SSbD: Innovation Beyond REACH

Exploring how Safe and Sustainable by Design is reshaping chemical innovation, regulation and sustainability.

ChIR Symposium 2026

Barcelona · 29–30 June 2026
Parc Científic de Barcelona

Book of Abstracts

https://www.emmcchir.org/symposia/symposium2026/welcome

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A meeting point for chemical innovation, regulation and sustainability

Since 2015, the ChIR Symposium has brought together students, researchers, academic staff, industry professionals and regulatory stakeholders to discuss current challenges in chemical innovation and regulation.

The 2026 edition will take place in Barcelona under the theme “SSbD: Innovation Beyond REACH”.

The symposium will explore how Safe and Sustainable by Design can support a shift from compliance-based chemical management towards earlier, more integrated decisions on safety, sustainability and innovation.

The event is also part of the transition from ChIR to ChIRS - Chemical Innovation and Regulation for Sustainability - reflecting the programme’s strengthened focus on sustainable chemistry, regulatory science, circularity and responsible innovation.

Through presentations, discussion and student research contributions, the symposium will provide a forum for exchanging perspectives across academia, industry and policy-oriented practice.

Scope

The symposium will address scientific, regulatory and innovation perspectives relevant to safer and more sustainable chemicals, materials, processes and technologies.

EU chemical policy and regulatory innovation	**Safe and Sustainable by Design**	**Sustainable materials and nanomaterials**
Microplastics and emerging contaminants	**Hydrogen production and energy conversion technologies**	**Circular economy and life-cycle thinking**
Biotechnology and bio-based products	**Computational chemistry and predictive assessment**	**Risk, hazard and sustainability assessment**

Symposium Committees

The ChIR Symposium 2026 is organised by academic staff from the ChIR/ChIRS consortium. The Local Organizing Committee coordinates the Barcelona edition of the event, while the International Committee supports the academic orientation and consortium-wide relevance of the symposium.

Local Organizing Committee

The Local Organizing Committee is responsible for the local coordination of the Barcelona edition, including venue arrangements, participant support and on-site organisation.

Daniel Sainz University of Barcelona **Spain**	**Carmen Gonzalez** University of Barcelona **Spain**

International Committee

The International Committee brings together representatives from ChIR/ChIRS partner universities and supports the academic scope, programme orientation and consortium-wide relevance of the symposium.

University of Barcelona **Daniel Sainz** **Carmen Gonzalez** **Spain**	University of Bologna **Emilio Tagliavini** **Paola Galletti** **Italy**	University of Algarve **Isabel Cavaco** **Ana Rosa Garcia** **Portugal**

Symposium Programme Timetable

Monday, 29 June

08:45	Registrations		
09:00	**Opening session**		
	Session 1 — Chemical Regulation, Product Information and Pharmaceutical Quality Chairperson: Emilio Tagliavini		
09:30	**Keynote 1**	Anna Białk-Bielińska Department of Environmental Analysis - University of Gdansk	Presentation title to be confirmed
10:10	**TP1**	Swapnil Bavane	Data, Traceability, and Transformation: The EU Digital Product Passport in the Chemical Industry
10:20	**TP2**	Giorgio Clarizia	The European Pharmacopoeia and the Quality of Medicines: Historical Perspective, Scientific Advancements, and Regulatory Milestones
10:30	**TP3**	Lame B. Selema	The International Pharmacopoeia: History, Functions and Role in Pharmaceutical Regulation
10:40	**TP4**	Ikenna Calvin Ugwoke	Diet–Gut Microbiome–CVD Axis: Molecular Dynamics-Guided Targeting of the CutC Choline Lyase Dimer Interface for Inhibition
10:50	*Discussion*	*Session speakers*	
11:10	**Coffee break**		
	Poster Session		
	Session 2 — Microplastics, Micropollutants and Sustainable Water Treatment Chairperson: Isabel Cavaco		
11:40	**TP5**	Adaeze Phoebe Njoku	Microplastic Removal from Waters by Coagulation–Flocculation–Sedimentation: Conventional and Natural Coagulants Compared
11:50	**TP6**	Ishita Sarkar	Multi-Scale Degradation of Polystyrene Micro- and Nanoplastics under O_3/UV Treatment
12:00	**TP7**	Ahmad Aakash	H_2O_2/UVC Advanced Oxidation Coupled with Nanofiltration for Micropollutant Removal from Secondary Wastewater Effluent: Dose Optimisation, Membrane Performance, and Treatment Configuration
12:10	**TP8**	Daniele Versura Jimenez	Process Integration for Enhanced Micropollutant Removal and Wastewater Reuse
12:20	*Discussion*	*Session speakers*	
12:40	**TP9**	Abrha Mengstu Leyu	Hexahydroxytriptycene-Based Metal-Organic Frameworks for Catalytic and Gas Sensing Applications
12:50	**TP10**	George Chidiebere Ezenwamadu	ZIF-8 and Truxene Thin Films for Gas Sensing Applications
13:00	**TP11**	M. Mustak Ahmed	Luminescent Gold(I) Complexes for Molecular Recognition of Environmental Contaminants
13:10	**TP12**	Md Abid Hasan	Hybrid Anisotropic Magneto-Optical Nano-Objects for Water Remediation Applications
13:20	*Discussion*	*Session speakers*	
13:30	**Lunch**		
	Poster Session		
	Session 3 — Sustainable Materials, Nanomaterials and Biomedical Chemical Innovation Chairperson: Alessandra Tolomelli		
15:30	**Keynote 2**	Elisabetta Petri Laboratory of Electrochemistry of Materials for Energetics (LEME) - University of Bologna	Presentation title to be confirmed
16:10	**TP13**	Francis Adjei	Sustainable Synthesis and Structural Evaluation of Alkali-Lanthanide Nanostructured Materials for Energy Storage Applications
16:20	**TP14**	Asim Mahmood	Colloidal Synthesis and Optoelectronic Characterization of Ternary Ag_3SBr Chalcohalide Nanocrystals for Energy Applications
16:30	**TP15**	Nadia Eka Wijaya	Synthesis and Characterization of Ternary Chalcogenide CuAuS Nanoparticles for Photothermal Cancer Therapy
16:40	**TP16**	Md. Saad Hossain	In Vitro Evaluation of Novel Metallodrugs as Cytotoxic Agents for Triple Negative Breast Cancer
16:50	*Discussion*	*Session speakers*	
17:10	***Closing of day 1***		

Tuesday, 30 June

Session 4 — Safe and Sustainable by Design, Bio-Based Products and Circular Food Systems
Chairperson: Daniel Sainz

09:00	**Keynote 3**	Mar Gonzalez OECD - Nanomaterials and Advanced Materials Programme	Presentation title to be confirmed
09:40	**TP17**	Deborah Chinwendu Ofoegbu	Formulation and Characterisation of a Fava Bean and Microalgae-Based Plant Yogurt
09:50	**TP18**	Deimantė Stankūnaitė	Life Cycle Assessment of an Integrated Multi-Trophic Aquaculture (IMTA) System: Fish and Algae Cultivation in Portugal
10:00	**TP19**	Catherine Angeli San Jose	Evaluation of Nitrates in Beetroot Juice and the Nutritional Characterization of Brewer's Spent Grain and Wine Lees
10:10	**TP20**	Sarah T. A. Zaza	Formulation and Rheological Characterization of Caseinate-Xanthan Gum Oleogels for Solid Fat Replacement
10:20	*Discussion*	*Session speakers*	*Discussion*

Session 5 — Energy Optimisation, Hydrogen Production and Sustainable Energy Materials
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10:50	**TP22**	Peter Obaloluwa Agboola	Hybrid Magneto-Semiconductor Nano-Objects for H_2 Production through Water Photocatalysis: Synthesis, Characterization, and TiO_2-Shell Engineering over Ni-Core Nanostructures
11:00	**TP23**	Sabrina Cervantes Vizcaino	TiO_2/(Ba,Sr)TiO_3/MXene Tertiary Heterojunction Photocatalyst for Hydrogen Generation
11:10	**TP24**	Mohammad Hamza	From Renewable H_2 to Grid-Compatible CH_4: Pilot-Scale Ex-Situ Bio-Methanation and Scale-Up Potential
11:20	*Discussion*	Session speakers	Discussion

11:40 **Coffee break**

Poster Session

Session 6 — Designing Sustainable Futures: Energy, Materials and Biomedical Innovation
Chairperson: Carme Gonzalez

12:10	**Keynote 4**	Jordi Falguera Garcia WATTEGA (ARCbcn & ERF)	Designing the Future of Local Energy Communities: Asynchronous Peer-to-Peer Trading in Multi-Energy Networks
12:40	**TP25**	Anđela Popović	Enhancing Anaerobic Biodegradation of Polylactic Acid (PLA) through Low-Intensity Chemical and Thermal Pretreatments
12:50	**TP26**	Nevil Jose	Metal Crosslinking of Peptide Hydrogels: Structural and Mechanical Effects
13:00	**TP27**	Ihsanti Fairuz Anatasya	Leptin Analogues Design, Synthesis, and Characterization for Alzheimer's Disease
13:10	*Discussion*	Session speakers	

13:30 **Lunch**

Poster Session

Session 7 — SSbD, Innovation Beyond REACH and the ChIRS Programme
Chairperson: Paola Galletti

15:30	**Round Table**	All the speakers	SSbD: Innovation Beyond REACH
16:00	**Keynote 5**	Isabel Cavaco ChIR Programme Coordinator	Chemical Innovation and Regulation for Sustainability: Responding to the Emerging Needs of SSbD

16:30 **Awards Session**

17:00 ***Closing session***

Research Theses and Poster Abstracts

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TP1 and P1

Data, Traceability, and Transformation: The EU Digital Product Passport in the Chemical Industry

Swapnil Bavane, Daniel Sainz
Facultat de Química, Universitat de Barcelona, Catalonia, Spain
Corresponding author: swbavanb7@alumnes.ub.edu

The Ecodesign for Sustainable Products Regulation (ESPR) introduced the Digital Product Passport (DPP), which marks a significant step in digitalizing product information to enable circularity, sustainability, and greater regulatory supervision in the European Union[1]. While comprehensive standards for several product categories are being developed, no chemicals-specific delegated act has yet been approved, therefore the future role of chemical product information within the DPP framework remains unknown. At the same time, broader EU initiatives like digital labelling under the revised CLP Regulation, the anticipated digitization of Safety Data Sheets (SDS) under the REACH revision, and cross-regulatory work on substances of concern, indicate a systemic shift toward a fully digital chemicals information ecosystem.

This work explores the ongoing phase of conceptual development of the DPP and related digitalization initiatives influencing chemical product information, as well as how these growing frameworks may interact with existing REACH and CLP duties. In addition to doctrinal and policy research, a case study of actual passport-like systems for consumer goods and materials is also considered to find real design and implementation lessons for the chemicals sector. Integrated methodologies, as well as a scenario-based investigation of probable future routes are used to analyze the benefits and problems that digitalization may offer for supply-chain communication, compliance monitoring, and hazardous material management. The goal of this work is to provide a structured foundation for understanding how chemical product information could eventually be integrated into the DPP once delegated acts are developed, as well as to outline considerations for policymakers and industry as the EU digital chemicals information landscape evolves.

Keywords: Chemical Management; Material Traceability; Digitalization; Circularity; EU DPP

[1] Council Regulation (EC) of 13 June 2024 establishing a framework for the setting of ecodesign requirements for sustainable products [2024] OJ L1781 art 9. https://eur-lex.europa.eu/eli/reg/2024/1781

TP2 and P2

The European Pharmacopoeia and the Quality of Medicines: Historical Perspective, Scientific Advancements, and Regulatory Milestones

Giorgio Clarizia[1,2*], Jaime Conceição[1,2,3]

[1] Faculty of Sciences and Technology, Universidade do Algarve, Faro, Portugal; [2] Algarve Biomedical Center Research Institute (ABC-Ri), Universidade do Algarve, Faro, Portugal, [3] Centre for Interdisciplinary Studies (CEIS20), Universidade de Coimbra, Coimbra, Portugal

Corresponding author: a90838@ualg.pt

Background: The European Pharmacopoeia is a regional pharmacopoeia that establishes quality standards for medicinal products and for raw materials (i.e., drugs, excipients, and primary packaging)[1,2]. The European Directorate for the Quality of Medicines & Healthcare (EDQM), an institution of the Council of Europe based in Strasbourg, France, is responsible for its publication. This entity includes, in addition to others, the European Pharmacopoeia Commission and coordinates the European Network of Official Medicines Control Laboratories.

Aim: The principal aim of this Master's Dissertation is to perform a historical and regulatory review of the European Pharmacopoeia, highlighting its history, functions, and constitution. In addition, its impact on emerging topics of pharmaceutical development and manufacturing is highlighted.

