirm the nanoparticles size in the 10 nm range. The electrocatalytic activity of Ag/ZnO nanoparticles was enhanced by the effective electron transfer between ZnO and Ag, promoting the multi-carbon Faradaic efficiency (FE) from (8 ± 1) % for ZnO to (17 ± 3) % for ZnAg1.5 over 10 minutes of chronopotentiometry. Operando diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and X-ray photoelectron spectroscopy (XPS) directly linked this enhancement to dynamic surface chemistry, revealing ZnO as the primary active site. Both techniques also suggested that surface- H_2O/OH^- can act as catalyst deactivators, leading to catalyst dissolution. Based on these insights the potential was pulsed between 0.82 and -0.63 V vs RHE to regenerate active sites. This increased FE to (54 ± 5) % with (37 ± 2) % selectivity towards ethanol. Together, these results demonstrate that rational interface design combined with dynamic potential modulation offers a powerful strategy for advancing syngas to multi-carbon electrocatalysis.[2]

References

[1] Du, H.; Fu, J.; Liu, L.-X.; Ding, S.; Lyu, Z.; Chang, Y.-C.; Jin, X.; Kengara, F. O.; Song, B.; Min, Q.; et al. Recent progress in electrochemical reduction of carbon monoxide toward multi-carbon products. *Mater. Today* **2022**, *59*, 182–199. DOI: 10.1016/j.mattod.2022.08.012.

[2] Villano, R.; Mutahir, S.; Fishler, Y.; Tan, J. Z. Y.; Villora-Picó, J. J.; Guo, X.; Sullivan, J. A.; Manyar, H. G.; Nicolosi, V.; Negahdar, L. Enhanced Multicarbon Production via Pulsed Syngas Electroreduction on Ag-Decorated ZnO Nanoparticles. *ACS Appl. Energy Mater.* **2026**, *9*, 4330–4342. https://doi.org/10.1021/acsaem.6c00220

HIGH ENTROPY METAL OXIDES AS ELECTROCATALYSTS FOR ALKALINE WATER SPLITTING

Praveen Kumar Selvam[1], Muhammad Sohail Riaz[1], Pau Farras Costa[1]
Presenter email address: p.kumars1@universityofgalway.ie

[1]*School of Biological and Chemical Sciences, University of Galway, Ireland*

Electrolysis of water to produce green hydrogen (GH_2) driven by renewable energy resources is one of the most attractive pathways toward a sustainable and renewable energy economy, as it significantly reduces the overall CO_2 emissions. Among the low-temperature water electrolysis technologies, anion exchange membrane water electrolysis (AEMWE) is considered the most promising due to its potential for high efficiency and low cost in GH_2 production. Fundamentally, water electrolysis systems involve two half-cell reactions, namely the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER), which occur at the cathode and anode, respectively. Earth-abundant transition-metal electrocatalysts and their synergistic effects with multiple elements in reaction intermediates play an essential role in the reaction mechanism, and their catalytic performance at both HER and OER sites can achieve the industrially required targets[1]. According to the literature, high-entropy transition metals oxides are the best alternatives to noble catalysts, as they reduce the system's capital expenditure. Moreover, the nanostructures of these electrocatalysts provide more active sites, thereby enhancing catalytic performance due to their increased surface-to-volume ratio[2]. Here, we report high entropy metal oxide (HEMO) nanoparticles as electrocatalysts for OER in AEMWE. Further, the electrochemical studies of the synthesized electrocatalysts were obtained in 1 M KOH and showed that FeCrMnCoTiOx achieved low overpotential of 329 mV at 10 mA cm^{-2}.

References

(1) Tong, W.; Forster, M.; Dionigi, F.; Dresp, S.; Sadeghi Erami, R.; Strasser, P.; Cowan, A. J.; Farràs, P. Electrolysis of Low-Grade and Saline Surface Water. *Nat. Energy* **2020**, *5* (5), 367–377. https://doi.org/10.1038/s41560-020-0550-8.

(2) Praveen Kumar, S.; Sharafudeen, P. C.; Elumalai, P. High Entropy Metal Oxide@graphene Oxide Composite as Electrocatalyst for Green Hydrogen Generation Using Anion Exchange Membrane Seawater Electrolyzer. *Int. J. Hydrogen Energy* **2023**. https://doi.org/10.1016/j.ijhydene.2023.06.121.

PHOTOOXIDATION OF NAPHTHALENE–BENZENE MIXTURES: PRODUCT DISTRIBUTIONS AND SOA FORMATION ACROSS DIVERSE ATMOSPHERIC CONDITIONS

A. Ben Brik[1], M. Polat[2,3], N. O'Sullivan[1], M. Campos-Pineda[4], M. Kieft [5], J. K. Nøjgaard [2,6], M. S. Johnson[2,3], A. A. Ruth[4], and J. Wenger[1]

Presenter email address: abrik@ucc.ie

[1] *School of Chemistry and Sustainability Institute, University College Cork, Cork, Ireland*
[2] *Department of Chemistry, University of Copenhagen, 2100, Copenhagen, Denmark*
[3] *National Research Centre for the Working Environment, 2100, Copenhagen, Denmark*
[4] *School of Physics and Sustainability Institute, University College Cork, Cork, Ireland*
[5] *Luper Technologies, 4545 AE Eindhoven, Netherlands*
[6] *Department of Environmental Science, Aarhus University, Roskilde, Denmark*

Pollutants released into the atmosphere do not remain in their original form; they undergo continuous chemical transformations that change their properties, lifetimes, and environmental impacts. Aromatic hydrocarbons such as naphthalene (Nap) and benzene (Bz) are important volatile organic compounds (VOCs) emitted from several sources, including fossil fuel and biomass burning. These compounds undergo photooxidation in the atmosphere to form secondary organic aerosol (SOA), which contains sub-micrometer sized particles that influence air quality and climate, and impact on human health.

In this study, we explore how environmental conditions affect these transformations. Experiments were carried out in a 27 m³ atmospheric simulation chamber, where reactions were initiated by hydroxyl (OH) radicals—highly reactive species that drive much of the chemistry in the atmosphere. Several reaction mixtures of Nap and/or Bz with different levels of nitrogen oxides (NO_x), sulfur dioxide (SO_2), and humidity were investigated.

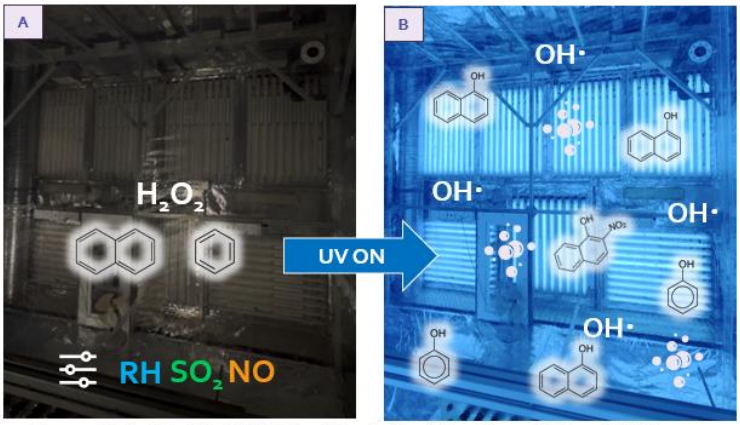


Figure 1: The inside of the IASC before (A) and after (B) turning on UV-A and UV-B lamps

To monitor the chemical changes of these species, we used chemical ionization mass spectrometry (CIMS), a sensitive analytical technique that allows us to detect and identify trace gases as they form and evolve, and a scanning mobility particle sizer (SMPS), which measures the formation and growth of SOA. Together, these techniques provide a direct link between changes in gas-phase composition and SOA formation.

Results showed that, as the reactions progressed, Nap and Bz decayed and produced a wide range of new chemical species, many of which contributed to SOA formation. The extent and nature of these transformations depended strongly on the simulated atmospheric conditions. Higher levels of NO_x led to the formation of nitroaromatic species, as well as earlier and more pronounced SOA formation, while SO_2 enhanced the total mass of SOA formed. In contrast, increased relative humidity generally delayed SOA formation in most cases.

These findings demonstrate that the fate of atmospheric pollutants highly depends on the environment in which they are produced. Investigating how these transformations occur is essential for understanding the physicochemical nature of air pollution and its broader impacts on climate and health.

Acknowledgments: This work has emanated from research funded by Taighde Éireann – Research Ireland under Grant number 21/FFP-A/8962. This work is also part of a transnational access project that is supported by the European Commission under the Horizon 2020 – Research and Innovation Framework Programme, H2020-INFRAIA-2020-1, ATMO-ACCESS Grant Agreement number: 101008003.

What To Do with Lightning in a Bottle: Non-Thermal Plasma for Treatment of Aqueous PFAS

Daniel Molloy [a], Gaurav Chugh [b], Eva Naughton [a], Jimmy Muldoon [a], Cormac D. Murphy [b,c], James A. Sullivan [a]
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[a] *UCD School of Chemistry, Belfield, Dublin 4, Ireland.*
[b] *UCD School of Biomolecular and Biomedical Science, Belfield, Dublin 4, Ireland.*
[c] *Conway Institute, Belfield, Dublin 4, Ireland*

Per- and polyfluoroalkyl substances (PFAS) represent a critical environmental challenge due to their extreme persistence and widespread contamination of global water supplies.[1] Conventional remediation methods, typically require a high energy input (e.g. high T incineration) or only sequester the pollutants (e.g. activated carbon adsorption or ion exchange) creating a secondary waste stream requiring further treatment[2]. Non-thermal plasma (NTP) offers a powerful alternative for treatment by generating highly reactive species that can mineralize PFAS at room temperature. Aqueous PFOA was effectively degraded *via* NTP treatment in a pulsed-discharge-over-water reactor. After 240 minutes of treatment, 97% of 100 ppm PFOA was degraded (with 71% defluorination). The extent of degradation and defluorination were increased when solution conductivity was increased following addition of NaCl to the PFOA solutions. At an optimized salinity of 200 mM, 74% degradation and 62% defluorination were achieved after 30 minutes of treatment. Other PFAS such as PFOS and shorter chain perfluorocarboxylic acids were also effectively degraded in this system, with enhanced rates of degradation in increased salinity. The results highlight the utility of NTP in treatment of PFAS and also the important influence of solution conductivity on effectiveness of the process.

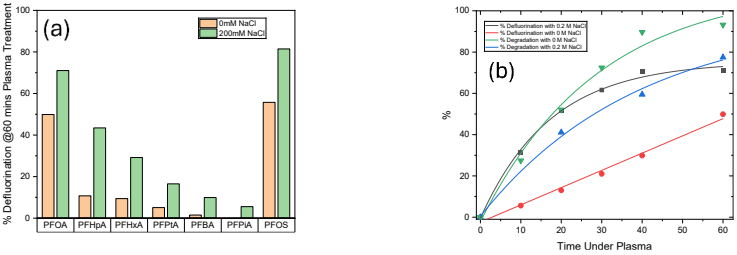

Fig 1 (a) % Defluorination of different PFAS after 1 hour plasma treatment with and without 0.2 M NaCl **(b) %** Degradation & defluorination of PFOA in 1 hour plasma treatment with and without 0.2 M NaCl

References

1. Tang, Kuok Ho Daniel. "Hidden Contaminants: The Presence of Per-and Polyfluoroalkyl Substances in Remote Regions." *Environments* 12, no. 3 (2025): 88.
2. Meegoda, Jay N, Bruno Bezerra de Souza, Melissa Monteiro Casarini, and Jitendra A Kewalramani. "A Review of PFAS Destruction Technologies." *International Journal of Environmental Research and Public Health* 19, no. 24 (2022): 16397.

A LOW-COST CEAS SPECTROMETER FOR IN-SITU ROADSIDE NITROGEN DIOXIDE

Conor W. Dorney[1], Meng Wang[1], Dean. S. Venables[1]

Presenter email address: 119474862@umail.ucc.ie

[1]Centre of Research into Atmospheric Chemistry/School of Chemistry, University College Cork, Ireland

Nitrogen dioxide (NO_2) is a major air pollutant and strongly associated with vehicle emissions. At present, there are no fast and low-cost instruments suited to mobile measurements or measurements at roadside sites. In this work, we describe a low-cost Cavity-Enhanced Absorption Spectrometer (CEAS) system for portable, in-situ measurements of NO_2 in urban environments. A blue LED centred at 440 nm was used as a light source with a 16 cm optical cavity, and transmitted light was detected with a silicon photomultiplier. Sensitivity to NO_2 at low ppb levels (3 ppb) was achieved at the instrument time resolution of 5 s. We discuss the application of the instrument to both stationary and mobile monitoring applications and present early work towards developing a backpack-mounted instrument.

References

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Tuesday 23rd June

11:45 – 13:30 WGB G03

Synthesis and Catalysis

Chair: *Dr Mary Deasy, TUD*

Amy Twomey (UCC)

Sustainable Synthesis of MOFs Using Deep Eutectic Solvents

Brian Durkan (RCSI)

N-FLUOROBENZENESULFONAMIDE AS A MILD IMIDATION REAGENT FOR THE PREPARATION OF N-SULFONYL SULFILIMINES

Ashwini Mishra (UCD)

Waste reduction and utilisation in alkyl halide synthesis: Development of "low waste" catalytic synthetic methodology

Fiona Kinsella (UCC)

EXPLORING THE POTENTIAL OF TECHNOLOGIES FOR MULTISTEP REACTION CASCADES

Aoibhínn Downes (UCD)

SYNTHESIS AND APPLICATION OF NOVEL AXIALLY CHIRAL P,N-LIGANDS

Rebecca O'Keeffe (UCC)

Asymmetric Intramolecular C–H Insertions with α-Diazosulfonates

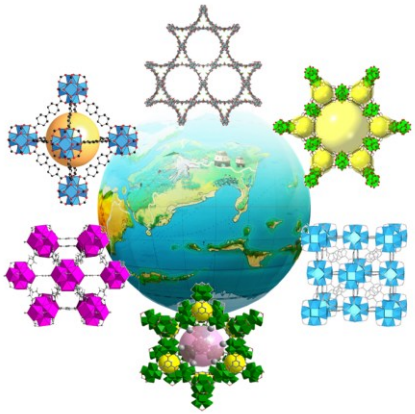
Sustainable Synthesis of MOFs Using Deep Eutectic Solvents

Amy Twomey,[1] and Davide Tiana[1*]
Email: 118386863@umail.ucc.ie

[1]*School of Chemistry, University College Cork, Cork, Ireland.*

Zirconium-based metal-organic frameworks (Zr-MOFs) are traditionally synthesised via solvothermal methods using the volatile organic solvent *N,N*-dimethylformamide (DMF). However, as of December 2023, the use of DMF has been restricted within the European Union due to its classification as a reproductive toxin, driving the need for safer and more sustainable solvent systems for MOF synthesis.[1]

In this study, six Zr-MOFs (UiO-66, UiO-67, MOF-801, MOF-808, MOF-545 and NU-1000) were synthesised using deep eutectic solvents (DESs) as an alternative to DMF.[2] This work demonstrates the versatility of DES-based synthesis routes and contributes to the development of greener protocols for the preparation of Zr-MOFs. Several frameworks were obtained with crystallinity and porosity comparable to those synthesised in DMF.



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[2] Smith, E. L.; Abbott A. P.; Ryder, K. S. *Chem. Rev.*, **2014**, *114*, 11060−11082.

N-FLUOROBENZENESULFONAMIDE AS A MILD IMIDATION REAGENT FOR THE PREPARATION OF N-SULFONYL SULFILIMINES

Brian Durkan[1], Mauro Adamo[1,2]
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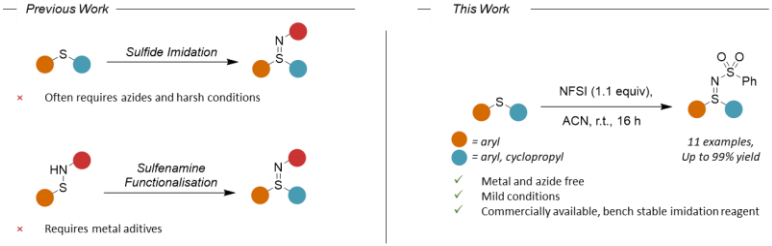
[1]*Dept. of Chemistry, Royal College of Surgeons in Ireland, Ireland*
[2]*Kelada Pharmachem, Ireland*

In spite of the emergence of sulfur and nitrogen containing functional groups as powerful pharmacores in medicinal chemistry,[1] the pharmaceutical potential of sulfilimines has remained relatively underexplored with recent reports identifying this group as a neglected pharmacore.[2]

Current routes to sulfilimines often rely on the use of transition metal additives and azides.[3] Thus, the development of more green and efficient methods for accessing sulfilimines is necessary in order to facilitate the synthesis and investigation of the pharmaceutical potential of such compounds.

In the course of our studies on the synthesis and reactivity of sulfonium salts, we discovered a novel route to N-sulfonyl sulfilimines through the reaction of sulfides and N-fluorobenzenesulfonamide (NFSI). Not alone does this represent a new route to this powerful functionality, it also provides direct evidence for the formation of the sulfur-nitrogen bond on reaction of NFSI and sulfides, with previous reactions of these reagents proposed to proceed through a fluorosulfonium intermediate.[4]

This mild, metal-free sulfide imidation is achieved using a bench-stable nitrogen source, accessing a diverse range of diaryl and aryl, cyclopropyl sulfilimines in up to 99% yield.



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(1)Lücking, U. *Chem. – Eur. J.* **2022**, *28* (56), e202201993.
(2)Greenwood, N. S.; Boyer, Z. W.; Ellman, J. A.; Gnamm, C. *J. Med. Chem.* **2025**, *68* (4), 4079–4100
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(4)Xu, X.; Yan, L.; Wang, S.; Wang, P.; Yang, A.-X.; Li, X.; Lu, H.; Cao, Z.-Y. *Org Biomol Chem* **2021**, *19* (40), 8691–8695.

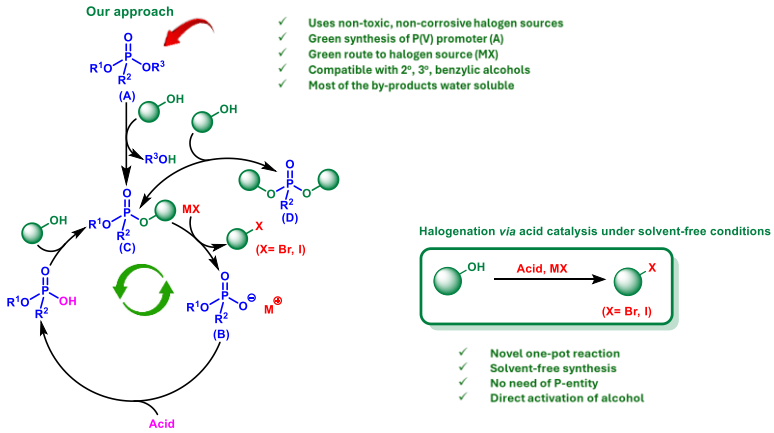
ICI Chemistry Colloquium
University College Cork 2026

WASTE REDUCTION AND UTILISATION IN ALKYL HALIDE SYNTHESIS: DEVELOPMENT OF "LOW WASTE" CATALYTIC SYNTHETIC METHODOLOGY

Ashwini Mishra[1], David Ryan[2], Aidan Cregan[2], Peter Byrne[1]*

[1]*School of Chemistry*, *University College Dublin, Ireland*;
[2]*School of Chemistry, University College Cork, Ireland*

Alkyl halides are essential intermediates in organic, medicinal, and materials chemistry, yet their preparation often relies on hazardous reagents such as thionyl chloride and PBr_3, generating toxic and acidic waste. Similarly, the Appel reaction[1] suffers from poor atom economy due to stoichiometric phosphine oxide by-products. Although catalytic Appel-type halogenations have improved efficiency[2], the synthesis of required phosphorus reagents still produces significant halogenated waste. To address these challenges, we developed a greener halogenation protocol based on a bench-stable phosphorus promoter (**A**), prepared through a non-PCl_3-dependent synthetic route.[3]



We report a one-pot halogenation method that enables *in situ* regeneration of promoter (**A**) from its phosphorus by-product (**B**). This operationally simple protocol is effective for primary, secondary, and tertiary alcohols and represents a key step toward catalytic turnover of (**A**) in halide synthesis. The methodology features several advantages: reduced waste generation, use of non-toxic halide sources, water-soluble by-products that simplify purification, and a modular one-pot setup. In addition, control experiments uncovered an unexpected acid-mediated halogenation pathway that proceeds without the phosphorus promoter. A subset of alcohols undergo efficient bromination and iodination under solvent-free conditions using only acid and metal halide, providing a complementary, minimal-waste strategy for specific substrates.

References:

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EXPLORING THE POTENTIAL OF TECHNOLOGIES FOR MULTISTEP REACTION CASCADES

Fiona Kinsella[1,2], Stuart Collins[1,2], Anita Maguire[1-3]
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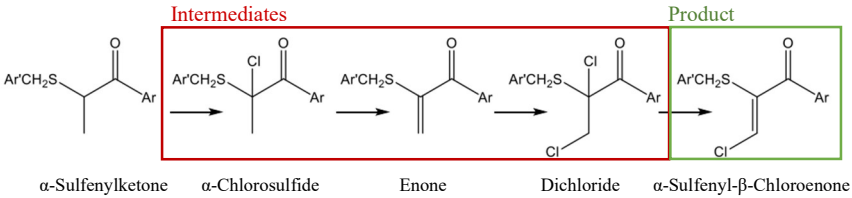
[1]School of Chemistry, University College Cork, Ireland, [2]ABCRF, University College Cork, Ireland, [3]School of Pharmacy, University College Cork.

The transition from traditional batch processing to advanced technologies such as flow chemistry and mechanochemistry is reshaping the landscape of synthetic methodology, offering powerful new opportunities for reactivity discovery and chemical innovation.[1] These modern platforms provide substantial advantages, including improved safety profiles, reduced waste generation, and enhanced reaction control.[1]



Within the Maguire–Collins group, previous studies established efficient routes to α-sulfenyl-β-chloroenones,[2] revealing a complex chlorination cascade that proceeds through multiple, observable intermediates.[2] The process displays notable stereoselectivity, with substituent effects, solvent choice, and reaction temperature influencing the resulting E/Z ratios. Building on this deep mechanistic understanding, we identified this transformation as an ideal candidate for enhancement through continuous flow and mechanochemical methodologies.

In the present work, we have optimised the synthesis of α-sulfenyl-β-chloroenones across batch, flow, and mechanochemical platforms, while significantly expanding the substrate scope. Notably, the mechanochemical protocol represents the first solvent-free route to these molecules, marking a meaningful step toward more sustainable and efficient synthetic strategies.

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ICI Chemistry Colloquium
University College Cork 2026

SYNTHESIS AND APPLICATION OF NOVEL AXIALLY CHIRAL P,N-LIGANDS

Aoibhínn Downes, Prof. Pat Guiry[2]
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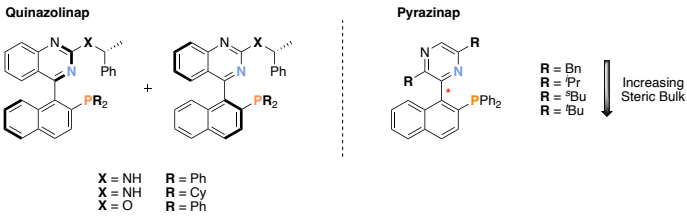
[1]*Centre for Synthesis and Chemical Biology, School of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland*

Axially chiral P,N-ligands have been shown to effectively induce stereoselectivity in a wide variety of transition metal-catalysed transformations.[1] Quinazolinaps are an example of such ligands, however, they have two key drawbacks, (1) they have long (7/8 steps) synthetic pathways and (2) they require stoichiometric amounts of an expensive palladium resolving reagent. [2,3] Three diastereomeric pairs of Quinazolinap analogues were accessed *via* a shorter 4-step synthetic pathway. In order to benchmark these novel ligands within their ligand class, they have been applied in Pd-catalysed AAA giving up to 81% *ee* and up to 98% yield. These ligands have also been applied in Cu-catalysed A^3 coupling giving up to 85% *ee* and up to 99% yield.

Pyrazine-based axially chiral P,N-ligands have also been reported to give excellent conversion and enantioselectivity in Pd-catalysed Asymmetric Allylic Alkylation (AAA).[4] The second aim of this project investigates the electronic and steric effects of substituents in the 2- and 5-poistions of Pyrazinap ligands. Four Pyrazinap ligands can be synthesised in 6 steps including key Suzuki-Miyaura coupling and Ni-catalysed phosphinylation steps from amino acid starting materials. These ligands will be applied in Pd-catalysed AAA, Cu-catalysed A^3 coupling and Ag-catalysed (3+2)-cycloadditions in order to assess their ability to induce stereoselectivity.



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Asymmetric Intramolecular C–H Insertions with α-Diazosulfonates

Rebecca O'Keeffe[1,2], Stuart G. Collins[1,2,3] and Anita R. Maguire [1,2,3,4]
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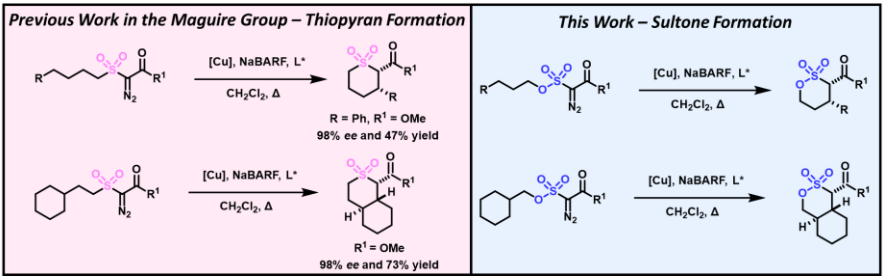
The formation of new carbon–carbon bonds is a powerful tool in organic synthesis. The Maguire/Collins team has published a series of papers over the past decade describing highly enantioselective intramolecular C–H insertion reactions with α-diazocarbonyl compounds, enabled by a copper-bis(oxazoline)-NaBARF catalyst system.[1-3] These studies demonstrated exceptional enantiocontrol in the construction of thiopyrans from α-diazosulfones, with desymmetrisation pathways delivering significantly higher efficiencies compared to simple substrates.[1-3] This work investigates whether the enantioselective copper catalysed C–H insertion can be extended to α-diazocarbonyl systems in which the sulfone substituent is replaced by a sulfonate group.



This modification is significant as the resulting sultones offer substantially greater synthetic versatility than thiopyrans. They can be readily functionalised via nucleophilic ring-opening reactions, leveraging the sulfonate as an excellent leaving group. Consequently, this approach has the potential to greatly expand the synthetic utility of copper-catalysed C–H insertion chemistry. The synthesis and handling of the sulfonates is considerably more challenging than the analogous sulfones due to their increased reactivity.

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Tuesday 23rd June

15:00 – 17:00 WGB G01

Materials Chemistry

Chair: *Dr Nikolay Petkov, MTU*

Yekaterina Tskhe (TCD)

STIMULI-RESPONSIVE HYDROGEL MICROSTRUCTURES: FABRICATION, PROGRAMMABLE ACTUATION AND SENSING

Amrutha Varshini Hariharan (UGAL)

DEVELOPMENT OF GLYCAN FUNCTIONALIZED IMMUNOMODULATORY BIOMATERIALS MITIGATING FOREIGN BODY RESPONSES

Kaynat Alvi (UCC)

Electrical and Optical Properties of Defect-Enhanced SiGe Heterostructures

Aodhán Dugan (QUB)

RETHINKING VANADIUM FLOW BATTERY ELECTRODE ACTIVATION: AN ELECTROCHEMICAL IMPEDANCE INVESTIGATION

Marilia Dalla Benetta (MU)

BRIDGING THE SCALE-UP GAP: SCHEELITE CATALYSTS FOR INDUSTRIAL AEM ELECTROLYSIS

Christian Corcoran (MTU)

Spatially Resolved Quantification of Molecular Functionalization Efficiency Using Thiol Marker Molecules

Joseph Monahan (MU)

The Benefit of Bling: Enhancing the Antibacterial Activity of MoS_2 Through Silver Nanoparticle Decoration

STIMULI-RESPONSIVE HYDROGEL MICROSTRUCTURES: FABRICATION, PROGRAMMABLE ACTUATION AND SENSING

Yekaterina Tskhe[1], Jing Qian[1], Enrique Azuaje Hualde[1,2], Nuwan Hegoda Arachchi[3], Michael J. Higgins[3], Colm Delaney[1], Larisa Florea[1]
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[2]Microfuidics Cluster UPV/EHU, BIOMICs Microfluidics Group, Lascaray Research Center, University of the Basque Country UPV/EHU, Vitoria-Gasteiz, Spain;
[3]ARC Centre of Excellence for Electromaterials Science, Australian Institute for Innovative Materials, University of Wollongong, Wollongong, Australia.

Recent advances in microfabrication technologies have enabled the development of soft micro-actuators for precise manipulation in aqueous environments. The integration of stimuli-responsive hydrogels allows controlled actuation under the applied stimuli such as light, temperature, magnetic or electric fields and chemical cues.[1]
In this work, we present the design and fabrication of micro-actuators incorporating pH-responsive hydrogels *via* direct laser writing (DLW). This high-resolution photolithography technique employs a femtosecond near-infrared laser to fabricate complex 3D architectures voxel-by-voxel.[2] The actuation was demonstrated on a microgripper design with thin cantilever arms and on bio-inspired designs featuring responsive joints. Their movement was driven by volumetric expansion of incorporated pH-responsive elements which swelled reversibly in response to local pH changes. The performance of such micro-actuators was evaluated in terms of structure design, photoresist formulation and fabrication parameters. Mechanical characterisation by atomic force microscopy (AFM) allowed to access the stiffness of the fabricated micro-actuators in dry and hydrated states. To combine actuation and sensing in one micro-actuator, the same pH-responsive hydrogels were employed to fabricate photonic microarrays for visual colour feedback enabling real-time optical readout of local pH.
In conclusion, DLW of novel micro-actuators composed of stimuli-responsive hydrogel provides potential for fabrication of high precision micro-tools that can be modulated based on hydrogel chemistry, structure design and fabrication parameters. These micro-actuators present applications for sensing, micro-object manipulation and as surgical microtools.

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Acknowledgements

Taighde Éireann – Research Ireland No. 18/EPSRC-CDT-3581, the Engineering and Physical Sciences Research Council No. EP/S023259/1, DeMANS grant No. 101007584.

