



ISSUE Q1 2023

NEWS UPDATE www.sspc.ie







challenge areas

Sustainability Molecule Molecule

Education & Public Engagement

Royal Irish Academy elects Prof. Pat Guiry as President

Health



Pat Guiry, full Professor of Synthetic Organic Chemistry at the University College Dublin (UCD) School of Chemistry, Director of the Centre for Synthesis and Chemical Biology and SSPC investigator, will take up the position as the 58th President of the Royal Irish Academy with immediate effect.

Pat has been a strand leader in SSPC since 2013. His group developed the first catalytic asymmetric synthesis of isoflavanones, an important class of natural products, with potential anti-cancer and anti-microbial therapeutic capabilities.

Now a Co-Principal investigator with SSPC, Pat's group works to develop new methodologies for the asymmetric synthesis of existing APIs and future drug candidates with particular focus on the discovery and application of organometallic complexes for industrially-relevant and small molecule organocatalysts for industrially-relevant, synthetic transformations. Read more here.

Prof. Damien Thompson appointed SSPC director



Professor Damien Thompson has been officially appointed the Director of SSPC. He is Professor of Molecular Modelling at the University of Limerick, managing the predictive materials modelling group at SSPC and the Bernal Institute. His research focus is in the area of modelling and design of nano-structured materials for health and sustainability. Read more here.



Dr Eoin Scanlan



Prof. Thorfinnur Gunnlaugsson

Chemical Society Reviews: Glycosidase activated prodrugs for targeted cancer therapy



Authors: Harlei Martin, Laura Ramírez Lázaro, Thorfinnur Gunnlaugsson and Eoin M. Scanlan, **Trinity College Dublin**

Many current therapeutic strategies, including the drugs used in chemotherapy, usually target cells that are proliferating. Hence, there is an urgent need to identify specific cancer-targeting therapies. In this review, glycosidase activated prodrugs that target cancer cells are discussed. Glycosylated prodrugs undergo enzymatic bioconversion, cleaving the prodrug to release the anticancer drug at the desired site of action, hence minimising the toxic side effects associated with many current anticancer drugs. In addition, the presence of the carbohydrate moiety increases the aqueous solubility of the drugs, allowing for a more effective treatment. In the past decade, significant advancements have been made in this field that have led to the development of many novel carbohydrate-based prodrugs - ranging from simple glycoconjugates to complex self-assemblies and materials, which are discussed in detail herein. Read full review here.

FUNDING HIGHLIGHT

SFI Infrastructure Awards: Prof. Andrew Kellett, DCU, AUTOPILOT: Automated High-Throughput Analysis of Cellular Phenotyping



PUBLICATION Alteration in Levels of Specific miRNAs and Their **Potential Protein Targets between Human** Pancreatic Cancer Samples, Adjacent Normal **Tissue, and Xenografts Derived from These Tumors** Life, 2023, 13(3), 608. Fiona O'Neill. | Taylor-Jade Coyle.| Sandra Roche.| Martin Clynes et al.



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Prof. Anne Marie Healy

PROJECT SPOTLIGHT Natural Product Extraction



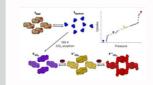
This work, led by Prof. Anne Marie Healy and Prof. Helen Sheridan with PhD student, Kate Tolan, at Trinity College Dublin, aims to apply processing and pharmaceutical formulation to traditional medicinal tinctures and create modernized, versatile and stable bioactive formulations. The project makes use of a metabolomics approach in the assessment of the impact of pharmaceutical manufacturing processing technologies on the phyto-chemical profile. This work has the potential to impact the quality, safety and efficacy of Echinacea purpurea products through an improved understanding of its photochemical profile and how to retain this during processing, as well as through optimising its formulation. Also, an investigation into the use of NADES (Natural Deep Eutectic Solvents) as a replacement for organic solvents in the tincturing process has the potential to have a significant environmental impact.