Method: A literature review was conducted between October 1, 2025, and June 30, 2026, using PubMed, Scopus, and Google Scholar, prioritizing scientific articles. The most recent edition of the European Pharmacopoeia[3] was used as the primary source of information. Additionally, official documents, regulatory reports, and online resources provided by EDQM, European Medicines Agency (EMA), International Council for Harmonisation (ICH) and World Health Organization (WHO) were consulted.

Results: Between 1969 to 2026, twelve official editions have been published, and the 12th Edition of the European Pharmacopoeia[3] is in force since January 1, 2026. Regarding the frequency of updating and revision, presently, the pharmacopoeia has a new edition every three years with eight additional supplements. The European Pharmacopoeia has evolved into a key regulatory framework ensuring the quality, safety, efficacy and harmonization of medicines throughout Europe and the world, as it belongs to the Pharmacopoeial Discussion Group (PDG). Its continuous evolution demonstrates the ability to address emerging challenges, such as the development of standards for biotherapeutics[4], nitrosamine risk management[5], and reducing of animal testing through alternative methods[6].

Conclusion: The European Pharmacopoeia is one of the world's leading pharmacopoeias, ensuring and harmonizing the quality specifications of medicines for human and veterinary use. Its history and performance demonstrate a continuous adaptation to key emerging issues in the manufacture of medicines, protecting public health. At the same time, its growing focus on innovation and sustainability highlights a commitment to keeping pace with advancements in science and technology while maintaining high regulatory standards.

Acknowledgements: Giorgio Clarizia thanks Professor Jaime Conceição for all the support provided during the completion of his master's dissertation, and to the Universitat de Barcelona, Universidade do Algarve and Università degli Studi di Bologna for hosting the ChIR 2024-2026 program.

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TP3 and P3

The International Pharmacopoeia: History, Functions and Role in Pharmaceutical Regulation

Lame B. Selema[1,2], Jaime Conceição[1,2,3]

[1] Faculty of Sciences and Technology, Universidade do Algarve, Faro, Portugal; [2] Algarve Biomedical Center Research Institute (ABC-Ri), Universidade do Algarve, Faro, Portugal; [3] Centre for Interdisciplinary Studies (CEIS20), Universidade de Coimbra, Coimbra, Portugal

Corresponding author: a90919@ualg.pt

Background: A pharmacopoeia is an authoritative compendium that establishes official quality standards and specifications, providing comprehensive details on the requirements and characteristics which medicinal products and their specific components [i.e., drug(s), excipients, and primary packaging], must meet to guarantee their safety, quality and efficacy.[1] According to the Index of World Pharmacopoeias,[2] there are currently a total of 61 pharmacopoeias globally which may be classified into national, regional and subregional, and international. The International Pharmacopoeia (Ph. Int.), published under the auspices of the World Health Organisation (WHO) since 1951, occupies a unique position as the only freely accessible, non-commercial pharmacopoeia with an explicit mandate to serve the needs of developing nations.[3,4]

Aim: The aim of this master's dissertation is to perform a historical and regulatory analysis of the Ph. Int. with a focus on its development, evolution, and role. Additionally, this research seeks to delve into the Ph. Int.'s function in the pharmaceutical field and decipher its influence and relationship to similar organisations dedicated to the legal and regulatory oversight of medicines.

Method: The methodology employed combined a historical analysis, literature and regulatory policy review, conducted between October 1, 2025, and June 30, 2026. The main sources of information included official WHO publications, editions of the Ph. Int., Expert Committee reports, International Council for Harmonisation (ICH) guidelines, and documents from the European Directorate for the Quality of Medicines & HealthCare (EDQM), Pharmacopeial Discussion Group (PDG), United States Pharmacopoeia (USP), and International Meetings of World Pharmacopoeias (IMWP). Other sources were identified through systematic searches of PubMed, Scopus, and Google Scholar.

Results: Between 1951 to 2026, thirteen official editions and a total of five supplements have been published. The Ph. Int.'s influence mainly lies within the context of low- and middle-income countries, where it is a practical regulatory tool due to its free accessibility and orientation to essential medicines. Beyond this, its harmonisation role is limited by its non-binding nature, irregular and resource dependent update cycle, narrow monograph coverage and limited oversight of emerging therapeutic technologies. Future research could focus on closing empirical gaps by assessing the practical uptake and application of the Ph. Int. in developing nations and how adequately the interest of countries dependent on international quality standards are represented in the PDG and IMWP platforms.

Conclusion: The Ph. Int. contributes significantly to global public health, specifically supporting WHO programmes, regulatory systems for developing countries, and establishing quality standards for essential medicines. To ensure its continued relevance, it will be necessary to protect and strengthen its fundamental principles, which are governed by health equity, commitment to public health, scientific rigor, and autonomy in the face of the constantly evolving pharmaceutical landscape.

Acknowledgements: Lame B. Selema sincerely acknowledges the financial support provided by the European Commission through the Erasmus Mundus Joint Master's Degree Scholarship (2024-2026).

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DIET-GUT MICROBIOME-CVD AXIS: MOLECULAR DYNAMICS-GUIDED TARGETING OF THE *CUTC* CHOLINE LYASE DIMER INTERFACE FOR INHIBITION

Ikenna Calvin Ugwoke[1,2], Carolina Estarellas[1,2,3]

[1]Department of Nutrition, Food Sciences and Gastronomy, Torribera Food Campus, University of Barcelona, Santa Coloma de Gramenet, Spain, [2]Institute of Theoretical and Computational Chemistry (IQTC), University of Barcelona, Barcelona, Spain, [3]Research Institute on Nutrition and Food Safety (INSA), University of Barcelona, Santa Coloma de Gramenet, Spain.

Corresponding author: iugwokug7@alumnes.ub.edu

Certain dietary nutrients and gut bacteria contribute to the risk of cardiovascular diseases (CVD). Choline-rich foods such as eggs, meat, and legumes can be metabolized by gut anaerobes carrying the choline utilization (*cut*) gene cluster, encoding the *CutC/D* enzyme complex. *CutC (choline TMA-lyase)* converts choline into trimethylamine (TMA), which is further oxidized in the liver to trimethylamine N-oxide (TMAO), a metabolite linked to CVD risks, including thrombosis and atherosclerosis.[1,2]

Our studies focus on understanding *CutC* as a therapeutic target to inhibit this pathway. Here, we investigated *CutC* from *Klebsiella Pneumoniae* in its dimeric biological assembly, focusing on structural stability, conformational plasticity and inter-subunit communication. While previous strategies mainly targeted the active site,[3] we propose that disrupting the dimer interface may provide an alternative strategy by weakening dimer stability or allosteric coupling between monomers.

Extensive molecular dynamics simulations were performed for both choline bound and free forms of the enzyme, using available *CutC* crystal structures, accounting for more than 20µs. Resulting trajectories were analysed using structural stability metrics, residue flexibility, interface residue distance monitoring, and network-based communication analysis (shortest-map path & weighted implementation of suboptimal paths). The simulations revealed an overall stable dimeric architecture, while maintaining flexibility in functional regions, including the glycyl radical domain and a proposed *CutD* approach region identified by our research group. In addition, key dimer interface residues that may contribute to dimer stability and/or allosteric coupling between monomers were identified. These residues represent crucial hotspots for inhibiting the dimer and will be further evaluated through single-point mutation calculations. Based on these results, additional biochemical assays involving the identified interfacial mutant residues will be performed to validate the therapeutic relevance of this approach.

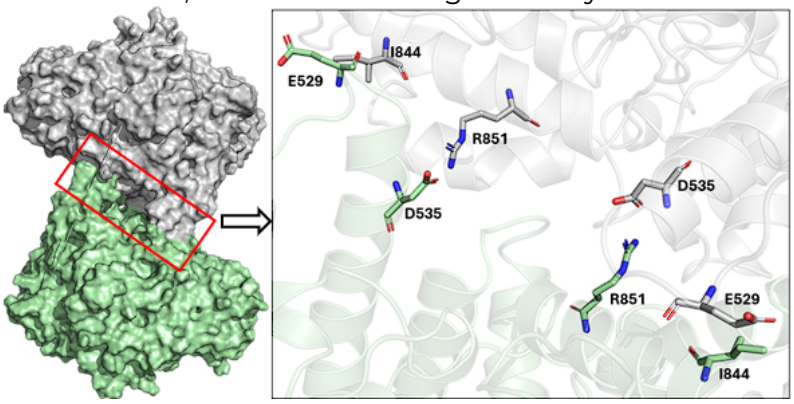

Figure 1. Choline TMA-layse (CutC) dimer highlighting key interface residues

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TP5 and P5

Microplastic Removal from Waters by Coagulation–Flocculation–Sedimentation: Conventional and Natural Coagulants Compared

Adaeze Phoebe Njoku[1], Margarida Ribau Teixeira[2]

[1,2]Erasmus Mundus MSc Environmental Chemistry and Regulations, [2]University of Algarve, Faro

Corresponding author: njayphoebe@gmail.com

Microplastic (MP) pollution is a well-established global concern, with fragments from the ~400 million tonnes of plastic produced annually accumulating across freshwater, marine, and terrestrial environments. Wastewater treatment plants are significant MP discharge pathways yet were not designed for these particle sizes. Chemical treatment to address this carries its own environmental costs, including residual metals, ecotoxicity, and accumulation in soils and sediments.[1] The metal-salt coagulants used here, however, are considered comparatively low-impact at standard doses. Natural, plant-derived coagulants offer an alternative, but their polymer-specific MP removal remains largely unexplored. This study compares polypropylene (PP) MP removal by two conventional coagulants, Polyaluminum Chloride (PAC) and $FeCl_3$, against Tanfloc SG 1500 (TANAC S.A., Brazil), a cationic tannin-based coagulant from *Acacia mearnsii* bark. PP fragments (<500 µm) were spiked at 100 mg/L into 800 mL jar tests of tap water and decanted secondary effluent (200 rpm/1 min, 20 rpm/15 min, 30 min settling; doses 0–50 mg/L). Turbidity-based removal was the primary endpoint, with pH, conductivity, and zeta potential; an elevated pH (9.0) condition was also tested for PAC to promote $Al(OH)_3$ sweep floc. Tanfloc SG achieved the highest tap-water removal (69.1% at 20 mg/L), outperforming both conventional coagulants and indicating charge neutralisation and bridging as effective for buoyant PP.[2] PAC at pH 9.0 reached 64.5% at 30 mg/L, consistent with enhanced sweep flocculation.[3] At natural pH, PAC and $FeCl_3$ peaked near 39–42% (10–30 mg/L) in tap water. In secondary effluent, $FeCl_3$ gave the clearest dose-response (40.3% at 50 mg/L; zeta potential between −10.3 and −14.7 mV, indicating sweep flocculation),[4] while PAC showed overdose restabilisation from 30 mg/L. These results identify pH management as a key determinant for conventional coagulants and position Tanfloc SG as a promising natural option. Ongoing trials include Tanfloc in secondary effluent, hybrid-coagulant setups, and FTIR polymer verification (polyethylene, possibly PET) toward a mixed-MP scenario.

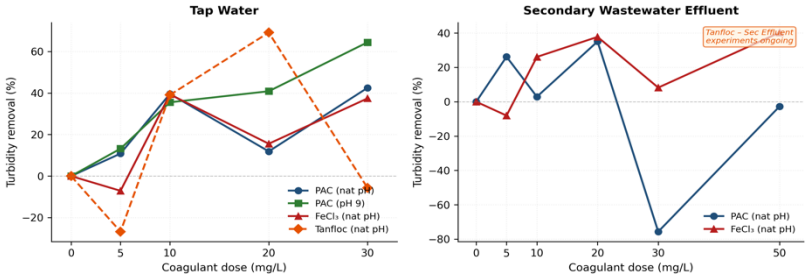

Figure 1: Turbidity removal vs coagulant dose. Left, tap water: PAC (natural pH and pH 9), FeCl3 and Tanfloc SG (natural pH). Right, secondary effluent: PAC and FeCl3(natural pH). PP spike 100 mg/L; negative values indicate turbidity increase above the unspiked control (under-dose destabilisation).