DEVELOPMENT OF GLYCAN FUNCTIONALIZED IMMUNOMODULATORY BIOMATERIALS MITIGATING FOREIGN BODY RESPONSES

Amrutha Varshini Hariharan[1], Matilde Gallani[2], Laura Russo[3,4], Abhay Pandit[1]
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[2]*Università degli Studi di Padova, Italy*
[3]*School of Medicine and Surgery, University of Milano-Bicocca, Milan, Italy*
[4]*Fondazione IRCCS San Gerardo dei Tintori, Monza, Italy*

The therapeutic potential of implantable biomaterials is often limited by the host immune response. Immune cells exhibit surface receptors that recognize and bind glycans. Glycans are carbohydrates that are linked together in a linear or branched configuration. In this study, we propose that the surface functionalization of biomaterials with immunomodulatory glycans can help mitigate immune rejection through interactions with glycan-binding receptors expressed from immunitary cells. Glycosylated biomaterial coatings were developed to present two distinct glycans: 2,3–sialyllactose and 2,6-sialyllactose. Sialic acids were conjugated to lactose in specific conformations using a one-pot, three-enzyme chemoenzymatic approach. These sialyllactoses were then functionalized onto a linear polyethylene glycol (PEG) backbone, which can be coated onto the material surface. The chemical synthesis was characterised and confirmed using infrared spectroscopy and Nuclear Magnetic resonance. Furthermore, immunostaining of human blood-derived macrophages revealed the presence of sialic acid-binding immunoglobulin-type lectins (SIGLECs) across macrophage phenotypes, suggesting that the glycol-functionalized biomaterials could modulate immune responses by the interaction with SIGLEC receptors.

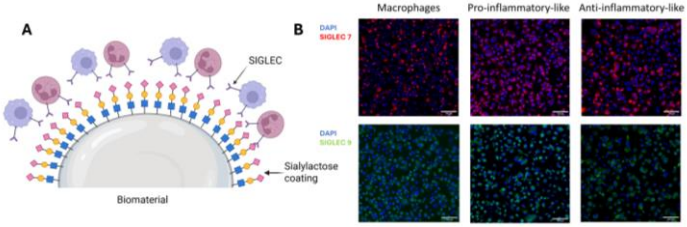

Figure 1:(A)Representation of sialylactose coatings interacting with SIGLECs on immune cells. (B)Immunostaining of macrophages and their activated phenotypes showing the expression of SIGLECs.

Acknowldgement
Research Ireland (Grant Number: 18/EPSRC-CDT/3583).

Electrical and Optical Properties of Defect-Enhanced SiGe Heterostructures

Kaynat Alvi[1,2], Liam O'Faolain[1] and Felipe Murphy-Armando[2]
Presenter email address: kaynat.alvi@tyndall.ie

[1]*Munster Technological University, Cork, Ireland*

[2]*Tyndall National Institute, University College Cork, Cork, Ireland*

Defect engineering provides a powerful route to tailor the electronic and optical properties of group-IV semiconductor heterostructures beyond conventional strain and compositional approaches. Here, we employ density-functional theory (DFT) to investigate Ge-Ge [110] split self-interstitial (SSI) defects in $Si_{1-x}Ge_x$ alloy supercells. A systematic analysis is performed across multiple alloy compositions and defect density to elucidate the evolution of defect-induced electronic structure and optical response. The introduction of SSI defects consistently generates localized states within the band structures, their dispersion, energetic separation, and hybridization are strongly governed by the underlying lattice symmetry. Face-centered cubic (FCC) supercell exhibits enhanced defect-defect interactions and more dispersive defect states, whereas the simple cubic (SC) supercell yields significantly flatter and more isotropic defect states due to reduced hybridization and distinct Brillouin-zone topology. Optical absorption calculations reveal the emergence of a sub-band-gap peak below the intrinsic direct transition of SiGe, confirming the optical activity of the defect-induced states. This indicates that Ge-Ge split interstitials can introduce effective direct-like transition pathways in otherwise indirect group-IV systems. This study establishes a symmetry-resolved understanding of defect-induced electronic and optical behaviour in SiGe alloys, offering a framework for defect-mediated design of CMOS-compatible photonic materials.

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(2) L. Spindlberger; J. Aberl; L. Vukušić; T. Fromherz; J. M. Hartmann; F. Fournel; S. Prucnal; F. Murphy-Armando;M.Brehm Mater. Sci. Semicond. Process. **2024**, 181, 108616.

RETHINKING VANADIUM FLOW BATTERY ELECTRODE ACTIVATION: AN ELECTROCHEMICAL IMPEDANCE INVESTIGATION

Aodhán Dugan[1], Josh J. Bailey, Hugh O'Connor, Paul Kavanagh, Oana Istrate[2], Peter Nockemann

Presenter email address: adugan02@qub.ac.uk

1 The QUILL Research Centre, School of Chemistry and Chemical Engineering, Queen's University Belfast, Belfast, UK

2 The School of Mechanical and Aerospace Engineering, Queen's University Belfast, Belfast, UK

Vanadium flow batteries (VFBs) show significant promise in stationary energy storage due to their durability, safety, high round-trip efficiency and scalability. However, lab-scale testing lacks standardised protocols, with significant inter-institutional variation limiting technological development.(1) A critical gap exists in understanding the electrode "wetting" or "activation" period required before reliable performance data can be obtained. Testing prior to full activation may yield unreliable results(2), yet no quantitative method exists to determine when systems are ready for analysis. To investigate this, time-resolved electrochemical impedance spectroscopy (EIS) was applied to pristine (P-GF) and thermally treated (H-GF) graphite felt electrodes over 30 h under continuous flow at 25°C, under two superficial velocities (v_s): 0.08 and 0.50 cm s^{-1}. The dominant resistance — conventionally attributed to mass transport — increased linearly for P-GF and oscillated for H-GF, contrary to expectations. Distribution of relaxation times (DRT) analysis deconvoluted the impedance into distinct contributions, identifying the dominant process as charge transfer rather than mass transport based on its flow rate independence and temporal behaviour consistent with surface degradation. Transmission line modelling confirmed this and revealed progressive loss of electrochemically active surface area for both electrode types, with thermal treatment providing ~40× greater initial active surface. These findings suggest that the dominant impedance in VFB graphite felt under flow may be kinetic rather than diffusive, with implications for how activation data is interpreted and how electrode optimisation is approached. Further work will extend this analysis to full-cell cycling conditions.

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BRIDGING THE SCALE-UP GAP: SCHEELITE CATALYSTS FOR INDUSTRIAL AEM ELECTROLYSIS

Marilia B. Dalla Benetta [1], Carmel B. Breslin[2] , Eithner Dimpsey [2] and Jonh Graves [2].
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[1] *Chemistry Department, Maynooth University, Ireland*
[2]*Advanced Manufacturing Engineering, Coventry University, England*

A key challenge in materials research is translating promising laboratory-scale developments into scalable, real-world technologies. While significant effort is devoted to designing novel electrocatalysts, many remain at the proof-of-concept stage and are not implemented in practical systems.

In this work, carried out in collaboration with Coventry University, catalysts developed at Maynooth University are evaluated for scalability, performance, and long-term stability under more application-relevant conditions. Scheelite and perovskite materials were selected due to their relatively straightforward synthesis, high yield, and suitability for producing the larger material quantities required for device-level testing. A major focus of this study was the development of catalyst inks with properties suitable for scale-up. Parameters such as dispersion stability, drying behaviour, and adhesion to the substrate were optimised. The incorporation of an ionomer into the ink formulation was also investigated to assess its influence on film formation and electrochemical performance. In parallel, the effect of substrate choice was examined, with comparisons made between carbon paper and carbon cloth in terms of coating quality and catalyst utilisation.

The performance of the scaled-up electrodes was assessed in the context of the hydrogen evolution reaction (HER) in anion exchange membrane (AEM)[1] electrolysers. Particular attention was given to understanding how formulation and processing parameters influence electrode structure and, consequently, catalytic activity and stability. Benchmark comparisons were carried out using Pt/C (both powder and supported on carbon paper) as a reference.

Overall, this work addresses key practical considerations in bridging the gap between material discovery and device integration, highlighting the importance of formulation, processing, and substrate selection in the successful scale-up of electrocatalysts for green hydrogen production.

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Spatially Resolved Quantification of Molecular Functionalization Efficiency Using Thiol Marker Molecules

Christian Corcoran[1], Nikolay Petkov[2]
Presenter email address: Christian.Corcoran2@mymtu.ie

[1]*Centre for Advanced Photonics and Process Analysis, MTU Bishopstown, Ireland*
[2]*Physical Sciences Dept, MTU Bishopstown, Ireland*

The functionalization of silica surfaces with molecules bearing various end-chain functionalities is an important method used in applications ranging from chromatography to biochemical sensing for early detection of biomarkers and pollutants removal and monitoring. Specifically, the biomarkers in the exhaled human breath are at extremely low concentrations and require selective pre-concentration of the targeted analytes for ultra-sensitive detection. Surface modification of Si films using organsosilanes is a pathway towards preconcentration. Alkoxysilanes featuring various end-chain functionalities can be exploited to covalently bind gaseous analytes during breath analysis to greatly increase the performance of the sensor. These can be referred to as anchor molecules. While the silica surface reaction with a silane molecule is well understood for bulk (powdered) materials the quantification of the functionalization efficiency for thin silica layers is limited.

Herein we demonstrate a method for the quantification of silane functionalization efficiency to the silica surface, based on Energy Dispersive X-Ray Spectroscopy (EDS). Taking advantage of the customizable silane synthesis process (alkane chain and reaction conditions), with an anchor molecule bearing a thiol terminal functional group (EDS marker entity) we established the limits vs the expected efficiency of the functionalization process. We also benchmark the enhancement of the functionalization process when comparing native and nanoporous silica surfaces, demonstrating the higher analyte pre-concentration efficiency for the nanoporous surfaces with accessible porosity.

References

Kumar. H & Mingdi Y., Mater. Interfaces 2025, 2(1), 66–83 https://doi.org/10.53941/mi.2025.100007

Karawdeniya B. et al. Chem. Rev. 2022, 122, 14990−1503 https://doi.org/10.1021/acs.chemrev.1c00990

THE BENEFIT OF BLING: *ENHANCING THE ANTIBACTERIAL ACTIVITY OF MOS_2 THROUGH SILVER NANOPARTICLE DECORATION*

Joseph Monahan[1,3], Fiona Walsh[2,3], Carmel Breslin[1,3]
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[1]*Chemistry Department, Maynooth University, Ireland*
[2]*Biology Department, Maynooth University, Ireland*
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The rise of antimicrobial resistance (AMR) has become one of the most pressing threats to global health[1]. This has highlighted the urgent need for alternatives to conventional antibiotics. The development of multifunctional nanomaterials offers a promising strategy to address the growing challenge of bacterial resistance.

In this work, we report the synthesis, structural characterization, and antibacterial performance of silver-decorated molybdenum disulfide (Ag@MoS_2) nanosheets as an advanced antimicrobial platform. Ag@MoS_2 nanocomposites were prepared via a chemical reduction approach[2], enabling uniform deposition of silver nanoparticles onto exfoliated MoS_2 surfaces. The synthesized material was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) and flame atomic absorption spectroscopy (FAAS).

Antibacterial activity was first assessed against susceptible Gram-negative and Gram-positive strains. Ag@MoS_2 exhibited significantly enhanced bactericidal activity compared to pristine MoS_2 and silver nanoparticles alone, as demonstrated by bacterial viability assays. The nanocomposites also showed significant inhibition of highly resistant strains. The antibacterial mechanism was studied by examining the oxidative capacity of the material, Ag^+ release and direct membrane damage.

This study highlights the potential of Ag@MoS_2 nanohybrids as versatile antimicrobial materials with applications in coatings, medical devices, and water treatment technologies.

References

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Tuesday 23rd June

15:00 – 17:00 WGB G03

Medicinal Chemistry

Chair: *Dr David Jones, UCC*

Emily Hill (UL)

AMORPHOUS SOLID DISPERSIONS FOR IMPROVED BCS CLASS II DRUG DISSOLUTION AND STABILITY

Sebastian Pim (RCSI)

USING ON/ON FLUORESCENCE LIFETIME MICROSCOPY TO OBSERVE BIOORTHOGONAL REACTIONS IN LIVE CELLS

Pei-Hsuan Wu (TUD)

LIGAND EXCHANGE OF COPPER COMPLEXES AND ITS EFFECTS ON DNA INTERACTIONS

Aoife Cotter (UL)

SPRAY-DRIED ENZYME-LOADED LIPOSOMES FOR PULMONARY DELIVERY

Andreea Cislaru (MU)

CONTROLLING THE SUGAR CODE: AN ENZYMATIC GLYCOENGINEERING APPROACH TO REMODELING THE IgG ANTIBODY GLYCAN LANDSCAPE

Surangana Kashyap (QUB)

TRANSFORMATION OF LIGNIN INTO INTRINSIC NITRIC OXIDE DONORS WITH TUNABLE RELEASE BEHAVIOR

Rebecca Lynn (DCU)

Copper Metallo-nucleases for Genome Editing

AMORPHOUS SOLID DISPERSIONS FOR IMPROVED BCS CLASS II DRUG DISSOLUTION AND STABILITY

Emily Hill[1,2], Maryam Karimijafari[1,2], Ayman Hijazi[1], Emmet O'Reilly[1,2]
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[2]*Research Ireland and SSPC SFI Research Centre*

The rising proportion of discovered drugs with poor solubility, known as BCS class II drugs, requires formulation scientists to overcome this limitation to make these drugs commercially viable. Amorphous solid dispersions (ASDs) have become a favored method for tackling this issue. Converting crystalline APIs into their higher energy amorphous form improves their solubility. Then dispersing this metastable form within a polymeric carrier alleviates stability and recrystallisation concerns[1]. ASD solubility, dissolution and stability were the focus of this work.

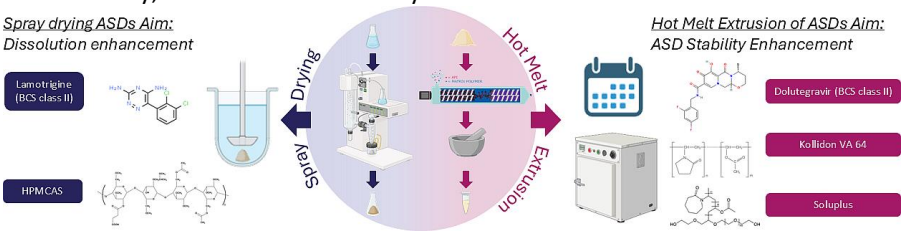

Fig 1: Overview of project aims and manufacturing methods used.

ASDs of lamotrigine, an epilepsy drug, were spray dried with HPMCAS. Varying the drug polymer ratio affected amorphisation and particle morphology, both of which impact dissolution. The dissolution profiles of the spray dried ASDs in simulated intestinal fluid were compared to the crystalline drug and showed improved release and greater overall dissolution. Then ASD stability was explored through the extrusion of ASDs with a significant focus on polymer choice. Theoretical approaches including Flory-Huggins (FH) theory and PC-SAFT modelling were applied to aid understanding of successful polymer selection. Dolutegravir, Soluplus and Kollidon VA 64 were investigated at various drug polymer ratios. Despite FH interaction parameter predicting immiscibility for both drug polymer systems, stability studies highlighted notable stability of all ASDs, with over six months stability for the Soluplus samples. These findings highlight the multi-faceted nature of ASD stability involving drug-polymer interactions, miscibility and glass transition temperatures.

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USING ON/ON FLUORESCENCE LIFETIME MICROSCOPY TO OBSERVE BIOORTHOGONAL REACTIONS IN LIVE CELLS

Sebastian Pim[1], Anaïs C. Bourgès[1], Dan Wu[1], Gonzalo Durán-Sampedro[1], Massimiliano Garre[1], Donal F. O'Shea[1]
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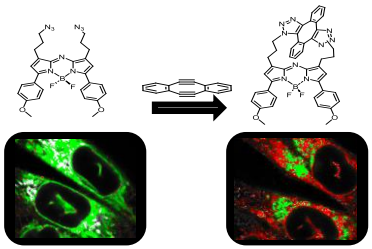
Bioorthogonal fluorescence imaging is an effective way of monitoring dynamic events in sub-cellular compartments in a non-destructive manner. The Sondheimer diyne allows for two sequential 1,3-dipolar cycloadditions under mild conditions without the need for a catalyst.[1] Previous work from the O'Shea research group has shown that this diyne can be used for bioorthogonal imaging in live cells.[2] To expand on these initial findings, the bis-azide substituted BF2-azadipyrromethene 1 was selected as an attractive candidate for bioorthogonal fluorescence imaging as it would emit in the advantageous near infrared spectral region and has bis-azide functionality allowing for two cycloaddition reactions (Figure). The synthesis of 1 was achieved in 10 steps starting from butan-1,4-diol and 2-bromo-4'-methoxyacetophenone. Photophysical characterization of 1 showed an emission □max at 677 nm with quantum yield of 0.49 in methanol. The reaction of 1 with Sondheimer diyne gave a mixture of cis and trans macrocyclization products 2 in excellent yield under mild room temperature conditions (Figure). The bioorthogonal reaction between 1 and the Sondheimer diyne has been observed in the nuclear envelope and nuclear invaginations of live cells, with the progress of these reactions being tracked by Fluorescent Lifetime Imaging Microscopy (FLIM).



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LIGAND EXCHANGE OF COPPER COMPLEXES AND ITS EFFECTS ON DNA INTERACTIONS

Pei-Hsuan Wu[1], Bernadette Creaven[1], and John Colleran[1]
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The anticancer properties of copper complexes are closely related to their ability to induce DNA cleavage and inhibit cancer cell proliferation.[1–3] However, the inherent lability of these complexes can significantly alter their therapeutic efficacy. Cyclic voltammetry[4] and DNA cleavage assays demonstrate that ligand exchange occurs readily, and that the efficiency of DNA cleavage is highly dependent on the coordination environment of the copper centre which in turn varies with endogenous anions. These results suggest that identifying the specific active species remains challenging, as the diverse array of endogenous ligands present under physiological conditions may facilitate continuous ligand substitution *in vivo*.[5,6]

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SPRAY-DRIED ENZYME-LOADED LIPOSOMES FOR PULMONARY DELIVERY

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Pulmonary delivery of enzyme therapies bypasses gastrointestinal and hepatic first-pass metabolism; however, free enzymes are rapidly cleared from the airways by mucociliary transport and immune cell uptake [1]. PEGylated liposomes can serve as sustained drug depots in the lungs, and dry powder liposomal formulations may enable shortened administration times versus traditional nebulised suspensions. This work developed a stable dry powder formulation of PEGylated liposomes encapsulating Bovine Deoxyribonuclease (DNase) as a model for recombinant human DNase, which is administered via nebuliser as a free enzyme to reduce mucus viscosity in patients with cystic fibrosis (CF).

Optimised DNase-liposomes demonstrated enzymatic activity upon disruption, >5% encapsulation efficiency (E.E%), 150–160 nm mean size, a low polydispersity index (PdI) (0.08-0.09) and a neutral surface charge. The formulation remained stable for 24 h at 37°C and 45 days at 4°C, as measured by size, PdI, protein-to-drug ratio, and enzyme activity. The liposomal formulation demonstrated <10% release of an indicator dye in a CF mucus model between 4-24 hours, suggesting controlled release capability in its target mucus. The mean size and enzyme activity were successfully preserved after spray drying followed by reconstitution, both immediately and following 6-week room temperature storage. Minor increases in PdI and slight decreases in E.E% were observed post-spray-drying ($p < 0.05$), likely reflecting bilayer rearrangement without expected impact on *in vivo* performance. Powders exhibited high yields (>80%), low residual moisture content (4–6w/w%) and favourable in *vitro* aerosolisation characteristics as assessed via Andersen cascade impactor. These spray-dried DNase-loaded liposomal powders demonstrate potential as a platform for pulmonary enzyme therapy delivery.

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CONTROLLING THE SUGAR CODE: AN ENZYMATIC GLYCOENGINEERING APPROACH TO REMODELING THE IgG ANTIBODY GLYCAN LANDSCAPE

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Monoclonal antibodies (mAbs) are the most widely used protein therapeutics in the treatment of cancers, arthritis, and other human disorders worldwide. Currently, the production of mAbs by mammalian (e.g., CHO cells) or alternative cell culture platforms gives rise to heterogeneous mAb structures (1). Contrastingly, homogeneous mAbs demonstrate higher specificity and selectivity to their ligands (FcRs) (2), allowing for reduced patient dosing and enhanced therapeutic value. N-glycans can fine-tune immunological responses such as antibody-dependent cellular cytotoxicity (ADCC) or anti-inflammatory properties. However, the formation of single glycoforms remains a challenge. Two current glycoengineering methods include a) cell line engineering and b) media supplementation and process parameter alterations (1). Here, we present an alternative chemoenzymatic workflow for the design and characterization of single glycoform mAbs using a previously developed N-glycoanalytical technology (3,4). This workflow sequentially removes key glycan motifs from the mAb originator molecules, followed by the addition of selective glycan epitopes using glycosyltransferase enzymes and sugar donors to generate a family of glycoengineered mAbs with improved pharmacokinetics and enhanced effector functions.

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TRANSFORMATION OF LIGNIN INTO INTRINSIC NITRIC OXIDE DONORS WITH TUNABLE RELEASE BEHAVIOR

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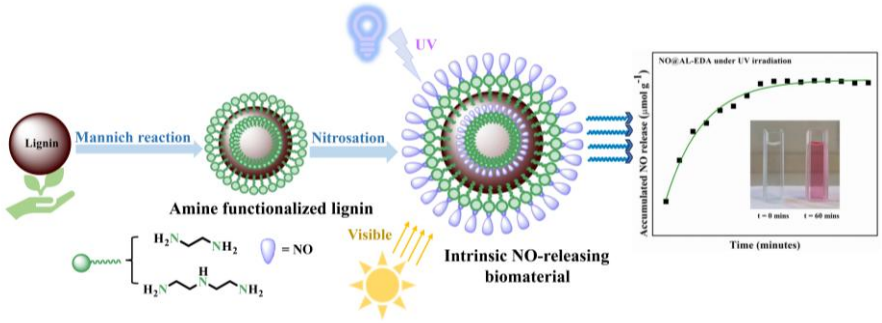
Nitric oxide (NO) delivery systems are widely explored for wound healing and antimicrobial applications, but current approaches based on small-molecule donors or nanoplatforms often suffer from undesirable leakage, instability, and poor biocompatibility. Lignin offers a sustainable alternative, yet its intrinsic NO-donor functionality remains largely unexplored. Herein, we report the direct transformation of lignin into an intrinsically NO-releasing biomaterial platform. Alkaline (AL) and organosolv (OL) lignins were functionalised through Mannich amination with ethylenediamine (EDA) or diethylenetriamine (DETA), followed by nitrosation to generate NO-donor groups in the lignin skeleton. Both AL- and OL-lignin showed efficient NO release profile, among which AL–EDA delivered ~250 µmol g^{-1} of NO over 240 minutes. The resulting materials exhibited tunable, light-responsive NO release, governed by lignin structure, amine type and site population, and irradiation conditions. This work establishes lignin as a sustainable platform for light-controlled bioactive nitric oxide delivery with potential biomedical applications.



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Copper Metallo-nucleases for Genome Editing

Rebecca Lynn[1], Alex Gibney[1], Eva Delahunt[1], Haydn Beaton[2], Stephen MacDonald-Brown[2], Carlos Lence[2], Miles Kenny[2], Matt Allen[2], Iva Lukac[2], Andrew Jordan[2] and Andrew Kellett[1]

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A nuclease is an enzyme that acts like molecular scissors to cleave DNA. There is a major interest in targeting DNA with directed nucleases for gene editing. This has been exploited in several state-of-the-art gene editing systems such as zinc finger nucleases (ZFNs), transcription activator-like effector nucleases (TALENs) and clustered regularly interspaced short palindromic repeats (CRISPR). However, despite their promising potential, they possess several undesirable side effects including low efficiency and off-target cleavage. A promising alternative is the development of artificial metallo-nucleases (AMNs) which, in the presence of catalytic first row transition metals such as copper, cleave DNA using an oxidative mechanism. This mechanism offers the opportunity for permanent gene knockout compared to the damage induced by Cas enzymes, the nuclease family recruited by CRISPR-Cas systems, which are amenable to repair. Herein we report the synthesis, characterisation, and preliminary activity of three new types of copper-based AMNs. The AMNs were designed to incorporate stable azide substituents for future incorporation into gene-targeting vectors via nucleic acid click chemistry. Of the three types of AMN, one class is based on an expansion of the Clip-Phen family, another utilises the 'Click to Chelate' strategy and the final focuses on the Phenanthroline-Oxazine ligand class.

Wednesday 24th June

09:45 – 10:40 WGB G01

Medicinal Chemistry

Chair: *Dr Lorraine Bateman, UCC*

Niamh Hickey (UL)

Development of molecular dynamics models of complex crystallisation mechanisms of pharmaceuticals

Ciara McEvoy (MU)

THE DESIGN AND SYNTHESIS OF PYRAZOLOPYRIMIDINONES AS POTENTIAL ANTI GLIOBLASTOMA AGENTS USING COLD ATMOSPHERIC PLASMA (CAP)

Karina Chan (RCSI)

DEVELOPMENT OF VHL BASED PT-PROTACS TO DEGRADE PT-BINDING PROTEINS

Development of molecular dynamics models of complex crystallisation mechanisms of pharmaceuticals

Niamh Hickey[1,2], Sarah Hudson[1,2], Pierre-Andre Cazade[3], Sarah Guerin[1,2]

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Molecular modelling can give critical insight into the properties and behaviour of pharmaceutical crystals[1]. Classical Molecular Dynamics enables modelling large systems accounting for solvent and thermodynamics effects. It also provides time resolved information otherwise inaccessible to stationary DFT calculations or Monte Carlo (simulations). In this present work, we will discuss our development of molecular dynamics (MD) simulations for studying the interaction of excipients with crystalline nanoparticles of drug products, based on the CHARMM/CGenFF[2] forcefield, to model the crystallisation of indomethacin using the LASP method (liquid-antisolvent precipitation)[3].

Experimentally there were challenges in obtaining the stable polymorphic form of the API. A seeding approach was experimentally successful in driving the solid-state transformation, which we then computationally redesigned. The two different excipient combinations that were successful in driving the solid-state form transformation also had to be modelled. Our aims were to model the impact and influence of the seeding approach on the system, as well as the difference between the two excipient combinations.

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THE DESIGN AND SYNTHESIS OF PYRAZOLOPYRIMIDINONES AS POTENTIAL ANTI-GLIOBLASTOMA AGENTS USING COLD ATMOSPHERIC PLASMA (CAP)

Ciara McEvoy[1,2], Natalia Bednarz[2,3], James Curtin[2,3], Gemma K.Kinsella[2,3], John C. Stephens[1,4].
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Glioblastoma multiforme (GBM) grade IV remains one of the most aggressive and lethal brain cancers, with a median survival of just 12 to 24 months despite standard therapy.[1] Pyrazolopyrimidinones, fused nitrogen-containing heterocycles, are common motifs in bioactive pharmaceutical agents. Cold atmospheric plasma (CAP), known for generating reactive oxygen species (ROS) with spatial and temporal precision, offers a novel strategy to enhance anticancer efficacy.[2]

In this study, a series of pyrazolopyrimidinone derivatives were synthesized via microwave-assisted condensation of 5-aminopyrazoles and β-ketoesters, which were then purified and structurally characterized using spectroscopic methods, including NMR and IR spectroscopy. Their cytotoxicity was evaluated against the U-251 MG human glioblastoma cell line, both alone and in combination with CAP treatment. CAP was applied in two modes: (i) direct irradiation and (ii) indirect treatment. To date, 56 compounds have been synthesized, with yields ranging from 15% to 99%. Preliminary results identify a lead compound that exhibits a 120-fold decrease in IC_{50} when combined with 30 s of direct CAP irradiation (IC_{50}: 453.3 to 3.8 µM). These results suggest that CAP can selectively potentiate the anticancer effects of pyrazolopyrimidinones at the tumour site, offering a novel approach to targeted glioblastoma therapy. Ongoing work includes expansion of the compound library and systematic structure activity relationship (SAR) studies to further optimize therapeutic efficacy.

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DEVELOPMENT OF VHL BASED PT-PROTACS TO DEGRADE PT-BINDING PROTEINS

Karina Chan,[1] Joshua McLean,[1] Alby Benny,[1] Keelan Farnan,[2] Triona Ní Chonghaile,[2] Darren Griffith [1]
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Platinum (Pt)-based drugs such as cisplatin, carboplatin and oxaliplatin play a very important and well-documented role in treating cancer and are employed in nearly 50% of all anticancer treatments. The primary mechanism of Pt-based drugs is associated with their ability to cross-link nuclear DNA; the Pt-DNA adducts interrupt transcription, generate DNA perturbation damage responses and ultimately induce apoptosis. Pt(II) anticancer drugs also interact with a range of other nucleophiles, including RNA, mitochondrial DNA and proteins. Of these, the role Pt protein binding plays in on- and off-target activity of Pt-based drugs has been of particular interest. [1]

Proteolysis-targeting chimeras (PROTACs) are bifunctional molecules that can hijack the ubiquitin proteasome system (UPS) to achieve targeted degradation of proteins of interest. [2] Our group recently reported the first example of a metallo-PROTAC that could successfully degrade known Pt-binding proteins. [3]

PROTAC activity can be fine-tuned through the selection of linker length, type of E3 ligase ligand and Pt complex. A novel class of VHL based Pt PROTACs will be reported together with results to date describing their synthesis, biological activity and a proteomic study on lead Pt PROTAC.

Acknowledgements
This research was conducted with the financial support of Taighde Éireann – Research Ireland under Grant number 22039A01.

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Wednesday 24th June

09:45 – 10:40 WGB G03

Synthesis and Catalysis

Chair: *Prof Declan Gilheany, UCD*

Oana Popa (UCD)

STEREOSELECTIVE GLYCOSYLATIONS

Éabha McMahon (UCC)

INTERMOLECULAR C-H INSERTION REACTIONS OF ACYCLIC α-DIAZO-β-OXO SULFONES USING ENANTIOSELECTIVE COPPER BIS(OXAZOLINE) CATALYSTS

Sarah Smoni Varghese (UCD)

DESIGN AND SYNTHESIS OF NOVEL AXIALLY CHIRAL P,N-LIGANDS EXPLOITING NON-COVALENT BONDING INTERACTIONS

STEREOSELECTIVE GLYCOSYLATIONS

Oana G. Popa[1], Eoghan M. McGarrigle[1]
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Oligosaccharide synthesis, which currently poses many difficulties, consists of multiple glycosylation steps.[1] A great amount of work has been carried out to improve the outcome of this type of reaction, however a complete chemo-, regio- and stereoselective glycosylation strategy remains difficult to achieve.[2]
Previously, a new class of tetramethyl *N*-methyliminodiacetic acid (TIDA) boronates has emerged as effective building blocks to automate the synthesis of small molecules.[3] Thanks to its property of binary affinity for silica-gel, this TIDA boronic ester tag can simplify the purification process by enabling a catch-and-release methodology. Herein, we report the synthesis of monosaccharide building blocks using a TIDA boronic ester tag and use of these building blocks in the further synthesis of oligosaccharides using the HPLC-based automated system.
1,2-*cis*-Glucosides were synthesized in high stereoselectivity, starting from hemiacetal donors. This work involves a one-pot chlorination (under Appel conditions), halide metathesis to iodide (with LiI), and glucosylation sequence.[4] A range of glycosyl acceptors and donors are shown to be suitable under the reaction conditions.
The picolinyl and picoloyl groups have been previously introduced by Demchenko *et al.* when a positively charged species was identified as an intermediate during glycosylations.[5] Getting inspiration from this work, we synthesized and tested several donors containing positively charged groups.