Trinity College Dublin are hosting the upcoming 71st Int. Congress & Annual Meeting of the Society for Medicinal Plant and Natural Product Research (GA), July 2-5, 2023. Registration and full details here.

FUNDING HIGHLIGHT

SFI Infrastructure Awards: Prof. Anita Maguire, UCC, Fast reaction kinetics in NMR Spectroscopy.

PUBLICATION



Reversible transformations between the non-porous phases of a flexible coordination network enabled by transient porosity Nature Chemistry, 2023. Varvara I. Nikolayenko, Dominic C. Castell, Debobroto Sensharma, Mohana Shivanna, Leigh Loots, Katherine A. Forrest, Carlos J. Solanilla-Salinas, Ken-ichi Otake, Susumu Kitagawa, Leonard J. Barbour, Brian Space & Michael J. Zaworotko



PROJECT SPOTLIGHT Modelling and Optimization of the Cryopreservation



O

Dr Jessica Whelan

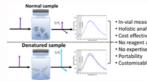
and Revival of Mammalian Cells

Cyopreservation is a key step that enables the commercial production and supply of traditional biopharmaceuticals and many emerging advanced therapeutics. Traditionally cryopreservation has been limited to low cell densities and small volumes due to the challenges associated with maintaining cell viability and functionality post-thaw. The capability to cryopreserve high density, high volume cell suspensions is highly desirable. It facilitates significant cycle time reduction, of up to 14 days, for recombinant protein biopharmaceuticals produced with mammalian cultures and allows for breakpoints and product supply where the medicine is a cell-based therapy. This project led by Dr Jessica Whelan at University College Dublin, aims to establish a model-supported process development approach for this essential step which will ensure reliable process performance based on fundamental understanding of the underlying phenomena.

FUNDING HIGHLIGHT

SFI Infrastructure Awards: Dr Luis Padrela and Prof. Vivek Ranade, UL. Next Generation Nanopharma Process **Development Platform (NaPRO).**

PUBLICATION



In-Vial Detection of Protein Denaturation Using Intrinsic Fluorescence Anisotropy

Analytical Chemistry, 2023, 95, 5, 2774-2782. Chullipalliyalil, K. Elkassas, K. McAuliffe, M.A.P. Vucen, S. Crean, A.



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Dr Constantina Papatriantafyllopoulou

FUNDING HIGHLIGHTS

SFI Infrastructure Awards: Prof. Peter McLoughlin, SETU Waterford, Nanoscale Chemical Imaging System

PROJECT SPOTLIGHT Metal-organic frameworks (MOFs)

Dr Constantina Papatriantafyllopoulou at the University of Galway, focuses on developing biocompatible drug carriers with enhanced adsorption capabilities and controlled release properties. Metal-organic frameworks (MOFs) are promising candidates due to their stability and tuneable porosity. The programme has led to the isolation of MOFs with an unprecedentedly high encapsulation of the anticancer drug doxorubicin. These MOFs exhibit a pH-controlled release mechanism, which enables targeted control in acidic tumour environments. Furthermore, some of the isolated MOFs display dual functionality as MRI contrast agents, depending on the type of metal ion present in their structure. This study lays the foundation for the development of efficient drug carriers and theranostics.

PUBLICATIONS

Thiourea-catalysed conjugate additions of amines to vinyl phosphonate and phosphinates†. Organic and Biomolecular Chemistry, 2023, 21, 1027-1032. Peter E. McDermott | Martin P. Ó. Fearraigh | Alexandra M. Horan | Eoghan M. McGarrigle



Third-Generation Sequencing of Epigenetic DNA Angewandte Chemie -International Edition, 2022. Searle, B. Müller, M. Carell, T. Kellett, A.