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TP6 and P6

Multi-Scale Degradation of Polystyrene Micro and Nanoplastics under O_3/UV Treatment

Ishita Sarkar, Reyhan Ammar, Carmen Sans, Julia Nieto-Sandoval

Department of Chemical Engineering and Analytical Chemistry. Faculty of Chemistry, University of Barcelona, C/ Martí i Franqués 1. 08028, Barcelona, Spain

Corresponding author: isarkasa7@alumnes.ub.edu

Microplastics (MPs) and nanoplastics (NPs) are persistent aquatic pollutants whose small size, mobility, and resistance to conventional wastewater treatment challenge both removal and risk assessment. This study evaluates combined ozone and ultraviolet treatment (O_3/UV) as a destructive advanced oxidation process for degrading polystyrene microplastics (PSMPs) and nanoplastics (PSNPs) in water, using four monodisperse fractions: 150 nm (NP 149), 900 nm (NP 919), 10 µm (MP 9.9), 100 µm (MP 101). PSMPs and PSNPs suspensions (50 mg L^{-1}) were treated separately in a semi-continuous reactor under controlled conditions (O_3 feed rate= 10 mg min^{-1}; T = 20 °C; pH = 7; UVC lamp (12 W)) for 120 min. To follow the reaction, an integrated characterization framework was employed covering particle-size evolution (LS, DLS), morphology and surface alteration (SEM, TEM, and AFM), optical behavior (turbidity and UV–Vis spectroscopy), structural and functional-group changes in MPs (Raman and FTIR spectroscopy), and carbon redistribution in NPs (TOC/DOC analysis). Volatile and semi-volatile intermediates were also identified by HS-SPME-GC-MS, while ECOSAR modelling was used to evaluate the potential aquatic toxicity of selected transformation products. In addition, scavenger tests were also performed to evaluate the contribution of reactive oxidative species (ROS) in PSNPs degradation. O_3/UV treatment induced size-dependent transformation across all fractions. MPs mass loss reached 52% for MP 101 and 27% for MP 9.9, while NPs showed marked colloidal and optical responses, including significant reductions of turbidity (> 97%) and hydrodynamic diameter (approximately 57% for NP 149 and 61% for NP 919). A 94.1% TOC reduction was achieved when treating NP 149, whereas persistent DOC accumulation was observed during the treatment of NP 919, indicating incomplete mineralization. The identification of intermediate by-products, together with scavenging assays, suggested the formation of volatile and semi-volatile intermediates (e.g., benzaldehyde, acetophenone) likely arising from radical oxidation pathways. ECOSAR modelling suggested that selected transformation products may retain aquatic toxicity, highlighting the need to assess treatment-derived ecological risk alongside degradation efficiency. Overall, this research, as exposed in Figure 1, proposes a stepwise O_3/UV degradation pathway for PSMPs and PSNPs, connecting particle-scale fragmentation, oxidative structural modification, intermediate by-product formation, and ecotoxicological relevance.

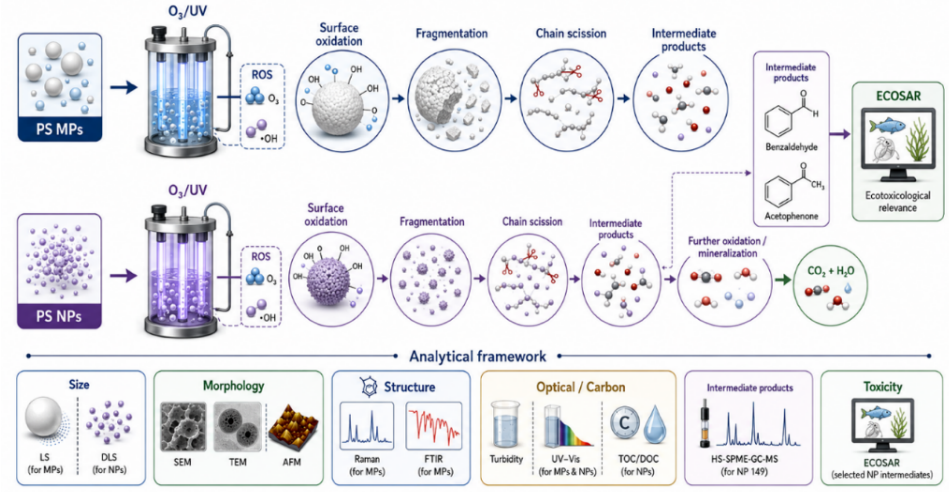

Figure 1. Graphical overview of O_3/UV-driven transformation of PS MPs and NPs.

H_2O_2/UVC ADVANCED OXIDATION COUPLED WITH NANOFILTRATION FOR MICROPOLLUTANT REMOVAL FROM SECONDARY WASTEWATER EFFLUENT: DOSE OPTIMISATION, MEMBRANE PERFORMANCE, AND TREATMENT CONFIGURATION

Ahmad Aakash, Alberto Cruz-Alcalde, Núria Lopez-Vinent, Jordi Labanda Angulo

Department of Chemical Engineering and Analytical Chemistry/ University of Barcelona / Spain

Corresponding author: ahmadaakash019@gmail.com

Micropollutants — pharmaceuticals, personal care products, and industrial chemicals — persist through conventional wastewater treatment, posing risks to aquatic ecosystems and human health. This study evaluated a hybrid H_2O_2/UVC advanced oxidation process (AOP) followed by nanofiltration (NF) for micropollutant removal from secondary effluent (Gavà-Viladecans WWTP, Barcelona), pretreated by multimedia sand filtration and spiked with nine compounds (metoprolol, carbamazepine, atrazine, naproxen, ibuprofen, gemfibrozil, 5-MeBT, sulfamethoxazole, metronidazole) at 100 µg/L each.

AOP experiments were conducted in a 1 L jacketed glass reactor (4 W UVC, 254 nm, 25°C, 120 min, n=3). At the optimal dose of 10 ppm H_2O_2, removal ranged from 21.1 ± 5.8% (atrazine) to 77.2 ± 6.7% (sulfamethoxazole). Both 5 ppm (11.3–72.7%) and 15 ppm (21.0–67.3%) performed worse, the latter due to H_2O_2 self-scavenging. Spectrophotometric monitoring (ammonium metavanadate) confirmed only 10–18% H_2O_2 consumption at 120 min; the dark control (~91% H_2O_2 remaining, no degradation) confirmed the photolytic mechanism. UVC alone showed direct photolysis only for sulfamethoxazole (66%) and gemfibrozil (41%); all others ≤15%. AOP effluent was processed through a flat-sheet NF270 crossflow membrane (15 bar, 25°C, 60 min). Feed conductivity (2.3–3.3 mS/cm) dropped to 70–88 µS/cm in the permeate (>96% ionic rejection), with 0 NTU turbidity. Seven of nine compounds achieved 100% rejection with only 4.7–7.4% flux decline (baseline ~46.9 LMH). Exceptions were 5-MeBT (54–78%; MW 133 g/mol, neutral at pH 8) and gemfibrozil (variable; log K_o^W 4.77, adsorption-breakthrough). The integrated train achieved >99% overall removal of six compounds; the NF-before-AOP configuration performed worse by co-concentrating matrix scavengers. These results establish the MMF→AOP→NF sequence as a robust multi-barrier strategy, while identifying 5-MeBT and gemfibrozil as priority targets for further optimisation.[1]

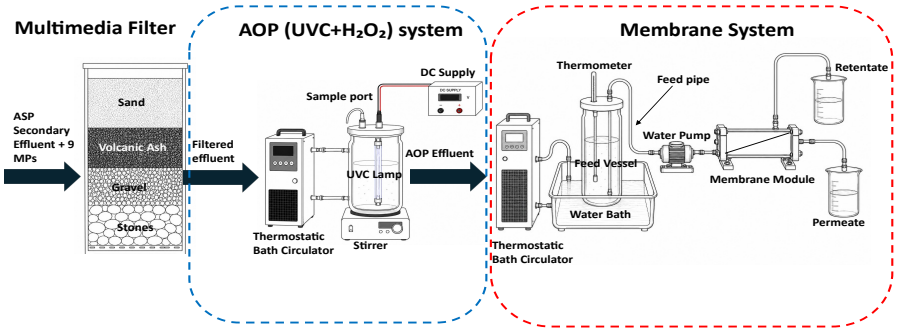

Figure 1. Schematic of the integrated MMF → H_2O_2/UVC AOP → NF membrane treatment train.

Keywords: micropollutants; advanced oxidation; nanofiltration; wastewater treatment.

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TP8 and P8

Process Integration for Enhanced Micropollutant Removal and Wastewater Reuse

Daniele Versura Jimenez, Prince Ebo-Donkor, Alberto Cruz Alcalde, Jordi Labanda Angulo, Nuria Lopez Vinent

Department of Chemical Engineering and Analytical Chemistry, Universitat de Barcelona

Corresponding author: daniele.versura@gmail.com

Water pollution has become an increasingly pressing global environmental challenge. Rising population density and rapid urbanization have intensified domestic wastewater discharge, increasing the presence of nutrients, organic matter, and micropollutants (MPs). Due to their persistence and bioaccumulation potential, MPs require improved treatment technologies, as conventional wastewater treatment plants (WWTPs) often fail to remove them effectively. Constructed wetlands (CWs) represent a sustainable and low-energy alternative for wastewater treatment, although their performance toward complex MPs can be limited.

This study evaluated the effect of two amendments - coconut fiber and biochar - on pollutant removal in laboratory-scale CWs. Systems were assembled in 5 L polyacrylate tanks containing layered substrates of cobblestones, volcanic rocks, fine gravel, and sand, with or without (control) a 5 cm amendment layer. Phragmites australis was selected for its high nutrient and MP removal capacity. Wastewater collected after secondary treatment from the Gavà-Viladecans WWTP (Barcelona, Spain) was spiked with nine MPs (herbicides, pharmaceuticals, and an anticorrosive compound) at 100 ppb each. MP concentrations were determined by HPLC-PDA using a Mediterranea Sea C18 column. To further improve MP removal, three post-treatment technologies were assessed: UVC/H2O2 oxidation (4 W irradiation; 10 and 15 ppm H2O2), nanofiltration with an NF90 membrane (15 bar, 1 h), and adsorption using four activated carbons with different physicochemical properties.

Results showed that CWs achieved over 96% total suspended solids removal, confirming effective filtration by the porous media. Electrical conductivity decreased from 3.75 to approximately 2.7 mS/cm in all treatments, indicating reduced salinity risk. Dissolved organic carbon decreased in the control and biochar systems, while a slight increase was observed with coconut fiber due to carbon leaching. Phytotoxicity tests using lettuce and radish seeds showed germination rates above 85%, suggesting suitability of the treated effluents for agricultural reuse. Among CW treatments, biochar achieved the highest MP removal efficiencies, likely due to its large surface area and abundance of functional groups. Atrazine and carbamazepine were the most persistent compounds.

Among post-treatments, UVC/H2O2 achieved near-complete degradation of most MPs after 120 min, although atrazine and carbamazepine remained more persistent, particularly in coconut fiber effluents because of competition for hydroxyl radicals by dissolved organic carbon. Nanofiltration provided complete MP removal together with strong reductions in conductivity, turbidity, and dissolved organic carbon. Activated carbon adsorption also showed excellent performance, with commercial powdered activated carbon removing nearly 100% of all MPs within a few hours, while pelletized and laboratory-prepared carbons required longer contact times and were less effective for atrazine and carbamazepine.

These findings demonstrate that intensified CWs can enhance micropollutant removal and support agricultural wastewater reuse. Among the post-treatments tested, nanofiltration and activated carbon adsorption showed the highest overall efficiency, whereas UVC/H_2O_2 provided rapid oxidation but may generate phytotoxic by-products and require higher energy input. Future studies should focus on optimizing hybrid treatment systems and evaluating the long-term performance of intensified CWs amended with different materials.

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TP9 and P9

HEXAHYDROXYTRIPTYCENE-BASED METAL-ORGANIC FRAMEWORKS FOR CATALYTIC AND GAS SENSING APPLICATIONS

Abrha Mengstu Leyu[1], Yuzelfy Mendoza Gamero[1,2,3], Albert Romano-Rodriguez[2,3], Daniel Sainz-García[1,2].

[1] Inorganic and Organic Chemistry Department, [2]Institute of Nanoscience and Nanotechnology (IN²UB), [3]Electronic and Biomedical Engineering Department. Universitat de Barcelona, Barcelona, Spain.