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INTERMOLECULAR C-H INSERTION REACTIONS OF ACYCLIC α-DIAZO-β-OXO SULFONES USING ENANTIOSELECTIVE COPPER BIS(OXAZOLINE) CATALYSTS

Éabha L. McMahon[1,2], Stuart G. Collins[1,2], Anita R. Maguire[1-4]
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The Maguire team has demonstrated highly enantioselective intramolecular C-H insertion reactions in acceptor/acceptor α-diazocarbonyl compounds using copper bis(oxazoline) catalysts with α-diazo-β-oxo sulfones and related compounds.[1–4]

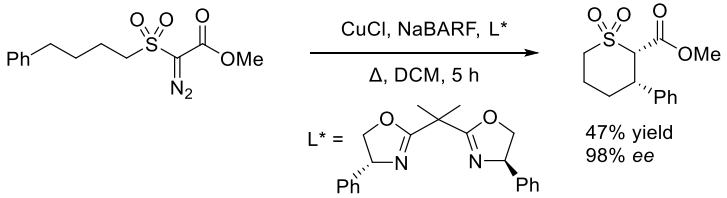

Figure 1: *Asymmetric copper catalysed intramolecular C-H insertion.*

This work is powerful novel methodology for the formation of new C-C bonds with an abundant metal copper catalyst and excellent enantiocontrol. Key to this methodology is the selective activation of previously unactivated C-H bonds through use of a catalyst with insertion of a carbene derived from an α-diazo-β-oxo sulfone.

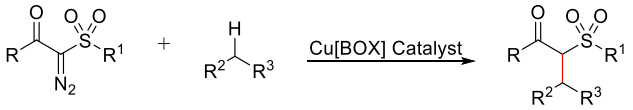

Figure 2: *Intermolecular C-H insertion reaction.*

The exploration of the impact of variation of the substrate and C-H source on the efficiency and selectivity of these transformations is discussed, as well as examining the role of the catalyst, ligand and counterion in the C-H insertion step.

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DESIGN AND SYNTHESIS OF NOVEL AXIALLY CHIRAL P,N-LIGANDS EXPLOITING NON-COVALENT BONDING INTERACTIONS

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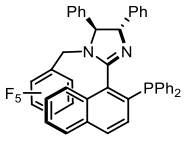
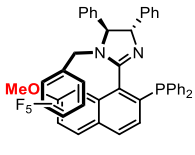
The synthesis and application of UCD-Phim, a P,N ligand containing both central and axial chirality, was reported by the Guiry group in 2017.[1] This ligand gave excellent applications in asymmetric catalysis however it starts to epimerise at temperatures greater than 40 °C. In order to increase the configurational stability of the ligand system, a library of novel axially chiral P,N-ligands have been synthesized. It was found that the novel ligands containing the heptafluoronaphthalene moiety showed higher barrier to rotation around the chiral axis which was calculated using VT-NMR spectroscopic techniques.



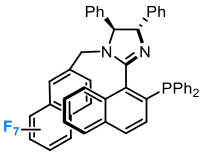
(*S,S,R*$_a$)-UCDPhim

Barrier to rotation
$\Delta G^{\ddagger}$ = 26.8 kcal/mol



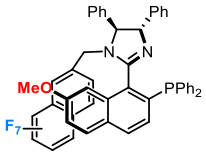
(*S,S,S*$_a$)-MeO-UCDPhim

Stable at room temp.
Epimerises at 40 °C



(*S,S,R*$_a$)-Kochi-UCDPhim

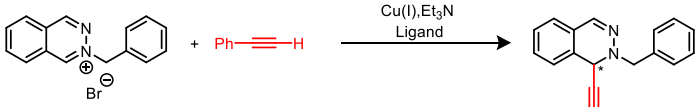
Barrier to rotation
$\Delta G^{\ddagger}$ = 27.2 kcal/mol



(*S,S,R*$_a$)-MeO-Kochi-UCDPhim

Barrier to rotation
$\Delta G^{\ddagger}$ = 27.5 kcal/mol

Application of the axially chiral ligands were analysed in the copper-catalysed alkynylation of phthalazinium salts in order to access 1-alkynyl-1,2-dihydrophthalazines enantioselectivity. This expands on the work done by Chen and co-workers, where the racemic alkynylation scope was explored.[2] Optimisation of the copper-catalysed alkynylation on the model substrate is described, obtaining the alkynylated product in high yields and enantioselectivities.



77% yield, 89% *ee*

References –

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Wednesday 24th June

11:00 – 12:15 WGB G01

Materials Chemistry

Chair: *Dr Brendan Bulfin, UCC*

Martina Piletti (UCC)

ORANGE PEEL EXTRACT AND NITROGEN-DOPED CARBON DOTS ENRICHED CHITOSAN FILMS FOR SMART PACKAGING AND CO2 LASER-INDUCED LABELLING

Niamh O'Shea (TCD)

The development of Ln-btp mechanically interlocked molecules and self-assemblies

Muhammad Adnan (UL)

Molten Salt Assisted Synthesis of Fluoride-free Mxenes and its application in Energy Storage

Neil Curtis (UCC)

MICROELECTRODE STUDY OF LITHIUM AND SODIUM PLATING KINETICS

ORANGE PEEL EXTRACT AND NITROGEN-DOPED CARBON DOTS ENRICHED CHITOSAN FILMS FOR SMART PACKAGING AND CO2 LASER-INDUCED LABELLING

Martina Piletti[1], Kaushani Kotuwegoda Guruge[2], Carlo Spadoni[3], Paola Carolina Alzate Calderon[2], Nilushni Sivapragasam[2], Daniela Iacopino[1]
Presenter email address: martina.piletti@tyndall.ie

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[2]School of Food & Nutritional Sciences, University College Cork, Cork, Ireland
[3]Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 3, Sesto Fiorentino, 50019 Florence, Italy

Active food packaging systems have gained significant attention due to their ability to extend shelf life and preserve food quality through the incorporation of functional agents[1]. In this study, environmentally friendly, photoluminescent, and transparent chitosan-based composite films were prepared by a simple aqueous solvent casting method. Electrochemically synthesized nitrogen-doped carbon dots (NCDs, 0.5–1% w/w of polymer) and orange-peel extract (OPE, 50% w/w of polymer) were embedded in the polymer and the resulting films exhibited high transparency (>80% transmittance at 600 nm), flexibility, and strong UV shielding performance. Compared with pure chitosan films, the incorporation of OPE and NCDs significantly enhanced UV-blocking efficiency, achieving 96% blocking in the UVC region, 89% in the UVB region, and 63% in the UVA region. The improved functionality was attributed to hydrogen-bonding interactions between chitosan, NCDs, and OPE, enabling effective dispersion of additives within the polymer matrix. Furthermore, the films demonstrated excitation-dependent photoluminescence, converting absorbed harmful UV radiation into lower-energy visible light in the blue–green region, thereby providing protective functionality[2]. Antimicrobial assays revealed selective activity against *Pseudomonas fluorescens*, Gram-negative bacteria. OPE contributed more significantly to antimicrobial activity than NCDs, while both additives synergistically enhanced antioxidant capacity. In addition to packaging performance, a laser-programming strategy using a 1064 nm CO_2 laser enabled direct writing of tunable fluorescent patterns on the films, providing dynamic information encryption and high-security anti-counterfeiting features. These multifunctional, sustainable composites show strong potential for advanced applications in food packaging, pharmaceuticals, and healthcare materials.

References

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The development of Ln-*btp* mechanically interlocked molecules and self-assemblies

Niamh A O'Shea[1,2], Oxana Kotova[1], Sandra Fernandez-Farina[1,3], Owen Oseghale[1,2], Bláithín Rawson[1], and Thorfinnur Gunnlaugsson[1,2]
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The world of interlocking molecules has continued to be developed due to their versatility and flexibility. Within the supramolecular chemistry world, the Gunnlaugsson group have utilised the [2,6-bis(1,2,3-triazole-4-yl) pyridine] (***btp***) binding motif, to create beautiful supramolecular architectures including mechanically interlocked molecules (MIMs) and Ln(III) self-assemblies. This work has focused on building ***btp*** rotaxanes and also utilising the syn-syn orientation of the ***btp*** for Ln(III) and Zn(II) complexes. Hence, building upon the work of McCarney and Byrne's,[1] we are developing a hydrogen bonding and active-metal templated psueodorotaxanes and rotaxanes. Rotaxanes are functional molecules in terms of molecular sensors and the nanomaterials world. Our aim is to create novel MIMs for use within the electronic, imaging and magnetic industries. The rotaxane is be based upon the building of a ***btp*** macrocycle and a ***btp*** thread with a different number of stations to shuttle the macrocycle, forming a switch mechanism.Our aim is to stopper the rotaxanes using Ln cyclen complexes which were previously designed by the Gunnlaugsson group[2] The fluorescence and delayed-fluorescence of the rotaxane and self-assemblies have been studied, both kinetically and thermodynamically with their lifetime's values being evaluated.

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Molten Salt Assisted Synthesis of Fluoride-free Mxenes and its application in Energy Storage

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Department of Chemical Sciences, University of Limerick, Limerick

Abstract:

The growing demand for efficient and sustainable energy storage systems has accelerated the search for advanced electrode materials for next-generation batteries. MXenes, a family of two-dimensional transition metal carbides and nitrides, have attracted significant attention due to their metallic conductivity, hydrophilic surfaces, and excellent mechanical stability. However, their practical application is often limited by compact multilayer stacking and poor delamination, which reduce active surface area and hinder ion transport. Among them, M_4X_3 MXenes are particularly promising because their robust structures enable efficient ion intercalation, high storage capacity, and rapid ion diffusion. Herein, we report for the first time the synthesis of $Nb_4C_3T_x$ MXene using a Lewis acid molten salt etching (LAMS) method. This approach uses molten salts in the presence of Lewis acids to selectively etch Nb-based precursors, producing high-quality few-layer MXene with enhanced active surface area. In addition, –Cl surface terminations increase interlayer spacing while preserving high electronic conductivity, leading to improved charge transfer kinetics and enhanced cycling stability. These findings highlight the strong potential of $Nb_4C_3T_x$ MXenes as versatile electrode materials for advanced battery technologies and provide a scalable synthesis route for future high-performance energy storage applications.

References:

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MICROELECTRODE STUDY OF LITHIUM AND SODIUM PLATING KINETICS

Neil Curtis[1], James Rohan[2]
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[1] *School of Chemistry, University College Cork, Ireland*
[2] *Electrochemical Materials and Energy, Tyndall National Institute, Ireland*

Lithium and sodium metal anode batteries have been the focus of research for decades thanks to their high energy density.[1] However, efforts to implement the technology have prevented by safety risks related to dendritic deposition. The underlying mechanism of this deposition may offer some solutions. This study investigated the electron transfer kinetics of the deposition for both lithium and sodium metal onto a nickel microelectrode array. The small electrode area allows for fast scan rates without incurrring large transient currents which would be seen on macroelectrodes.[1] Faster scanning allows measurement of the deposition reactions while minimising effiects from side reactions, particularly the formation of a solid-electrolyte interface which would convolute the measured kinetics.[2] Better understanding of this underlying deposition mechanism could further the development of improved electrolyte/additive combinations.

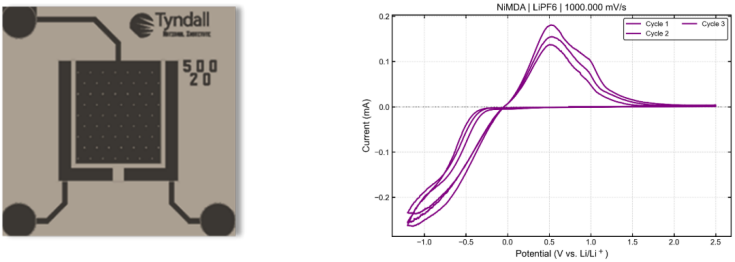

Figure 1: Schematic of an MDEA (left). CV results of Ni MDEA in 1 M $LiPF_6$ electrolyte scanned at 1 V/s (right)

References

ACS style text (Calibri, 8 pt, single line spacing, aligned left)

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Wednesday 24th June

11:00 – 12:15 WGB G03

Analytical Chemistry

Chair: *Dr Eoin McGillicuddy, TUD*

Edel Whelton (UCC)

Characterisation of Tissue Type in Breast Disease via Bioimpedance Measurements

Emily Harlin (MU)

DEVELOPMENT OF ORTHOGONAL FLUORESCENT PROBES AND GREEN LABELLING STRATEGIES FOR N-GLYCAN ANALYSIS

Devansh Shah (UCC)

NON-POROUS SILICA FOR PROTEIN-A HIGH-PERFORMANCE AFFINITY CHROMATOGRAPHY OF MONOCLONAL ANTIBODIES

Md Rasel (UCC)

Laser-Induced Graphene Based Sustainable Platform for Wearable Health Monitoring

Characterisation of Tissue Type in Breast Disease via Bioimpedance Measurements

Edel Whelton [abcd], Eva Flynn [abc], Dr. Yineng Wang [ab], Dr. Martin O'Sullivan [c], Dr. Justina Ugwah [ab], Dr. Peter Ryan [d], Mr. Ray Burke [b], Dr. Brian O'Donnell [c], Prof. Eric Moore*[ab]

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Abstract

Breast cancer remains a significant health concern, with diagnostic pathways often relying on invasive biopsies that can cause patient discomfort and anxiety. The development of non-invasive, reliable methods to distinguish benign from malignant breast tissue is crucial for improving patient outcomes and streamlining clinical workflows.

This study investigates the use of bioimpedance technology—specifically the SMARTBiop method—for the characterisation of tissue in breast disease. The SMARTBiop system is a two-electrode set up on a biopsy needle tip. The primary objective is to establish a comprehensive reference database of bioimpedance measurements, enabling clinicians to differentiate tissue types with greater accuracy and reduce unnecessary biopsies. The creation of a tissue data bank is anticipated to facilitate early identification of benign disease, potentially eliminating the need for biopsy and expediting the investigation of suspicious lesions.

Bioimpedance measurements consistently revealed distinct electrical properties among benign, healthy, and cancerous tissue types. These findings support the hypothesis that bioimpedance can serve as a reliable marker for tissue characterisation.

DEVELOPMENT OF ORTHOGONAL FLUORESCENT PROBES AND GREEN LABELLING STRATEGIES FOR N-GLYCAN ANALYSIS

Emily Harlin[1], Fergal Byrne[1], Robert Elmes[1,2,] Róisín O'Flaherty[1,2,3]
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[3]CÚRAM, SFI Research Centre for Medical Devices, Biomedical Sciences Building, University of Galway, Ireland, H91 W2TY.

Over 50% of human proteins are glycosylated, and more than 80% of biopharmaceuticals contain N-glycans. These glycans are frequently altered in immune dysregulation and can significantly affect therapeutic safety and efficacy, driving demand for sensitive, robust, and sustainable analytical tool[1]. This work presents an integrated approach to advanced N-glycan analysis by developing novel fluorescent probes and greener labelling strategies. A panel of structurally diverse fluorophores was designed, incorporating chemistries for lanthanide complexation, tetrazine-based bioorthogonal reactivity, and squaramide-mediated conjugation. These probes provide orthogonal alternatives to established labels such as 2-aminobenzamide (2-AB) and aminoquinoline carbamate (AQC), improving flexibility in fluorescence-based detection. Among them, the squaramide-based probe showed the highest labelling efficiency and sensitivity. In parallel, the sustainability of the glycan labelling workflow was evaluated by replacing acetonitrile with bio-derived solvent systems. Cyrene and 2,2,5,5-tetramethyloxolane (TMO) delivered comparable performance in labelling efficiency, reproducibility, and glycan profile integrity, while reducing environmental impact. Quantitative robustness was further enhanced using an internal standard and validated by HILIC-UPLC[2]. Together, these advances establish a versatile and scalable platform that integrates novel probe design with sustainable methodology, expanding analytical capabilities while reducing the environmental impact of glycoanalytical workflows.

References

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NON-POROUS SILICA FOR PROTEIN-A HIGH-PERFORMANCE AFFINITY CHROMATOGRAPHY OF MONOCLONAL ANTIBODIES

Devansh Shah[1,2], Dr. John Hanrahan[2], Prof. Eric Moore[1]
Presenter email address: 121102582@umail.ucc.ie

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[2]*Glantreo Limited, Cork, Ireland*

Accurate quantification of monoclonal antibodies (mAbs) is critical at all stages of biopharmaceutical development, particularly for monitoring cell culture harvest samples during upstream processing. High-performance affinity chromatography (HPAC) using immobilised Protein-A ligands offers improved speed, robustness and reproducibility over traditional immunoassays such as enzyme-linked immunosorbent assay (ELISA)[1]. Non-porous silica was chosen as the chromatographic support due to the absence of internal pore structures, which eliminates intraparticle diffusion limitations and enables faster mass transfer, especially when handling complex biomolecules such as IgG.[2]

In this study, Solad™ non-porous silica particles were successfully functionalised with recombinant Protein-A using a sulfhydryl-reactive coupling chemistry[3], and characterised by SEM and BCA assay. Initial column evaluation by HPAC with rabbit immunoglobulin G (IgG) standard demonstrated excellent chromatographic efficiency. Further evaluation with a monoclonal antibody feedstock sample confirmed effective separation of IgG from cell culture components, achieving a resolution of over 31 while maintaining high efficiency. Independent evaluation at WuXi Biologics, China, confirmed strong system suitability, linearity, and accuracy across multiple antibody formats, further demonstrating the robustness and industrial applicability of the non-porous Protein-A silica column for quantitative antibody analysis.

These findings highlight the potential of the non-porous Protein-A silica column as a robust and high-resolution tool for rapid mAb titre analysis. Ongoing work aims to broaden the platform's applicability to a wider range of antibody formats through the immobilisation of alternative ligands, such as Protein-G and Protein-L.

References

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Laser-Induced Graphene Based Sustainable Platform for Wearable Health Monitoring

Md Rasel[1], Jahidul Islam[1], Hassan Hamidi[1], Sofia Rodrigues Teixeira[1], Aidan J. Quinn[1], Daniela Iacopino[1]
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Wearable electrochemical sensors are emerging tools for continuous, non-invasive health monitoring in applications such as infant health care and chronic wound management. In this work, we present a flexible, low-cost multisensing platform based on laser-induced graphene (LIG) for the detection of pH and uric acid, targeting integration into wearable systems including baby diaper–based urine monitoring and smart bandage devices. The sensors were fabricated using a rapid, chemical-free direct laser writing process on polyimide substrates with a 450 nm visible laser, enabling scalable and sustainable production of conductive graphene structures.

The pH sensor was developed by modifying the LIG electrode with polyaniline nanostructures via electropolymerization. It demonstrated a near-Nernstian sensitivity of 56.7 mV/pH over a wide range (pH 4–10), with low hysteresis (2.29 mV) and minimal drift, indicating strong stability and reproducibility.[1] The uric acid sensor was developed without further modification on LIG, exhibited a good sensitivity covering the physiological range and good selectivity against common interfering species presents in biological fluids. Both sensing modalities were validated in artificial urine and artificial wound exudate, maintained stable and reliable performance, confirming suitability for realistic biological environments. The flexibility of the platform enables seamless integration into wearable formats for continuous monitoring of infant and wound-related biomarkers.

Overall, this study demonstrates a sustainable LIG-based multisensing strategy for dual wearable applications in infant urine diagnostics and chronic wound management, offering a promising route toward low-cost, real-time healthcare monitoring.

References

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77th Chemistry Colloquium
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A Rapid and Green HPLC Method Development Strategy for Pharmaceutical Compounds

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High-performance liquid chromatography (HPLC) remains the cornerstone analytical technique for the separation and quantification of pharmaceutical compounds. However, conventional method development approaches are often time-consuming, solvent-intensive, and environmentally burdensome. This project aims to develop a rapid and sustainable method development strategy by extending the Stationary Phase Optimised Selectivity LC (SOS-LC) concept to incorporate green mobile phase systems. Originally introduced as a forward-thinking tool employing serially coupled low-volume cartridges packed with chemically diverse stationary phases, the SOS-LC approach demonstrated the capacity to achieve robust separations through systematic optimisation of stationary phase selectivity across up to five coupled columns. Building upon this foundation, the present work seeks to evaluate the compatibility of the SOS-LC framework with environmentally friendly mobile phases for the analysis of pharmaceutical compounds.

A range of pharmaceutical test mixtures will be designed to encompass both structurally and physicochemically diverse compounds as well as closely related substances, such as active pharmaceutical ingredients (APIs) and their associated impurities. The performance of the green SOS-LC approach will be rigorously assessed through method validation and benchmarked against traditional HPLC method development strategies and the selectivity of the approach assessed for green mobile phases. The outcomes of this study will contribute to the advancement of greener analytical practices in the pharmaceutical industry, offering a time-efficient and environmentally conscious alternative to established method development workflows.

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BARDS -UV Characterisation of a dual formulation of mircrospheres as a Quality Control Tool

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Microspheres are spherical particles used as carriers for active pharmaceutical ingredients (APIs), typically composed of natural or synthetic polymers, and are widely employed to achieve controlled and targeted drug delivery. Cariban, indicated for the treatment of nausea and vomiting in pregnancy, utilizes a modified-release formulation in which its active ingredients, are incorporated into a polymer enabling delayed and sustained drug release and improving therapeutic efficacy and patient compliance. Such formulations are particularly useful for maintaining consistent plasma drug concentrations over extended periods. Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS) is an analytical technique that monitors changes in acoustic resonance during the dissolution of solid dosage forms in a liquid medium.

In this study BARDS-UV will be used to track the disintegration and dissolution of two API's in a mixture of microspheres made for each drug. The correct ratio of microspheres can potentially be tracked using this combined acoustic and light spectroscopy simultaneously in a rapid, real-time manner.

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DEVELOPMENT AND ASSESSMENT OF AN IMMERSIVE VIRTUAL REALITY EXPERIMENT FOR CHEMISTRY EDUCATION

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As part of the Virtual Labs Initiative, a suite of highly immersive and interactive virtual reality applications has been developed to address key gaps in chemistry students' hands-on experience with advanced analytical instrumentation, which are often expensive and have limited physical access. Among these applications is a VR experiment focused on Capillary Zone Electrophoresis, a technique with which few incoming postgraduate students have prior experience. Thus, they can benefit from the additional experience VR offers to prepare them for their degree examinations and industry challenges. Two cohorts of postgraduate students were involved in the development of the VR experiment, and their feedback was captured through surveys. The final cohort was split into a VR group and a control group, the latter watching a 2D video covering the same information as the VR experiment. Although the control group performed better in a theory quiz, students in the VR group found practical tasks easier. The student's self-reported confidence increased by the same amount for both groups and both groups gave positive feedback on their respective pre-lab interventions.

New Polycyclic Guanidine Alkaloids from Brazilian Porifera *Monanchora arbuscula*

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Brazil contains a highly biodiverse coastline and marine environment, with confirmed 612 species of porifera identified, 310 of which are endemic to Brazil[1]. *Monanchora arbuscula* from Brazil has been a rich source of polycyclic guanidine alkaloids (PGAs), with potent anti-viral, anti-bacterial and cytotoxic metabolites[2]. Dimeric PGAs, containing two cyclic guanidine moieties have been noted for potent anti-viral activity, such as batzelladine A[3]. In this study, the chemical diversity of *M. arbuscula* was analysed in order to isolate and elucidate new bioactive PGAs. The methods utilised were mass spectrometry ((+)-UPLC-ESI-MS/MS), preparative-HPLC-UV-ELSD for the annotation and purification of new PGAs, and 1D/2D NMR for structural elucidation. Two new PGAs were isolated from the methanolic fraction of *M. arbuscula* and MS/MS analysis revealed some homologues and analogues which will be targeted for future purification and elucidation. The reported PGAs mirabilin B, monaladine A, clathriadic acid and batzelladine C were also isolated. The isolated compounds will be tested for anti-bacterial bioactivity.

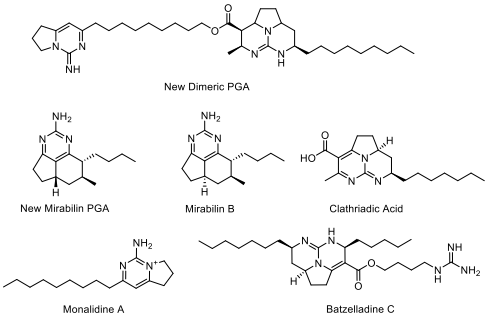

Figure 1: The structures of isolated PGAs from Brazilian M. arbuscula

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THE IMPACT OF STORAGE CONDITIONS ON INSULIN SOLID-STATE STABILITY

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Background: Therapeutic peptides in the solid-state are incorporated into various drug delivery systems. However, most research to date has focused on stabilising peptides in solution. The aim of the work presented was to investigate how solid-state morphological differences in peptide samples, using insulin as a model system, influence moisture uptake and physical stability upon exposure to environmental temperature and humidity.

Methods: The solid-state properties of recombinant human insulin powder supplied by Novo Nordisk and Merck were determined as received and following storage at 40°C/75% relative humidity (RH) for four weeks. A range of techniques were employed including flame atomic absorption spectroscopy (AAS), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC) and dynamic vapour sorption (DVS). Additional analyses are ongoing.

Results: Flame AAS confirmed an insulin: zinc ratio of approximately 3:1 for both sources of insulin. SEM revealed that the Novo Nordisk insulin particles have a more homogeneous morphological appearance while also revealing that Merck insulin particles appear to aggregate to a much higher degree post storage. DVS revealed differences in moisture interactions with Merck and Novo Nordisk insulin samples. The FTIR spectra of Merck and Novo Nordisk insulin samples post storage were altered compared to their starting materials and when compared to each other. The DSC thermograms indicate a key thermal event at 60°C, which likely represents an enthalpy relaxation in the solids. This thermal transition was still present but shifted to a lower temperature in the samples post storage.

Conclusion: Differences in insulin solid-state morphology influence moisture uptake and associated physical changes, with DSC and FTIR providing key insights into these stability effects. Ongoing work involving High-Performance Liquid Chromatography (HPLC), Nuclear Magnetic Resonance (NMR) and surface area analysis may reveal further chemical and physical stability insights for these samples.

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INVESTIGATION IN THE FORMATION OF TOXICANTS DURING THE PYORLYIS OF SYNTHETIC COMPONENTS OF E-LIQUIDS.

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The prevalence of e-cigarette use across Europe has risen significantly, with recent data indicating that up to 44% of 15–16-year-olds in Europe have reported previous use.[1] While often perceived as a safer alternative to combustible tobacco, the thermal degradation of synthetic flavouring agents in e-liquids remains a critical, yet under-characterized, source of potential pulmonary toxicity.

Graph Convolutional Neural Networks (GC-NN) were utilised to generate a library of predicted pyrolytic products which was then validated by APCI/ESI-MS, NMR and Bond Dissociation Energy calculations.[2] APCI/ESI-MS are employed as a screening technique to identify potential fragmentation patterns observed during vaporisation while NMR allows for product elucidation of vaporised synthetic flavour samples.[3-4] Bond Dissociation energies allowed for the energy required for a bond to break and therefore the temperature required to impart that amount of thermal energy, with this temperature identified it could then be seen if that specific mechanistic pathway was feasible under the typical conditions seen within an e-cigarette. Temperatures between 150°C–250°C primarily causes initial evaporation. [4]

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PH-DEPENDENT SWITCHABLE DNA ORIGAMI IN NANOCONFINEMENT

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Nanopipette sensors are an emerging class of low-cost, rapid sensing devices that provide a unique opportunity to expand the scope of electrochemical biosensors. These types of sensors work by measuring changes to the surface charge of the internal walls of an easy-to-fabricate nanopipette. When the surface of the pipette is charged, it creates an electrical double layer (EDL) overlap at the tip, resulting in a non-ohmic electrical response known as ion current rectification (ICR). This allows for a highly sensitive and tunable biosensor. This technology was combined with a switchable DNA origami zipper that undergoes a pH-dependent conformational change.[1] These conformational changes are monitored by a significant change in rectification. Conformational change can also be induced by changing the local pH inside the nanopipette by applying a voltage.[2]

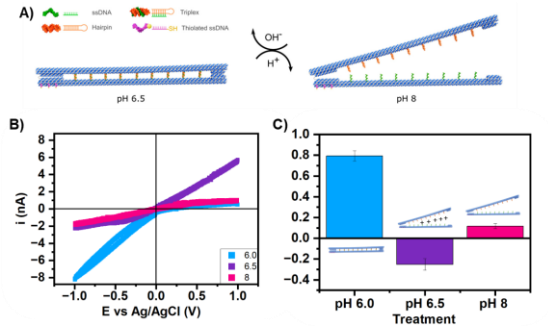

Figure 1. A) Conformational states of pH-dependent DNA origami zipper. B) CVs of nanopipettes functionalized with DNA origami zippers in different conformational states. C) Comparison of RR of each conformational state.

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SUSTAINABLE THERMO-RESPONSIVE 3D PRINTED MEDIA FOR ORGANIC SOLVENT-FREE HPLC SEPARATION

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Thermally Responsive Polymers are an emergent class of stationary phase materials for reverse phase liquid chromatography (LC). The phase of these polymers is temperature dependent, transitioning from a hydrophilic phase at low temperature to a hydrophobic phase at higher temperatures above Lowest Critical Solution Temperature (LCST).[1] The modulation of a stationary phases' behaviour via temperature control allows for optimization of elution times for target analytes and for the use of a thermal gradient in separations, replacing solvent gradients in RPLC within entirley aqueous separations.[1] Poly(N-Isopropyl Acrylamide) (PNIPAM) is an attractive material for this application due to its low LCST of c.32˚ C[1] and the wide availability of synthetic routes of PNIPAM films and hydrogels used in applications such as drug delivery and bioseparations.[1,2] Advancements in 3D printing technology have greatly improved the viability of 3D printed materials for use in LC systems.[2] Masked Stereolithography (MSLA) which utilizes high definition UV-LCD screens to create parts from photopolymer resin has greatly reduced the cost of Vat printing while maintaining the ability to create parts with high accuracy and small feature sizes. The main aim of this work is to fabricate 3D printed columns packed with well-characterized thermo-responsive PNIPAM stationary phase for chromatographic separations, utilizing a thermal.We aim to design and characterise a synthetic pathway for PNIPAM monoliths crosslinked with N'N methylbisacrylamide via a photoinitiated free radical polymerisation in a transparent 3D printed column. We will also evaluate the thermal response and chemical composition of these PNIPAM monoliths and apply them in separation of modular mixtures of pharmaceutically active compounds.

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ICI Chemistry Colloquium
University College Cork 2026

Method development for a bench top NMR and adaptation of this experiment towards a virtual reality laboratory

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This project aims to develop and validate optimized nuclear magnetic resonance spectroscopy protocols for the Spinsolve 90 Ultra multi-X system and to translate these protocols into a virtual reality laboratory training environment. The optimized procedures will be designed with reference to industrial experience and an existing NMR method, providing a validated foundation for both analytical application and educational translation.

NMR spectroscopy is a central technique for molecular characterization in modern chemistry, providing essential structural and quantitative information across pharmaceutical, chemical, and academic contexts[1]. However, practical NMR training remains challenging because of instrument cost, limited accessibility, safety considerations, and the conceptual difficulty of interpreting spectroscopic data. Virtual reality offers a promising approach to laboratory education by providing a safe, accessible, and repeatable training environment, while also supporting the visualization of abstract concepts and molecular-level phenomena[2].