EPE BURSARY

Crystal Clear Project





Co-funded by the Erasmus+ Programme of the European Union



DiSSI (our EPE EU ERASMUS+ funded project on dimensions of diversity for social inclusion) will be collaborating with the SSPC EPE Bursary Crystal Clear Project (aligned with ACTUATE ERC work) led by **Dr Sarah Guerin** at the University of Limerick to flesh out the design and implementation of a citizen science experiment. The experiment will ask the public to grow piezoelectric crystals at home using a kit. The initial kit are being developed and tested by students in Coláiste Nano Nagle, Limerick. The goal is for students to stress test the kits and work out the most efficient way to grow the crystals. Over 10 weeks, their refined protocol will then be upscaled by the DiSSI and Crysal Clear project teams to produce hundreds of kits ready for dissemination to the wider public with **Dr Genco Gurulp** and **Dr Martin McHugh**.



PUBLICATION



Developing student codesigned immersive virtual reality simulations for teaching of challenging concepts in molecular and cellular biology

FEMS Microbiology Letters, 369, (1), 2022. Jerry Reen, F.| Jump, O.| McEvoy, G.| McSharry, B.P.| Morgan, J.| Murphy, D.| O'Leary, N.| O'Mahony, B.| Scallan, M.| Walsh, C.| Supple, B.



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INDUSTRY CORNER

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UPCOMING EVENTS

April	Knowledge Day: Continuous Reactors & Processes for Pharma, April 19th. Register here. Modelling & Molecule Theme Meeting, April 18th, UCC
Мау	Training: Intro to Stats & R, May Event: Recruitment Drive, May 17th, UL Molecules II Theme Meeting I May 9th, UCD Molecules III Theme Meeting I May 26th, Virtual Manufacturing Theme Meeting I May 31st, UL
June	Knowledge Day: Long Acting Injectables, June 1st. Materials & Medicine I Theme Meeting, June 7th, UL Training: ESGI Working group with MACSI, June 19th, UL
Aug.	Training: Chemometrics, August 17th
Sept.	Training: Small Molecule DP Formulation Knowledge Day: Molecular Modelling
Nov.	Knowledge Day: Synthetic Peptides

Knowledge Day Ideas? Sustainable, Chemistry, CSR, EDI, Process Modelling.... 'Let us know what other topics would be of interest to you for future Knowledge Days or training sessions – contact Aisling or Jamie

Flow Knowledge Day and Community of Practice

SSPC, in partnership with **Pfizer** hosted a Flow Knowledge Day on the 15th of February. The format of the event comprised both academic and industry presentations, poster session and panel discussion providing opportunity for an engaging session and knowledge sharing across the sector. Presentations on the day catered to all levels of expertise and topics included:

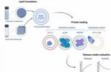
- Introduction to Flow Aoife Kearney, UCC
- Hazardous Reagents, Telescoping and PAT Prof. Anita Maguire, UCC
- Photochemistry, High Energy, Catalysis, Green Chemistry Dr Marcus Baumann, UCD
- Engineering continuous processes, Mixing, RTD, heat and mass transfer Prof. Vivek Ranade, UL
- Scale-up and Hydrogenation Dr Megan Smyth, Almac
- Flow chemistry for safe sustainable and intensified processes Dr Philippe Roth, Corning



If you'd like to get involved in the Community of Practice or would like more information on any of the content contact Aisling.Arthur@ul.ie or Jamie.Guidera@ul.ie



PUBLICATION



Save the Date, May 17th RECRUITMENT DRIVE

We are hosting a Recruitment Drive on **Wednesday, May 17** in the University of Limerick. This will be an excellent opportunity for our member companies to meet with our researchers in years 3 and 4 of their studies and preparing for employment. The format of the day will include poster sessions, career talks and industry stands.

PLACEMENT UPDATE Monika Myślińska, TCD, SK biotek



"I think that the broadening your skillset, adding to your experience, meeting new professionals with very different expertise is really worth it." **Read more here**



Long acting injectables for therapeutic proteins Ryan, S.| Shortall, K.| Dully, M.| Djehedar, A.| Murray, D.| Butler, J.| Neilan, J.| Soulimane, T.| Hudson, S.P. Cook Medical (2022) Colloids and Surfaces B: Biointerfaces.