Corresponding author: aleyuley197@alumnes.ub.edu

Metal-organic frameworks (MOFs) are crystalline porous materials that have attracted a lot of attention due to their unique properties, which include high surface areas, significant porosity, a variety of chemical functionalities, tunable structures, and wide-range of applications in gas storage, sensing, catalysis, and energy-related technologies. In this study, a series of transition metal-based MOFs were synthesized using hexahydroxytriptycene (HHTT) ligand and evaluated for their thermal, electrical, structural, catalytic, and gas-sensing properties. The HHTT linker was synthesized from triptycene through bromination, methoxylation, and demethylation reactions, yielding a highly functionalized linker containing six hydroxyl coordination sites. The synthesized HHTT was coordinated with Ni(II), Cu(II), Zn(II), and Co(II) acetate salts under isothermal conditions to produce four different MOFs. The synthesized MOF materials were characterized using powder X-ray diffraction (PXRD), infrared spectroscopy (IR), scanning electron microscopy coupled with energy dispersive X-ray spectroscopy (SEM-EDX), thermogravimetric analysis (TGA), and electrical conductivity measurements. PXRD analysis revealed distinct low-angle reflections characteristic of framework formation. IR spectra confirmed coordination between the ligand and metal ions through the disappearance of the phenolic O-H band and the appearance of oxygen-metal vibrational bands. SEM-EDX analysis revealed the incorporation of the metal centers within the framework and distinct metal-dependent morphologies. TGA analysis revealed that all synthesized MOFs have good thermal stability with framework integrity maintained up to approximately 300-350 °C before gradual decomposition. Electrical measurements demonstrate that there is a significant difference in resistance among MOFs, indicating the effect of the coordinated metal center on charge transport properties, and all the MOFs are conductive. Finally, the MOFs were investigated further for catalytic and gas sensing applications. Catalytic studies focused on alcoholysis of ring-opening reactions of cyclohexene oxide and gas sensing towards CH_4 and CO_2. Generally, this study demonstrates the successful synthesis of HHTT-based Ni, Cu, Zn, and Co MOFs with tunable structure, crystalline, thermally stable, conductive, and catalytic properties.

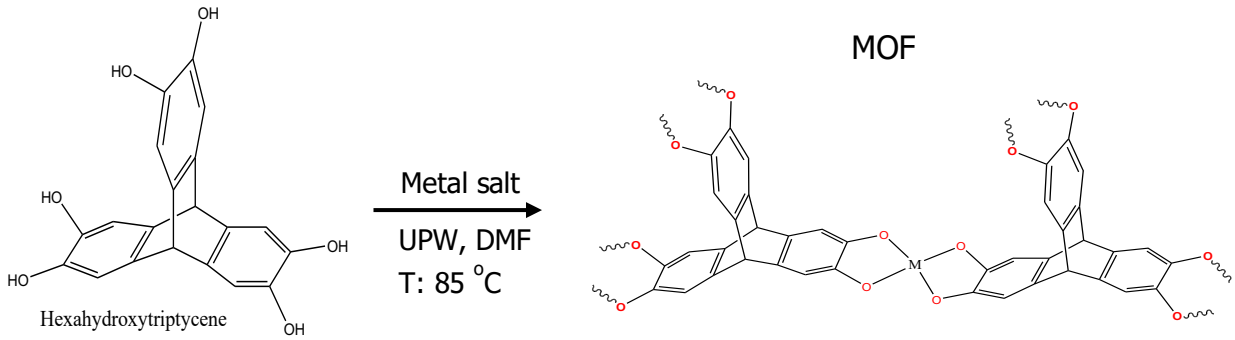

Figure 1. Synthesis of MOFs using HHTT

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ZIF-8 AND TRUXENE THIN FILMS FOR GAS SENSING APPLICATIONS.

George Chidiebere Ezenwamadu[1,2,3], Sergi González Martínez[1,2,3], Sonika Sharma[1,2,3], Mauricio Moreno Sereno[1,2], Albert Romano Rodriguez[1,2], Daniel Sainz García[2,3]

[1]Dept Electronic and Biomedical Engineering, Universitat de Barcelona, Barcelona, Spain. [2]Institute of Nanoscience and Nanotechnology (IN^{2}UB), Universitat de Barcelona, Barcelona, Spain. [3] Dept Inorganic and Organic Chemistry, Universitat de Barcelona, Barcelona, Spain.

Corresponding author: gezenwez7@alumnes.ub.edu

Metal Organic Frameworks (MOFs) have emerged as promising, tunable materials for next-generation gas sensing applications due to their chemical versatility, intrinsic porosity, and structural modularity. This thesis presents two objectives. Objective 1: The SPR grating sensors were enhanced by functionalising them with homogeneous ZIF-8 thin films grown through the dip coating method. Gas sensing occurs through the refractive index (RI) modulation caused by analyte adsorption inside the porous ZIF-8 framework for the detection of ethanol under 2-and 5-minute exposure cycles, and Objective 2: Chemiresistive MOFs synthesized from hexahydroxytruxene ligand (HHTx) and coordinated with copper (Cu) transition metal (HHTx – Cu) for the detection of greenhouse gases. The HHTx - Cu MOFs were synthesized through the interfacial route and deposited on interdigitated electrodes (IDEs) by drop-casting to form conductive sensing films. The chemiresistive sensing occurs through the resistance modulation caused by exposure to carbon (IV) oxide (CO_2) and methane (CH_4) pulses.

For the SPR platform, Au chips were cleaned by sonication in acetone, isopropanol, distilled water (DI), and dried under nitrogen flow. The fresh precursor solutions of $Zn(NO_3)_2{\cdot}6H_2O$ (25 mM) and 2-methylimidazole (50 mM) were used for 3 growth cycles (30 minutes each) to obtain homogeneous and reproducible ZIF-8 layers. Methanol rinsing and nitrogen drying are critical to remove loosely bound crystallites. The ZIF-8 free reference area was etched using diluted nitric acid. Ethanol sensing was done under optimal flow conditions. For the chemiresistive platform, the HHTx - Cu MOFs were synthesized, dried, and characterized using IR and PXRD. The films were fabricated by drop casting of the HHTx – Cu MOF in ethanol solution (0.3 mM). CO_2 and CH_4 sensing were done under optimal flow conditions.

The step height measurement of the ZIF-8 thin films in the profilometer indicates a homogeneous film of 146 nm thickness. The functionalized ZIF-8 SPR chips detected ethanol concentrations at the SPR resonance wavelength of 642 nm. This measurable redshift was observed at 80 ppm (VMF=0.2V). This is within the laser diode interrogation range of 635 - 780 nm. The cycles of 5 minutes show a more stable horizontal baseline, indicating an optimal performance. Furthermore, the HHTx – Cu MOFs were crystalline and electrically active through measurable resistance changes on exposure to CO_2 and CH_4. The optical and chemiresistive MOF-based platforms demonstrate great performance for gas sensing. Finally, future work is needed to improve the performance and scalability of the gas sensors.

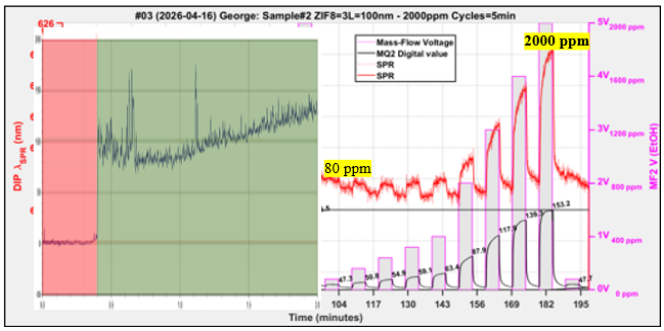

Figure 2: Step-height measurement and SPR sensorgram of ethanol exposure for the 5-minute cycle.

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TP11 and P11

Luminescent Gold(I) Complexes for Molecular Recognition of Environmental Contaminants

M. Mustak Ahmed[1], A. Pinto[1,2], A. Lázaro[1,2], I. Angurell[1,2], L. Rodríguez[1,2]

[1]Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Martí i Franquès 1-11, 08028, Barcelona, Spain. [2]Institut de Nanociència i Nanotecnologia de la Universitat de Barcelona (IN^{2}UB)

Corresponding author: mdahmeda101@alumnes.ub.edu

Environmental contamination by hazardous species such as polyaromatic hydrocarbons (PAHs), anions, and metal cations poses a raising challenge for water systems, environmental safety and public health. There is an increasing demand for sensitive, rapid, and cost-effective detection technologies capable of identifying these at low concentrations. In this context, luminescent materials offer a promising platform for the development of next-generation sensing systems.

This study focuses on the rational design and synthesis of luminescent systems based on gold(I) organometallic complexes that give rise to functional fluorescent materials when they are linked into a polymeric structure. Phosphine ligands incorporating chromophoric units such as carbazole and pyrene were synthesized and coordinated to Au(I) centers to obtain a series of Au(I) complexes.[1] In parallel, a light active molecular probe was synthesized via a Sonogashira coupling strategy and integrated into a fluorescent cellulose matrix.[2,3] Consequently, the presence of a terminal alkyne functionality facilitates coordination to gold(I), allowing for the creation of hybrid luminescent systems for sensing applications. All systems were characterized using ^{1}H and ^{31}P NMR, IR, UV-Vis and photoluminescence measurements.

Photophysical investigations demonstrate that coordination to gold(I) substantially alters the emission properties of these systems, resulting in enhanced excited-state interactions and tunable luminescence. These materials display pronounced sensitivity to their chemical environment, as interactions with target analytes produce quantifiable changes in emission intensity and spectral characteristics. Consequently, these responses facilitate the selective detection of environmental contaminants via luminescence signaling at low concentrations. Overall, this work illustrates how molecular design and metal coordination can be combined to create efficient and adaptable sensing platforms. And this highlights their potential for real world applications in environmental monitoring.

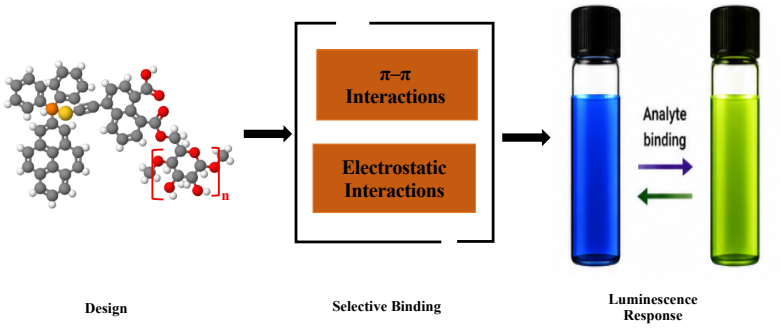

Figure 1. Schematic illustration of Au(I)-based luminescent sensing platform for the selective detection of environmental contaminants.

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HYBRID ANISOTROPIC MAGNETO-OPTICAL NANO-OBJECTS FOR WATER REMEDIATION APPLICATIONS

Md Abid Hasan, Gara Jiminez Ortega, Marta Estrader Bofarull
Laboratory of Nanostructured and Nanocomposite Materials (LM2N), Dept. of Inorganic and Organic Chemistry, Universitat de Barcelona, Barcelona, Catalonia, Spain
Corresponding author: mdhasanh49@alumnes.ub.edu

Anisotropic magneto-plasmonic hybrid nanostructures are gaining attention for their tunable synergetic features.[1] Among magneto-plasmonic nanomaterials, Fe_3O_4@Au has been found prominent in detecting contaminants and biomolecules, thereby extending their applications in sensing technologies.[2,3] In Fe_3O_4@Au core-shell nanostructure, the Fe_3O_4 nanorods (NRs) are the core while the Au counterpart is the shell. While isotropic Au NPs shell exhibits the Local Surface Plasmon Resonance (LSPR) in its fixed optical region, the rod-shaped Fe_3O_4 serves as elongated template where the Au-shell grows, thus providing with longitudinal and transverse directions LSPR (which arises from differential length to width size (aspect ratio) of the nanorods). Thus, by adjusting the Fe_3O_4 nanorod's aspect ratio (Figure 1a), a diverse spectral range up to the Near Infrared Ray (NIR) region can be gained efficiently for the longitudinal LSPR of the Au-shell.[4-7] This phenomenon in combination with the magnetic properties of the Fe_3O_4-core could provide better opportunity to exploit and make better use of the hybrid Fe_3O_4@Au nano-ojects in sensing applications. Hence, controlling the synthesis parameters to obtain Fe_3O_4 NRs with tunable aspect ratios is crucial.

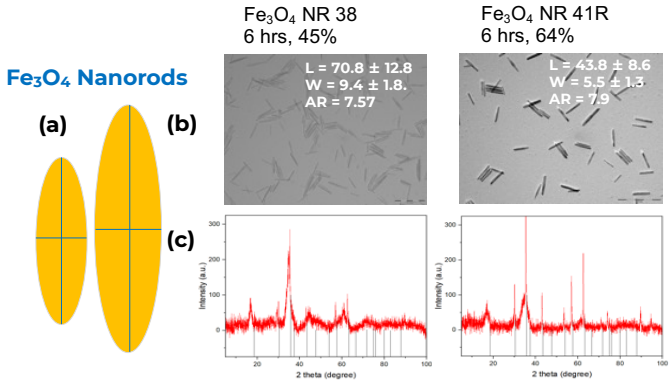

Figure 1: (a) Fe_3O_4 NR (b) TEM Images (c) XRD Patterns

In this work, Fe_3O_4 nanorods with tunable sizes were synthesized using a solvothermal method. Two different synthesis parameters: 1) filling percentage of the reactor vial and 2) time reaction were varied in order to study their effect in the NRs aspect ratio. X-ray diffraction analysis (Figure 1c) matches well with the reference XRD pattern, confirming the cubic spinel structure of the nanorods. Three filling percentages of 26%, 45% and 64% were tested for 6, 18 and 24 hours, each, at 200^0 C. Three different aspect ratio levels were obtained when the filling percentage changes from 26% to 64%. At 26% of filling percentage, the aspect ratio ranges from 3.6 to 6.4 when the reaction time increases from 6 to 24 hours. Similarly, at 45% and 64% of filling percentage, within the same time period, the aspect ratio varies from 5.5 – 7.9 and 6.5 – 9.9 respectively. In case of 45% and 64%, although the aspect ratios did not show much coherence with the alternation of time (6 to 24 hours), it is evident (Figure 1b) that higher filling percentage gives rise to higher aspect ratio in all the three experimented time of 6, 18 and 24 hours. Therefore, it is possible to tune the LSPR region of Fe_3O_4 nanorods by changing filling percentage of the reactor.