In collaboration with Fourth Reality, this project will adapt the validated NMR procedures into an interactive VR laboratory. The final outcome will be an integrated analytical protocol and virtual training tool that supports both reliable NMR workflow development and innovative chemistry education.

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Title: "Development of High efficiency column packing for the production of 5um Non porous silica SOLAD by Normal phase HPLC Column".

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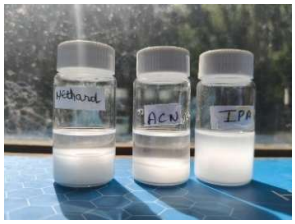
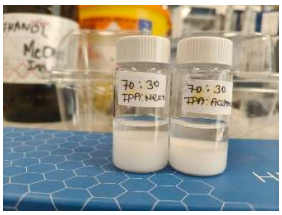
Introduction:

High performance liquid chromatography is a widely used analytical technique in pharmaceutical, chemical and research laboratories for the separation, identification and quantification of compounds. Silica is widely used as a stationary phase material in HPLC due to its strong mechanical stability and its surface area.

Selection of solvent is one of the critical steps in slurry preparation. It plays a major role in particle dispersion, sedimentation Rate and improves the overall packing uniformity. Therefore, solvent behaviour is crucial during the initial stages of the column packing.

The present study mainly focuses on the development of 5um non porous silica based normal phase HPLC columns. As part of the work, solvent selection was performed by using the sedimentation test to identify the most suitable solvents for the slurry preparation. The organic solvents such as Isopropyl alcohol, Acetone, Methanol, Acetonitrile, Hexane, 70:30 of IPA: Methanol, 70:30 of IPA: Methanol were tested based on their ability to controlled settling of particles. Sedimentation behaviour was monitored visually to identify the settling characteristics. The images include:





Further work: Based on the results of sedimentation test, the most suitable solvent was selected for the column packing with 5um non porous silica particles. The selected solvent was used to evaluate the packing efficiency and uniformity. Further studies mainly focus on the optimization of packing parameters such as concentration of slurry, packing pressure to achieve the reliable column performance. Furthermore, the optimized slurry packing system plays a major role in multi column packing tool, which enables the simultaneous packing of multiple HPLC columns with enhanced efficiency and stability.

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2. P. Keller, F. Ernl, H. R. Linder, and R.W. Frei*1 Analytical Research and Development, Pharmaceutical Division, Sandoz, Ltd., 4002-Basle, Switzerland.

3. Stan Perche pied, Harald Ritchie, Gert Desmet a, Sebastiaan Eeltink www.elsevier.com/locate/aca

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Characterisation of Dominant N- and O-Glycans in Uterine Tissue

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Infertility has been recognized as a significant global health concern for decades, affecting approximately 8–15% of couples worldwide and involving multiple contributing factors[1]. Among these, compromised endometrial receptivity in females is considered a critical underlying cause. Numerous proteins are expressed on the endometrial cell surface, and glycosylation serves as a key post-translational modification that plays an essential role in enhancing endometrial receptivity, promoting embryo apposition, and facilitating trophoblast adhesion and invasion, processes which are essential for successful embryo implantation[2].

In the proposed study, we characterised the major glycan motifs associated with uterine receptivity by analysing the dominant N- and O-glycans in uterine tissue obtained from fertile, subfertile, and infertile cohorts (n=20). A novel workflow was developed, adapted from established N-glycomics methodologies, to incorporate additional steps for comprehensive O-glycan characterisation. This includes the use of endoglycosidases and a non-reductive β elimination glycan release approach for the sequential release of glycans[3], followed by analysis using HILIC-UPLC.

Preliminary results indicate successful optimisation of the sequential glycan release protocol and demonstrate distinct glycan profiling patterns across cohorts, highlighting the potential role of glycosylation in modulating endometrial receptivity.

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The use of thermally responsive polymers in 3D printed columns for HPLC applications

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One of the major developments in Reversed Phase HPLC (RP-HPLC) is the use of mobile phase gradients, compared to isocratic mobile phases, to improve the peak quality for analyte measurements[1], particularly analytes with wide variances in hydrophobicity. While this mobile phase gradient usage is highly valuable in refining the separation performance of RP-HPLC, its usage of organic solvents, such as methanol and acetonitrile, is undesirable due to their toxicity and environmental impact. A less considered approach which would solve this issue is the development of a selectivity gradient within the stationary phase of a RP-HPLC system, eliminating the necessity for organic solvents.

Thermally responsive polymers appear to be a useful material class to achieve this, as their hydrophilicity is dependent on temperature, with the behaviour rapidly changing once the Lower Critical Solution Temperature (LCST) is exceeded. Of these materials, one of the most studied and practical polymers is poly(N-isopropylacrylamide) (pNIPAAm) due to its LCST of 32 °C[3], which makes it useful for biological activity in addition to practical LCST manipulation. In this work we explore the RAFT polymerisation of the NIPAM derivatives to form a modular monolith within 3D printed columns. These columns are fabricated using Masked Stereolithography (MSLA), a vat-based technique chosen for high precision and low cost that can be easily scaled up. The stability of the as synthesized monolith is examined via degradation studies, with the eluent of these studies examined via UV-Vis spectroscopy. The polymer synthesised for RP-HPLC use is to be characterised by a variety of techniques, such as Contact Angle wetting technique to determine its altering hydrophilicity in response to temperature, in addition to examinations of its swelling behaviour. Chemical and morphological characterization of the polymer is to be examined by FTIR, in conjunction with techniques such as SEM and NMR. Finally, the capacity for the polymer monolith to separate analytes is to be examined using a variety of pharmacological compounds with variable physicochemical properties.

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ICI Chemistry Colloquium
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DESIGN AND DEVELOPMENT OF AN IMMUNOSENSOR ASSAY FOR THE DETECTION OF ESTRONE IN WATER

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,Estrone is an endogenous estrogenic hormone, and its presence in aquatic environments may have harmful effects on aquatic ecosystems. Detection of estrone levels in water is important for assessing water quality, establishing and evaluating advanced water treatment, and complying with environmental regulations. This project focuses on evaluating the Enzyme-Linked Immunosorbent Assay (ELISA) for detecting estrone in water and on developing electrochemical immunoassay protocols for point-of-care aquatic ecosystems. The initial evaluation of estrone in water is performed by ELISA, which detects the antigen in water using an antibody-coated microplate. The validated ELISA protocol is then transferred to the electrochemical method and evaluated using gold nanoparticle-modified gold screen-printed electrodes. A gold nanoparticle-modified electrode is conjugated with estrone antibodies to selectively detect estrone. Detection sensitivity is evaluated using both physical and covalent antibody immobilization methods. This developed assay protocols for the detection of estrone in water, achieving lower detection limits, simpler sample preparation, and greater cost-effectiveness than conventional estrone detection methods, such as chromatographic methods, making it suitable for routine screening of estrogenic contaminants in the aquatic environment for point-of-care aquatic care.

SOLUBILITY OF GEFITINIB IN ORGANIC SOLVENTS: EXPERIMENTAL AND THEORETICAL INVESTIGATION OF STABLE AND METASTABLE FORMS

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Crystallisation is the dominant separation and purification technique in pharmaceutical manufacturing, with ~90% of active pharmaceutical ingredients (APIs) purified using this process *[1]*. Control of nucleation, crystal growth, and polymorphic form requires an understanding of solubility behaviour.

The solubility of gefitinib, a BCS Class II drug, was investigated in organic solvents, with ongoing work to isolate and characterise the metastable form and construct a complete solubility phase diagram and metastable zone width (MSZW).

Gefitinib shows strong temperature-dependent solubility, ranking 2-MeTHF > ethyl acetate > acetonitrile > toluene, correlating with solvent greenness *[2]* and hydrogen-bond acceptor ability, indicating enhanced solvation via interactions between the drug's hydrogen-bond donor functionality and more basic solvents *[3, 4]*. MSZW varies with saturation temperature, ranking 2-MeTHF > ethyl acetate > toluene > acetonitrile, indicating both thermodynamic and kinetic effects.

COSMOtherm (COSMO-RS) predictions using TZVP and TZVPD-FINE reproduced solvent ranking and temperature dependence; TZVP showed better agreement, while TZVPD-FINE overestimated intermolecular interactions.

Thermodynamic modelling identified the Yaws equation as the best-fitting correlation. Dissolution is endothermic and strongly enthalpy-driven, with $\Delta G°$ and $\Delta H°$ following the same solubility trend, while entropic contributions remain small.

Solubility differences are governed primarily by the enthalpic penalty of disrupting crystal lattice interactions, supporting greener solvents and improved, reproducible crystallisation design through solvent choice and seeding strategies.

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Analysis of residual solvents present in pharmaceutical products using HS-GC-FID

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Residual solvents are volatile organic solvents which are used or produced during the manufacturing of pharmaceutical products. These solvents are undesired and are not completely removed from the final products. This can affect the product quality, stability, and effectiveness if their levels exceed the acceptable limits established by the ICH.

This work will focus on nanoformulations and analysing residual solvents ethanol and acetone potentially present using gas chromatography-flame ionisation detection (GC-FID). Direct injection can be used when the tested sample is soluble in the organic solvent, while headspace (HS) injection is a good technique for semi-volatile and volatile solvents. HS-GC is the preferred technique for analysis of residual organic solvents in nanoformulations as it offers several advantages over direct injection. In using HS, only volatile components are introduced into the GC system, resulting in extended column lifetime and reduced instrument maintenance, providing superior sensitivity and reproducibility. Headspace sampling is conducted by placing a liquid or solid sample in a sealed vial until a thermodynamic equilibrium between the sample and gas phase is reached. A known aliquot of the gas phase analyte is then transferred to the GC for analysis.

HS-GC-FID is an effective and reliable technique for the analysis of residual solvents such as ethanol and acetone in nanoformulations to determine the quantity of these solvents and whether it follows the ICH guidelines.

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DEVELOPMENT AND VALIDATION OF A SEMI-TARGETED SCREENING METHOD FOR ANIMAL FEEDING STUFFS BY UHPLC-HRMS.

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Sources of animal feed contamination can be introduced by intentional adulteration, natural occurrences, or through accidental misuse. There is legislation in place that outlines the requirements for feed testing.[1] However, veterinary drugs and naturally occurring prohibited substances (NOPS) can enter the food chain through their presence in animal feed. Currently, there is no method available in Ireland that screens for feed contaminants on the Irish market. Samples are analysed for contaminants using confirmatory methods, which can be time-consuming and limiting.

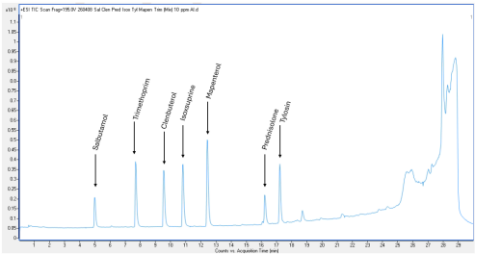

Figure 1. Separation of Salbutamol, Trimethoprim, Clenbuterol, Isoxsuprine, Mapenterol, Prednisolone and Tylosin in a 10 ppm mix.

A reverse phase chromatography method, employing a mobile phase gradient is currently being developed which screens for various β-agonists, antibiotics and NOPS in feed by UHPLC-HRMS. Initial work has taken place on a Thermo Ultimate 3000 HPLC and Agilent UHPLC-QTOF system, using an Eclipse Plus C_{18} column (100 x 2.1 mm, 1.8 µm), with the aim to optimise separation and fragmentation of the included analytes. Work will continue on a Thermo Orbitrap Exploris UHPLC-HRMS system to further improve the selectivity and specificity of the method. A QuEChERS-based sample preparation method will also be optimised. Once a suitable method has been developed and validated, it will be used to screen routine samples entering the Irish market.

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University College Cork 2026

Novel C4D Electrode Performance Analysis for Simultaneous Detection of Heavy Metals

Sri Navaneetha Krishnan K.S[1], Abhishesh Pal[2], Yineng Wang[2], Eric Moore[1,2] Alan O'Riordan[2]

[1] School of Chemistry, University College Cork, [2] Tyndall National Institute

Abstract:

Monitoring heavy metal contamination requires rapid, low-cost field analysis. Current portable microchip capillary electrophoresis methods lack the signal-to-noise ratio of benchtop laboratory equipment. This work evaluates the effects of dielectric layer composition and planar microelectrode geometry on the resolution of heavy-metal electropherograms using Capacitively Coupled Contactless Conductivity Detection (C4D). To characterize its analytical capabilities, the custom microfluidic platform is benchmarked against a laboratory-standard Agilent Technologies 7100 CE system using a priority heavy-metal mixture (Pb^{2+}, Cd^{2+}, and Cu^{2+}). Utilizing a fixed, optimized external readout interface, the study maps how microfluidic channel dimensions and electrode topology adjustments influence peak resolution, sensitivity, and separation efficiency relative to the commercial benchtop system. This systematic evaluation establishes design rules for optimizing chip-scale architectures, delivering a path toward laboratory-grade precision in a portable footprint without compromising hardware proprietary assets.

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Evaluating the impact of Green Mobile phases on HPLC Separation Selectivity for Pharmaceuticals.

Amal Raj[1], Melissa Hanna-Brown[1]
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In high-performance liquid chromatography (HPLC), selectivity is a major influence on the overall resolution of mixtures. The practical implications of selectivity are onerous for method developers as experimental optimisation involves changing mobile phase (buffer, pH, organic solvent, flow profile) and stationary phase (dimensions, morphology, derivatisation chemistry). Method development activities therefore are environmentally impactful and given the growing regulatory and environmental restrictions encouraging reduction in use of hazardous organic solvents, and promotion of more environmentally friendly methods in chromatography, separation science is looking to change its practices around selectivity optimisation. Swapping to green solvents however is not straightforward as instrumental pressure limitations, solvent cut-off wavelengths and reductions in selectivity space can influence chromatographic performance which is resulting in slow translation of method development practices.

This study is focused on the evaluation of the influence of green mobile phases on the separation selectivity in HPLC applications for pharmaceutical analysis. Conventional solvents are being compared with green solvents approaches for method development benefits and limitations together with alternative stationary phase base particle materials (non silica based including graphitic carbon and titanium materials) as well as particle morphologies (different porosity).

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ICI Chemistry Colloquium
University College Cork 2026

IDENTIFICATION AND QUANTITATION OF SYNTHETIC COOLANTS IN E-LIQUIDS USING GC-MS/MS

Laura Regan[1,2], Maureen Walsh[2], Reeta Joshi[2], Colmán Ó Ríordáin[1]
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E-liquids are a regulated substance in Ireland and are monitored by the HSE Tobacco Control Network Support Unit with analytical assistance provided by the State Laboratory. The device used to transform e-liquid into a vapour is known as an Electronic Nicotine Delivery System (ENDS). These devices and the liquid inside them are regulated under *S.I. No. 271 of 2016, European Union (Manufacture, Presentation and Sale of Tobacco and Related Products) Regulations 2016*. [1] Part of this legislation is the prohibition of any compounds that facilitate nicotine uptake or are known or suspected carcinogens.

The objectives of this research project are to develop GC-MS/MS methods suitable for the identification and quantification of hazardous analytes found in commercially available e-liquids for ENDS and to establish a profile of compounds in e-liquids available on the current Irish market.

A GC-MS/MS method has been developed to identify nine synthetic coolants that could potentially be used in ENDS. These coolants have the potential to facilitate nicotine uptake and there is very little research to date regarding the safety of these compounds when used in e-liquids. [2] GC-MS/MS was chosen as the analytical method as it provides greater selectivity and sensitivity compared to GC-MS and requires less sample preparation than LC-MS/MS. [3]

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ICI Chemistry Colloquium
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Nitrate and Nitrite Analysis in the Pharmaceutical Industry using Ion Chromatography

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Nitrate and nitrite are chemicals frequently and naturally found but can be react to form nitrosamines during pharmaceutical manufacturing. It is important to monitor the levels of nitrite and nitrate as nitrosamines are chemical compounds classified as probable human carcinogens. They form when nitrites, which can stem from nitrates, react with amines. Even trace amounts are very vital in pharmaceutical industry as it can affect the quality and safety of the final drug, hence it is necessary to detect and measure them accordingly.

The aim of this project is to detect nitrate and nitrite in pharmaceutical ingredients and products using ion chromatography (IC) with conductivity detection, a well-accepted technique for the determination of ions. One potential issue is some drugs contain a lot of chloride which can mask very small amounts of nitrite/nitrate interfering with the small nitrite/nitrate signal, making it difficult to detect and accurately measure nitrite and nitrate. To overcome this, samples will be prepared prior to analysis to avoid interference and improve results.

It is expected that this IC method will give consistent and reliable results even at low levels in pharmaceutical matrices, showing IC is a reliable technique for testing nitrates and nitrates in the pharmaceutical sector.

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Development of pipette-tip-based electrochemical sensors

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Many diseases are difficult to analyze due to the complex matrices of the body or the low concentration. Moreover, existing analytical methods are costly, time-consuming and require extensive sample preparation. Therefore, a novel pipette-tip-based electrochemical biosensor technique was developed to enable the detection of diseases and cancers in blood samples through a simple pipetting. The sensor quantifies a specific biomarker, a protein antibody naturally present in the blood, of patients carrying carcinogenic or disease-related molecules. This detection is achieved through a key combination of electrochemical properties and biomarker capture. The biosensor was fabricated from gold nanoparticles (AuNPs) co-functionalized with dopamine moieties, which provide traceable redox activity, along with target protein-specific antibodies. This approach offers a promising, highly sensitive single-step assay applicable to complex matrices such as blood. Furthermore, it requires less analysis time, lower cost, and smaller sample volumes compared to existing biomarker detection techniques.

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A Novel Green Fast HPLC Method Development Strategy for Biomolecules.

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Developing reliable LC methods for complex biomolecules is often slow, expensive, and technically demanding. This project explores an innovative approach by experimenting with the SOS-LC (Serially Optimized-Selectivity Liquid Chromatography) strategy, which combines stationary phases of different selectivity in series to achieve rapid optimal separations of complex mixtures. This concept, originally introduced by Sandra and co-workers[1,2], enables rapid optimization of chromatographic selectivity by connecting complementary stationary phases to create a broader and more flexible separation space. This approach has been shown to improve resolution and reduce method development time compared to traditional single-column strategies.

In this work, we are evaluating the POP-LC principle using conventional short HPLC columns connected with zero-dead-volume connectors for biomolecule separations. This poster will detail the background to the research, current progress and contextual benefits of such an approach.

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Exploring thermo-responsive polymers for green organic solvent-free HPLC

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Introduction:

High-Performance Liquid Chromatography (HPLC) plays a major role in pharmaceutical analysis, drug discovery, bioavailability studies, and clinical diagnostics. However, its dependence on hazardous organic solvents poses environmental and safety concerns. Thermoresponsive polymers offer a greener alternative by acting as smart materials that undergo reversible phase transitions in response to temperature changes, making them promising stationary phases in Temperature-Responsive Liquid Chromatography (TRLC).

Thermo-responsive polymers that undergo structural changes at certain temperatures offer a potential alternative to current LC separation strategies that rely mainly on the modulation of mobile phase polarity for elution compounds retained on stationary phases. Some of these polymers undergo a reversible change in their polarity in response to temperature change. This reversible switching enables analyte retention to be controlled solely By completely eliminating hazardous organic solvents from mobile phase and replacing temperature gradients. Although Poly(N-isopropylacrylamide) PNIPAm dominates this field, limitations in tunability and biocompatibility have encouraged exploration of alternatives such as Poly N-vinylcaprolactam (PNVCL), Pluronic F127, Poly(2-(2-methoxyethoxy) ethyl methacrylate ($PMEO_2MA$), Elastin-Like Polypeptides (ELPs), and Perfluoro (methyl vinyl ether) PMVE these polymers grafted silica beds are packed into a stainless-steel column for sustainable next-generation chromatographic applications.

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ICI Chemistry Colloquium
University College Cork 2026

Determination of Residual Solvents in Pharmaceuticals using Gas Chromatography-Mass Spectrometry

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Gas chromatography-mass spectrometry (GC-MS) is widely used for the identification and quantification of residual solvents due to its high sensitivity and selectivity. The residual solvents are volatile organic compounds that can remain in the pharmaceutical products after manufacturing or purification processes. Mainly, these solvents can easily affect the safety, efficacy and stability of pharmaceutical formulations. Commonly used solvents are methanol, acetone, and ethanol and so will be the targets of this work.

The main objective of this work is to detect and quantify the residual solvents in pharmaceutical products that have potentially undergone degradation due to incorrect storage, extreme conditions and beyond expiration using an optimised GC-MS method.

The separation of volatile compounds from the matrices is achieved by gas chromatography, while mass spectroscopy it is used for compound identification as accurate identification and quantification of residual solvents is essential in pharmaceutical quality control.

The GC-MS is a highly sensitive, accurate, and reliable technique for monitoring residual solvents in the pharmaceutical sector. It plays a significant role in ensuring compliance with regulatory standards and improving product safety.

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Industrial applications of Broadband Acoustic Resonance Dissolution Spectroscopy

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Abstract:

Broadband Acoustic Resonance Dissolution Spectroscopy is a spectroscopic analytical technique that monitors the change in the speed of sound in water. As soluble material is added to a glass vessel with a spinning stir bar near a microphone, a decrease in frequency will be detected immediately upon addition of the sample, due to an increase in compressibility caused by generation of microbubbles in the medium. The acoustic response is unique and reproducible for different materials and amounts of such at standardised conditions. This phenomenon is useful in the identification of counterfeit pharmaceuticals, measuring thickness of enteric coated particles and identifying if a solid blend is of uniformity. The first part of this project is about the method development of analysis of a range of samples provided to the lab by an undisclosed company in pharmaceutical manufacturing, with concerns of the quality of materials they are receiving from a new supplier. The samples which are not particularly soluble in water do not give great BARDS responses and are not giving consistent results across different experiment runs. A 20% 1-propanol mixture in de-ionised water was employed as the medium for each sample and yielded distinguishable and reproducible results for most of the samples. Each was run in duplicate or triplicate across a range of concentrations.

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Thermo-responsive polymers for HPLC applications

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Abstract: Thermo-responsive polymers have emerged as an important group of smart stationary phases in high-performance liquid chromatography (HPLC), which can be modulated by temperature instead of organic solvent gradients[1]. Previous research has focused on grafting them on silica beads which can undergo reversible conformational changes around their lower critical solution temperature (LCST) or upper critical solution temperature (UCST)[2]. At LCST, polymers exist as hydrophilic in nature (expanded) whereas at UCST, they exist as hydrophobic in nature (collapsed). They have demonstrated promising applications in biomolecule separation, therapeutic drug monitoring by reducing organic solvents [3]. In this study, we are focused on the development of a plethora of temperature-responsive polymers responsible for altering their hydrophilicity and porosity in response to temperature. The main aim of this study is to establish efficient synthetic routes for potential thermo-responsive polymers. In parallel, the project focuses on the evaluation of changes in hydrophilicity and porosity of polymer across a defined temperature range.

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BARDS -UV Characterisation of MUPS formulation of Omeprazole Tablets as a Quality Control Tool

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Disintegration and dissolution testing are fundamental to pharmaceutical quality assessment, yet conventional methods remain slow, separate, and offline, limiting their ability to capture dosage form behaviour in real time. Here we present BARDS-UV-Vis, an integrated analytical platform combining Broadband Acoustic Resonance Dissolution Spectroscopy (BARDS) with ultraviolet-visible spectroscopy for continuous, in situ monitoring of tablet disintegration and active pharmaceutical ingredient release. Using Losec MUPS (Multiple Unit Pellet System) tablets containing omeprazole as a model formulation, the system captures the complex two-stage release process involving initial tablet disintegration followed by microsphere dissolution under changing pH conditions. We show that BARDS-UV-Vis enables second-by-second monitoring of both physical dosage form breakdown and dissolution kinetics within a single workflow, providing enhanced temporal resolution and improved process understanding compared with conventional USP dissolution testing. By directly correlating disintegration behaviour with drug release profiles, the platform offers a more comprehensive and information-rich approach to pharmaceutical quality control. These findings demonstrate the potential of BARDS-UV-Vis for real-time quality monitoring, process analytical technology, and future GMP-compatible pharmaceutical manufacturing applications

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Electrochemically Deposited Ag and Cu Nanostructures for Surface-Enhanced Raman Scattering Sensors

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Surface-enhanced Raman scattering (SERS) is a powerful analytical technique for trace chemical detection, relying on plasmonic enhancement at nanostructured metallic surfaces. The interplay between surface morphology and chemical functionality is critical in governing analyte adsorption and signal amplification.

Here, we report the electrochemical fabrication of silver (Ag) and copper (Cu) nanostructures on microelectrodes and evaluate their performance as SERS-active substrates. Ag electrodeposition produces fractal nano dendritic structures, while Cu forms nanostructured roughened films, offering distinct surface chemistries and enhancement properties.

Functionalization with 4-mercaptobenzoic acid (4-MBA) yielded pH-responsive SERS substrates. The protonation state of the carboxylic acid group was monitored spectroscopically, enabling pH sensing in buffered solutions and in complex media such as milk, where spoilage-related changes were tracked. Additionally, 4-MBA-modified Au substrates were used to probe local pH variations during electrochemical reactions.

These results highlight the importance of combining controlled nanostructure fabrication with tailored surface chemistry to develop selective and versatile SERS-based chemical sensors.

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Deep Eutectic Solvent Mediated Synthesis of Spinel Oxide Nanomaterials

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Deep Eutectic Solvents (DES) are an emerging class of solvents formed from mixtures of hydrogen bond donors (HBD) and hydrogen bond acceptors (HBA), which exhibit melting points significantly lower than those of their individual components due to strong intermolecular interactions[1]. Since their introduction, DESs have attracted increasing interest as sustainable and versatile media for materials synthesis, offering advantages such as low toxicity, biodegradability, and tunable physicochemical properties.[2]

Here, a series of magnetic ferrite spinels (MFe_2O_4; M = Fe, Co, Ni, Zn) have been synthesised using DES-based approaches, with particular emphasis on investigating the effects of reaction temperature and time on phase and size control. The obtained materials have been characterised XRD, IR, TGA, and electron microscopy. These studies reveal that DES are a viable medium for the environmentally benign, tuneable, production of functional mixed metal oxides nanomaterials.

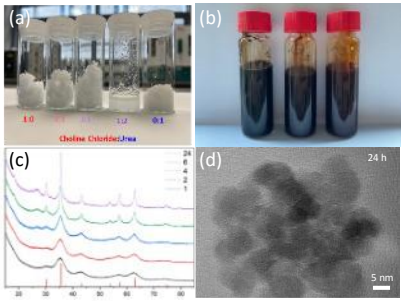

Figure 1: Choline chloride/urea DES (a), dispersions of DES synthesised magnetic nanoparticles (b), XRD patterns showing particle size evolution (c), and TEM image of $NiFe_2O_4$ (d).

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SOLID STATE Cu_2O@METAL CATALYSIS OF THE CO_2 REDUCTION REACTION

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The carbon dioxide reduction reaction (CO_2RR) is an electrochemical process that enables carbon capture and utilization, turning waste CO_2 into useful chemicals *e.g.* CO, methane, ethylene, or ethanol.[1] A key component of this process is a catalyst, as it provides active sites to absorb and bend the very stable CO_2 molecules making them easier to reduce.[2] The resultant products of reduction are heavily dependent on the type of catalyst that is used. Recently a solid state core-shell catalyst (Cu2O@Pt shell) was produced by the immobilisation of 30 nm Pt nanoaprticles on a Cu^0 layer and subsequent annealing at 350 ^oC yielding immobilised 60 nm nanocubes with a Pt core/Cu_2O shell.[3] These substrates showed excellant activity for methanol fuel cells. Growing interest in Cu_2O for the CO_2RR reaction has been seen in the last decade due to it being expensive, tunable, and capable of forming valuable C_1 and C_2 products. The work presented here will look at the effectiveness of this solid state core-shell nanostructured catalyst for the CO_2RR using an electrocatalytic H-cell. Also, recent reports on the use of Cu_2O-Ag alloyed have demonstrated to greatly enhance the CO_2 electrochemical performance as Ag boosts CO generation.[4] Preliminary results will be presented on the replacement of Pt with Ag with the hope that positive results would enable moving from the expensive rare earth metal Pt.

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'From Fashion to Function: Recycling Polyester into High-Value Materials'

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In recent decades, the global fashion industry has shifted toward rapid consumption and fast-changing trends, increasing textile waste.[1] Clothing purchases in Europe rose from 17 to 19 kg per person between 2019 and 2022.[2] This highlights the need for scalable recycling strategies for polyester (PET), a widely used synthetic fibre.

Current PET recycling includes mechanical and chemical approaches. Mechanical recycling reduces fibre length and material quality upon repeated processing.[3] Chemical recycling, particularly PET glycolysis, offers high monomer recovery under mild conditions. However, industrial application is limited by long reaction times and energy-intensive heating.[4]

This work investigates microwave-assisted glycolysis of dyed PET post-consumer textiles using ethylene glycol and a non-toxic catalyst to produce bis(2-hydroxyethyl) terephthalate (BHET), a valuable monomer for upcycling. The method improves heating efficiency, reducing reaction time and energy consumption while maintaining high monomer yields.

In this work, minimal variation in BHET yield was observed between dyed and undyed fibres, indicating dyes do not significantly inhibit depolymerisation. An in-process method for removing residual dyes from BHET crystals was also demonstrated. Additionally, selective depolymerisation of PET in polycotton blends enabled full cotton recovery.

Future work will focus on functionalising BHET for 3D-printable polymer materials. Overall, this work presents a faster, more energy-efficient, and scalable recycling strategy for real-world textile waste, supporting circular economy solutions.

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Development and Comparative Electrochemical Characterisation of Iron-Nickel Alloy Microelectrodes for Electrochemical Microsensors

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Abstract:

This study investigates iron-nickel alloy as a cost-effective alternative to noble-metal electrode materials for electrochemical microsensor applications. This research focuses on the fabrication and electrochemical characterisation of iron-nickel electrodes on both macroelectrode substrates and microfabricated electrode arrays alongside conventional noble-metal-based systems in order to evaluate electrochemical activity, stability, and overall electrochemical performance.

Microelectrode arrays are fabricated using photolithographic patterning and thin-film deposition techniques to produce structured electrode surfaces for electrochemical analysis. Surface behaviour and electrochemical performance are investigated profilometric, microscopic, potentiostatic, and voltammetric techniques, with cyclic voltammetry being utilised to characterise the electrochemical behaviour of both iron-nickel and noble-metal electrode systems. Electrochemical glucose detection is being used to validate electrochemical performance and assess the suitability of iron-nickel alloy for sensing applications.

Through comparison of the electrochemical analysis, this study aims to determine the potential of iron-nickel alloy as a low-cost alternative to conventional noble-metal electrode materials for future electrochemical microsensor technologies.