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TP13 and P13

Sustainable Synthesis and Structural Evaluation of Alkali-Lanthanide Nanostructured Materials for Energy Storage Applications

Francis Adjei[1], E. Carolina Sañudo[1,2]

[1] Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, C/Martí i Franqués 1-11, 08028, Barcelona, Spain, [2] Institut de Nanociències i Nanotecnologia, Universitat de Barcelona (IN2UB), 08028 Barcelona, Spain

Corresponding author: fradjeia70@alumnes.ub.edu

The development of cost-effective, structurally tunable nanomaterials is critical to advancing next-generation battery technologies.[1] Alkali-lanthanide-based coordination materials have attracted attention for their structural versatility and potential electrochemical functionality; however, their synthesis often relies on solvent-intensive methods and expensive rare-earth elements. Addressing these limitations requires developing environmentally benign synthesis strategies and exploring more abundant metal alternatives.

In this work, a series of alkali-metal coordination frameworks incorporating lithium or sodium with terbium, yttrium, and zirconium were synthesized using two complementary sustainable approaches: mechanochemical and microwave-assisted synthesis. Both methods significantly reduce reaction times and solvent consumption compared with conventional synthetic routes, while enabling rapid formation of crystalline or amorphous coordination architectures.[2] Structural and physicochemical characterisation was performed using powder X-ray diffraction (PXRD) to assess phase formation and crystallinity, and infrared (IR) spectroscopy to confirm ligand coordination and bonding environments.

Ongoing electrochemical investigations are evaluating the influence of alkali-ion selection, synthesis route, and lanthanide-to-zirconium substitution on ionic conductivity and charge transport mechanisms. These studies will establish structure-property relationships that guide the rational design of sustainable coordination-based materials for solid electrolytes for future solid-state battery applications.

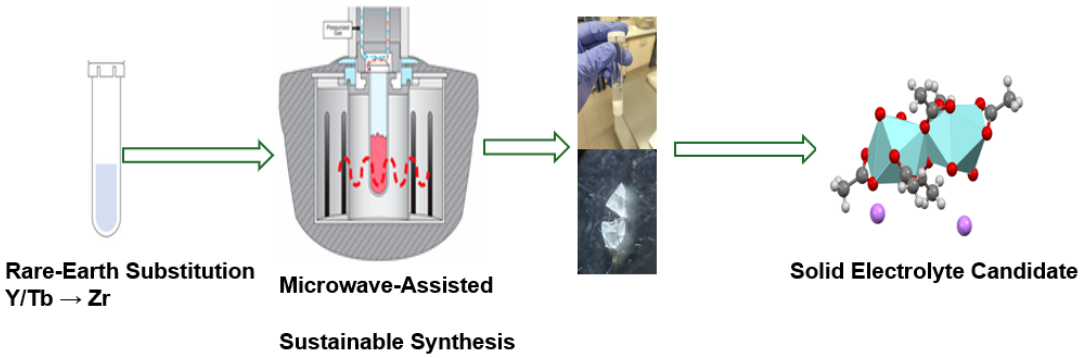

Figure 1: Schematic representation of rare-earth substitution and sustainable synthesis of alkali-metal coordination frameworks, highlighting their development as solid electrolyte candidates for solid-state battery applications.

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TP14 and P14

Colloidal Synthesis and Optoelectronic Characterization of Ternary Ag_3SBr Chalcohalide Nanocrystals for Energy Applications

Asim Mahmood, Dr. Albert Figuerola Silvestre

Laboratory of Nanostructured and Nanocomposite Materials (LM2N), Dept. of Inorganic and Organic Chemistry, Universitat de Barcelona, Barcelona, Catalonia, Spain

Corresponding author: amahmoma139@alumnes.ub.edu

The growing global demand for clean energy has driven extensive research into photovoltaic technologies across multiple generations of solar cell materials. Crystalline silicon, which dominates over 90% of the commercial market with efficiencies up to 27.3% [1], is limited by its indirect bandgap, thick wafer requirements, and high fabrication costs. On the other hand, thinfilm alternatives are extensively under ongoing research such as, CdTe and CIGS offer cost advantages but are compromised by cadmium toxicity and indium scarcity, respectively. Currently some researchers are studying organic solar cells, though these materials are flexible and solution-processable with efficiencies reaching ~19.7% [2], but degrade rapidly under moisture and oxygen exposure. Halide perovskites have shown remarkable progress, surpassing 25% efficiency within a decade [3], yet lead toxicity and poor environmental stability remain critical barriers to commercialization. These cumulative limitations have motivated the search for lead-free, stable, and compositionally tunable semiconductors. Chalcohalide semiconductors, characterized by their mixed chalcogen-halide anion chemistry, high carrier mobility, intrinsic defect tolerance, and wide bandgap tunability, have recently emerged as a compelling alternative for next-generation energy applications including photodetectors, photocatalysis, thermoelectric, and solar cells [4]. Among this emerging class, ternary silver-based chalcohalides of the formula Ag_3SBr remain entirely unexplored at the nanoscale to the best of our knowledge, no prior synthesis or optoelectronic characterization of this compound has been reported through Colloidal or Hot-Injection route.

This work addresses that gap by reporting, for the first time, the colloidal synthesis and preliminary optoelectronic characterization of Ag_3SBr nanocrystals. Silver acetate and dodecanethiol in octadecene were heated to form a transparent yellow complex at 127 °C, followed by hot-injection of a bromide-sulfur precursor (benzoyl bromide and bis(trimethylsilyl) sulfide) at 140 °C under nitrogen for one hour, with the reaction maintained for one hour under nitrogen. The resulting nanocrystals were characterized using X-ray diffraction (XRD), energydispersive X-ray spectroscopy (EDX), high-resolution transmission electron microscopy (HR-TEM), and selected area electron diffraction (SAED), collectively confirming phase purity, elemental composition, and crystalline quality. Solid-state optical absorption measurements performed using a UV-Vis-NIR spectrophotometer revealed a bandgap falling in the near-infrared region, indicating that Ag_3SBr nanocrystals can harvest light beyond the visible spectrum a characteristic particularly relevant for broad-spectrum photodetection and thermoelectric energy conversion. This study provides a foundational understanding of Ag_3SBr at the nanoscale and opens a pathway for broader investigation of ternary silver-based chalcohalides as functional materials for sustainable energy technologies.

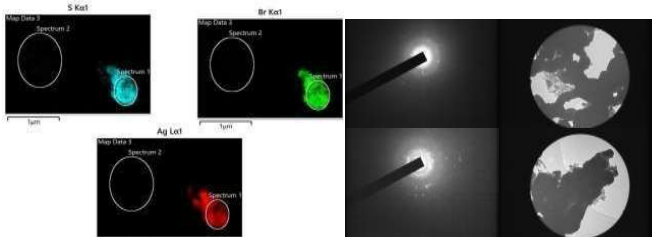

Figure 1. STEM-EDS Elemental Mapping and SAED Characterization of Ag_3SBr Nanocrystals.

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TP15 and P15

SYNTHESIS AND CHARACTERIZATION OF TERNARY CHALCOGENIDE AuCuS NANOPARTICLES FOR PHOTOTHERMAL CANCER THERAPY

Nadia Eka Wijaya, Albert Figuerola

Laboratory of Nanostructured and Nanocomposite Materials (LM2N), Department of Inorganic and Organic Chemistry, Universitat de Barcelona, Catalonia, Spain

Corresponding author: nwijaywi117@alumnes.ub.edu

Synthesis and Characterization of Ternary Chalcogenide CuAuS Nanoparticles for Photothermal Cancer Therapy has been conducted. The aims of this research were to synthesize novel ternary CuAuS nanoparticles using colloidal synthesis method and to characterize the structure, morphology, chemical, and optical properties of AuCuS for its potential application as a photothermal cancer therapy agent. This research started with the synthesis of binary copper sulfide ($Cu_{2-x}S$) by colloidal heat-up method followed by the introduction of gold (Au^{+}) via cation exchange reaction. Materials obtained from synthesis were characterized using XRD, TEM, and HRTEM-EDX, while UV/Vis/NIR spectrophotometer was used for optical characterization of the material. Results of this research were ca. 9.7 nm nanoplates with atomic ratio of Cu : Au : S = 50% : 28% : 21%. XRD analysis shows that the copper sulfide produced was a mixture of roxbyite and djurleite crystal structures based on ICDD references. Since there are no references for AuCuS crystal structures, comparison using similar ternary materials was carried out, suggesting the presence of ternary phases. The synthesized nanoplates are plasmonic and absorb near infrared light at around 1185 nm, wavelength suitable for photothermal cancer therapy.

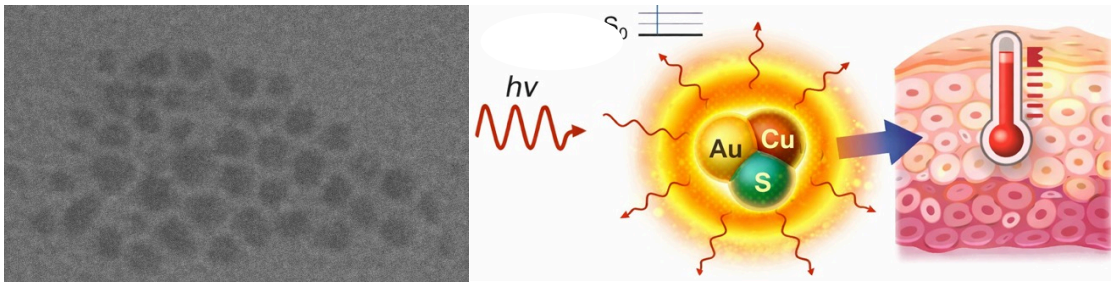

Figure 1. Schematic illustration for the mechanism of photothermal therapy agent

TP16 and P16

In Vitro Evaluation of Novel Metallodrugs as Cytotoxic Agents for Triple Negative Breast Cancer

Hossain, Md. Saad[1,2]; Pinto, Tiago[1]; Sampayo Andrade, Berenice[3]; Ramírez Monroy, Armando[3]; Valente, Andreia[1]

[1] Centro de Química Estrutural, Institute of Molecular Sciences and Departamento de Química e Bioquímica, Faculty of Sciences, University of Lisbon, Lisbon, Portugal. [2] Faculty of Sciences and Technology, University of Algarve, Portugal. [3] Centro de Química del Instituto de Ciencias, Benemérita Universidad Autónoma de Puebla, 72570, Puebla, Puebla, México.

Corresponding author: a90922@ualg.pt

Cancer remains a major health problem worldwide, and breast cancer is one of the most common cancer types[1]. Among the different breast cancer subtypes, triple-negative breast cancer (TNBC) is considered one of the most aggressive because of its high recurrence risk, metastatic potential, and poor response to conventional chemotherapy[2,3]. Although chemotherapy is still widely used, many conventional drugs are limited by poor selectivity, severe side effects, and the development of resistance[4]. Platinum-based drugs have also played an important role in cancer treatment, but their use is limited by toxicity and resistance in several breast cancer models[5]. These drawbacks support the search for new metal-based compounds with different chemical properties and biological activity. Among metallodrugs, ruthenium- and iron-based organometallic complexes have attracted increasing interest as non-platinum anticancer candidates. In organometallic Ru(II)- and Fe(II)-cyclopentadienyl complexes, small changes in the coordinated ligands can strongly affect stability, lipophilicity, cellular uptake, and cytotoxic activity[6]. Based on this chemical rationale, this thesis evaluates thirteen newruthenium (Ru)- and iron (Fe)-based metallodrugs in MDA-MB-231 cells, a widely used TNBC model. Cytotoxicity was assessed using the MTT assay, followed by dose-response analysis and IC_{50} determination. Most of the tested compounds showed cytotoxic activity, with IC_{50} values between 0.2 and 4 μM, whereas carboplatin, a clinically used platinum-based drug, showed IC_{50} > 100 μM. Further work will investigate long-term proliferative effects and intracellular distribution to better understand the anticancer potential of the most promising metallodrugs.

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TP17 and P17

FORMULATION AND CHARACTERISATION OF A FAVA BEAN AND MICROALGAE-BASED PLANT YOGURT

Deborah Chinwendu Ofoegbu[1,2], Kricelle Deamici[2], Hugo Perreira[2]

[1]University of Algarve, Department of Chemical and Pharmacy, Portugal. [2]GreenCoLab, Portugal

Corresponding author: deborah.ofoegbu@studio.unibo.it

The growing demand for sustainable, nutrient-dense dairy alternatives has spurred interest in legume and algal proteins as plant-based substitutes for cow's milk in fermented products. Faba bean (*Vicia faba* L.) is a protein-rich, low-fat legume with strong gelling potential, while microalgae provide a complete amino acid profile enriched with polyunsaturated fatty acids, pigments, and bioactive compounds. The combination of these raw materials offers a promising route for developing a novel, functional, plant-based yoghurt with reduced environmental impact compared with dairy yoghurt.

This work focuses on understanding how faba bean and microalgae interact in an acid-induced fermented gel system. Here, we developed and characterised yogurt produced from faba bean milk fortified with microalgae biomass, aiming to assess the influence of microalgae inclusion on the physicochemical and textural properties of the final product. Fava bean isolates and concentrates are commonly used for their high protein content, which produces a creamy yogurt; however, their production is costly, creating a need for a simpler, cheaper processing method. Also, plant-based yogurt suffers from low protein solubility, phase separation, particle sedimentation, and high syneresis, all of which worsen during storage. These structural problems arise because plant proteins are less soluble than dairy proteins and form weaker gel networks upon acidification. Yellow *Chlorella spp.*, as an active structural ingredient, may contribute to gel network formation, but this has not been investigated in combination with faba bean protein during LAB fermentation, and it is unclear whether its inclusion can improve textural properties to levels acceptable to consumers. Faba bean milk was prepared at a bean-to-water ratio of 1:3, yielding a total solids content of more than 8.5%, then heat-treated at 90 °C for 10 minutes. Microalgal biomass was incorporated at 1, 2, and 3% prior to inoculation with a commercial starter culture (*Streptococcus thermophilus* and *Lactobacillus delbrueckii* subsp. *bulgaricus*), and fermentation was continued until the pH reached 4.5. The resulting yogurts were evaluated for pH, titratable acidity, syneresis, water-holding capacity, gel strength and colour (L*, a*, b*) with formulations optimised by response surface methodology.

Figure 1: Yellow *Chlorella spp*

Life Cycle Assessment of an Integrated Multi-Trophic Aquaculture (IMTA) System: Fish and Algae Cultivation in Portugal

Stankūnaitė Deimantė[3,4,5], Lima Alexandre[1], Santos Rui[2], Speranza Lais[1,2]

[1]GreenCoLab – Associação Oceano Verde / Portugal, [2]CCMAR - Center of Marine Sciences / Portugal
[3]University of Algarve / Portugal, [4]University of Bologna / Italy, [5]University of Barcelona / Spain

Corresponding author: deimante.stankunaite@studio.unibo.it

Aquaculture is a fast-growing sector as food demand is increasing alongside global population growth.[1] As a result, pollutants from the offshore fish cultivation sites negatively affect surrounding water bodies. Compared to monoculture, IMTA systems have various benefits, from reducing environmental pollution and creating a more resilient ecosystem, to social and economic advantages.[2] IMTA under this study incorporates two types of fish (seabream and seabass) and golden kelp (*Laminaria ochroleuca*) cultivation. Life cycle assessment (LCA) was used to quantitatively evaluate the sustainability of fish and macroalgae co-cultivation in open water system. The goal of this LCA was to assess environmental hotspots of the IMTA system and study the potential of seaweed to recycle nutrients originating from the fish farm. The assessment was performed in accordance with ISO 14040/44 guidelines. Therefore, this study was conducted in 4 steps: goal and scope definition, inventory analysis, impact assessment, and interpretation. The IMTA system modelling was done using OpenLCA software together with the Ecoinvent database, and the impacts were quantified using the Environmental Footprint 3.1 methodology. Cradle-to-gate approach with a functional unit (FU) of 1 kg of product was used. The identified hotspots of the assessed IMTA system were fish feed, fuel, and infrastructure materials. Climate change (CC), Eutrophication: freshwater (EP-fw), and Eutrophication: marine (EP-m) environmental impacts were reduced by 2.63-3.10% compared to monoculture (Figure 1). Reduction of fish aquaculture effects was not substantial due to an insufficient ratio of species co-cultivation. Further LCA studies could analyse indicated hotspots, investigate different cultivation scenarios to optimise IMTA systems, and explore a meaningful nutrient removal threshold that is beneficial for the environment or operating business.[3]

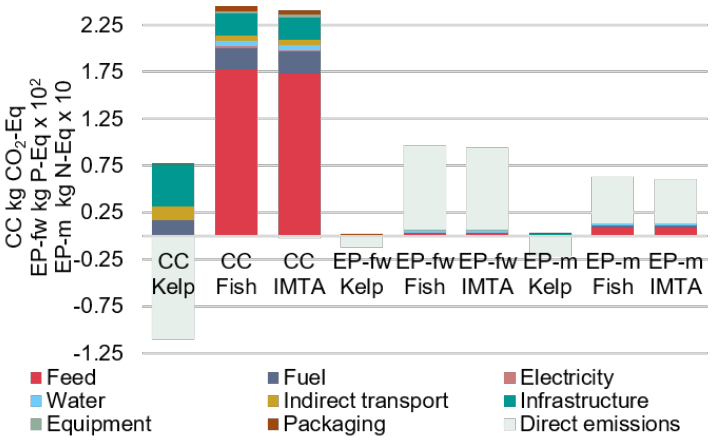

Figure 1. *Environmental impacts comparison in kelp, fish and their production combined in an IMTA system per 1 kg*

Acknowledgements: Acknowledgment: This work was financially supported by "Pacto da Bioeconomia Azul" (Project No. C644915664-00000026) within the WP5 Algae Vertical, funded by Next Generation EU European Fund and the Portuguese Recovery and Resilience Plan (PRR), under the scope of the incentive line "Agendas for Business Innovation" through the funding scheme C5 - Capitalization and Business Innovation."

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TP19 and P19

Evaluation of Nitrates in Beetroot Juice and the Nutritional Characterization of Brewer's Spent Grain and Wine Lees

Catherine Angeli San Jose[1], Yana Tronina Tronin,[1,2] Cristina Pubill-Ulldemolins[1]

[1]University of Barcelona: Campus de l'Alimentacio de Torribera, Department of Nutrition, Food Science and Gastronomy, Santa Coloma de Gramenet, Barcelona, Spain; [2]CETT Barcelona School of Tourism, Hospitality and Gastronomy (CETT), Barcelona, Spain

Corresponding author: csanjosa90@alumnes.ub.edu

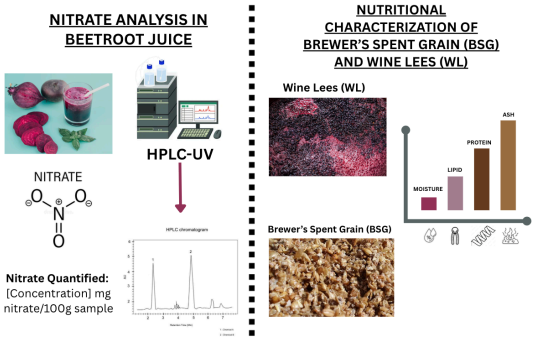

Figure 1. Main research aims of the study.

Non-communicable diseases (NCDs), particularly cardiovascular diseases (CVDs), account for at least 70% of deaths worldwide which is equivalent to about 40 million people[1,2]. Researchers have focused on modifiable factors that lower the prevalence of NCDs such as diet and diet processing. Various dietary patterns have been proposed for NCD prevention such as the Mediterranean diet which has been associated with reduced NCD incidence and mortality.[1] There has been an increasing demand for functional foods which are not only robust but also address the critical concern of food waste by utilizing by-products from the food industry. This interdisciplinary study has two aims:

- To quantify dietary nitrates and nitrites in beetroot juice, which have been proved to improve cardiovascular function due to its high inorganic nitrate content;[3]
- To explore the nutritional potential through the nutritional characterization of agro-industrial by-products such as brewer's spent grain (BSG) and wine lees (WL), known for their significant protein, fiber and phenolic content.

Nitrate & Nitrite Quantification in Beetroot Juice

Nitrate and nitrite content in beetroot juice was quantified and detected via a direct method using HPLC-UV using a common reverse phase C18 column and an ion pair mobile phase. Four samples were analyzed in triplicates: commercially available beetroot juice, laboratory produced beetroot juice and its freeze-dried counterpart and lastly, a beetroot juice combined with other fruits (made by our collaborators at CETT). This method successfully determined direct quantification of nitrates, which were abundant in all samples rather than nitrites.

Nutritional Characterization of Brewer's Spent Grain (BSG) and Wine Lees (WL)

Nutritional characterization of BSG and WL were carried out using methods from the Association of Official Analytical Collaboration International (AOAC) including moisture determination, protein determination, total lipid content and ash content. The reference sample was store bought dulce de leche. These methods have been successfully applied for the dulce de leche and BSG samples.

Keywords: Functional foods; beetroot juice; dietary nitrate; wine lees (WL); brewer's spent grain (BSG); food waste valorization

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Formulation and Rheological Characterization of Caseinate-Xanthan Gum Oleogels for Solid Fat Replacement

Sarah T.A. Zaza[1], Saskia Speed[2], Helena Esplugas[1], Teresa Calvet[2], Esther Santamaría[1,3], Laura Bayés-Garcia[2], Carmen González[1,3] Alicia Maestro[1,3]

[1] Departament d'Enginyeria Química i Química Analítica, Facultat de Química, Universitat de Barcelona; [2]Departament de Mineralogia, Petrologia i Geologia Aplicada, Facultat de Ciències de la Terra, Universitat de Barcelona; [3] Institute of Nutrition and Food Safety, Universitat de Barcelona, Spain

Corresponding author: Szazazaz7@alumnes.ub.edu

The food industry faces a critical need to replace saturated and trans-fats with healthier lipid alternatives without compromising macroscopic functionality and product stability. This research investigates the emulsion-templated "oleogelation" of liquid extra virgin olive oil (EVOO) to create a functional, semi-solid gel network. The primary objective was to develop and optimize a fully natural, "clean-label" oleogel by replacing synthetic surfactants with a food-grade biopolymer mixture of sodium caseinate and xanthan gum.

Oil-in-water emulsions with varying lipid loads were prepared and structurally evaluated. Particle size distribution analysis of the optimized 50% liquid oil emulsion revealed a single bell-shaped curve (a unimodal distribution), proving that the biopolymer matrix successfully stabilized the oil into highly homogeneous droplets without any significant coalescence or clumping. Optical microscopy further confirmed that the droplets were forced into a highly dense arrangement. Following dehydration via freeze-drying, the resulting oleogels and subsequent chocolate spread formulations were comprehensively characterized. The mechanical and macroscopic properties were evaluated using Texture Profile Analysis (TPA) and spreadability testing. Furthermore, the structural and physicochemical integrity of the matrices was thoroughly examined through rheological measurements, scanning electron microscopy (SEM), differential scanning calorimetry (DSC), colorimetric analysis, and oxidative stability testing.

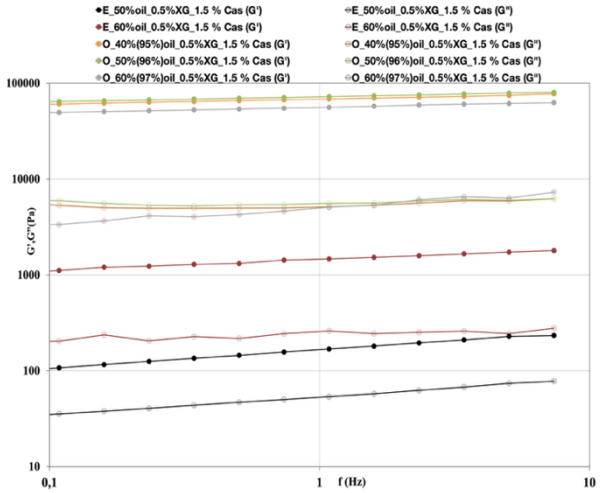

Figure 1. Frequency sweep profiles of the optimized oleogel containing 50% oil (96% final oil yield), 0.5% xanthan gum, and 1.5% sodium caseinate (50% oil, 0.5% XG, 1.5% CAS), along with the corresponding emulsion. The figure also includes 40% (95%) and 60% (97%) oleogels, as well as the emulsion corresponding to the 60% formulation.