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SYNTHESIS AND OPTICAL PROPERTIES OF UNSYMMETRIC AROMATICALLY π-EXTENDED BODIPY

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BODIPY dyes are widely used across sensing, imaging and photochemical applications,[1] yet access to compact dyes that absorb and emit in the red/NIR region remains limited. Recent work has highlighted that introducing asymmetry into the BODIPY core can influence photophysical behaviour allowing for fine-tuning of optical properties and enhancement of intersystem crossing.[2] In this study we use asymmetrical substitution to redshift BODIPY absorption/emission maxima using an optimised modular route to asymmetrical BODIPYs (**aBDPs**) through condensation of corresponding pyrrole carboxaldehydes with alkyl-substituted pyrroles. This designed approach recorded increased yields of the target **aBDP** (41-75%), improved isolation and purification efficiency and reduced yields of undesired symmetrical BODIPY by-products. A library of **aBDPs** was synthesized, and subsequent aromatization yielded asymmetrical benzo- (**aBBDP**) and naphtoBODIPYs (**aNBDP**).

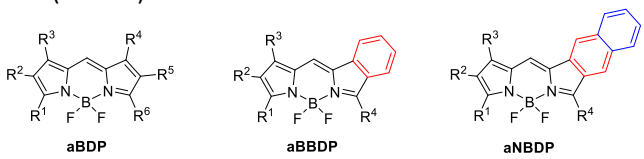

Figure 1. General structures of **aBDPs**, **aBBDPs** and **aNBDPs**.

Synthesized **aBBDPs** and **aNBDPs** displayed intense fluorescence in the red region with emission maxima panning 590-680 nm and fluorescence quantum yields ranging from 27% to 84%, while selected **aBDPs** demonstrated triplet formation and singlet oxygen generation quantum yields up to 20% in toluene. This work provides an effective route to asymmetrical BODIPYs and shows how controlled substitution can shift absorption toward the red/NIR while retaining compact structures.[3]

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NICKEL BASED ELECTRODEPOSIT CATALYSTS FOR OXYGEN EVOLUTION REACTION

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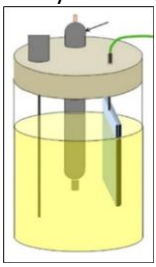
Oxygen Evolution Reaction (OER) is the anodic half-cell reaction involved in electrochemical processes, in this project the relevant process is water splitting [1]. OER requires a four-electron transfer process, contrasting with the comparatively simple Hydrogen Evolution Reaction (HER) process which is the corresponding half-cell reaction. This leads to problems such as high energy loss, poor chemical kinetics and the requirement of a large overpotential to function [2] necessitating the development of stable and efficient electrocatalysts with improved chemical kinetics for use in energy applications of OER such as fuel cells [1]. One method of synthesis of electrocatalysts is electrodeposition using metallic salts. Here, a fixed potential is applied to an electrode as the electrode sits in a solution of metal ions. An electrodeposit (ED) is formed directly at the surface of the electrode from the nitrate salts used as the source of metals in this project. Figure 1.1 [3] shows a sample Electrodeposition cell with porous Nickel Foam working electrode. The method for the electrodeposition can be seen in Figure 1.2. Optimisation of the parameters for deposition, for example, deposition time, potential, ion concentration and ion ratio has led to the optimisation of the catalyst for OER in terms of onset potential, high peak current density and a steep rise in current density.

Figure 1.1



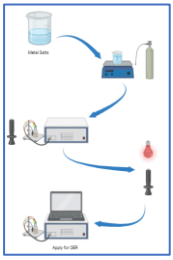


Figure 1.2

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ADVANCING CIRCULAR ECONOMY IN THE TYRE INDUSTRY VIA GREEN CHEMISTRY UPGRADING OF RECOVERED CARBON BLACK

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The accumulation of end-of-life tyres (ELTs) presents a significant environmental challenge due to their large-scale production and resistance to degradation.[1] Conventional disposal methods, including landfilling and incineration, contribute to pollution and the loss of valuable resources, underscoring the need for more sustainable and circular management strategies. Pyrolysis offers a promising route for ELT valorisation, producing recovered carbon black (rCB) with potential as a sustainable alternative to fossil-derived virgin carbon black (vCB).[2,3] However, rCB typically exhibits high ash content, low surface area, and limited surface reactivity due to residual inorganic species, restricting its application as a high-value material. Conventional demineralisation methods often require harsh conditions, including high temperatures and concentrated acids or bases, leading to environmental concerns such as hazardous effluent generation.[3] In this work, hydrogen peroxide-based treatments were investigated under ambient and microwave-assisted conditions as a more sustainable strategy for rCB upgrading. Reaction parameters were evaluated to obtain optimal ash loss. Reduction in ash content is expected to improve pore accessibility and surface functionality, key factors governing its performance as an advanced carbon material.

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HETEROMETALLIC PORPHYRIN DIMERS FOR APPLICATIONS IN QUANTUM TECHNOLOGIES

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Quantum computers are built of quantum bits (qubits). Paramagnetic coordination compounds of Cu^{II} or V^{IV} can be used as qubits since their projection of S = ½ can be used as basis states for quantum computation.[1] Porphyrin complexes of these ions have attracted a great interest due to their good quantum properties like long coherence times.[2] Modifications of the porphyrin scaffold with organic synthetic approaches enable the merging of paramagnetic centres in multi-qubit architectures, i.e., quantum logic gates. Magnetic interactions between the two metallic centres can be tuned to match the requirements of quantum computing.[2] An example is represented by the heterometallic meso-meso linked porphyrin dimer of Ranieri *et al.*[3], which combines the right intensity of magnetic coupling interaction (10^{-3} cm^{-1}) with the single spectral addressability through EPR spectroscopy of Cu and V ions.

To move a step further, here we present a similar approach to investigate the possibility of including within the same architecture a coherent ion, i.e., V^{IV} or Cu^{II}, and Cr^{III} ion characterized by a S = 3/2 state. The second ion can be used as a multilevel qubit to increase the number of logical operations.[4] Tuning of the magnetic interactions will be pursued with the architectures shown in Figure 1.

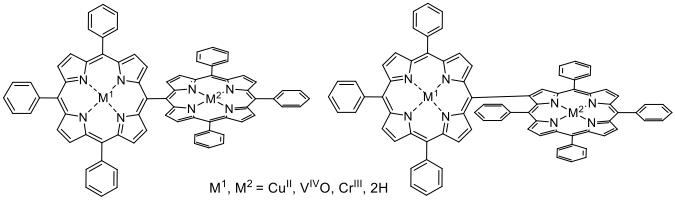

Figure 1. Targeted heterometallic meso-meso and meso-beta linked porphyrins.

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Bicyclo[1.1.1]pentane building blocks as material isosteres in metal-organic framework

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Metal-organic frameworks (MOFs) are known for their selective absorption and high surface area and find application in energy storage, gas storage and separation, purification, catalysis, sensing, and drug delivery.[1] Traditionally, alkynes and aromatics are used as organic ligands as their rigidity facilitates the formation of a highly ordered structure. However, the use of alkynes and aromatics limits the functionality of the pore to π-π interaction, ionic-π interactions, metal-π interactions, polar-π interactions, and σ -π interaction.[2] To eliminate the use of aromatics and alkynes, rigid aliphatic compounds such as bicyclo1.1.1pentan (BCP) can be used.

BCP is a rigid, aliphatic, three-dimensional hydrocarbon, which is used in medicinal chemistry as a bioisostere for phenyl rings and alkynes.[3] Recently, this concept was transferred to material science, where BCP containing MOFs showed improved adsorption selectivity due to the tuning of the pore topography, and pore shape.[4,5] So far, only commercially available bicyclo[1.1.1]pentane-1,3-dicarboxylic acid has been used as a linker in MOF generation. Therefore, the synthesis of more advanced linkers with various angles is in demand and is the target of this work. Here, we present such advanced linkers developed from BCP aldehyde **1** and BCP alkyne **2**.

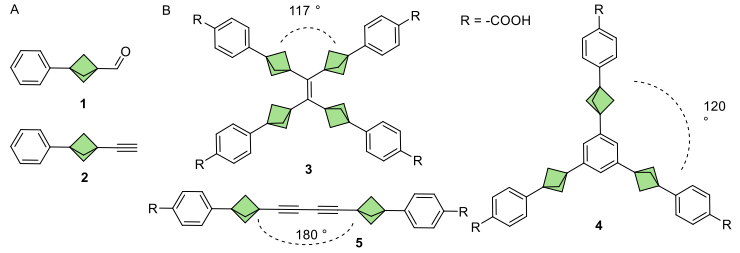

Figure 1: Targeted MOF linkers (B) and their key precursors (A)

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DEEP EUTECTIC SOLVENT MEDIATED SYNTHESIS OF CADMIUM SULFIDE QUANTUM DOTS

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Deep Eutectic Solvents (DES) are a novel class of solvents comprised of a mixture of two or more hydrogen bond donors (HBD) and hydrogen bond acceptors (HBA). These solvents have a melting point significantly lower than that of their individual components, owing to strong hydrogen bonding interactions. Since their introduction, DESs have been widely studied for a range of applications such as electrodeposition, extractions, battery technologies and nanomaterials synthesis.

DESs are widely considered to be "green" solvents for a number of reasons. Depending on the choice of HBA and HBD, DESs can be non-toxic, biodegradable and inexpensive solvents. In addition to addressing sustainability concerns, careful choice of the HBA and HBD can allow the tuning of the physicochemical properties of nanomaterials synthesised in the DES. In conventional nanomaterials synthesis, such control requires precise manipulation of reaction conditions. The highly tuneable nature of DES can simplify this process, as swapping the HBA or HBD of the solvent can alter its viscosity, ion mobility, solvation ability and coordination ability.

Quantum dots (QDs) are semiconducting nanoparticles with a diameter of between 2-10 nm. They have a wide range of applications, including QLED displays, sensitised solar cells and photoluminescence sensing. The optical properties of QDs depend strongly on the particle size, highlighting the need to be able to carefully control the nucleation and growth of these particles. Hot-injection synthesis is widely accepted as the conventional method for the size-controlled synthesis of QDs. While control over particle size can be obtained, there are sustainability concerns relating to the use of organic solvents and the elevated temperatures and therefore high energy costs associated with the synthesis.

Here, we report the use of a choline chloride-urea DES for the synthesis of cadmium sulfide QDs. The effects of precursor ratio and synthesis temperature on the nucleation and growth of the QDs have been evaluated and it has been shown that this DES can act as a viable solvent for the size-controlled synthesis of cadmium sulfide QDs.

EVOLUTION OF CRYSTAL PHASE COMPOSITIONS IN Fe-Ni (OXYHDR)OXIDE SYSTEM

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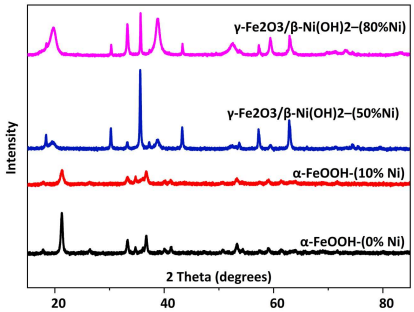
Iron-Nickel (oxyhydr)oxides have proven to be one of the most promising platinum-group-metal-free (PGM-free) electrocatalysts for oxygen evolution reaction (OER) in water [1]. However, there remain knowledge gaps regarding structural and phase transitions as Ni/Fe synthesis ratios are varied. Literature has so far not been able to clarify whether single or multiple crystalline phases are formed when different Ni-Fe synthesis ratios are varied at constant hydrothermal conditions [2]. Herein, we present a study demostrating crystalline phase transformations in Ni-Fe (oxyhydr)oxide systems induced by varying Ni content ($n_{Ni}=n_{Ni}/[n_{Ni}+n_{Fe}]$) at constant hydrothermal conditions.



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EXPLOITING COCCOLITH SCAFFOLDS FOR ENGINEERED MICRO-DEVICES

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Coccoliths produced by coccolithophore algae are naturally occurring calcite calcium carbonate ($CaCO_3$) scaffolds with intricate micro- and nanoscale morphologies that are difficult to reproduce synthetically[1]. Previous work from CerebroMachines Lab demonstrated that polydopamine (PDA)-functionalized *Emiliania huxleyi* coccoliths, termed *Robocoliths*, can convert light into heat and collective swarming motion, with PDA acting as the light-responsive component with the coccolith asymmetry contributing to enhanced motion[2]. This project investigates coccolith-derived $CaCO_3$ scaffolds with further morphology-defined substrates for PDA functionalization. Selected coccolithophore strains were cultivated and screened for their ability to provide recoverable calcified material. Coccolith isolates from *Chrysotila carterae* and *Hymenomonas lacuna* were assessed by SEM-EDX and FTIR to evaluate morphology, elemental composition, and calcium-carbonate-associated spectral signatures. Recovered samples showed morphologically interpretable coccolith structures and reproducible calcite $CaCO_3$-associated signatures. Preliminary PDA functionalization experiments indicated coccolith-associated deposition; however, aggregation and coating heterogeneity remain important parameters for further optimization. Overall, these findings support the development of coccolith-derived $CaCO_3$-PDA hybrids as biomaterials that combine natural mineral architecture with functional surface chemistry for potential applications in light-responsive microdevices.

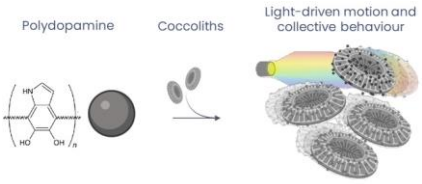

Figure 1. Robocoliths created via organic-inorganic hybrid combination (coccolith-polydopamine) display micromotor-like movement upon light excitation.

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Ceria nanoparticle on alumina as highly tuneable and portable colour comparator essay for gas phase H2O2.

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The rapid and reliable detection of hydrogen peroxide (H_2O_2) vapours is of increasing importance in occupational safety, industrial hygiene, and homeland security, owing to both its widespread use as a disinfectant and its infamous role as a precursor in improvised explosives. Conventional electrochemical sensors, while effective, require continuous power and frequent calibration, limiting their reliability for continuous deployment. Here, we present a tuneable, portable and reusable colourimetric sensing platform based on cerium oxide (CeO_x) nanoparticles immobilised within an anodic aluminium oxide (AAO) substrate for the detection and quantification of gaseous H_2O_2.

CeO_x tags were made using sol–gel synthesis of a cerium precursor directly within the porous AAO matrix, followed by calcination to form nanoparticles assembled within the substrate channels. Exposure to H_2O_2 vapour induces a concentration dependent colour change arising from oxygen buffering properties of nano-scale ceria associated to the redox transitions between Ce^{3+} and Ce^{4+} species, enabling quantification through digital image analysis using a camera or RGB sensor. The tuneable performance is achieved by varied calcination temperature (350 °C, 400 °C, and 430 °C) affecting the nanoparticle crystal size, morphology, and redox behaviour. Structural and chemical characterisation was performed using X-ray diffraction, scanning electron microscopy, and X-ray photoelectron spectroscopy.

The AAO substrate provides high thermal stability, allowing complete regeneration and reuse of the sensing tags via low-temperature heating, representing a significant advantage over single-use paper-based systems. This passive sensing approach offers continuous assay readiness without the need for power or frequent calibration and demonstrates strong potential for low-cost, scalable deployment in industrial environments and security screening applications.

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A PORPHYRIN POLYETHYLENIMINE POLYMER AS AN EFFECTIVE PHOTOSENSITISER FOR HYDROGEN EVOLUTION

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Increased CO_2 concentrations in the atmosphere have contributed greatly to the greenhouse gas effect and subsequently climate change.[1] Thus, there has been growing interest in renewable energy sources including hydrogen gas. TiO_2 semiconductors have been used to photocatalytically reduce water to hydrogen.[2] However, as a broad band-gap semiconductor TiO_2 is limited to the absorption of UV light, which only accounts for 4% of all light emitted by the sun.[3] Visible light represents a larger portion of the solar irradiance spectrum at 46%. Hence, we have synthesized a porphyrin-appended polyethylenimine polymer, **PEI-ZnTPP**, (see **Figure** 1 for structure) with strong light absorption properties in the visible region, and have utilized this polymer in the preparation of nanocomposites with TiO_2 thus increasing the overall solar energy harvesting capability of the semiconductor material.[4] When tested for photocatalytic hydrogen evolution (PHE), in conjunction with platinum as a catalyst, the prepared nanocomposites had an impressive PHE rate of 36,750 μmol g^{-1} h^{-1}. This disproportionately high rate is attributed to favorable electron transfer from the **PEI-ZnTPP** polymer to the TiO_2 surface following photoexcitation, which is evident through thermodynamic and electrochemical analysis of the nanocomposites.

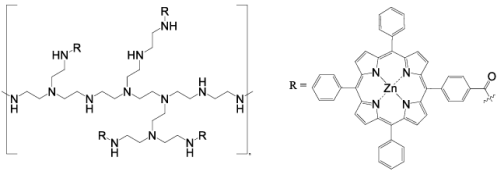

Figure 1: Structure of PEI-ZnTPP polymer used to prepare nanocomposites for PHE.

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UNDERSTANDING THE CHEMISTRY OF IRON-SULPHUR CLUSTERS USING MACHINE-LEARNT INTER-ATOMIC POTENTIALS

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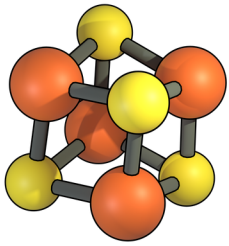

Figure 1: A small iron-sulphur cluster. Iron atoms are shown in orange, sulphur in yellow.

The industrial conversion of nitrogen to ammonia, an essential component of fertiliser, is energy intensive due to the high pressures and temperatures required. Nature achieves this reaction under milder conditions using the nitrogenase enzyme, which incorporates iron-sulphur clusters (Figure 1) at the active sites. The theoretical study of iron-sulphur clusters is impeded by the extreme complexity of their electronic structure, with computational studies through density functional theory (DFT) rapidly becoming unfeasible for larger clusters approaching the size of those found in nature.[1] Acceleration of the required calculations can be achieved through machine-learnt inter-atomic potentials (MLIPs), however no MLIPs with support for such spin coupled systems have been developed thus far. The work presented includes a new MLIP based upon SpookyNet[2] and extended to model the spin-coupling behaviour of such systems. By training the MLIP on a sample of DFT calculations and then applying it to example iron-sulphur clusters, the nature of their ability to bind nitrogen has been explored. The technique also finds broader application in reaction discovery and catalyst design.

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Thiol-yne Mediated Covalent Conjugation-Induced Self-Assembly for Multiscale Polymeric Biomaterials

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Polymeric Nanoparticles (PNPs) are promising for drug delivery due to versatility. Traditional preparation, such as self-assembly of amphiphilic block copolymers and emulsification polymerisation, have poor control and surfactant toxicity. Conjugation induced self assembly (COSA) is an emerging alternative to prepare PNPs. This study reports the synthesis of new water soluble and alkyne derived-polymer that undergo COSA based on UV-light mediated thiol-yne click chemistry. We uncovered the role of molar mass, crosslinking density and irradiation time on the formation of PNPs along with the possibility to load doxorubicin in-situ. DTT and LAP were the crosslinker and photo-initiator. The TEM images in figure 1a) confirm the NP formation over time as by two minutes of irradiation the polymer has assembled into spherical NPs of about 200 nm with the size increasing to just under 1 µm by 5 minutes. The DLS results in figure 1b) also confirm this result. The alkyne band is still present in the Raman spectrum in figure 1c) indicating that functionalisation of NPs is possible. We report an approach to control the formation of functional polymeric materials based on thiol-yne click chemistry which is appealing for drug delivery and imaging.

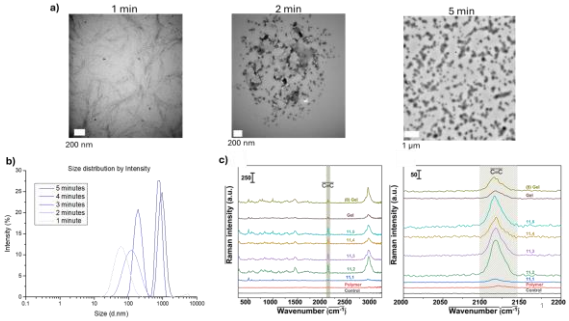

Figure 1: *a) TEM images of the polymer forming nanoparticles, b) DLS size distribution by intensity at a polymer concentration of 50 mg/ml and 50% cross linking density c) Raman spectrum highlighting the decrease in intensity of the alkyne bond.*

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HARVESTING THE MINERALIZATION ABILITY OF STONY CORAL PROTEINS TO CREATE BONE-MIMETIC CALCIUM PHOSPHATE COMPOSITES

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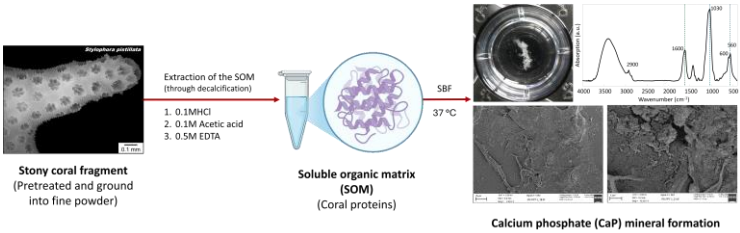
Developing scalable bone-mimetic composites that reproduce the hierarchical structure and physicochemical and biological performance of native bone remains a major challenge in regenerative biomaterials [1]. Here, we investigate whether soluble skeletal organic matrix (SSOM) proteins extracted from the scleractinian corals *Pocillopora damicornis* and *Stylophora pistillata* can be redirected to mediate calcium phosphate mineralization for bone-like material fabrication. SSOM proteins were isolated by decalcification using HCl, acetic acid [2], and EDTA; extracts were compared in terms of protein yield, molecular weight distribution by SDS-PAGE, and mineralization ability. HCl extraction produced the highest protein recovery. The mineralization potential of HCl-derived SSOM proteins was evaluated in simulated body fluid against control systems comprising bovine serum albumin and synthetic polyelectrolyte analogues. Only coral-derived SSOMs promoted rapid deposition of bone-like calcium phosphate. Characterizations by FTIR, SEM, TEM, and solid-state NMR suggest intimate association between the proteinaceous matrix and calcium phosphate nanoparticles, while potentiometric Ca^{2+} binding measurements showed strong and selective calcium affinity. Together, these findings show that coral skeletal proteins direct calcium phosphate mineralization and represent promising biomolecular agents for collagen-based scaffolds, offering a route toward next-generation bone repair materials with improved matrix–mineral integration.



Graphical Abstract. Coral-derived SOM proteins guide calcium phosphate mineralization in SBF

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Investigating the photophysical properties and photocatalytic activity of Re(I) complexes with D-π-A ligands towards the reduction of CO_2 to formic acid.

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Today, fossil fuels account for approximately 80% of the global energy supply.[1] This overdependence on burning fossil fuels to meet global energy demands and the associated emission of greenhouse gases such as CO_2 has been the primary contributor to climate change. Hence, there has been a push towards more sustainable energy solutions, such as green H_2, to mitigate its adverse effects. Inspired by photosynthesis, photocatalytic CO_2 reduction is seen as a potential approach to convert CO_2 into formic acid, a H_2 storage medium. Re(I) α-diimine complexes have been known to facilitate photocatalytic CO_2 reduction but are typically selective for CO and have poor visible light absorption.[2] Herein, to tune the selectivity towards formic acid and to enhance their visible light absorption, a series of Re(I) phenanthroline complexes bridged to a phenoxazine moiety (Figure 1), in a donor-π-acceptor system (D-π-A), were synthesized and assessed for their photocatalytic activity. These results alongside their steady state and time-resolved photophysical properties will be presented.

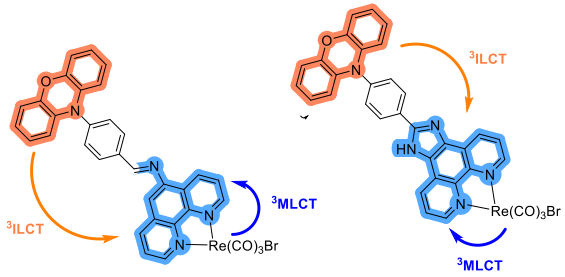

Figure 1: Structures of D-π-A Re(I) complexes. (Donor in orange and acceptors in blue).

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Porous Anodic Alumina Templates for Magnetic Micro/ Nano-wires for Biomedical Application.

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Porous anodic alumina (AAO) templates were fabricated using a two-step anodization process to develop magnetic micro/nanowires for biomedical applications. AAO provides a cost-effective and highly ordered nanoporous platform whose pore diameter, interpore distance, and length can be precisely tuned by adjusting anodization voltage, time, electrolyte composition, and temperature.[1] In this procedure, the aluminium foil is initially pre-textured through degreasing with acetone followed by electropolishing of the surface. The first stage of anodization produces a textured concave pattern on the aluminium substrate, achieved after the oxide layer is removed. Subsequently, the second anodization step is conducted under identical conditions, leading to the self-organized formation of nanopores at the base of each convex.[2]The surface is then protected from etching, and any remaining aluminium is eliminated. The template's excellent physical and chemical stability also enables its use as an efficient drug reservoir and enhances sensor performance when coated with metals. Magnetic nanowires grown within these nanopores exhibit strong shape anisotropy, resulting in high coercivity values desirable for targeted drug delivery, hyperthermia, and magnetic manipulation. [3]The deposition of magnetic materials into the AAO channels significantly influences their magnetic behaviour, allowing tunability similar to core–shell Fe–Fe_3O_4 nanowires reported in recent studies, where controlled oxidation and structural characteristics enable adjustable magnetic properties and improved biocompatibility. [4]The AAO template and its magnetic nanowires offer a flexible platform with significant potential for advanced biomedical and sensing uses.

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ROLE OF SUPPORTING ELECTROLYTES IN MODULATING ACTIVITY AND SELECTIVITY OF 5-HMF ELECTROOXIDATION ON GOLD

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The transition toward low-carbon energy systems necessitates efficient and sustainable energy conversion technologies. Electrochemical valorisation of biomass-derived molecules has emerged as a promising strategy, particularly through coupling organic electrooxidation with hydrogen production in hybrid electrolysis[1]. 5-Hydroxymethylfurfural (HMF) is a key platform molecule that can be electrochemically oxidized into 2,5-furandicarboxylic acid (FDCA), a value-added monomer with the potential to replace terephthalic acid in polyethylene terephthalate (PET) production. While gold catalysts exhibit high activity and stability in the electrooxidation of small organic molecules, they typically show poor selectivity toward FDCA during HMF electrooxidation[2].

Here, we present a detailed electrochemical investigation of HMF oxidation on gold in alkaline media. Cyclic voltammetry and chronoamperometry reveal that the reaction is limited by the formation and reactivity of key intermediates, leading to sluggish reaction kinetics and incomplete oxidation. By introducing ionic additives, we demonstrate that the interfacial behaviour can be tuned, significantly altering intermediate activity. This approach enables enhanced selectivity toward FDCA on gold. These findings provide new insights into the mechanistic pathways of HMF electrooxidation and highlight the critical role of electrolyte composition in controlling activity and selectivity.

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DEVELOPING NOVEL RHENIUM(I) TRICARBONYL THERANOSTIC LUMINESCENT PROBES AS ANTICANCER AGENTS

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Ovarian cancer is one of the most common forms of gynaecologic malignancies, currently having the highest mortality rate. Recently there has been a rise in platinum-resistant recurrent ovarian cancer. In 70% of cases, the cancer initially responds to platinum-based treatments, but returns within six months, having become more aggressive and resistant to platinum-based treatments such as cisplatin. This is concerning as ovarian cancer already accounts for 4.3% of female cancer related deaths worldwide.[1] This data highlights the need for new compounds that move away from the typical platinum-based treatments and drives the development of novel treatment methods using alternative metal centres and effective ligands. Rhenium complexes have shown promising results due to their low in-vivo toxicity, highly tuneable structures and exceptional spectroscopic properties. These complexes have shown activity not only as anticancer agents, but also as antimicrobial agents.[2] Our research group is currently investigating the activity of rhenium tricarbonyl complexes containing phenanthroline-derived ligands against ovarian cancer cell lines. Results show promising activity against cisplatin resistant cell lines. Tetrazolate rhenium tricarbonyl complexes are well known to have luminescent properties that allow their potential use as diagnostic agents. By combining both classes of heterocyclic ligands (phenanthroline and tetrazolate) within the rhenium tricarbonyl complex framework, we are developing a new family of compounds that have the capability of anticancer activity. In addition, their pH-responsive luminescence indicates their potential utility to act as theranostic agents. Here we will present data on the synthesis, characterisation, anticancer activity and luminescent properties of our novel complexes.

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MULTIFUNCTIONAL NUIG4 METAL–ORGANIC FRAMEWORK FOR ANTIBIOTIC DELIVERY: ADSORPTION, RELEASE, AND ANTIBACTERIAL ACTIVITY

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Metal–organic frameworks (MOFs) have gained increasing attention as promising platforms for drug delivery due to their high porosity, tunable structures, and ability to enable controlled release. In this study, the multifunctional MOF **NUIG4** was evaluated as a carrier for antibiotic delivery, focusing on tetracycline (TET), isoniazid (INH), and pyrazinamide (PYZ).NUIG4 demonstrated high drug loading capacities, achieving up to 1327.5 mg g^{-1} for TET, 212.8 mg g^{-1} for INH, and 166.7 mg g^{-1} for PYZ, indicating strong interactions between the framework and the antibiotic molecules. The kinetic analysis showed that the adsorption process follows a pseudo-second-order model with a high correlation coefficient ($R^2 \approx 0.99$), suggesting a chemisorption mechanism. Drug release studies revealed a clear pH-responsive behaviour. At physiological pH (7.4), TET release reached approximately 54% over 3 hours, whereas under acidic conditions (pH 5.5), rapid release was observed, reaching ~85% within 180 minutes. PYZ exhibited nearly complete release (~100%) within 7 minutes, indicating diffusion-controlled release behaviour. Importantly, antibacterial studies confirmed that TET@NUIG4 retained full antimicrobial activity against Escherichia coli and Staphylococcus aureus, with minimum inhibitory concentration (MIC) values of 1.56 µg mL^{-1} and 0.39 µg mL^{-1}, respectively, matching those of the free drug. These results highlight NUIG4 as a promising platform for controlled and targeted antibiotic delivery, with potential applications in the treatment of infectious diseases.

Acknowledgements

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Design and Synthesis of Tetraphenylethylene based Glycoclusters

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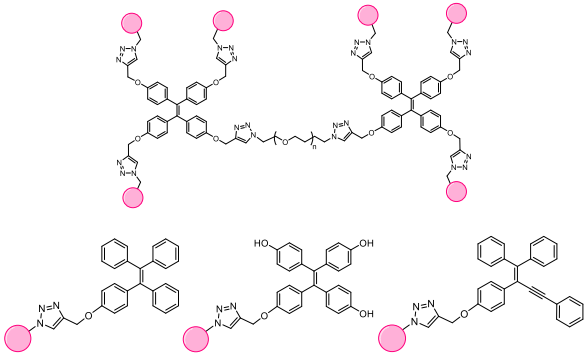
Carbohydrate–lectin interactions regulate essential cellular processes including cell signaling, immune responses, and cell adhesion. Dysregulated lectin activity has been linked to cancer, inflammation, and fibrosis, spurring interest in synthetic lectin ligands capable of modulating these processes. Multivalent glycoclusters exhibit enhanced lectin binding through the multivalency effect, with TPE-based glycoclusters showing particular promise as lectin inhibitors. However, their interaction mechanisms remain underexplored.