Crucially, rheological evaluations physically validated the success of this structural transformation. Dynamic frequency sweeps revealed that the storage modulus (G′) of the dehydrated matrices approached 10^5 Pa, strictly dominating the loss modulus (G″) by over an order of magnitude with virtually no frequency dependence, which is the definitive hallmark of a true, highly stable solid-like gel. Impressively, this extreme mechanical strength was remarkably resilient, with G′ the curves for the 40%, 50%, and 60% EVOO formulations clustering tightly together at maximum strength, proving the biopolymer network could effectively entrap massive lipid loads without structural collapse (Figure 1). This exceptional mechanical strength allowed the oleogel to firmly entrap the liquid oil, achieving a near 100% Oil Binding Capacity (OBC).

Finally, the optimized oleogels were incorporated into a complex chocolate spread matrix to evaluate their technological viability. This study proves that clean-label, emulsion-templated EVOO oleogels can successfully replicate the physical mechanics of traditional solid fats, offering a highly functional and trans-fat-free technological solution for the food industry.

Acknowledgments: I would like to express my sincere appreciation to the Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD.

Energy Optimization and Process Integration Strategies for Industrial Operations: A Case Study in a Company

Abdallah Essam Elbassiouny[1,a], Renato Carvalho[2,a], Ana Rosa Garcia[1]

[1]University of Algarve / Portugal, [2]University of Lisbon/ Portugal; [a]For confidentiality reasons, the company analyzed in this study will be referred to as "the Company"

Corresponding author: Abdallah.elbassiouny@studio.unibo.it

In the highly competitive food processing and biofuel production sectors, energy costs play a critical role in maintaining a company's economic performance. In the past few years, with the increasing prices of energy sources due to geopolitical conflicts, global crises, and stricter chemical regulations and aggressive carbon pricing, the company aims to reduce its fuel consumption and optimize its energy usage as this step is essential not only to lower the operational costs but also to decrease greenhouse gas emissions in line with government targets and industry regulations. Additionally, the company has steam consumption levels exceeding the industrial benchmarks according to the latest energy audit done in 2023. Since steam is one of the major contributors to variable operating costs in the company, this led to a strong demand for improved management and optimization of thermal energy systems. This study focuses on improving energy efficiency and resource utilization within the industrial operations of the company by identifying energy management opportunities then developing process integration and optimization strategies.

The methodology combined energy auditing, process analysis, and process simulation to identify energy saving opportunities and evaluate their feasibility. Four industrial projects were carried out to provide both technical improvements in thermal energy management and lower the greenhouse gas emissions rate while having positive economically viable solutions for the industrial application and implementation. Applications ranging in different periods of payback time are shown in the techno-economic study for each project.

The first project focused on optimization of the steam boilers in the utility plant. This was achieved by recovering and integrating the superior blowdown of the boilers into other processes; leading to a 55k€ of annual savings and a payback time of 19 months with reduction of CO_2 emissions of 391 ton/yr.

The second project involved the development of a new condensate recovery system with an estimated annual savings of 27k€ per year, a payback period of one-month, and a reduction of CO_2 emissions at 106 ton/yr. As part of this project, key performance indicators (KPIs) were also developed to monitor steam usage and condensate recovery in the different operating units.

For the third project, an underperforming clogged plate heat exchanger for 7 years was assessed and planned to be maintained through operational and maintenance strategies, with the introduction of a new clean-in-place (CIP) system to serve not only this heat exchanger but all the ones in operation inside the preparation and extraction plant. This project has a CAPEX of 83k€ and a payback period of 34 months. In addition to a CO_2 reduction of 185 ton/yr. Finally, process simulation using Aspen HYSYS was conducted for (project 4) to evaluate the performance of condensers system in the extraction unit, leading to the identification and recommended removal of redundant and underutilized condensers with low heat recovery efficiency. Overall, the projects resulted in total energy savings of approximately 982.44 MWh/yr, across thermal energy, natural gas usage, and electricity consumption.

Keywords: energy efficiency, process integration, steam optimization, condensate recovery, heat integration, process simulation, techno-economic analysis, greenhouse gas emissions reduction.

HYBRID MAGNETO-SEMICONDUCTOR NANO-OBJECTS FOR H_2 PRODUCTION THROUGH WATER PHOTOCATALYSIS SYNTHESIS, CHARACTERIZATION, AND TiO_2-SHELL ENGINEERING OVER NI-CORE NANOSTRUCTURES

Peter Obaloluwa Agboola, Eloi Ros Costals, Marta Estrader Bofarull

Laboratory of Nanostructured and Nanocomposite Materials (LM2N), Dept. of Inorganic and Organic Chemistry, Universitat de Barcelona, Barcelona, Catalonia, Spain

Corresponding author: pagbooag67@alumnes.ub.edu

The global drive to decarbonize energy systems has intensified interest in solar-driven hydrogen (H_2) production via photocatalytic water splitting. TiO_2 remains the benchmark photocatalyst, yet its wide bandgap (~3.2 eV) restricts absorption to UV light (<5% of the solar spectrum) and fast electron-hole recombination limits efficiency.[1,2] Coupling TiO_2 with a ferromagnetic Ni core in a core@shell geometry is expected to address both: the internal magnetic field prolongs e-/h+ lifetime via Lorentz/spin-polarization effects[3] and enables broadband plasmonic absorption. This work presents a multi-route platform for hybrid Ni/NiO@TiO_2 core@shell nanostructures via electrodeposition, solvothermal, and ALD routes; the native NiO shell may further enhance OER kinetics via Ni(III)-O radical formation.[4]

Ni nanowires (NWs) were grown by electrodeposition into AAO templates pre-sputtered with Au/Ag seed layers[5], while spherical Ni nanoparticles (NPs) were obtained via solvothermal hydrazine reduction[6]. Electrodeposition at -1.2 V gave polycrystalline Ni NWs (SAED/HRTEM) with a ~15 nm NiO shell (EELS). Solvothermal Ni NPs were quasi-spherical (90-154 nm), enabling TiO_2-shell growth via two hydrothermal routes: (i) sol-gel + hydrothermal crystallization at 160 °C, 20h (Route 1)[7], and (ii) Ti-glycolate boiling-water reflux at 100 °C, 2 h (Route 2).[8] NH_3 concentration was identified as critical for uniform shell formation.

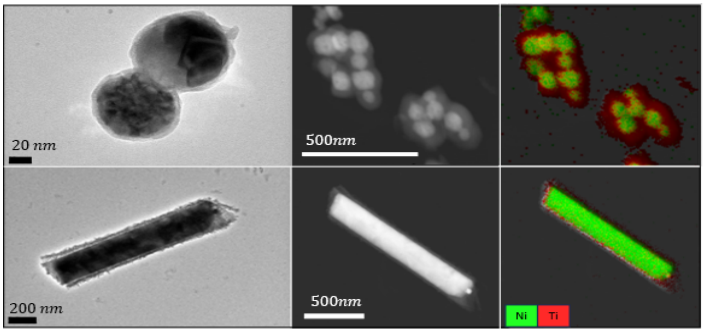

Figure 1. *TEM bright field*, *dark field,* and *EDX* mappings of synthesized Ni/NiO@TiO_2 nanostructures: nanoparticles (top row) and nanowires (bottom row). Ni (green), Ti (red).

ALD-grown TiO_2 shells offered a controlled-thickness alternative: (1) ALD inside AAO pores (inside-out NW geometry, Fig.1 bottom), and (2) direct ALD onto Ni NPs (thickness-tunable, Fig.1 top)[9]. Materials were characterized by powder XRD.

A robust multi-route platform for Ni/NiO@TiO_2 hybrid nanostructures has been established. EELS confirms a ~15 nm NiO shell on polycrystalline Ni NWs, providing built-in OER-active sites. The 'inside-out' ALD-on-AAO route is a conceptual advance, enabling intimate magneto-semiconductor contact from the outset of NW growth.

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TP23 and P23

TiO_2/(Ba,Sr)TiO_3/MXene Tertiary Heterojunction Photocatalyst for Hydrogen Generation

Sabrina Cervantes Vizcaino[1], Jaroslaw Serafin[1], Xavier Vendrell[1]

[1]Department of Inorganic & Organic Chemistry and Institute of Nanoscience and Nanotechnology (IN2UB) University of Barcelona, Spain

Corresponding author: scervace7@alumnes.ub.edu

The growing environmental impact of fossil fuel consumption has heightened interest in sustainable energy solutions. Hydrogen poses a promising energy alternative due to its high energy density and potential for carbon-neutral production.[1] Although conventional hydrogen production methods, like steam methane reforming, remain carbon-intensive, photocatalytic water splitting (PWS) has attracted considerable interest as a sustainable generation pathway.[2] The efficiency of PWS is primarily determined by light absorption, charge separation, charge transport, and surface reaction kinetics intrinsic to the photocatalytic material. To this end, a diverse range of materials have been investigated for such applications including metal oxides, metal sulfides, carbon-based materials, metal-organic frameworks, and nanomaterials.[2]

Among these materials, TiO_2 presents a promising candidate due to its cost effectiveness, abundance, non-toxicity, and chemical stability and resistance. However, its narrow light-absorption range and rapid charge recombination rate hinder photocatalytic efficiency.[3] Numerous approaches, including use of co-catalyst, doping, and creation of heterojunctions, have been pursued to enhance photocatalytic activity.[4] Despite significant advances through these modification strategies, current studies demonstrate 1-2% hydrogen production efficiency while 10% efficiency is required to compete in the current hydrogen market.[5]

Accordingly, this study aims to explore the synergistic relationship of a novel TiO_2-based composite composed of Barium Strontium Titanate (BST) perovskite and MAX/MXene phases for increased photocatalytic efficiency in hydrogen production. The incorporation of the selected materials capitalizes on the ferroelectric properties of BST to enhance charge separation and the high electrical conductivity of MAX/MXene phases to facilitate charge transport.[6,7] The composite was synthesized through solid-state impregnation and characterized using FTIR, XRD, SEM-EDX, Raman, Photoluminescence, and UV-Vis spectroscopy. The photocatalytic performance was evaluated using a gas-flow photoreactor equipped with a 200 W mercury-xenon UV lamp as irradiation source where the optimized composite exhibited a significantly increased hydrogen production rate of 5.09 mmol/g/h compared to 0.01 mmol/g/h of sole TiO_2.

This study contributes to the development of more efficient photocatalysts for the advancement and practical implementation of solar-driven hydrogen production technologies.

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From Renewable H_2 to Grid-Compatible CH_4: Pilot-Scale Ex-Situ Bio-methanation and Scale-Up Potential

M. Hamza[1], P. Gil[1,2], J. Guilera[1,2], S. Astals[1]

[1] Universitat de Barcelona, Spain, [2] Institut de Recerca en Energia de Catalunya, Spain

Corresponding author: sastals@ub.edu

The increasing utilization of renewable electricity requires energy storage pathways that are technically robust and infrastructure-compatible. Power-to-Methane offers a promising route by converting renewable hydrogen and carbon dioxide into methane, enabling long-term energy storage through existing gas infrastructure.[1] In parallel, the transition of wastewater treatment plants into water resource recovery facilities creates new opportunities to integrate anaerobic digestion, biogenic CO_2 utilization, renewable hydrogen and circular energy production. Within this context, ex-situ biological methanation is an attractive technology because it operates under mild conditions, uses hydrogenotrophic microorganisms as biocatalysts and can valorize CO_2 streams while avoiding the harsher operating requirements of thermochemical methanation.[2]

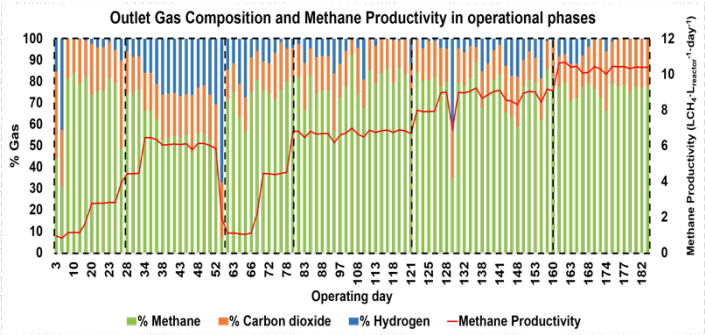

Figure 3. Gas composition and productivity in operational phases

This work presents the pilot-scale operation of a thermophilic ex-situ trickle-bed reactor for H_2 and CO_2 bio-methanation, with emphasis on renewable hydrogen utilization, hydrodynamic optimization and scale-up relevance. A 40 L packed-bed reactor was operated in counter-current mode at near-atmospheric pressure and 55–58 °C for more than six months. The system was inoculated with sieved and diluted digestate from a full-scale anaerobic digester and progressively exposed to increasing hydrogen loads. Hydrogen feed was increased from 100 to 1000 mL·min^{-1}. Liquid recirculation was varied between 45 and 200 L·h^{-1} to investigate the influence of wetting regime and gas–liquid contact on reactor performance.