This project focuses on synthesizing novel TPE-based glycoclusters with valencies exceeding four to investigate how higher multivalency affects galectin binding affinity. We also explore different TPE core structures to examine their aggregation properties and influence on binding behavior, alongside the effect of PEG linker length variation. Preliminary data indicates that higher valency leads to stronger binding, consistent with biological multivalent binding patterns. This research may advance TPE-based tools for studying carbohydrate–lectin interactions and inform therapeutic strategies for lectin-mediated diseases.



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STUDYING THE NUCLEATION BEHAVIOUR AND KINETICS OF NUCLEOBASES

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Nucleobases plays a critical role in therapeutic applications such as anti-viral and anti-cancer drugs, where efficient purification is essential for their development[1]. Crystallisation offers a promising alternative to conventional purification techniques. A systematic study was performed to investigate the crystallisation behaviour of cytosine, contemplating solubility measurements, metastable zone determination and crystallisation experiments, analysing induction times and kinetic parameters of the process. The solubility trend observed (water–ethanol > water > methanol) highlights not only the influence of solvent polarity, but also the hydrogen bonding and solvent structure on the nucleobase solubility. The MSZW was narrower in aqueous solutions, and presented a broader limit in methanol (Figure 1). The induction time was measured under different conditions to evaluate the effect of supersaturation, solvent type and the presence of impurity on the crystallisation of cytosine. The presence of thymine as an impurity acted as a nucleation inhibitor, as increasing its concentration progressively delayed induction times and the effect was more pronounced in organic solvents (Figure 1).

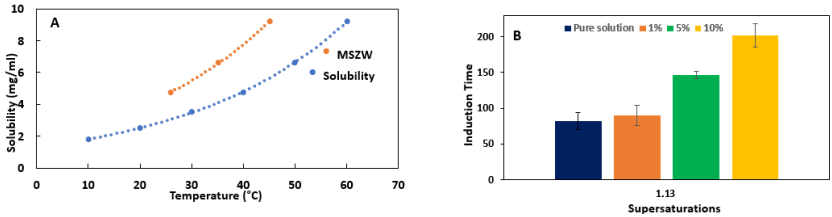

Figure 1: (A) Solubility and MSZW for cytosine in methanol. **(B)** Induction time of cytosine in water with different concentration of thymine.

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COMPUTATIONAL DISCOVERY OF METAL-ORGANIC FRAMEWORKS AS DRUG CARRIERS FOR ANTICANCER DRUGS

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Cancer is one of the most pressing health concerns worldwide, resulting in millions of deaths annually.[1] Conventional treatments, such as chemotherapy, suffer from a lack of selectivity and have significant side effects. The use of Metal-Organic Frameworks (MOFs) as nanocarriers for anticancer drug delivery shows promise as MOF characteristics make it possible to specifically tailor their properties for controlled and targeted delivery of therapeutic agents. MOFs are crystalline porous materials that consist of metal ions or clusters bonded coordinatively to organic ligands.[2] Therapeutic agents, such as doxorubicin, can be loaded into the MOF either through encapsulation within the pores or attachment via a surface. An improvement in efficacy, reduced side effects and reduced pharmacokinetic problems can provide safer and more effective therapy methods. This work focuses on studying existing MOFs, such as UiO-variants, for potential multi-drug delivery to enhance treatment efficiencies and combat increasing drug resistance.

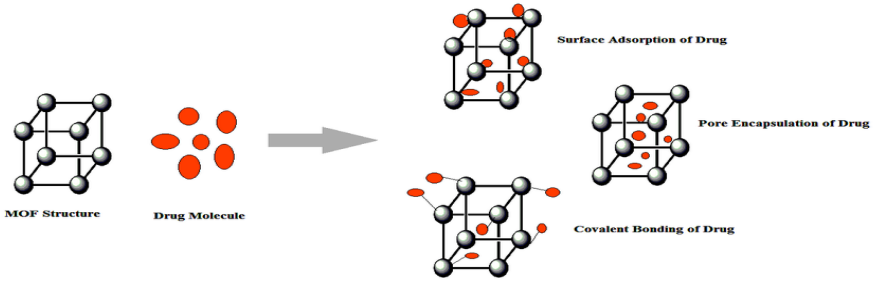

Figure 1. Schematic of drug loading in a MOF.[3]

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Complex Matters: Structural Activity of N,N-disubstituted-N'-acylthiourea Cu(II) Antifungals

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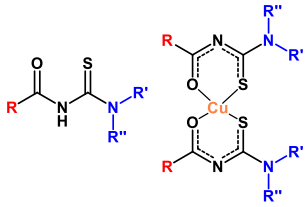
Antifungal resistance is an escalating global health challenge, creating an urgent need for new therapies. Among fungal pathogens, infections caused by Candida albicans remain a major source of morbidity, particularly in immunocompromised patients.[1] Metal-based therapeutics offer a promising yet underexplored strategy for antifungal drug discovery.

This study investigates a series of Cu(II) complexes bearing N,N-disubstituted-N'-acylthiourea ligands as potential antifungal agents. By systematically varying the acyl and amine substituents, the steric, electronic, and lipophilic properties of the ligand framework can be finely tuned.[2] Antifungal screening against Candida albicans established clear structure–activity relationships, demonstrating how ligand design influences biological potency. These findings highlight the potential of rationally designed Cu(II) acylthiourea complexes as a platform for combating antifungal resistance.[3]



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Making a Peptide Therapeutic More Sustainably: A Greener Approach to Solid-Phase Peptide Synthesis

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Peptide therapeutics are a rapidly growing class of medicines for cancer, hormonal, and metabolic disorders, with the global market projected to reach $76 billion by 2029.[1,2] As demand rises, sustainable manufacturing becomes critical. This project focuses on developing a greener synthesis of a peptide therapeutic, using Fmoc-based solid-phase peptide synthesis (SPPS). Unlike traditional Boc-SPPS, which relies on strong acids and hazardous solvents, the Fmoc strategy eliminates the need for harsh reagents such as hydrofluoric acid (HF), improves waste management, and enables the integration of greener solvent systems.[3]

To further reduce environmental impact, greener reagents and solvents such as dimethyl sulfoxide (DMSO), ethyl acetate (EtOAc) and alternative acids are being examined to replace dimethylformamide (DMF), dichloromethane (DCM), and trifluoroacetic acid (TFA), all of which pose toxicity and/or persistence concerns.[4]

The goal is to deliver a high-yield, high-purity protocol aligned with green chemistry principles, providing a model for sustainable peptide production in the pharmaceutical industry.

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DEVELOPMENT OF NOVEL ARYL PHOSPHONATE NUCLEOTIDE ANALOGUES

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Without proper treatment, human immunodeficiency virus (HIV) infection can progress to acquired immunodeficiency system (AIDS), which can be fatal.[1] Infections are generally lifelong, but can be managed with the use of highly active antiretroviral therapy (HAART). Several antiviral drug classes are used in combination as part of HAART, with nucleoside/nucleotide reverse transcriptase inhibitors (NRTIs) often forming the backbone of the regimen.[2] Of the drugs which inhibit HIV reverse transcriptase (RT), a subclass called the acyclic nucleoside phosphonates (ANPs) exist. Of particular importance in this class are the antiviral drugs adefovir and tenofovir.[3] This work is concerned with the design and synthesis of aryl-linked analogues of the aforementioned ANPs.[4] An advantage of the aryl linker moiety is the presence of sp^2-hybridised carbon atoms, which can be installed *via* Chan-Lam coupling.[5] This could provide access to a broad range of novel phosphonate prodrugs for future evaluation.[6]

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Synthesis and Evaluation of Novel Lipids Based on Quinolones and Their Evaluation as RNA Delivery Vehicles with Dual Effect

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Lipid nanoparticles (LNPs) are the most clinically sucessful delivery platform of RNA therapeutics to date. However, their application is constrained by the safety, potency, and limited functionality of currently available ionisable lipids.[1]

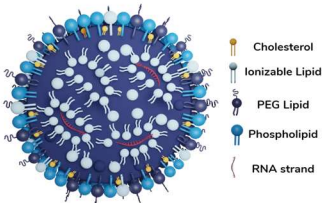
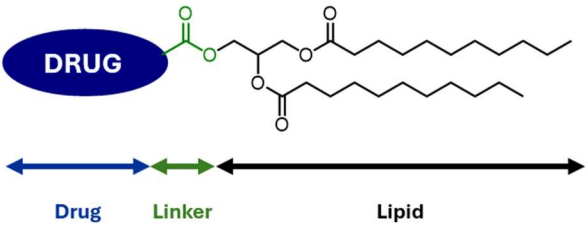


Figure 1: mRNA LNP composition [2]

This project aims to develop novel multifunctional lipids by integrating bioactive molecular scaffolds into the lipid design. By enabling the co-delivery of RNA and bioactive molecules, this dual-targeting approach seeks to improve treatment efficacy, reduce LNP toxicity and improve drug biocompatability.



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iEDDA "Click-to-Release" Activation of TCO-caged Pt(II) Prodrug for Targeted Cancer Therapy

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Platinum (Pt)-based chemotherapy drugs remains an integral part of anticancer therapeutics and are still widely used today. Despite the widespread use of Pt(II) drugs, there are many downfalls, such as inherent and acquired resistance and serious side effects. [1] There is an urgent need to develop Pt drugs with enhanced selectivity for cancer cells to minimise toxic side effects and enhance efficacy.

The biorthogonal inverse-electron-demand Diels-Alder (iEDDA) cleavage reaction between tetrazines and transcyclooctene (TCO) is a powerful chemical strategy allowing for controlled release of drugs, such as doxorubicin [2]. The reaction of TCO with a suitable tetrazine results in the formation of the free-amine containing drug, CO_2, and a dihydropyridazine. The main objective of this work is to develop a Pt based iEDDA click-to-release platform between a cancer targeting tetrazine and a TCO-caged Pt prodrug, allowing for selective activation of a Pt anticancer drug candidate directly at the tumour site. We hypothesis that the bulky TCO ligand will cage the Pt complex, making it inactive until reaction with a suitable tetrazine.
We report the successful synthesis of a TCO caged Pt(II) drug candidate and ongoing efforts are now focused on demonstrating iEDDA "click-to-release" of the TCO caged Pt prodrug using suitable tetrazines. This has been successfully demonstrated by UV-Vis spectroscopy by following the attenuation of the n- π* tetrazine band. Cytotoxicity studies will be carried out to determine the cytotoxicity of the TCO caged Pt prodrug with and without a tetrazine present.

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Developing a Gold(I) PROTAC to Degrade Thioredoxin Reductase

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Cisplatin and its derivatives have proven instrumental in improving cancer mortality over the past 75 years, and have become the gold-standard in treating numerous solid tumors; however, a non-selective mechanism of action has limited clinical use. Therefore, it is of interest to design metal-based drugs accessing novel mechanisms of action by harnessing the well-established capability of transition metals to selectively bind intracellular protein targets.[1, 2] Particularly, gold(I) complexes bearing N-heterocyclic carbene ligands have been found to strongly inhibit thioredoxin reductase, a key enzyme in cellular redox metabolism commonly overexpressed in cancer.[3] This offers a powerful tool to be exploited in developing gold(I) proteolysis-targeting chimeras (PROTACs) capable of eliminating disease-associated proteins by recruiting and hijacking the Ubiquitin-Proteasome System (UPS). The Au(I)-PROTAC and respective parent complex were synthesized with >95% purity in high yield. *In vitro* cytotoxicity studies and quantification of TrxR degradation via western blot are currently being undertaken in HT-29 colorectal adenocarcinoma cells.

This research was conducted with the financial support of the Fulbright Commission and RCSI.

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DEVELOPMENT OF GALLIUM ANTIMICROBIAL DRUG CONJUGATES TARGETING ESKAPE PATHOGENS

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Antimicrobial resistance (AMR) has become a rapid emergency to the global healthcare system, causing over 5 million deaths worldwide per year.[1] In clinical practice, a large proportion of multidrug resistant (MDR) infections are caused by "ESKAPE" pathogens; *Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acinetobacter baumannii, Pseudomonas aeruginosa* and the *Enterobacter* species. These MDR pathogens are found in the WHO's priority pathogen list, highlighting the need for urgent therapeutic development.[2] In search of novel therapies to overcome MDR, metallo-antimicrobials have attracted great attention. Their multitargeted mechanisms can deter the onset of drug resistance in pathogens.[3] Ga(III) holds great potential as an antimicrobial agent, it closely resembles Fe(III) in size and charge, allowing it to compete for Fe(III) binding sites in microorganisms as a non-functional Fe(III) analogue. Being redox inert under physiological conditions, Ga(III) hinders essential metabolic processes in pathogens when substituted in Fe(III) redox-cycling dependent enzymes.[4] 5-fluorouracil (5-FU) and 5-fluorocytosine (5-FC) exhibit antifungal activity and are more recently being investigated for their antibacterial activity. Being a fluorinated cytosine analogue, 5-FC acts as a prodrug that is converted into 5-FU by cytosine deaminase. Both 5-FU and 5-FC act as antimetabolites given they inhibit nucleic acid synthesis. 5-FU has also been reported to inhibit biofilm creation and decrease bacterial virulence.[5] This project aims to (i) develop Ga(III) antimicrobial drug-conjugates that possess the unique antibacterial properties of Ga(III) and the antimicrobial effects associated with 5-FU and 5-FC, and (ii) investigate the drug conjugates' antimicrobial properties against ESKAPE pathogens.

This research was conducted with the financial support of Taighde Éireann – Research Ireland under Grant number GOIPG/2025/5609.

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DEVELOPMENT OF HIGH-THROUGHPUT SCREENING METHODOLOGY TO IDENTIFY RNA-BINDING PROTEIN VIA 19F NMR

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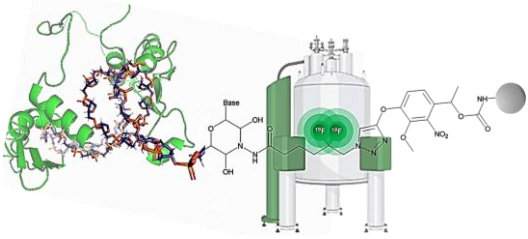
Protein-RNA interactions regulate fundamental biological processes and are increasingly implicated in cancer, neurodegeneration, and chronic disease[1]. However, robust methods to validate these interactions remain limited by cost, throughput, and analytical complexity[2]. ^{19}F NMR provides a sensitive, background-free readout of RNA structure and binding-dependent changes under physiological conditions. Previous collaborative work demonstrated that ^{19}F-labelled RNA efficiently detects protein-RNA interactions. RNA-binding domains from double-stranded and single-stranded RNA-binding proteins were recombinantly expressed and purified, while cognate RNA partners were chemically synthesised with a 3'-terminal 5-fluorouridine label. Protein binding produced diagnostic shifting and broadening of the RNA ^{19}F resonance, enabling interaction validation within an hour and in a single experimental attempt.

This project develops a high-throughput platform for identifying RNA-binding proteins using ^{19}F NMR. The approach bridges organic and physical chemistry with molecular and structural biology through a solid-supported, photocleavable fluorinated linker. The linker is assembled through convergent synthesis and designed for 3'-end conjugation to single- and double-stranded RNA. Following photocleavage, fluorinated RNA constructs are analysed by ^{19}F NMR before and after protein addition, while positive interactions are validated by mass spectrometry.



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A SUPRAMOLECULAR APPROACH TO TARGETED ANTI-MICROBIALS

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Antimicrobial resistance (AMR) is a major threat due to the increasing number of pathogens becoming resistant to traditional antimicrobial agents, such as antibiotics and antifungal treatments. It is predicted to cause 10 million deaths annually by 2050.[1] Anti-adhesion agents bearing carbohydrates have been shown to be an effective non-toxic strategy to circumvent infection, whilst novel supramolecular approaches disrupting ion balance, prove to be a novel cytotoxic approach.[1,2]

Following this we have developed a novel peptidomimetic which consists of a peptide squaramide hybrid termed 'squaratide'. These squaratide core may possess many benefits including better *in vivo* stability, increased hydrogen bonding ability and a versatile and straightforward synthesis. The squaratide core can then be functionalized with glycans to form glycoconjugates capable of targeting lectins of key bacteria and fungi. We have also exploited supramolecular chemistry by demonstrating the ability of these compounds to bind known antimicrobial agents. This poster will outline the preliminary results of the work carried out on this project to date.

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SYNTHETIC STUDIES ON A NOVEL CYCLOPEPTIDE FROM *STREPTOMYCES NODOSUS*

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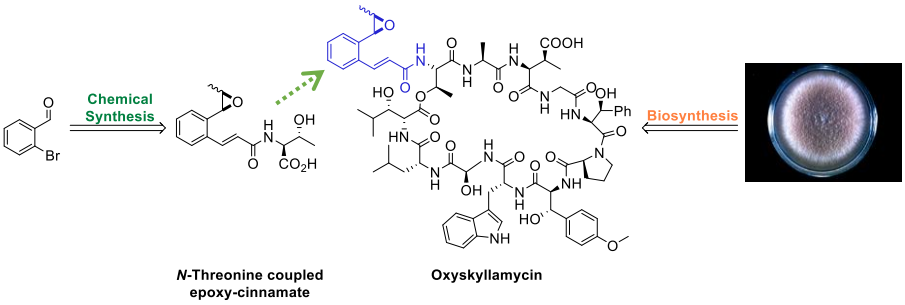
Oxyskyllamycin is a newly discovered analogue belonging to the skyllamycin family of cyclic lipopeptides.[1] Compounds from the skyllamycin family are known to possess interesting biological activities, such as biofilm dispersion, anti-cancer activity and others.[1,2] Although the gross structure is confirmed the stereochemistry about the cinnamate-based epoxide is not known. Thus, one main goal of this project is the structural elucidation of oxyskyllamycin, and the epoxy motif found on the cinnamoyl chain.

Herein we report a route for the synthesis of stereoisomers of the *N*-threonine linked epoxy-cinnamate starting with 2-bromobenzaldehyde. The biosynthesis of oxyskyllamycin is also shown with the optimisation of growth, isolation and purification of the novel cyclopeptide.



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REGIOSELECTIVE IRIDIUM-CATALYSED C(7)-H BORYLATION & CHAN-LAM COUPLING OF 6-FLUOROQUINOLONES

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Fluoroquinolone antibiotics are one of the world's most commonly prescribed classes of antimicrobials and are among the World Health Organisation's (WHO) Model List of Essential Medicines.[1,2]

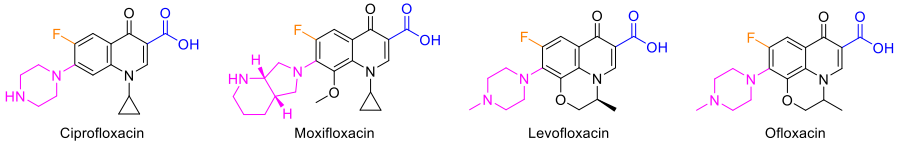
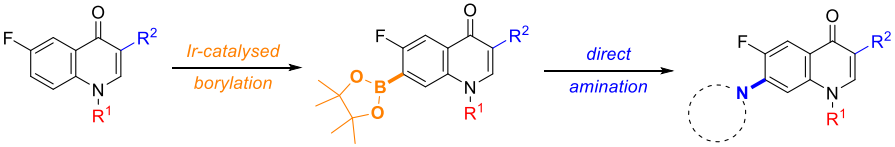


Figure 1. WHO Model List of Essential Medicines containing 6-Fluoroquinolones (2024)

Modulation of the substituent at the 7-position of quinolone antibiotics is well recognised for enhancing potency and pharmacokinetics.[3]

In this work, we utilise an iridium-catalysed C–H borylation strategy of the C-7 position of 6-fluoroquinolones, achieving good yields and enabling an efficient amination protocol *via* the Chan-Lam-Evans coupling, thereby expanding the accessible substitution space at C-7 beyond traditional amines.



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SYNTHESIS OF α-ALLYL ESTERS THROUGH Pd-CATALYSED ALLYLIC ALKYLATION OF DISUBSTITUTED KETENES

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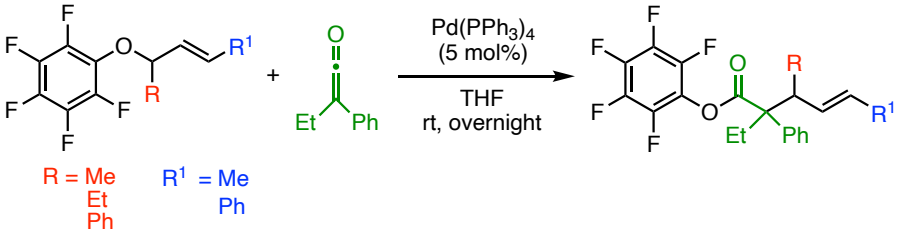
α-Allylic esters are an important group of compounds with potential to access pharmacologically active nucleoside analogues (possessing anti-viral and/or anti-cancer properties), as well as providing a new route to already approved/explored medicines, such as the serotonin antagonist LY426965.[1] Previous work has focused on investigating enantioselective palladium catalysis with varying success (47-93% yield for 19 examples, 34-83% ee for 12 examples).[2] The current direction of our work has entailed developing more substituted allyl ethers to expand the substrate scope of the reaction, and furthermore explore regio- and diastereoselective aspects. Non-enantioselective Pd-catalysed studies have revealed the potential for the development of the catalytic asymmetric synthesis of α-allyl esters from newly developed starting materials.



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SYNTHESIS AND CHARACTERISATION OF BIOTINYLATED CU(II) SUBSITUTED DIPYRIDOPHENAZINE COMPLEXES.

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Copper(II) complexes are known to display a wide range of biological activities. Their ability to display various geometries as well as their redox properties make them an attractive choice in medicine. Copper is abundant in the human body and plays major roles in various biological processes and therefore does not face toxicity issues that other metal-based complexes do, such as platinum or gold-based molecules. Biotin is involved in a very large number of biological processes, such as mediating gene regulation and fatty acid synthesis[1] in the human body. The synthesis of biotin-containing drugs has been carried out as both anti-microbial agents[2] via the inhibition of biotin protein ligase and anti-cancer[3]. Moreover, studies have shown that the biotin receptor is overexpressed in several types of tumors, leading to better specificity and greater drug uptake[4]. The promising effects that biotin displayed in previous studies[5] as well as the well-known efficacy of Cu(phen) complexes as both anti-bacterial and anti-cancer agents have led us to the synthesis of a family of biotinylated Cu(II) substituted dipyridophenazine complexes as both potential anti-microbial and anti-cancer agents.

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Chemoenzymatic glycoengineering: A Novel Solution-Phase Approach for Developing Single Glycoform Therapeutics

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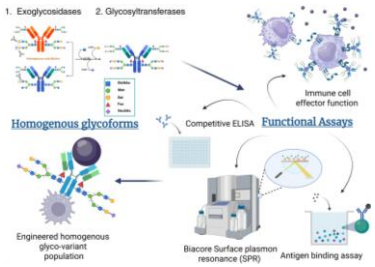

Current approaches for generating single glycoform monoclonal antibodies (mAbs) include genetic manipulation, cell culture modification, and chemoenzymatic methods. While genetic approaches offer precision when target glycan modifications are predetermined, they are costly and time-intensive. Metabolic approaches provide financial advantages but rarely achieve homogeneity. Chemoenzymatic methods, though expensive, can be retrospectively applied to various therapeutics [1]. Recent chemoenzymatic glycoengineering strategies utilize glycosyl transferases and hydrolases on solid support membranes or employ endo-β-N-acetylglucosaminidase (ENGases) with monosaccharyl transferase mutants [2][3]. Our proposed methodology advances beyond these approaches via 1) implementation in solution phase, offering cost advantages and avoiding glycan-site accessibility limitations on intact proteins (associated with solid support coupling) and 2) utilization of a unique combination of glycosyl transferases and endoglycosidases to generate novel mAb glycoforms. We will describe results on the development of an innovative in-vitro glycoengineering technology enabling solution-phase creation of single glycoform mAbs with enhanced safety, efficacy, and effector functions compared to heterogeneous counterparts . We will develop this technology using two different antibodies; an IgG2a mAb developed against the Aspergillus fumigatus siderophore TAFC [4][5] and a polyclonal IgG.

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SYNTHESIS OF RESOLVIN D2 ANALOGUES AND DETERMINATION OF STEREOCHEMICAL CONFIGURATION

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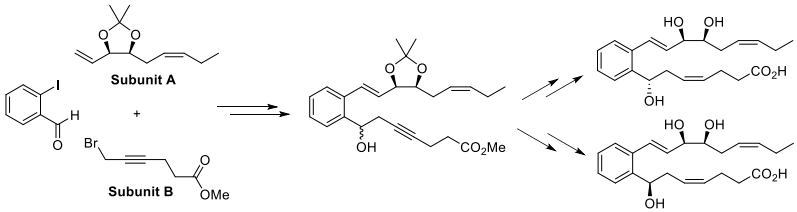
Chronic inflammation is the underlying cause of serious conditions such as Alzheimer's disease and Crohn's disease.[1] Pro-resolving mediators are produced by the body to resolve inflammation but are often absent in chronic inflammation. Such compounds are of interest as potential novel anti-inflammatories. Resolvin D2 (RvD2) is active at nanomolar concentrations, resolving inflammation by increasing macrophage effercytosis.[2] However, its use as an anti-inflammatory drug is limited by a short half-life. This is partly due to the presence of a reactive triene system, which is prone to metabolic degradation. To develop longer lasting analogues while retaining anti-inflammatory activity, we have designed aromatic analogues of RvD2. Replacement of the reactive triene core structure with a benzene ring should improve the molecular stability. Presented here is the coupling of two key subunits to a benzene ring to form a core aromatic structure. Subsequent partial hydrogenation[3] and deprotection steps afford the key RvD2 analogue structure. Two epimeric analogues have been synthesised and isolated, and their absolute stereochemical configurations have been determined using Mosher's acid.[4] Sufficient quantities have also been prepared for biological testing.



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INVESTIGATING SILVER PHENANTHROLINE COMPLEXES AS POTENTIAL ANTIFUNGAL AGENTS

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The Candida genus is responsible for causing over 150 million fungal infections annually, with *Candida albicans* being the most clinically significant member of the genus. It is responsible for approximately 40% of fungal bloodstream infections and is particularly problematic in immunocompromised patients. Rising antimicrobial drug resistance has intensified the need for new antifungal agents with alternative mechanisms of action capable of bypassing existing resistance pathways. Silver-based complexes have emerged as promising antimicrobial candidates due to their ability to coordinate with biologically active ligands, including 1,10-phenanthroline and its derivatives. Two such derivatives, phenanthroline-oxazine and pyrido-phenanthroline, have shown notable antifungal potential. Previous studies demonstrated the *in vitro* activity of the phenanthroline-oxazine derivative PPO and its silver complex, $Ag(PPO)_2$, against *C. albicans*. However, their *in vivo* efficacy and mechanism of action remained unclear. In this study, label-free quantitative proteomics was used to investigate the antifungal mechanism of $Ag(PPO)_2$. Proteomic analysis revealed that the silver complex disrupted fungal respiration, with treated *C. albicans* cells showing reduced abundance of key respiratory enzymes, including succinate dehydrogenase and NADH-ubiquinone reductase. Treatment also caused major changes in fungal cell wall structure and altered the abundance of adhesins, including adhesin 2 and adhesin 5. The *in vivo* efficacy of $Ag(PPO)_2$ was assessed using the *Galleria mellonella* infection model, where treatment provided 80% protection against C. albicans infection. Additionally, the pyrido-substituted phenanthroline silver complex $Ag(PPP)_2$ has also demonstrated potent antifungal activity.

SYNTHESIS AND BIOLOGICAL ACTIVITY OF DEAZAGUANINES

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The enzyme TGT (tRNA guanine transglycolase) exchanges a nuclear encoded guanine at position 34 (the wobble position) of tRNA for the hypermodified nucleobase queuine in the tRNA of four amino acids: histidine (His), asparagine (Asn), aspartic acid (Asp) and tyrosine (Tyr). Queuine is produced by bacteria and cannot be synthesised by eukaryotes, in the case of mammals queuine must be obtained from the bacteria in the gut or food.

The TGT enzyme has been shown to have strict specificity for its tRNA substrates but it will accept a large variety of synthetic queuine analogues as false substrates which are inserted at position 34 of the previously mentioned tRNAs. (1) A subset of these false substrates have shown promising results in disease models for multiple sclerosis and rheumatoid arthritis. (2)

A novel library of synthetic queuine analogues has been prepared to gain further understanding of the biological processes that are influenced by the tRNAs modified by TGT false substrates.

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Design, Synthesis and Evaluation of Novel Glycomimetic Compounds as Galectin 8N antagonists

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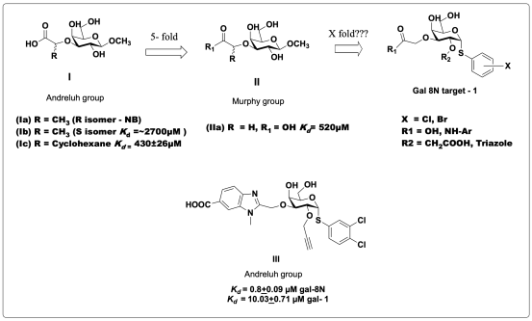
Galectins are an important class of carbohydrate-binding proteins that have been shown to play various roles in regulating the immune system and inflammatory response, with diverse functions and activities. Galectin activity has been implicated in the development of cancer, heart failure and autoimmune conditions such as rheumatoid arthritis, making them attractive molecular targets for drug design and development.

The Andreluh group synthesised ligands based on 3-lactoylgalactoside **(I),** where the lactic acid derivative **(Ia)** gave a K_D = ~2700 µM for the S-isomer, while the *R*-isomer did not bind[1]. Later, modifications on **(Ic)** the C3 position with a (i) benzyl group and (ii) the anomeric position with an α-*S*-glycoside led to enhanced binding towards galectin 8N. This modified compound showed a K_D of 12±0.9 µM for galectin 8N, representing a 40-fold improvement[1]. Later, the Murphy group modified the lactic acid derivative preparation **(IIa)**, and this gave a 5-fold improvement in the K_D value (520 µM), when compared to **(II).** On the contrary to expectations, 2-*O*-propargyl-D-galactoside **(III)** was found to strongly increase binding enthalpy to galectin-8N. This could be attributed to non-canonical cation-π interactions in giving a nanomolar inhibitor of galectin-8N terminal[2]. In this work, we are aiming to modify further the groups at the galactopyranoside C2, C3 and anomeric positions with a view to improving further binding to galectin- 8N.



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DESIGN AND SYNTHESIS OF AN IMPDH INHIBITOR LIBRARY WITH ANTIMICROBIAL POTENTIAL

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Antibacterial drugs are fundamental to modern medicine, but their overuse has driven the rise of antimicrobial resistance (AMR), which is associated with increased mortality and healthcare costs worldwide. New treatments with novel mechanisms of action are needed to combat AMR. Inosine monophosphate dehydrogenase (IMPDH) catalyses the rate determining step of guanine nucleotide biosynthesis, which is vital for DNA/RNA synthesis. Shared critical residues in *Pseudomonas aeruginosa*, *Streptococcus aureus*, and *Cryptosporidium parvum* may indicate the potential for IMPDH inhibitors to exhibit broad-spectrum antimicrobial effects[1]. Gorla *et al.* identified a potent *C. parvum* inhibitor by high throughput screening, but this scaffold contained a metabolically unstable oxime group[2]. This project replaces the unstable oxime with a series of more stable heterocycles to improve pharmacological behaviour. Initially, a series of urea-based IMPDH inhibitors was synthesised and evaluated for activity against bacterial IMPDH[3]. A second series of bioisosteric analogues was subsequently prepared where the urea scaffold was replaced with a corresponding squaramide[4]. Introduction of a squaramide in this fashion should confer improved pharmacokinetic properties and increased hydrogen bonding ability[5].