The reactor achieved stable high-rate bio-methanation, reaching methane productivities of ~10 L CH_4·L$^{-1}_{reactor}$·day^{-1} at high hydrogen loading. Methane concentrations varied between approximately 65 and 90% as shown in Figure-1, depending on gas loading, hydrogen availability and liquid recirculation conditions. The results demonstrate that high methane productivity can be maintained under thermophilic and near-atmospheric operation, supporting the technical feasibility of biological Power-to-Methane at pilot scale. Hydrodynamic operation played a critical role in reactor performance. Adjusting liquid recirculation affected wetting efficiency, liquid-film resistance and biofilm–gas contact within the packed bed. Excessive recirculation may increase liquid-film thickness and limit hydrogen diffusion, whereas insufficient recirculation may reduce effective wetting and active mass-transfer area. Optimizing this balance is therefore essential for improving hydrogen utilization and designing larger trickle-bed bio-methanation systems.[3] The pilot-scale results provide practical evidence for scaling ex-situ bio-methanation from laboratory systems toward demonstration plants integrated with wastewater resource recovery, anaerobic digestion and renewable hydrogen infrastructure.

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ENHANCING ANAEROBIC BIODEGRADATION OF POLYLACTIC ACID (PLA) THROUGH LOW-INTENSITY CHEMICAL AND THERMAL PRETREATMENTS

Anđela Popović[1], Carlos Mario Olaya Rincón [1], Sergi Astals [1]

[1] Dept. Chemical Engineering & Analytical Chemistry, Universitat de Barcelona, Spain

Corresponding author: apopovpo91@alumnes.ub.edu

Total global plastic production reached 430.9 million tonnes in 2024, with 89.8 % of this plastic produced from fossil fuels, driving the search for sustainable alternatives. Bioplastics such as polylactic acid (PLA) have risen as promising substitutes for conventical plastics.[1] However, despite its classification as biodegradable, PLA degrades slowly under anaerobic conditions. Achieving approximately 75 % degradation can take over 400 days under mesophilic conditions, and even thermophilic anaerobic digestion (AD) requires large treatment times of 32-52 days for complete biodegradation. Therefore, pretreatments are a strategy to make AD a viable end-of-life pathway for PLA products.[2]

This study evaluates the effects of low-intensity chemical and thermal pretreatments on the anaerobic biodegradation of commercially available PLA cups, cut into 1 cm^2 pieces, under both mesophilic (35 °C) and thermophilic (55 °C) conditions. Nine pretreatment conditions were applied for one hour each: (1) immersion in water (hydrolysis control); (2) hydrolysis at 70 °C; (3) thermal treatment alone at 70 °C; (4–6) alkaline pretreatment with KOH at 1 M, 2 M, and 3 M; and (7–9) combined alkaline and thermal pretreatment with KOH at 1 M, 2 M, and 3 M at 70 °C. Biochemical methane potential (BMP) tests were set up by placing half the bottles under mesophilic conditions and the other half under thermophilic conditions. Methane production was monitored periodically by weighing the bottles and measuring gas volume.

Preliminary results after 65 days (thermophilic) and 80 days (mesophilic) of experimentation show the influence of both pretreatment type and temperature. Under thermophilic conditions, all pretreatments significantly increased methane production, compared to untreated PLA. The best-performing condition so far was KOH 2 M with thermal treatment at 70 °C, yielding of 375 mL CH_4/g VS (Figure 1). Under mesophilic conditions, PLA showed very limited biodegradation. Untreated PLA produced 0 mL CH_4/g VS, while the KOH 2 M at 70 °C condition achieved the highest methane yield of 80 mL CH_4/g VS (Figure 2). Overall, thermophilic conditions produced 4.7-fold higher methane yields than mesophilic conditions, underlining the temperature as a determining factor for PLA biodegradation, and demonstrating that the combination of alkaline treatment under thermophilic conditions is an avenue to maximising PLA biodegradability.

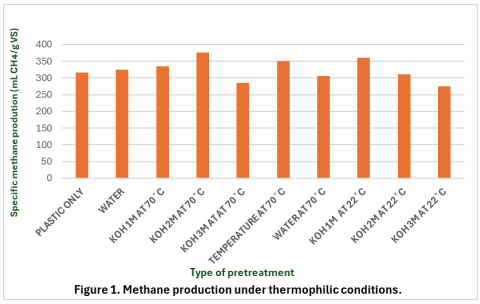

Figure 1. Methane production under thermophilic conditions.

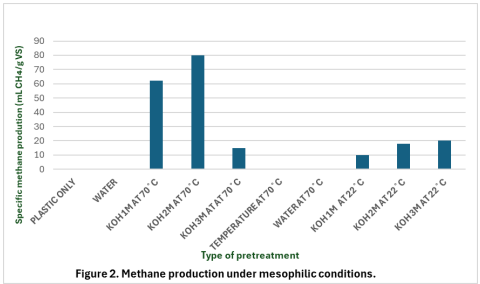

Figure 2. Methane production under mesophilic conditions.

These findings demonstrate that low-intensity, one-hour pretreatments can substantially enhance PLA biodegradability under practical operational conditions, supporting the development of sustainable end-of-life solutions for bioplastic waste.

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TP26 and P26

Metal Crosslinking of Peptide Hydrogels: Structural and Mechanical Effects

Nevil Jose[1], Pol Barcelona[2], Elena Xuriguera[2], Patrick Gamez[1,3], and Ana B. Caballero[1]

[1]Departament de Química Inorgànica i Orgànica. Facultat de Química, UB, [2]Departament de Ciencia dels Materials i Química Física. Facultat de Química, UB; [3]Catalan Institution for Research and Advanced Studies (ICREA), Passeig Lluís Companys 23, 08010, Barcelona, Spain

Corresponding author: nevil.jose@studio.unibo.it

Hydrogels are hydrophilic polymeric networks characterized by high water content, permeability, and tunable properties, which make them attractive materials for biomedical applications such as drug delivery, tissue engineering, wound healing, biosensors, bioinks, and catalysis.[1] Within this framework, peptide-based hydrogels are particularly appealing due to their mild fabrication conditions, biocompatibility, biodegradability, and functional versatility. However, their limited mechanical strength and slow gelation kinetics remain major challenges that restrict their biomedical applicability.[2] Tightly-controlled metal coordination offers a strategy to modify peptide assembly, since metal ions can introduce additional crosslinking points and influence the supramolecular organization of the peptide network.

This thesis investigates the effect of Cu(II) binding on the structure and properties of hydrogels formed by two amphiphilic Fmoc-protected histidine-containing peptides. The peptides were selected because the Fmoc group can promote aromatic interactions, while histidine residues provide metal-binding sites through imidazole coordination. Cu(II) complexation was first studied by UV-Vis spectroscopy and ESI-MS to evaluate metal binding and identify peptide-Cu(II) species. The gel formation was then compared for the free peptides and their Cu(II)-bound forms. The resulting assemblies were characterized using spectroscopic, microscopic and rheological techniques, including circular dichroism, fluorescence spectroscopy, FTIR, TEM and rheology.

The preliminary results indicate that Cu(II) coordination modifies peptide self-assembly and can alter the structural organization of the hydrogel network. These changes are expected to affect fibril formation, secondary structure and mechanical behaviour. Overall, this work explores metal binding as a tool to tune the properties of short peptide hydrogels and to improve their potential relevance as functional biomaterials.

Keywords: Peptide hydrogel, Metal coordination, Cu(II) coordination, Self-assembly, Supramolecular biomaterials

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LEPTIN ANALOGUES DESIGN, SYNTHESIS, AND CHARACTERIZATION FOR ALZHEIMER'S DISEASE

Ihsanti Fairuz Anatasya[1], Cristina Pubill Ulldemolins[1]
[1]University of Barcelona / Spain
Corresponding author: ianataan61@alumnes.ub.edu

Alzheimer's disease (AD) is a neurodegenerative disease that is characterized primarily by the formation of tau and amyloid beta aggregate in the brain. There are scientific evidences suggesting that leptin, an adipocyte-derived hormone, has a bidirectional role in AD by providing neuroprotective effect and regulating cognitive function.[1] Hence, this thesis aims to design, synthesize, and characterise leptin peptide, starting from its building block of amino acid, as well as evaluating the synthesis process sustainability using green and hazard metrics.

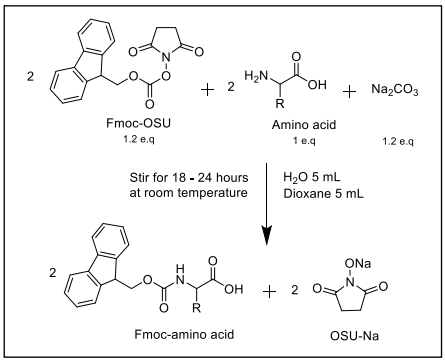

Figure 1. Fmoc-amino acid protection

Leptin analogues design are developed based from the suspected neuroprotective epitope from literature studies. Several modified analogues were generated after analyzing Ala-substitution effect on the fragments towards Aβ aggregation and the leptin interaction on the active sites of human leptin receptor. Modification strategies included the incorporation of terminal capping, non-natural amino acid, and residue substitution, to make the structure more polar, and hence would be able to cross the blood-brain-barrier more effectively.

The most commonly used peptide synthesis strategy is solid- phase peptide synthesis (SPPS).[2] In this method, it is important to ensure that -NH_2 group in amino acid to be protected prior to the peptide synthesis to ensure the reaction selectivity. Fmoc protecting group was selected due to its superiority on orthogonal protection.[3] A one-pot amino acid -NH_2 protection method was developed using Fmoc-OSU and tested on five different L-amino acids with varying polarity. The process yields on 47 – 78% product and 79 – 95% purity, with non-polar amino acid residue has a higher yield, implicating that the reaction or purification design favouring specific polarity profile. Peptide synthesis is still attempted using solid-phase peptide synthesis (SPPS), both in manual and automatic mode, and is awaiting purification.

Polarimetry and NMR analysis confirmed that the products have the same stereochemistry as the raw material and structure as the commercial reference after 4 weeks. Impurities profile were analyzed using 1D and 2D NMR, which found that most of them were originated from purification solvent.

Green metrics analysis on amino acid protection were done using kernel and composite metrics.[4] The product mass intensity (PMI) value for synthesis and extraction ranging from 93 – 239 mg/mg product, while the total PMI ranging from 1824 – 3084 mg/mg, which is dominated by the purification process. Theoretically, the designed synthesis is efficient with maximum reaction mass effectivity (RME) ranging 67 – 75%, but the actual RME only reached 30 – 55%, suggesting that the practical aspect of the reaction could be improved. Chloroform as the main purification solvent dominate the solvent intensity by 87% on total consumption, constituting almost 80% of the solvent PMI. This solvent also poses the biggest normalized hazard score of all materials, considering the volume and exposure throughout use. Future improvement on the amino acid protection should be focused on the optimizing the purification process with chloroform alternative.

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PLASTIC: PERCEPTION & IMPACT

An MSc Study Investigating Public Awareness of Environmental Risks and Potential Circular Solutions

Elena Berselli, Silvia Boldorini, Isabella Correa Caicedo, Valentina Felchero, Sally Howard Ihle, Benedetta Lauria, Refilwe Mmopiemang, Ashwini Nirbail, Kelvin Otieno, Lydia Rupprecht

Erasmus Mundus Master's in Chemical Innovation and Regulation. Alma Mater Studiorum, University of Bologna, Italy

This study, developed within the course Environmental Risk of Plastic Materials (ChIR), Alma Mater Studiorum – University of Bologna, investigates public awareness of plastic pollution, with a focus on microplastics and circular solutions. Survey results from a diverse international cohort reveal uneven understanding: although many correctly identify that "Microplastics are small plastic particles (<5 mm)" and originate from plastic breakdown, misconceptions persist regarding their harmlessness and their exclusive association with marine environments. Significant knowledge gaps also emerge around bioplastics, as several respondents remain unaware that "'Biobased' does not equal 'biodegradable'" and that biodegradation depends on chemical structure rather than resource origin. While reducing plastic use, recycling, and adopting non fossil materials are widely perceived as effective strategies, the findings highlight a clear mismatch between public perception and scientific evidence, emphasizing the need for targeted educational initiatives.

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