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Synthesis of novel quinoline-5,8-diones as inhibitors of Anaplastic Lymphoma Kinase (ALK) and cancer cell growth

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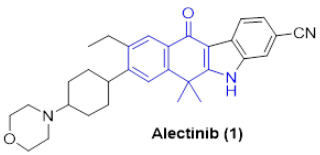
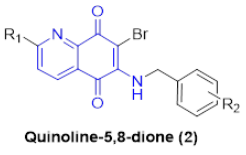
Anaplastic Lymphoma Kinase (ALK) is a membrane tyrosine kinase receptor which is a target in approximately 5% of all non-small cell lung cancer (NSCLC) cases. NSCLC accounts for 80-85% of all lung cancer cases and is unfortunately responsible for a very poor prognosis.[1] Three generations of ALK inhibitors have been reported resulting in life prolonging treatment.[2] However, the majority of patients acquire chemoresistance to these treatments, which has developed through gene amplification and secondary mutations on the enzyme.[3] Alectinib (1) is an example of a second-generation treatment which displays structural similarities to the quinoline-5,8-dione system. This project outlines the synthesis of quinoline-5,8-diones (2), which have been synthesised from cheap and readily available quinolinols via bromination and oxidation reactions. These have then been successfully derivatised at the C(6) position with a wide range of benzylamines to generate a library of novel compounds. Computational studies have successfully shown that these compounds display favourable binding interactions to the ALK enzyme. Future work will involve the evaluation of all novel compounds for their antiproliferative activity.



Alectinib (1)



Quinoline-5,8-dione (2)

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IDENTIFICATION OF PROTEIN TARGETS OF THE 2-AMINOINDOLINES IN MELANOMA

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Melanoma (a form of skin cancer) claims the lives of approximately 60,000 people annually worldwide. The 2-aminoindoline family of compounds were previously shown to selectivity inhibited the growth of nine different melanoma cell lines. This effect was selective towards melanoma cell lines, with other cancer cell lines displaying significantly less growth inhibition compared to the melanoma cell lines. X-ray crystal structures have shown that the 2-aminoindoline family of compounds) mimic parts of histone proteins[1]. Histones are proteins found in the nucleus of cells. DNA coils around them, and the (*N*-terminal) ends of histone proteins can be modified. These post-translational modifications (PTMs) are recognised by other proteins that control the expression of different genes based on environmental factors. This is called epigenetic regulation and the proteins involved are called epigenetic proteins. Since the 2-aminoindoline family of compounds mimic the modified *N*-terminal ends of histones, they can bind to and inhibit epigenetic proteins. There are close to 1,000 reported epigenetic proteins. It is likely that the compounds that are active on melanoma cell lines work by inhibiting epigenetic proteins, but we do not know the exact epigenetic proteins being inhibited. My PhD project aims to determine which epigenetic proteins are being inhibited in melanoma. Compounds will be synthesised, attached to beads (immobilised) and incubated with lysed cells (ruptured to expose the proteins). Proteins that bind to the immobilised compounds can be isolated and identified by mass spectrometry proteomics. Once these proteins are identified, the compounds can be modified to enhance their activity and selectivity towards these newly identified epigenetic proteins. These newly identified epigenetic proteins can then be targeted by the molecules to treat melanoma.

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SYNTHESIS OF FIRST DIIRIDIUM BRIDGING CARBIDO COMPLEX USING CARBODISULFURANE AS A CARBON ATOM TRANSFER REAGENT

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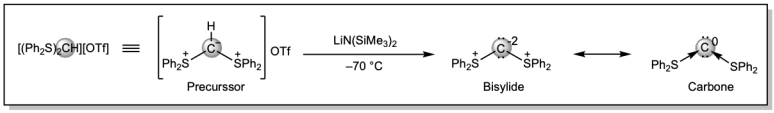
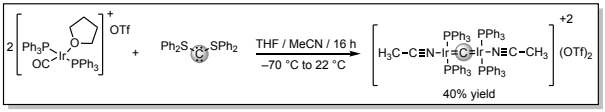
Introducing atomic elements into molecules is an elusive transformation. While atomic hydrogen and oxygen are routinely used in synthesis, transferring higher-valent atoms like nitrogen or carbon is far more challenging. Although true atomic carbon can be generated by the carbon arc method[1], its extreme reactivity demands specialised conditions. A practical workaround is to stabilise atomic carbon with two donor ligands, forming divalent carbon(0) complexes (carbones) or bis-ylides. Our interest lies in using **carbodisulfurane** as a carbon-atom-transfer reagent.



Reaction of the monocationic iridium complex with carbodisulfurane produced an immediate colour change from yellow to orange-red when warmed to 22 °C. Characterisation by NMR, IR, mass spectrometry, and finally by X-ray diffraction confirmed the formation of the first diiridium bridging carbido complex.



Overall, the formation of diiridium bridging carbido complex demonstrates that carbodisulfurane can enable carbon-atom transfer to late transition metals beyond the previously explored systems, highlighting its broader potential in metal–carbide chemistry.

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ASYMMETRIC HYDROGEN ATOM TRANSFER USING CHIRAL P-H DONOR

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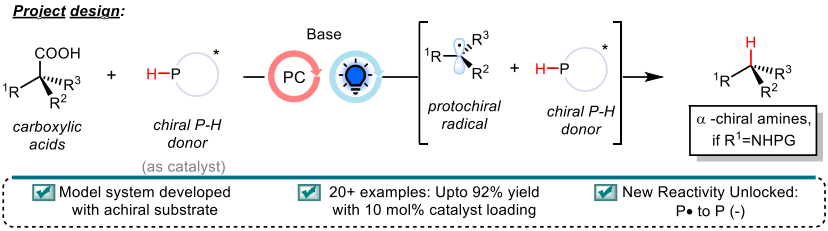
Chiral amines are omnipresent among natural products and APIs.[1] Despite continued interest, methods for their asymmetric synthesis are still lacking.[2] Herein, we report a dual catalytic system, which allows the synthesis of chiral amines via hydrogen atom transfer (HAT). A photocatalyst works in tandem with catalytic P-H* donors, opening the possibility of enantioselective HAT between a pro-chiral radical and chiral H-atom source (Scheme 1). To date, only reagents derived from Sn, S, and Si have been used for the asymmetric HAT reaction, but they are far from providing a general solution.



Scheme 1: Project Design

Phosphorus is an excellent and yet unexplored alternative.[3] Organophosphorus compounds have weak P-H bonds, P-centered radicals are well studied and asymmetric chemistry of P-compounds is well-established, with many chiral scaffolds available.

We have successfully developed a model system and we discovered unprecedented catalysis with a P-H donor, facilitated by the previously elusive reduction of P-centered radical to P-centered anion[4]. The preliminary screening has been performed across > 20 substrates, with yields > 92%. Currently, we are optimizing the enantioselective variant of the reaction.

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SMALL NITROGEN BICYCLES: CONSTRAINED MOLECULAR GEOMETRY FOR AZA BIOISOSTERES AND PENTAVALENT, PENTACOORDINATE NITROGEN

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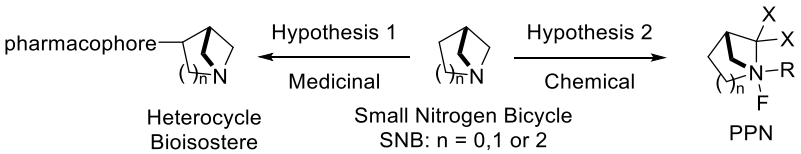
There is a presently undeveloped class of molecules with nitrogen at the bridgehead of two small rings. These small nitrogen bicycles (SNBs) have a crucial structural attribute in which nitrogen bond angles are significantly reduced, yet not to the extent of inducing instability towards ring opening. This molecular geometry leads to two hypotheses, one with very wide pharmaceutical application and the other disrupting conventional ideas about chemical valence and reactivity.



Hypothesis 1 – Medicinal. It is known that the cubyl and bicyclopentyl molecular fragments act as bioisosteres of the phenyl fragment in various pharmaceuticals and that this unexpected effect derives from their compact size. We report progress towards testing the hypothesis that, since our target small ring nitrogen compounds have the same compactness, they can also act as bioisosteres of the multiple heteroaromatic fragments that occur in >50% of all pharmaceuticals (e.g. pyridyl or imidazolyl) [1].

Hypothesis 2 – Chemical. Over the last 20 years, the non-existence of pentavalent pentacoordinate nitrogen (PPN) has been recognised as due mainly to lack of space around the nitrogen atom. Spatial constriction stabilised by SNB's may allow space to bond a fifth atom. We report initial calculations supporting this hypothesis and progress towards the synthesis of relevant small nitrogen bicycles.

We report simple methodologies for the synthesis of SNBs and derivatives towards bioisosteres and pentavalent pentacoordinate nitrogen

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DESIGN AND SYNTHESIS OF A PORPHYRIN-BASED PHOTOCATALYTIC DYAD FOR VISIBLE-LIGHT DRIVEN CO_2 REDUCTION TO FORMATE

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The selective photocatalytic reduction of carbon dioxide to formate represents an opportunity to simultaneously combat increasing levels of atmospheric CO_2 while at the same time generating a useful chemical feedstock.[1] In this work, a photocatalyst based on a porphyrin-bipyridine dyad with a naphthalimide bridging ligand [Figure 1] is being developed for visible-light-driven reduction of CO_2 to formate. The approach combines a metalloporphyrin photosensitiser with a rhenium bipyridine catalytic centre, which will enable light absorption and electron transfer within a single molecular system. The poor absorption of rhenium tricarbonyl diimine complexes in the visible region limits their efficiency under solar irradiation, however, the incorporation of a porphyrin unit, with its highly conjugated 18π electron system and strong visible light absorption [Figure 2], enhances light harvesting and promotes electron transfer to the catalytic centre through photoexcitation. Bridging ligands, such as the naphthalimide, can aid in facilitating efficient charge transfer from the porphyrin photosensitiser to the rhenium catalyst while suppressing wasteful electron back transfer. Moreover, extending the conjugation within the photocatalyst helps create a broader absorption spectrum, thereby allowing the dyad to absorb more visible light. Initial synthetic stages have been successfully completed with high yields, and spectroscopic characterisation confirmed the synthesis of the photocatalyst and key intermediates. The resulting porphyrin derivatives exhibit strong visible-light absorption, and intramolecular photocatalytic studies have shown CO_2 reduction to carbon monoxide and formate.

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SYNTHESIS OF CAERULOMYCIN NATURAL PRODUCTS

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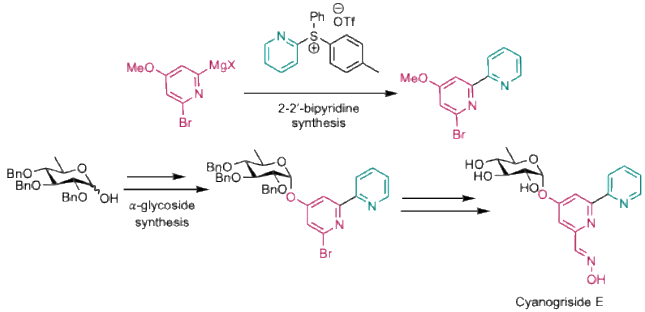
This work merges two areas of organic synthesis to access target natural products of the caerulomycin families.[1] Sulfonium salts have been utilised in various C-C bond forming reactions, including the synthesis of synthetically challenging 2,2'-, 2,3'- and 2,4'-bipyridine linkages reported by McGarrigle et al.[2] These 2,2'-bipyridine motifs are found in various areas of chemistry including ligands, photocatalysis, and medicinal chemistry. Caerulomycin natural products contain these 2,2'-bipyridine skeletons. Notably the cyanogrisides family (isolated from *A. cyanogriseus*) also feature α-glycosidic linkages between these bipyridines and various sugar moieties. While 1,2-cis-glycosidic bonds are synthetically difficult linkages, various methods have been developed for their synthesis.[3] Our group has recently published a stereoselective α-glucosylation method, which can be applied to a range of alcohol acceptors.[4] These two synthetic methods have been employed in synthesis of target natural products including cyanogriside E.



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A NEW APPROACH TO THE SYNTHESIS OF PHOSPHINOYL OXIMES USING DISULFIDE ORGANOCATALYSIS

Meadhbh Coomey[1], Dr Eimear Courtney[1], Aoibhe O'Donnell[1], Dr Tim O'Sullivan[1,2] and Dr David J. Jones[1]
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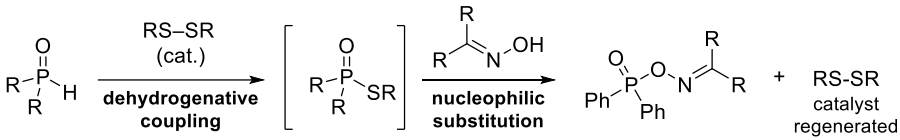
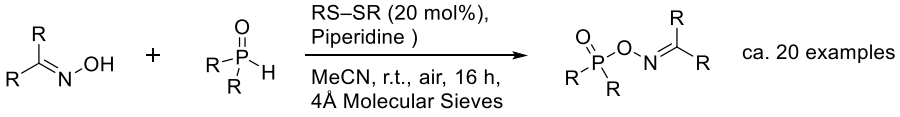
Compounds with P–O–N bonds (*e.g.*, phosphinoyl oximes) are increasingly significant due to their physical, chemical and biological properties. Despite this, their organocatalytic synthesis remains underexplored. Previous work by Goulart[1] and Handoko[2] explores the formation of P–O bonds using tellurium and selenium as organocatalysts and alcohol nucleophiles. However, both tellurium and selenium are toxic to humans, and these methods are not very general.[3] In this work, we present a new method for the efficient dehydrogenative phosphinoylation of oximes using readily available disulfides as the organocatalyst.



The utility of this approach is demonstrated by its tolerance to a broad range of oxime substrates, including alkyl-, aryl-, cyclic-, and heterocyclic- substituted oximes. Future work will expand the scope of organophosphorus coupling partners as well as targeting medicinally relevant examples.



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TAILORING MOF-BASED ELECTROCATALYSTS FOR CO_2 ELECTROCHEMICAL REDUCTION

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As society aims to decarbonise its material and energy sources, the capture of CO_2 and the potential to recycle the CO_2 using renewable energy sources may provide a clean carbon source for feedstock in industry or fuel. Electrochemical CO_2 reduction (CO_2RR) is a method of re-utilising CO_2 gas in the atmosphere to generate value-added products. Whilst there has been a significant amount of research into CO_2RR, making the process economically viable has still not occurred to the large energy costs associated with converting CO_2.[1] In particular, producing more complex hydrocarbon molecules in economically feasible amounts remains a challenge due to the complex nature of CO_2 gas reduction. The products of CO_2RR are in large part controlled by the electrocatalyst, which through surface chemistry with CO_2RR intermediates can control the final product.

This oral presentation will discuss multi-metallic metal-organic-framework (MOF) based electrocatalysts for CO_2RR. MOFs are crystalline, porous materials which can host a variety of metal sites. They are good gas adsorbents due to their porous cage-like frameworks, which can be used to trap the CO_2 gas for electrochemical reduction. MOF-based electrocatalysts were synthesized from Zn, Cu and Ag to take advantage of synergistic effects between these metals and the MOF structure. Electrodes were created by depositing a MOF-catalyst ink onto a conductive substrate. The MOF-based catalyst materials were tested in a custom electrochemical CO_2RR flow cell reactor to evaluate their performance for CO_2RR and water splitting. The MOF-based electrocatalysts were characterised through a variety of methods to understand their structure, electronic environment and how this contributes to their electro catalytical performance.

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IRON-SULFUR CARBIDE CLUSTERS AS MODELS OF TH ENITROGENASE ACTIVE SITE

Emer Doyle-Neilon[1], Justin Henthorn[2]
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Nitrogenase has been of great interest in bioinorganic chemistry for the last few decades as this biological system is vital for all life through its action as the catalyst for the reduction of dinitrogen to ammonia[1]. Nitrogenase is a complex biological system that requires multiple proteins to function, with FeMoco (Iron Molybdenum cofactor) the primary cofactor of nitrogenase. Molybdenum-dependent nitrogenase enzymes use a Fe_7MoS_9C active site to enable nitrogen fixation[2]. Since the discovery of the interstitial carbide in FeMoco,[3] many researchers have been attempting to synthesise a suitable mimic for the nitrogenase active site[4,5] but these attempts are limited due to the challenge of synthetically incorporating a carbide into iron-sulfur clusters. Hence, these clusters have been unable to replicate the geometrical structure of FeMoco and are therefore unable to sufficiently mimic the electronic structure and reactive properties of FeMoco. Our understanding of FeMoco will be enhanced by investigating these properties using a synthetic mimic of FeMoco derived from Iron-Sulfur carbide clusters. This work reports the synthesis and characterisation of a series of iron-sulfur carbide clusters which have been designed as structural and electronic mimics of FeMoco. Together with a powerful carbodisufurane as a carbon atom transfer source, these mimics tackle two current issues in this field; the carbodisufurane allows for easy insertion of a central carbide into the clusters which in turn allows for the synthesise of high fidelity FeMoco mimics.

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Enantioselective 1,4 and 1,2-additions on free anilines and derivatives

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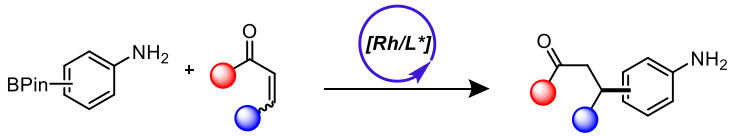
Nitrogen-containing motifs are ubiquitous in pharmaceuticals with anilines constituting a key class of intermediates in their synthesis.[1] A straightforward approach to building molecular complexity on the aniline moiety would be to employ aniline boronates in Rh-catalysed asymmetric 1,4-addition reactions.[2] However, free amines are notoriously difficult substrates for metal-catalysed reactions, as the N–H groups are well-known to poison catalysts, with the nitrogen lone pair further increasing complexity through competitive coordination.[3,4] Herein, we present a protecting-group-free strategy for the synthesis of enantioselective novel aniline-derived scaffolds.



20 examples
up to 96% yield
up to 98:2 *e.r.*

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GREEN SYNTHESES TOWARDS RUTHENIUM(II) POLYPYRIDYL COMPOUNDS

Rebecca Galway[1,2], Prof. Eric Moore[1], Dr Christopher Burke[1,2].
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Ruthenium(II) polypyridyl complexes (RPCs) of the type $[Ru(N^N)_3]^{2+}$, where N^N denotes a bidentate nitrogen-donor ligand, are being investigated due to their easily tuned photophysical and physiochemical properties. Such complexes have applications in sensing, cellular imaging and as anti-cancer therapeutic agents.[1]

Synthetic strategies are reliant on hazardous solvents, toxic reductants and energy intensive heating. These drawbacks underscore the need to develop more sustainable synthetic strategies.[2] Herein, greener approaches to syntheses of RPCs are described, including preparation of homoleptic complexes. Protocols developed include the exploration of surfactant mediated syntheses in water, and the use of auxiliary anionic agents, to provide the complexes from common precursors; $RuCl_3.nH_2O$, $[Ru(bpy)_2Cl_2]$ and $[Ru(DMSO)_4Cl_2]$.

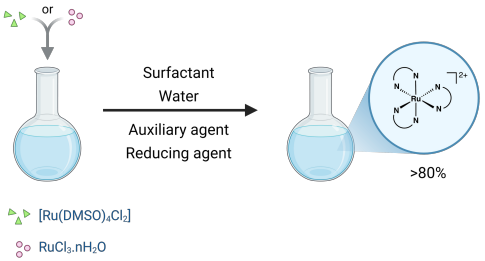

Figure 1. Illustration of the green syntheses of Ru(II) polypyridyl complexes

Acknowledgements
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ASYMMETRIC SYNTHESIS OF CYCLOBUTANONES WITH QUATERNARY α-ARYL STEREOCENTRES VIA DAAA

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Strained ring systems hold a key role in the discovery of novel reactivity due to their unique, rigid, puckered conformation which infers esoteric properties.[1] Despite being more stable than cyclopropanone, cyclobutanones' unique and similar reactivity has been underutilized. Additionally, compared to its five-, six-, and seven-membered relatives, cyclobutanone and its derivatives have been significantly overlooked in organic transformations despite being prevalent in biologically active molecules.

Many medicinally relevant compounds also contain enantioenriched quaternary α-aryl stereocentres, with their construction being considered one of the most difficult challenges in organic chemistry. Pairing this challenge with the difficult handling and manipulation of cyclobutanones, the need for the development of synthetic routes to generate cyclobutanones with quaternary α-aryl stereocentres is showcased. An effective way to install these stereocentres is via Pd-catalysed Decarboxylative Asymmetric Allylic Alkylation (DAAA) of α-aryl-β-keto allyl esters, which is a methodology well explored within the group on various substrates.[2]

Herein, we report the synthesis of a cyclobutanone with an enantioenriched quaternary α-aryl stereocentre via DAAA, achieving yields of up to 100% and enantioselectivity of 97% *ee* after optimization. Currently, a substrate scope is underway where the α-aryl substituent is being varied.

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CYCLOMETALATED IRIDIUM (III) SOLVATE COMPLEXES: DEVELOPMENT OF GREENER ROUTES TO THEIR SYNTHESIS AND THEIR APPLICATIONS IN LABELLING OF RECOMBINANT PROTEINS

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Iridium(III) solvates are an emerging area of interest for switch-on luminescence labelling of histidine rich proteins. [1] These complexes exhibit aqueous solubility, and selective and direct binding to di-histidine motifs via ligand substitution with labile solvent ligands such as acetonitrile. [2]
In this work, we present and compare different synthetic routes to iridium solvate complexes, including the traditional route via iridium dimer intermediate versus new approaches using green solvents developed in our lab that proceed via acetylacetonate intermediates and/or use of acid reagents that preclude the use of silver activation steps. The Ir-acac intermediate was found to be easily isolated, purified and characterised, and thus simplifies follow-on reaction steps.
We also report preliminary results on the application of the synthesised iridium solvate complexes, including their histidine-targeting and light-switch capabilities in naturally His-rich bovine serum albumin (BSA) and bacteriophage derived cell binding domain (CBD) protein at a genetically encoded His-tag. Future directions for the project will explore application of iridium solvates within biomolecular condensates as sensing and photodynamic therapy agents.

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DEVELOPMENT OF A CHIRAL AUXILLARY STRATEGY FOR THE DIASTEREOSELECTIVE SYNTHESIS OF P-STEREOGENIC NATURAL PRODUCTS

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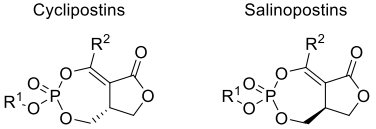
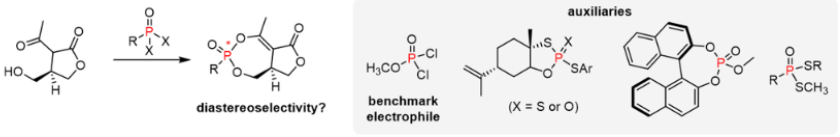
Cyclipostins and Salinipostins are natural products originating from soil and marine based microorganisms with the former acting as acetyl cholinesterase inhibitors and the latter possessing antimalarial activity.[1] Both classes of compounds contain a stereogenic phosphotriester motif in a bicyclic structure but differ in their stereochemical configurations. The total syntheses of these compounds were first reported in 2011 and 2018 respectively[2,3] with both approaches utilising a racemic mixture of the below gamma butyrolactone to couple to the phosphorus centre.



This work explores the effect of an enantioenriched butyrolactone on the diastereoselectivity of the reaction when combined with different chiral phosphorus auxiliaries. With the reaction proceeding via two subsequent substitution steps and the use of Neighboring Group Participation, an increased reaction rate is expected to result in diastereocontrol.



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REDUCTION OF RESOURCE USE AND WASTE GENERATION IN SYNTHESIS: DEOXYGENATIVE FUNCTIONALISATION OF ALCOHOLS WITH H-PHOSPHONATES

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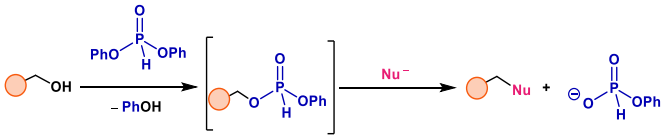
The development of sustainable and low-waste methodologies in chemical synthesis is a key objective for modern synthetic chemistry. Nucleophilic substitution reactions are one of the most widely used classes of reaction in organic synthesis.[1] However, traditional methods often generate significant waste and utilise reagents that generate large quantities of waste in the upstream processes used to synthesise the required starting materials. The American Chemical Society Green Chemistry Institute Pharmaceutical Roundtable (GCIPR) highlighted the direct substitution of alcohols as one of their ten key green chemistry research areas for the period 2018 - 2028.[2]



A sustainably derived H-phosphonate promotor was identified as a general reagent to enable the activation of alcohols towards nucleophilic substitution for a range of nucleophiles such as halides, amines, and phosphines. A process was developed, combining diphenyl H-phosphonate-mediated deoxygenative halogenation of alcohols with subsequent nucleophilic substitution, enabling substitution using amines and phosphine nucleophiles in high yields (80% - 99%). Use of iodide as a catalyst has been demonstrated to enhance product formation in instances in which low yields are otherwise obtained.

A chromatography-free isolation protocol for solid alkyl iodide substrates was established, significantly reducing the waste generation in the isolation process, and the resulting process mass intensity (PMI) values are competitive with the best current green protocols for alkyl halide synthesis.[3, 4]

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Synthesis of *γ*-Lactones and δ-Lactones from Ketenes and Epoxides or Oxetanes

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γ-Lactones and δ-lactones have been synthesised in our lab through a new catalytic intermolecular reaction. An epoxide or oxetane and a ketene are the two starting material substrates used by our group in the synthesis of *γ*-lactones and δ-lactones. *γ*-Lactones/δ-lactones have been reported to have multiple applications. The Corey lactone is a pivotal intermediate in prostaglandin synthesis [1]. Additionally, a *γ*-lactone has been used as an intermediate in the synthesis of Gemcitabine, a nucleoside analogue [2]. Baba et al synthesised a *γ*-lactone or δ-lactone from diphenylketene and a phenyl-substituted epoxide/oxetane through Ph_4SbI catalysis [3]. However, the catalyst used in the latter reaction is toxic and the scope of the reaction is quite limited. Hence, further research has gone into the synthesis of *γ*-lactones/δ-lactones by using an abundant environmentally benign catalyst, with the ultimate plan to develop a stereoselective variant of broad substrate scope. Our group has explored a number of different catalytic systems and it was concluded from our preliminary studies that LiI is the optimal catalyst for the desired reaction.

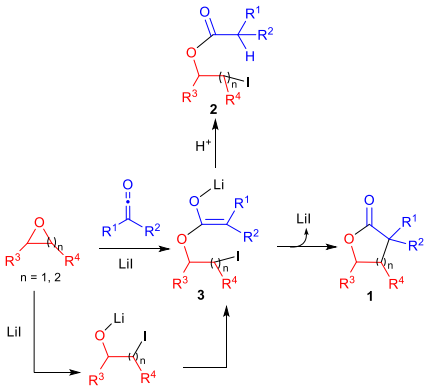

Figure 1: LiI-catalysed methodology

A range of epoxides/oxetanes have been investigated for the reaction shown in **Error! Reference source not found.**. The study of this reaction showed that under appropriate conditions the *γ*-lactones and δ-lactones (**1**) were formed in good yield. However, with certain epoxides/oxetanes an acyclic ester product **2** was formed (derived from enolate intermediate (**3**)). The epoxide and oxetane scope was explored by using diphenylketene or ethylphenylketene as the reactant partner. Further research is being carried out to enable cyclisation of the ester enolate intermediate **3**, for those examples where cyclisation does not currently readily occur. We will present our preliminary results on the new synthetic methodology**.**

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TIME-RESOLVED IR SPECTROSCOPY FOR EVALUATION OF PHOSPHINE COLIGAND EFFECTS ON THE ULTRAFAST BEHAVIOUR OF MN(I) PRECATALYSTS

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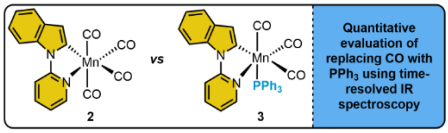

The use of Mn(I) carbonyl catalysts for C–H functionalisation reactions has received much attention in the last decade.[1] Simple pre-catalysts [$MnBr(CO)_5$] and [$Mn_2(CO)_{10}$)] have proven extremely effective and are used extensively in the literature. However, carbonyl ligands cannot be tuned to affect the activity of the metal centre while the popular use of pincer complexes with various coordinating heteroatoms[2] often requires multi-step syntheses and inert storage. Despite some recent examples[3], there is a distinct lack of simpler pre-catalysts, such as air-stable Mn-phosphine complexes. Understanding the effect of a phosphine coligand on the behaviour of Mn(I) pre-catalysts could enable access to a versatile class of ligands with tuneable steric and electronics.[5] We have investigated the photochemical activation of the pre-catalyst fac-[$Mn(inpy)(CO)_3(PPh_3)$] **3** by time-resolved infra-red spectroscopy (TRIR).[6] This reveals that light-induced dissociation of a CO ligand occurs preferentially over loss of the phosphine. The ultra-fast dynamics of complex formation with toluene, pyridine, and phenylacetylene are described. The alkyne undergoes a migratory insertion reaction into the Mn–C bond on a µs timescale with a similar first order rate constant to [$Mn(inpy)(CO)_4$], **2**, demonstrating that this key step in Mn-catalysed reactions is not affected by the presence of the phosphine ligand.

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Bioinspired Radical 1,2-Amino Migrations for Synthesis of Amines and Chiral Amino Acids

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Nature achieves highly selective construction of nitrogen-containing molecules through enzymatic transformations such as amino-group transposition catalysed by aminomutases.[1]Inspired by these processes, this work explores photochemically driven, enzyme-free radical 1,2-amino migrations as a strategy for skeletal reorganisation. This approach enables the conversion of readily available α-amino alcohol derivatives into valuable β-amino frameworks, offering an alternative to de novo synthesis.[2] Central to this study is the development of C–O bond activation methods to generate β-amino radical intermediates that undergo rearrangement via a radical transposition pathway (Figure 1).

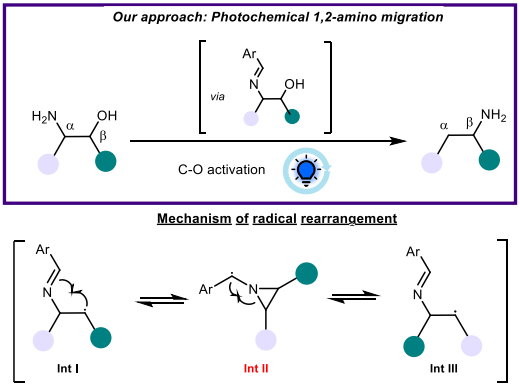

Figure 1. Our approach: Photochemical 1,2-amino migration

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TOWARDS THE SYNTHESIS OF TRIAZOLE-CONTAINING LIPOXIN A_4 MIMETICS

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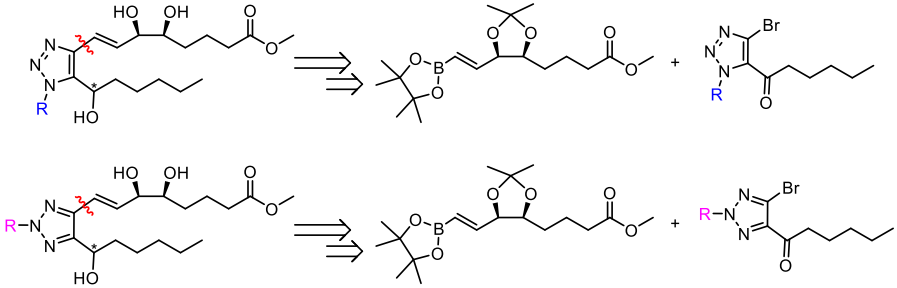
Lipoxins are a family of specialised pro-resolving mediators (SPMs) involved in inflammation resolution in the body.[1] Lipoxin A_4 is a naturally occurring member of this family which acts to resolve inflammation through a range of bioactions triggered upon binding to its cognate receptor.[2] LXA_4 is metabolised to several inactive metabolites rapidly in vivo so a significant amount of research has focused on the synthesis of mimetics with greater metabolic stability.[3]

Previously a range of LXA_4 analogues that incorporate various different functionalities to grant the compound greater metabolic stability have been synthesised.[4] This work details efforts made to expand this library of LXA_4 analogues and specifically focuses on the synthesis of five sets of triazole-containing LXA_4 analogues with varying substitution at different positions on the triazole ring.

To date the upper chain fragment has been synthesised in 27% yield and three out of five of the lower chain fragments have been synthesised in yields of up to 35%. Suzuki coupling of two of the lower chain fragments with the upper chain has been successful with yields of up to 84% obtained.



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PALLADIUM-CATALYSED DECARBOXYLATIVE ASYMMETRIC ALLYLIC ALKYLATION TO PREPARE STERICALLY HINDERED α-ARYL CYCLIC KETONES

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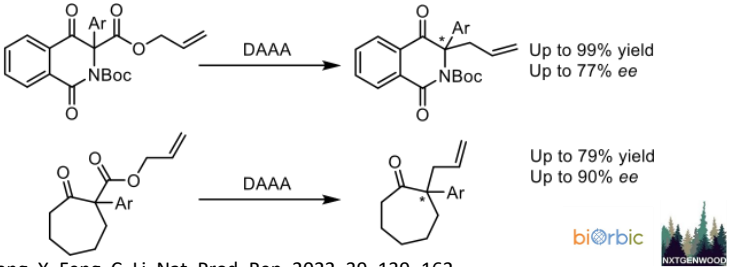
N-Heterocycles and carbocycles are motifs commonly seen in natural products, several of which have the potential to be used in the treatment of diseases such as cancer.[1] Many of these products are difficult to access synthetically due to the presence of quaternary stereocentres. The Pd-catalysed decarboxylative asymmetric allylic alkylation (DAAA) has been explored for the synthesis of quaternary α-allyl cyclic ketones with small alkyl and carbonyl substituents at the α-carbon.[2] Our group has expanded on this methodology, applying decarboxylative transformations to include sterically hindered α-aryl substrates.[3]

In this work, the DAAA reaction is effectively applied to previously unexplored *N*-heterocycles and carbocycles in order to access enantioenriched α-aryl containing products. Dihydroisoquinolinedione and cycloheptanone substrates have been synthesised for application in DAAA. The dihydroisoquinolinedione model substrate has been applied to this transformation, and the DAAA reaction of this substrate has been optimised to access the desired product, achieving yields of up to 99% and enantioselectivities of up to 77% *ee*. The results of our substrate scope, focusing on varying both sterics and electronics of the aryl ring on the α-carbon, are also described. The cycloheptanone model substrate has also been applied to the DAAA reaction, and conditions have been optimised to access the product in a 79% yield and 90% *ee*. The results of these investigations will be discussed.



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A NEW APPROACH FOR THE SYNTHESIS OF MEDICINALLY RELEVANT ORGANOPHOSPHORUS COMPOUNDS

Lauren Walsh[1], Dr. Eimear Courtney[1], Prof. Anita Maguire[1,2] and Dr. David Jones[1]
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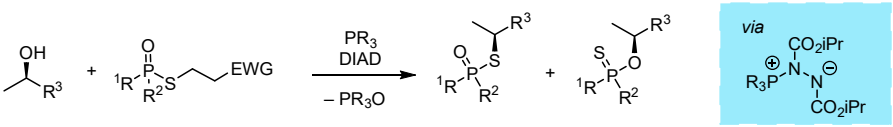
Sulfur-containing organophosphorus compounds are gaining increasing importance in organic synthesis due to their applications in anti-cancer, anti-viral and antimicrobial treatments. These compounds also hold significant value in agrochemistry as insecticides, while phosphorothioate compounds have applications in antisense oligonucleotide therapies due to their enhanced pharmacokinetic properties[1].

Previous group research has shown the possibility to functionalise P-S compounds by β-elimination and alkylation steps using alkyl hailides[2]. In this work, we progress on this research by use of the Mitsunobu reaction to complete both the β-elimination and alkylation in one singular reaction. This approach is distinct as it produces both *S*-alkylated and *O*-alkylated structural isomers, and uses sustainable, ubiquitous alcohol substrates in lieu of alkyl halides.



Previous literature[3] suggests the possibility to invert selectivity between structural isomers. The project aims to gain understanding of the reaction mechanism and kinetics to control the selectivity and afford the desired product. Future work will expand the substrate scope and further mechanism studies.

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FROM WASTE TO RESOURCE: METAL-ORGANIC FRAMEWORKS FOR POLYPHENOLS REMOVAL FROM WATER

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Among the wide varieties of pollutants in water, polyphenols are the most monitored for their double property: at high concentration their toxicity can alter the microbic balance and remove the oxygen in aqueous environment. On the other hand, polyphenols can be exploited due to their antimicrobic, antioxidant and nutraceutical properties for food, pharmaceutical and cosmetic industries [1,2]. MOF (metal organic frameworks) are highly porous compounds with a metal center and organic ligands in a tridimensional network. During the synthesis, the chemical and physical properties of MOF can be monitored by changing the metal nodes and the ligands of the structure [3]. Zirconium metal centered MOFs and modulated organic ligands were selected to study the adsorption efficacy of polyphenols. The synthetized materials were analyzed with various analytical techniques, then they were tested for water stability and adsorption efficacy. Computational chemistry was found to be useful for this purpose, modulating the functional organic groups on the MOFs' ligand to foresee the adsorption energy of polyphenols in the pores. Studies on $-NH_2$, $-NH_3^+$ (according to pH) and -OH functionalities were submitted on zirconium centered MOFs, structures were optimized starting from 3D visualization software, and the corresponding geometric optimization, single point energy calculations and solvent correction calculations were submitted to obtain the final energy interaction between the MOF and the polyphenol. Looking at the results, we could be able to foresee the polyphenol adsorption-desorption energy in the pores of the MOF to evaluate which is the most favorable for our application, this can speed up the optimization process considering the large variety of these materials.

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BODIPY PHOTOSENSITISERS FOR DEGRADATION OF ANTIBIOTICS IN WATER

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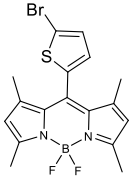
Water is a limited resource which is contaminated daily by antibiotics, pesticides, perfluorinated compounds, among other pollutants. According to the Environmental Protection Agency, the quality of Irish waters is declining.[1] Amoxicillin is a widely prescribed β- lactam antibiotic, a class of antibiotics which accounts for approximately 70 % of all antibiotics prescribed.[2] Antibiotics enter waterways through wastewater effluent, agricultural runoff, and improper disposal.[3] Even at low environmental concentrations, antibiotics can contribute to antimicrobial resistance. Therefore, sustainable solutions are required for the removal of antibiotics from water.

Photodegradation offers a promising approach, as it can be driven by harnessing solar energy. The first step in photodegradation is the absorption of light by a photosensitiser, leading to the production of reactive oxygen species (ROS) for the remediation of environmental pollutants, including antibiotics. BODIPY dyes are an attractive family of photosensitisers for photodegradation due to their absorption within the visible region, and therefore high energy light sources are not required.[4] This work focusses on the synthesis of BODIPY-based photosensitisers which were assessed for photodegradation of antibiotics. Their photophysical properties were studied using steady-state and time-resolved spectroscopy, and the types of ROS generated were identified. The ability of the BODIPYs studied to degrade amoxicillin will be presented.



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DEVELOPMENT OF A FLUORESCENCE-BASED LAMP ASSAY FOR *ESCHERICHIA COLI* DETECTION IN DAIRY-SOILED WATER

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The EU Water Reuse Regulation (EU) 2020/741[1] mandates routine monitoring of *Escherichia coli* (*E. coli*) as an indicator of faecal contamination in reclaimed water for agricultural irrigation. Current compliance testing relies on weekly culture-based enumeration (ISO 9308-2:2012)[2], which is reliable but requires more than 24 hours to obtain results, making it difficult for rapid decision making for water reuse management. In this work, Loop-Mediated Isothermal Amplification (LAMP) is investigated as a rapid, low-cost alternative for *E. coli* detection. LAMP enables highly specific DNA exponential amplification under isothermal conditions, eliminating the need for thermal cycling and supporting point-of-care deployment.[3] While common LAMP readouts such as fluorescence and gel electrophoresis are effective, their cost and limited scalability pose challenges for portable sensing formats. To address the limitations of conventional optical readouts, this study explores electrochemical detection using a DNA-intercalating redox reporter, providing a scalable and portable sensing strategy. Initial optimisation employed spectrofluorimetric monitoring to refine reaction conditions, achieving a limit of detection of 1–5 copies μL^{-1}. The optimised LAMP assay was successfully applied to dairy-soiled water, demonstrating robust *E. coli* amplification in a complex, inhibitor-rich matrix. Ongoing work focuses on integrating electrochemical detection with LAMP to enable rapid (<1 h), sensitive (<0.1 CFU mL^{-1}), and on-site monitoring for sustainable water reuse compliance.

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Nano-Enabled Sensor Development for Arsenic Detection in Water

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Arsenic contamination in drinking water remains a major global health concern, with As(III) being particularly important due to its high toxicity and mobility in aqueous environments. The World Health Organization and Environmental Protection Agency guideline/limit for arsenic in drinking water is 10 µg L^{-1} (10 ppb), but many affected regions still struggle with reliable monitoring and compliance. Although conventional analytical techniques provide sensitive detection, they are often expensive, time-consuming and require skilled operation. Therefore, rapid, low-cost and field-adaptable sensing approaches are needed for practical water monitoring. This work focuses on nano-enabled sensing platforms for As(III) detection using complementary colorimetric and electrochemical strategies.

In the colorimetric approach, polyvinylpyrrolidone-capped silver nanoprisms were synthesised and investigated for As(III) detection through arsenite-silver interactions, producing visible and measurable optical responses. In parallel, drop-cast gold nanoparticle-modified glassy carbon electrodes were developed and characterised by cyclic voltammetry, followed by square-wave anodic stripping voltammetry for trace As(III) determination. These findings support the further development of nano-enabled optical and electrochemical approaches for As(III) detection in water.

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LIGHT ACTIVATED BODIPY COPOLYMERS FOR HERBICIDE REMEDIATION IN WATER

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Water is an essential resource which is becoming increasingly threatened by human activities. Contaminants from industrial and agricultural processes readily leech into our waterways, and as many of these pollutants have adverse biological and environmental effects, it damages the ecosystems and our health.[1] Herbicides in particular are known as endocrine disruptors and are suspected to contribute to reproductive and developmental disorders as well as some cancers.[2] In Ireland, in 2025 alone there were almost 70 instances where pesticides were detected above the limits set by the EU, and 70% of these detected breaches were from 2-methyl-4-chlorophenoxyacetic acid (MCPA), one of the target herbicides in this study.[3] Novel remediation approaches to treat water contaminated with such pollutants are urgently needed. A sustainable approach is to design materials (photosensitisers) that harvest solar energy, and produce reactive oxygen species (ROS), which can degrade these pollutants. We have designed and assessed BODIPY polymers (such as shown in Figure 1) to generate ROS, and degrade herbicides using visible light as the energy source. The results of these studies together with the photophysical properties of the polymers will be presented.

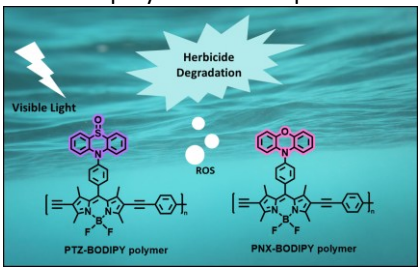

Figure 1. Schematic of ROS mediated photodegradation of herbicides in water.

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Application of fast, low-cost spectroscopic sensors to measure nitrogen dioxide in small towns in Ireland

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Nitrogen dioxide (NO_2) is an environmental pollutant released into the atmosphere predominantly by the automotive industry. Traditionally, NO_2 is more closely monitored in cities and larger urban areas and as a result its levels in smaller urban clusters are not as well documented despite many seeing high traffic volumes due to commuters passing through to the larger the cities. This work presents the application of a fast, low-cost cavity-enhanced absorption spectroscopy (CEAS) sensor monitoring of NO_2 levels in three small towns in County Cork, Ireland: Macroom, Killeagh and Millstreet. The respective populations of these towns are approximately 4100, 900, and 1800. The spatial and temporal characteristics of NO_2 in these towns, and the influence of highly polluting vehicles on local air quality are presented. The potential of the novel CEAS system for characterising NO_2 pollution in small population centres is discussed.

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Environmental monitoring of estrone in river water using point of concern electrochemical immunosensors.

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Abstract:

Estrone (E1), as a defined endocrine disruptor, affects the endocrine system of humans and animals, such as interfering with hormone synthesis and metabolism. While traditional LC-MS/MS facilitates the quantitative determination of E1 in complex aqueous matrix's, its utility is often constrained by serial sample processing and protracted analytical durations. Alternatively, immunochemical method are rapid, cost-effective and offer high sample throughput, demonstrates significant potential for measuring E1 in natural water bodies. Enzyme-linked immunosorbent assay (ELISA) is a sensitive and specific method for detecting E1 in water and can be used to monitor endocrine disruptors in environmental samples. Traditional ELISA utilizes antibody-antigen specific binding, amplifying the signal through an enzyme-catalysed colorimetric reaction, thus enabling qualitative or quantitative detection of E1 in natural water samples. This project will investigate carbon screen-printed gold nanoparticle coated electrochemical sensors, and compared with ELISA kits. Also innovatively develop an immunosensor detection method using screen-printed electrodes, comparing and optimizing it with traditional ELISA kits.

DATA-DRIVEN INSIGHTS INTO PIEZOELECTRICITY: MACHINE LEARNING FOR SUSTAINABLE MATERIALS

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A key challenge in ML-driven materials discovery is moving beyond "black-box" models to extract physically meaningful trends [3]. To address this, techniques such as feature importance analysis are used to identify the atomic and structural factors that most strongly influence piezoelectric response. These insights can guide the rational design of next-generation materials with tailored properties, impacting applications in self-powered sensors, biomedical actuators, and sustainable energy solutions.

In this work, a rigorous and reproducible ML framework is developed to predict piezoelectric coefficients, leveraging large inorganic material databases [1] and the recently introduced organic piezoelectric dataset, CrystalDFT [2]. Beyond prediction, this approach also emphasizes interpretability, providing insights into the underlying structure–property relationships that govern piezoelectric behavior. Unlike previous studies focused primarily on inorganic materials, this work incorporates both inorganic and organic piezoelectrics, which offer advantages such as mechanical flexibility, biocompatibility, and tunable molecular structures. However, their complex chemistry presents challenges for traditional screening approaches. By integrating organic materials into the ML framework, this study broadens predictive modelling and offers new insights into structure–property relationships that differentiate organic and inorganic piezoelectrics.

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GREEN CHEMISTRY UPGRADING OF BIO-BASED CARBON FOR CATALYTIC APPLICATIONS

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Global plastic consumption is ever-increasing, and efforts to mitigate plastic pollution have driven advancements in the field of recycling and the production of biodegradable alternatives.[1] Polyhydroxyalkanoates (PHAs) are a promising class of bioplastics, noted for their biodegradability and polyolefin-like mechanical properties.[1] Whilst exhibiting many benefits, PHAs are costly to produce when compared to traditional plastics. This highlights the need for effective recycling technologies to support a circular life cycle.[2]

This research focuses on the development of a feasible and sustainable heterogeneous catalyst to be used for the hydrolytic degradation of PHAs. Biochar is an inexpensive and renewable carbonaceous material[3]. This was the support material for the catalysts developed in this project, as its porous structure is well-suited to catalytic applications. To enhance its surface area and catalytic performance, the biochar was modified using $Ca(NO_3)_2$ and $Mg(NO_3)_2$ treatments. Catalytic characterisation was performed with use of many analytical techniques, including Fourier Transform Infrared Spectroscopy (FTIR), X-ray Fluorescence (XRF) and Scanning Electron Microscopy (SEM). The catalytic activity was assessed through hydrolytic reactions of PHAs. Investigating degradation was monitored via mass loss measurements, High-Performance Liquid Chromatography (HPLC), and FTIR analysis to evaluate changes in polymer structure and product formation. This work demonstrates the potential of modified biochar as an efficient and sustainable catalyst for PHA degradation, contributing to the advances of greener recycling technologies and promoting circular life-cycle strategies for PHAs.

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CATALYTIC PYROLYSIS OF POLYPROPYLENE USING A MICRO-MESOPOROUS ALUMINOSILICATE CATALYST

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Polypropylene (PP) is the 2nd most used plastic globally, after polyethylene.[1] Pyrolysis is a chemical recycling method used for plastic waste management, which involves heating plastic waste to temperatures of 300 – 800 ˚C in the absence of oxygen and ideally generates useful condensable and non-condensable products. Pyrolysis of PP in the presence of a catalyst has been shown to produce a number of valuable hydrocarbon products.[2]

Heterogenous aluminosilicate catalysts have been shown to increase the rate of plastic degradation during pyrolysis, facilitating degradation at lower temperatures.[3] They also alter the selectivity of the pyrolysis products observed. Zeolites are aluminosilicate catalysts made up of a network of tetrahedral SiO_4 and AlO_4^- units, connected through their oxygen atoms. Zeolites are known to effectively catalyse plastic pyrolysis by partaking in reactions with the plastic polymer at their surface acid sites, which are generated when H^+ is used as the AlO_4^- counterion.

A micro-mesoporous aluminosilicate catalyst was prepared using a one-pot hydrothermal modification of a HY zeolite seed. Mesopores were introduced using cetyltrimethylammonium bromide as a templating species, and their generation was confirmed using N_2 physisorption. TEM identified the formation of mesopores throughout the catalyst and also showed the presence of crystalline and amorphous phases in the material. XRD also confirmed the presence of the crystalline phase. Ammonia TPD was used to analyse the Bronsted acid sites in the catalyst.

The performance of the micro-mesoporous aluminosilicate catalyst in the cracking of PP was investigated using thermogravimetric analysis and within a lab-scale pyrolysis reactor. The pyrolysis products were analysed using FTIR, GC, and GC-MS.

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DEVELOPMENT OF AN IN-SITU CHLOROPHYLL-A FLUORESCENCE DETECTOR FOR THE EARLY ONSET DETECTION OF ALGAE

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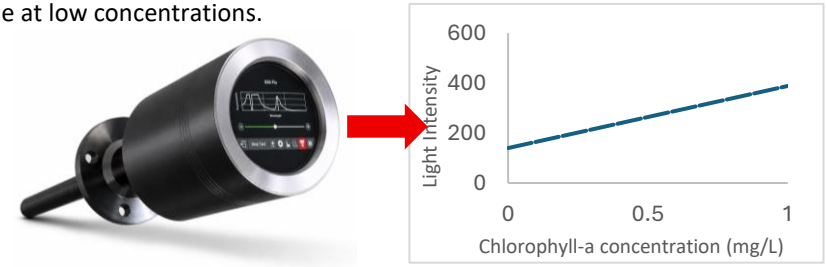
Early and accurate detection of algae has become an increasing priority for many fields, including water treatment, aquaculture, and the food and beverage industries. Particularly within Northern Ireland, there has been a significant increase in harmful algal blooms[1] but the increasing frequency & size of algal blooms generally has led to the demand for devices which can detect and quantify algae at low concentrations.



Chlorophyll-a (Chl-a) is the standard choice for algal detection since it is the prevalent pigment within all species of algae.[2] In this work two different Chl-a fluorescence sensors have been developed; one is an easily portable mobile system which measures samples in cuvettes and one can be deployed as a long-term fixed probe. Detection limits were found to be in the parts per billion scale. Tests on both chlorophyll-a solutions and on environmental water samples showed a strong correlation between concentration and fluorescence intensity. Several factors and their effect on fluorescence were tested on the environmental samples, such as temperature and light availability over time.

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SYNTHESIS OF POLY(ETHYLENE FURANOATE) FOR FOOD PACKAGING APPLICATIONS

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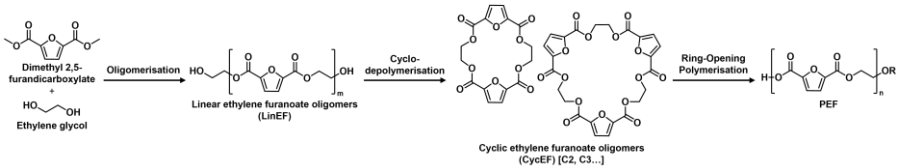
Global plastic production exceeds tens of millions of tonnes annually, with petroleum-derived poly(ethylene terephthalate) (PET) alone reaching over 55 million tonnes per year[1]. Poly(ethylene furanoate) (PEF), produced from renewable biomass feedstocks, has emerged as a promising candidate to replace PET for food packaging applications. PEF offers a reduced carbon footprint, superior gas barrier properties, high tensile strength, and the potential to be recycled with PET waste streams or biodegraded. However, the widespread adoption of PEF remains limited by several key challenges; namely, the low molecular weight achieved via traditional polycondensation routes, and its brittle mechanical properties, making processing difficult. This work focuses on the synthesis of cyclic ethylene furanoate oligomers and their subsequent ring-opening polymerisation as a potential route to produce high molecular weight PEF[2]. PEF blends and composites will be formulated to improve mechanical and physical properties, with the resulting PEF materials assessed for their viability as single-layer barrier film packaging and their potential end-of-life options. Overall, this research seeks to advance scalable, sustainable PEF synthesis for next-generation food packaging applications.



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Remote sensing of NO_2 across Cork city using a Low- Cost Long Path DOAS system.

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Differential Optical Absorption Spectroscopy (DOAS) is a long-standing remote sensing technique used to measure many absorbing trace gases. To attain the necessary sensitivity to weak absorptions from trace gases, conventional DOAS systems normally have kilometre-long path lengths and a large telescope to maximise the collected light. Such systems are expensive and largely limited to research applications. This work describes a low-cost, long path DOAS system with a 1.5 km path length in Cork city, Ireland, specifically to measure nitrogen dioxide (NO_2) for air quality monitoring. The system consists of a temperature-stabilised 0.8 W blue LED (peak wavelength at 435 nm), 5 cm diameter transmitting and receiving telescopes, and a compact spectrometer. A bandpass filter (420 nm – 460 nm) is used to eliminate stray light. The system is much smaller than conventional DOAS configurations and is relatively straightforward to assemble. The outlook for using the approach to monitor the contribution of NO_2 to urban air quality is discussed.

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IRON AS A SEASONAL ENERGY CARRIER

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Renewable energy sources have long been acknowledged as necessary for fighting climate change. However, renewable energy production rates vary seasonally, with production peaks often offset from when energy demand peaks[1,2,3]. Consequently, long-term storage solutions are key to renewable energy integration because they can balance these mismatches between production and consumption time periods[1,2].

Hydrogen is a commonly used energy carrier because of its high energy density[1,2,3]. However, its physical properties make long term storage difficult, with current solutions focused on geographically limited options or expensive materials[1,2,4]. These difficulties can be mitigated by chemically storing hydrogen, reacting hydrogen with another material in a reversible reaction[1,4].

Iron is an ideal such material due to its abundance, low cost, and lack of major safety risks[1]. The presented work analyses the release of hydrogen via the oxidation of iron in liquid water. This offers energy savings when compared to current state-of-the art systems which use steam[1] because the solid-liquid phase reaction reduces heating requirements and phase-separation challenges for the products. Results are presented for the iron-water oxidation rates under varying temperature and iron particle size and are discussed in the context of seasonal energy storage.

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Porous Anodic Alumina Templates for Magnetic Micro/ Nano-wires for Biomedical Application.

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Porous anodic alumina (AAO) templates were fabricated using a two-step anodization process to develop magnetic micro/nanowires for biomedical applications. AAO provides a cost-effective and highly ordered nanoporous platform whose pore diameter, interpore distance, and length can be precisely tuned by adjusting anodization voltage, time, electrolyte composition, and temperature.[1] In this procedure, the aluminium foil is initially pre-textured through degreasing with acetone followed by electropolishing of the surface. The first stage of anodization produces a textured concave pattern on the aluminium substrate, achieved after the oxide layer is removed. Subsequently, the second anodization step is conducted under identical conditions, leading to the self-organized formation of nanopores at the base of each convex.[2]The surface is then protected from etching, and any remaining aluminium is eliminated. The template's excellent physical and chemical stability also enables its use as an efficient drug reservoir and enhances sensor performance when coated with metals. Magnetic nanowires grown within these nanopores exhibit strong shape anisotropy, resulting in high coercivity values desirable for targeted drug delivery, hyperthermia, and magnetic manipulation. [3]The deposition of magnetic materials into the AAO channels significantly influences their magnetic behaviour, allowing tunability similar to core–shell Fe–Fe_3O_4 nanowires reported in recent studies, where controlled oxidation and structural characteristics enable adjustable magnetic properties and improved biocompatibility. [4]The AAO template and its magnetic nanowires offer a flexible platform with significant potential for advanced biomedical and sensing uses.

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Development of a Pt-NP microchip sensor for electrochemical detection of Ammonium

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Abstract:

Excess ammonium (NH_4^+) poses a significant threat to ecosystems and human health, making its monitoring essential for environmental protection and agricultural management. This study presents the development and evaluation of an electrochemical sensor for ammonium detection in real-world samples. Conventional sensors often suffer from poor selectivity due to cross-sensitivity to interfering ions such as potassium, chloride, sulphate, and other nitrogen species, resulting in inaccurate measurements in complex matrices like wastewater and soil extracts. In this study, an electrochemical sensing platform based on a platinum nanoparticle (Pt-NP) modified interdigitated electrode will be developed. The deposition of Pt-NPs will be employed to enhance the electrochemical active surface area (ECSA) and roughness improving sensitivity and selectivity. Key factors influencing sensor behaviour, including pH effects and interferents, will be systematically investigated, and a pH modulation strategy will be employed to ensure measurement conditions will be consistent and repeatable. The proposed sensor will demonstrate improved selectivity and robustness, highlighting its potential for reliable ammonium monitoring in complex environmental samples.

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Nanoporous metals for electrochemical sensing

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This research project explores the development of nanoporous metals, specifically nanoporous gold (NPG) and nanoporous copper (NPC), as high-performance electrochemical sensing platforms. Utilizing a 3D bicontinuous, sponge-like architecture, these materials offer significant advantages over traditional planar electrodes, including an increased density of catalytically active sites, high specific surface areas, and tailorable pore sizes. The project focuses on the fabrication of these materials via controlled selective dealloying of precursor metal alloys, integrated with state-of-the-art micro- and nanofabrication techniques. The electrochemical performance of the developed nanoporous materials will be assessed against a range of niche target analytes critical to the environmental, food, and biomedical sectors. Building on preliminary demonstrations of enhanced sensitivity for phosphate, nitrate, heavy metals, and dissolved oxygen at NPG, as well as non-enzymatic glucose detection at NPC, this work will further investigate the "nanoconfinement effect" and its role in analyte discrimination within complex matrices. A key objective is to evaluate the anti-biofouling characteristics of these 3D structures in challenging biological environments such as blood, saliva, and urine, where non-specific protein adsorption typically limits sensor longevity.

Structural characterization will be conducted using advanced nanovisualization equipment to correlate ligament morphology and pore distribution with electrochemical sensitivity and stability. The outcomes of this project will contribute to the design of robust, miniaturized
sensing technologies for real-time monitoring in animal welfare and clinical diagnostics, bridging the gap between laboratory-scale material science and portable, on-site analytical applications.

Keywords: Nanoporous Gold, Nanoporous Copper, Electrochemical Sensing, Dealloying, Anti- biofouling, Microfabrication, Point-of-Care Diagnostics

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Metal Organic Frameworks (MOF)-Coated IDT Resonance Sensors for Fast, Selective Gas Detection.

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Acetone sensing is important for applications spanning industrial monitoring, environmental control, and biomedical diagnostics. In particular, acetone is abundant in human breath, and its elevated concentration has been associated with diabetes, motivating the development of noninvasive sensing approaches for early detection and disease management. Existing detection strategies include resistive, capacitive, gravimetric, and analytical techniques such as gas chromatography-mass spectrometry (GC-MS), proton-transfer-reaction mass spectrometry (PTR-MS), and selected ion flow tube mass spectrometry (SIFT-MS). While analytical methods offer high accuracy and sensitivity, they are typically bulky, expensive, and often unsuitable for portable, real-time deployment. Unlike conventional DC chemiresistive sensors, which rely on steady-state resistance changes, the present platform transduces analyte adsorption through microwave-frequency resonance shifts, enabling a fast and potentially more stable electrical readout. Here, we introduce a resonance-based acetone sensing strategy that couples the molecular selectivity of a metal-organic framework with the rapid electrical readout of a microwave-frequency interdigitated device, providing an alternative to conventional DC chemiresistive sensing. Specifically, we develop a selective acetone sensing platform based on a ZIF-8/multi-walled carbon nanotube (MWCNT) composite coated onto an interdigitated transducer (IDT) fabricated on silicon. The sensing mechanism relies on the electrical resonance of the coated interdigitated structure, with resonance frequency given by $f_0 = 1/(2\pi\sqrt{LC})$. Upon acetone adsorption, the dielectric and electrical loading of the ZIF-8/MWCNT layer changes, leading to a measurable resonance shift, approximately described by $\Delta f/f_0 \approx -\frac{1}{2}(\Delta C/C + \Delta L/L)$. ZIF-8 provides selective adsorption sites for volatile organic molecules, while MWCNTs improve electrical transport and signal transduction. The proposed platform targets a limit of detection of 100 ppb or lower, together with a response time of less than 30 s. Planned cross-sensitivity studies against common interferents such as ethanol, methanol, isopropanol, ammonia, and humidity will further establish the selectivity of the proposed platform toward acetone. By combining MOF-based molecular selectivity with resonance-based electrical transduction, this approach offers a promising route toward compact and potentially low-cost acetone sensing, while also providing a broader platform for selective volatile organic compound detection.